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ORTHOGONAL RATIONAL FUNCTIONS: ASYMPTOTIC BEHAVIOUR AND COMPUTATIONAL ASPECTS

Promotor:
Prof. Dr. A. Bultheel

Proefschrift voorgedragen tot
het behalen van het doctoraat
in de toegepaste wetenschappen

door

Joris VAN DEUN

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Jury:
Prof. Dr. ir. J. Berlamont, voorzitter
Prof. Dr. A. Bultheel, promotor
Prof. Dr. ir. R. Cools,
Prof. Dr. W. Van Assche,
Prof. Dr. P. González Vera,
(Universidad de La Laguna, Tenerife)
Prof. Dr. O. Njåstad, (NTNU, Norway)

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Joris Van Deun
Departement Computerwetenschappen, K.U.Leuven
Celestijnenlaan 200A, B-3001 Heverlee, België

Abstract

Orthogonal rational functions with fixed poles are a natural generalization of orthogonal polynomials. Most attention so far has gone to the case of orthogonality on the complex unit circle or on the real line, where many polynomial results have been generalized to the rational case. In this thesis we extend several of these results to the case of orthogonality on a finite interval. First we study different types of convergence. Ratio asymptotics are derived and then used to obtain the asymptotic behaviour of the recurrence coefficients. We conclude this part with some strong and weak-star convergence results. Next we briefly study the convergence of gaussian quadrature formulas on the interval and their relation with formulas on the unit circle. A substantial part of this thesis is devoted to computational aspects of orthogonal rational functions, both on an interval and on a halfline. We give some interpolation algorithms and generalize the method of modified moments to the case of rational functions. Next, a generally applicable and numerically stable algorithm is provided to compute the recurrence coefficients, together with computable error bounds. The case of poles close to the interval of integration is treated separately, because of the additional numerical difficulties. Finally, as a case study we generalize the well-known Chebyshev polynomials to the rational situation and present some related quadrature formulas which allow fast and efficient computation.

Preface

Deze thesis is het neergeschreven resultaat van vier jaar onderzoekswerk. Veel van dat werk is, tot mijn grote vreugde, kunnen gebeuren in eerder solitaire omstandigheden – onontbeerlijk voor elke vorm van fundamenteel onderzoek – maar een minstens even belangrijk deel is het gevolg van nauwe samenwerking en intense communicatie met een aantal mensen die ik hier expliciet wil bedanken.

In de eerste plaats denk ik dan aan mijn promotor Adhemar Bultheel. Het is dankzij hem dat ik in contact kwam met dit onderzoeksgebied en dat ik na mijn studies op het departement ben gebleven. Ik waardeer enorm het vertrouwen dat hij stelt in mijn capaciteiten als onderzoeker, impliciet aanwezig in de vrijheid die hij me laat in mijn dagelijkse activiteit.

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También es un gran placer agradecerle a Pablo González Vera de la Universidad de La Laguna. Me ayudó mucho durante mi estancia en Tenerife, no sólo profesionalmente, sino también en la vida cotidiana. Fue una experiencia muy agradable trabajar con él, y una experiencia inolvidable pasar cuatro meses en esa isla. Aquí no hacen chuletadas como en la casa de Pablo. También se lo agradezco mucho estar en el tribunal de mi tesis. Espero que esto sea el comienzo de una colaboración fructuosa.

I also would like to thank Olav Njåstad of the NTNU, not just for being part of my jury, but also for the few but valuable conversations we have had together. The Røros conference in honour of his 70th birthday was a decisive moment in my scientific career.

Tenslotte wil ik ook mijn familie en vrienden bedanken. Ze hebben weliswaar hoegenaamd niets bijgedragen aan deze thesis, maar ze zijn een conditio sine qua non voor een leven waarin orthogonale rationale functies niet het belangrijkste zijn.

Joris
Mei 2004

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Nederlandse samenvatting

Orthogonale Rationale Functies: Asymptotisch Gedrag en Berekeningsaspecten

Inhoudsopgave

1 Inleiding

1.1 Situering

Orthogonale rationale functies (ORF) vormen een natuurlijke veralgemening van orthogonale veeltermen, in die zin dat we altijd het veeltermgeval terugkrijgen door alle polen op oneindig te plaatsen. De studie van orthogonale veeltermen kent reeds een lange geschiedenis met zeer uiteenlopende resultaten. In deze thesis zullen we ons voornamelijk bezighouden met asymptotisch gedrag enerzijds en numerieke aspecten (waaronder ook kwadratuurformules) anderzijds.

Sinds het pionierswerk van Szegő in verband met sterke convergentie van orthogonale veeltermen, heeft de studie van asymptotisch gedrag een hoge vlucht genomen, met onder andere relevante bijdragen van Rakhmanov (verhoudingen) en López Lagomasino (variërende maten). Deze laatste is van bijzonder belang voor orthogonale rationale functies.

De numerieke aspecten van orthogonale veeltermen (efficiënte berekening van recursiecoëfficiënten en Gauss-kwadratuurformules) zijn voornamelijk bestudeerd door Gautschi. Ondertussen zijn er ook verschillende veralgemeningen gemaakt van de traditionele Gauss-formules, vb. naar formules gebaseerd op Laurent-veeltermen.

1.2 Bestaande resultaten

Het onderzoek naar orthogonale rationale functies heeft zich tot dusver voornamelijk gericht op theoretische aspecten. Orthogonaliteit op de complexe eenheidscirkel en op de reële rechte zijn uitvoerig bestudeerd en vele eigenschappen van orthogonale veeltermen zijn veralgemeend naar het rationale geval. Wat het asymptotisch gedrag betreft, vermelden we resultaten omtrent asymptotiek van de verhoudingen, sterke en zwakke-sterasymptotiek. Het geval van een eindig interval is nog niet bestudeerd.

Gaussische kwadratuurformules, analoog met het veeltermgeval, zijn bestudeerd, maar meer algemene interpolerende formules nog niet. Ook de numerieke kant heeft nog bijzonder weinig aandacht gekregen. Wel is er een veralgemeend eigenwaardenprobleem gevonden dat als oplossingen de knooppunten in deze kwadratuurformules geeft.

In feite zijn de berekeningsaspecten van orthogonale rationale functies nog helemaal niet bestudeerd. Verschillende toepassingen in systeemtheorie zijn onderzocht en er zijn interessante verbanden met de theorie van semiseparabele matrices, maar de efficiënte berekening van orthogonale rationale functies ten opzichte van een willekeurige (niet-discrete) maat, voor hoge graad, is nog open voor onderzoek.

Ook expliciete voorbeelden zijn er bijna niet. De Malmquist-basis op de complexe eenheidscirkel (ten opzichte van de Lebesgue-maat) is een van de weinige gevallen waar voor willekeurige polen de ORF gekend zijn. Voortbrengende functies of differentiaalvergelijkingen zijn evenmin gekend.

1.3 Overzicht van de thesis

In hoofdstuk 2 geven we de nodige theoretische achtergrond en introduceren we de orthogonale rationale functies. Een belangrijk verband tussen functies op de eenheidscirkel en het interval besluit dit hoofdstuk.

Dit verband gebruiken we in het volgende hoofdstuk om het asymptotisch gedrag van orthogonale rationale functies op een eindig interval te bestuderen. Zowel asymptotiek van de verhoudingen en de recursiecoëfficiënten als sterke en zwakke-sterconvergentie komen aan bod. Enkele open problemen geven we in de appendix.

Kwadratuurformules op $[-1, 1]$ en hun convergentiegedrag bestuderen we in hoofdstuk 4. Ook het verband tussen formules op de cirkel en het interval wordt afgeleid. Uiteindelijk komen kort interpolerende formules aan bod.

De efficiënte berekening van ORF op een eindig interval neemt een zeer belangrijke plaats in in deze thesis. In hoofdstuk 5 geven we een algoritme om de recursiecoëfficiënten te berekenen, gebaseerd op interpolatie-eigenschappen van de Riesz-Herglotz-Nevanlinna-transformatie. We tonen met een foutenanalyse aan dat dit algoritme numeriek onstabiel is. Verbanden met kettingbreuken en Padé-benaderingen worden kort aangehaald.

Dit interpolatie-algoritme is in essentie gebaseerd op het gebruik van de momenten van de maatfunctie. In hoofdstuk 6 wordt aangetoond dat momentengebaseerde algoritmes onbruikbaar zijn, omwille van de slechte conditie van het probleem. De methode van de gewijzigde momenten voor het veeltermgeval wordt hier ook veralgemeend naar het rationale geval.

De meest algemene methode om ORF te berekenen wordt uiteengezet in hoofdstuk 7, samen met een gedetailleerde foutenanalyse. Het geval van polen dicht bij de rand verdient een aparte behandeling omwille van de intrinsieke moeilijkheden. Het gebruik van Laurent-veeltermen biedt hier een interessante uitweg.

Daarna volgt een kort hoofdstuk dat toelaat om het geval van een halfrechte terug te brengen naar het geval van een eindig interval via een gepaste transformatie.

In het laatste hoofdstuk geven we een rationale veralgemening van de Chebyshev-veeltermen. In deze gevalstudie is er bijzonder veel aandacht voor numerieke aspecten en efficiënten berekening van de gerelateerde kwadratuurformules.

2 Definities en begrippen

We veronderstellen dat de lezer vertrouwd is met de belangrijkste begrippen en resultaten uit de maattheorie en de theorie van L^p- en Hilbertruimtes, reproducerende kernfuncties en Fourieranalyse.

2.1 Orthogonaliteit op de eenheidscirkel

Veronderstel een maatfunctie $\mathring{\mu}$ gedragen op de eenheidscirkel en een rij van complexe getallen $B = \{\beta_1, \beta_2, \ldots\}$ volledig gelegen binnen de eenheidsschijf $\mathbb{D}$. De orthonormale veeltermen $\phi_{n,m}(z)$ ten opzichte van de variërende maat $d\mathring{\mu}/|w_n(z)|^2$ met $w_n(z) = (z - \beta_1)\ldots(z - \beta_n)$ zijn gekend. Ze zullen nuttig blijken voor de studie van het convergentiegedrag van orthogonale rationale functies.

Het (eindige) Blaschke product geassocieerd met de eerste n punten uit B wordt genoteerd als $B_n(z)$. Dit zal convergeren naar een van nul verschillende waarde enkel indien $\sum(1-|\beta_n|) < \infty$. De ruimte van rationale functies $\mathring{\mathcal{L}}_n$ is dan $\mathring{\mathcal{L}}_n = \text{span}\{B_0, B_1, \ldots, B_n\}$. Door te orthonormalizeren met betrekking tot $\mathring{\mu}$ verkrijgen we de ORF $\{\phi_n\}$ op de eenheidscirkel. Het verband met de variërende orthonormale veeltermen $\phi_{n,n}$ wordt gegeven door

$$g_n(z) = \frac{1}{z-\beta_n}\frac{\tau_n}{\nu_{n,n}}\left(z\phi_{n,n}(z) - \beta_n\frac{\phi_{n,n}(\beta_n)}{\phi^*_{n,n}(\beta_n)}\phi^*_{n,n}(z)\right)$$

waar $g_n(z) = \tau_n z^n + \ldots$ de tellerveelterm van $\phi_n(z)$ is en $\nu_{n,n}$ de hoogstegraadscoëfficiënt van $\phi_{n,n}(z)$.

De reproducerende kernfunctie voor $\mathring{\mathcal{L}}_n$ stellen we voor door $\mathring{k}_n(z,w) = \sum_{k=0}^n \phi_k(z)\overline{\phi_k(w)}$. Deze kunnen we ook schrijven als

$$\mathring{k}_n(z,w) = \left[\sum_{k=0}^n \phi_{n,k}(z)\overline{\phi_{n,k}(w)}\right](w_n^*(z)\overline{w_n^*(w)})^{-1}.$$

De formules van Christoffel-Darboux voor het rationale geval luiden dan

$$\begin{aligned}\mathring{k}_n(z,w) &= \frac{\phi_n^*(z)\overline{\phi_n^*(w)} - \zeta_n(z)\overline{\zeta_n(w)}\phi_n(z)\overline{\phi_n(w)}}{1-\zeta_n(z)\overline{\zeta_n(w)}},\\ &= \frac{\phi_{n,n}^*(z)\overline{\phi_{n,n}^*(w)} - z\overline{w}\phi_{n,n}(z)\overline{\phi_{n,n}(w)}}{(1-z\overline{w})(w_n^*(z)\overline{w_n^*(w)})},\end{aligned}$$

waarbij $\zeta_n(z)$ de Blaschke factor is die hoort bij β_n.

De Szegő-functie $\sigma(h,z)$, tenslotte, wordt gedefinieerd voor elke nietnegatieve meetbare functie h met $\log h \in L^1[0,2\pi]$ als

$$\sigma(h,z) = \exp\left(\frac{1}{4\pi}\int_0^{2\pi}\frac{u+z}{u-z}\log h(\theta)d\theta\right), \quad u = e^{\mathbf{i}\theta}, z \in \mathbb{D}.$$

2.2 Orthogonaliteit op een deelverzameling van de reële rechte

In dit geval wordt de maatfunctie μ gedragen op (een deel van) de reële rechte. Neem een rij van polen $A = \{\alpha_1, \alpha_2, \ldots\}$ gelegen buiten de drager van de maat, alle reëel en verschillend van 0. Definieer dan de factoren $Z_n(z) = z/(1-z/\alpha_n)$ en de basisfuncties

$$b_0 = 1, \quad b_n(z) = b_{n-1}(z)Z_n(z), \quad n = 1, 2, \ldots$$

De corresponderende ruimte van rationale functies stellen we voor door $\mathcal{L}_n = \text{span}\{b_0, \ldots, b_n\}$. Opnieuw verkrijgen we de ORF $\{\varphi_n\}$ door het orthonormalizeren van deze basis. De φ_n hebben reële coëfficiënten ten opzichte van de basis $\{b_k\}$. Van deze functies kan men aantonen dat ze (onder bepaalde voorwaarden) voldoen aan de volgende drietermsrecursiebetrekking,

$$\varphi_n(z) = \left(E_n Z_n(z) + F_n \frac{Z_n(z)}{Z_{n-1}(z)} \right) \varphi_{n-1}(z) - \frac{E_n}{E_{n-1}} \frac{Z_n(z)}{Z_{n-2}(z)} \varphi_{n-2}(z)$$

met beginvoorwaarden $\varphi_{-1}(z) \equiv 0$ and $\varphi_0(z) \equiv 1/\sqrt{\mu_0}$ waarbij μ_0 het totale gewicht van de maat is. De coëfficiënten E_n zijn verschillend van nul en we normalizeren ze positief. Indien de drager van μ verbonden is, geldt deze recursiebetrekking.

We kunnen eenvoudig expliciete uitdrukkingen vinden voor de recursiecoëfficiënten door links en rechts inwendige producten te vormen. Als resultaat vinden we dan

$$F_n = -E_n \frac{\langle Z_n \varphi_{n-1}, \varphi_k \rangle - \frac{1}{E_{n-1}} \left\langle \frac{Z_n}{Z_{n-2}} \varphi_{n-2}, \varphi_k \right\rangle}{\left\langle \frac{Z_n}{Z_{n-1}} \varphi_{n-1}, \varphi_k \right\rangle} = -E_n \hat{F}_n,$$

$$E_n = \frac{1}{\|\hat{\varphi}_n\|},$$

waar

$$\hat{\varphi}_n(x) = \left(Z_n(x) - \hat{F}_n \frac{Z_n(x)}{Z_{n-1}(x)} \right) \varphi_{n-1}(x) - \frac{1}{E_{n-1}} \frac{Z_n(x)}{Z_{n-2}(x)} \varphi_{n-2}(x)$$

en $k < n$.

Ook in dit geval is er een Christoffel-Darbouxformule die de reproducerende kernfunctie uitdrukt in termen van de φ_n.

2.3 Een verband tussen het interval en de cirkel

Door middel van de Joukowski-transformatie $x = J(z) = \frac{1}{2}(z + z^{-1})$ kunnen we de ϕ_n op de cirkel en de φ_n op het interval aan elkaar relateren. Hiervoor definiëren we eerst $B = J^{-1}(A)$ en $\hat{B}$ is de rij die we verkrijgen door in B de meervoudigheid van elk getal te verdubbelen. De maatfunctie $\mathring{\mu}$ op de cirkel nemen we als

$$\mathring{\mu}(E) = \mu(\{\cos\theta, \theta \in E \cap [0, \pi)\}) + \mu(\{\cos\theta, \theta \in E \cap [\pi, 2\pi)\}).$$

Dan kunnen we φ_n voorstellen in termen van $\hat{\phi}_{2n}$, de functies geassocieerd met $(\hat{B}, \mathring{\mu})$ door

$$\varphi_n(x) = \delta_n (2\pi)^{-\frac{1}{2}} \left\{ 1 + \frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}^*_{2n}(\beta_n)} \right\}^{-\frac{1}{2}} \frac{\hat{\phi}_{2n}(z) + \hat{\phi}^*_{2n}(z)}{B_n(z)}$$

waar $\delta_n = \pm 1$ is zodanig dat $E_n > 0$.

3 Asymptotisch gedrag

In dit hoofdstuk bestuderen we verschillende vormen van convergentie voor de ORF. We kijken achtereenvolgens naar asymptotiek van de verhoudingen en de recursiecoëfficiënten, sterke convergentie en zwakke-sterconvergentie. Alle resultaten werden afgeleid onder de veronderstelling dat de polen wegblijven van de randen van het interval $I = [-1, 1]$ (of van de cirkel).

3.1 Asymptotiek van de verhoudingen

De belangrijkste en meest algemene stelling in deze paragraaf is de volgende. Merk op dat we een klassiek resultaat uit de veeltermsituatie verkrijgen door alle polen op oneindig te plaatsen.

Stelling 1. *Veronderstel dat de rij $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I = \mathbb{R} \cup \{\infty\} \setminus I$ wegblijft van I en dat μ voldoet aan de Erdős-Turán-voorwaarde $\mu' > 0$ a.e. Dan geldt gelijkmatig op compacten van $\overline{\mathbb{C}}^I = \mathbb{C} \cup \{\infty\} \setminus I$ dat*

$$\lim_{n\to\infty} \frac{z - \beta_{n+1}}{1 - \beta_n z} \sqrt{\frac{1 - \beta_n^2}{1 - \beta_{n+1}^2}} \frac{\varphi_{n+1}(x)}{\varphi_n(x)} = 1$$

met $z = J^{-1}(x)$ en $\beta_k = J^{-1}(\alpha_k)$ voor $k = n, n+1$.

Voor het geval van een asymptotisch periodieke poolrij kunnen we een expliciete limiet geven.

Stelling 2. *Veronderstel dat de rij $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ asymptotisch m-periodiek is met limietwaarden $\{\alpha_i^0\}_{i=1}^m \subset \overline{\mathbb{R}}^I$ en veronderstel dat μ voldoet aan de Erdős-Turán-voorwaarde $\mu' > 0$ a.e. Dan geldt er dat*

$$\lim_{n\to\infty} \frac{\varphi_{nm+i}(x)}{\varphi_{nm+i-1}(x)} = \frac{1 - \beta_{i-1}^0 z}{z - \beta_i^0} \sqrt{\frac{1 - (\beta_i^0)^2}{1 - (\beta_{i-1}^0)^2}}, \quad i = 1, \ldots, m$$

gelijkmatig op compacten van $\overline{\mathbb{C}}^I \setminus \{\alpha_i^0\}$ met $z = J^{-1}(x)$, $\beta_k^0 = J^{-1}(\alpha_k^0)$ voor $k = i, i-1$ en $\alpha_0^0 = \alpha_m^0$.

Indien $m = 1$ wordt dit nog eenvoudiger.

Stelling 3. *Veronderstel dat de rij $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ zodanig is dat $\lim_{n\to\infty} \alpha_n = \alpha \in \overline{\mathbb{R}}^I$ en veronderstel dat μ voldoet aan de Erdős-Turán-voorwaarde. Dan geldt er voor $|\alpha| < \infty$*

$$\lim_{n\to\infty} \frac{\varphi_{n+1}(x)}{\varphi_n(x)} = \frac{1 - \alpha x}{x - \alpha} - \frac{\sqrt{(x^2 - 1)(\alpha^2 - 1)}}{x - \alpha}$$

gelijkmatig op compacten van $\overline{\mathbb{C}}^I \setminus \{\alpha\}$ *waar de tak van de wortel zodanig gekozen is dat de uitdrukking aan de rechterkant groter is dan 1 in modulus voor* $x \in \overline{\mathbb{C}}^I$.

Indien $|\alpha| = \infty$ *dan geldt er*

$$\lim_{n\to\infty} \frac{\varphi_{n+1}(x)}{\varphi_n(x)} = x + \sqrt{x^2 - 1}$$

gelijkmatig op compacten van $\overline{\mathbb{C}}^I$, *met dezelfde conventie voor de tak van de vierkantswortel.*

3.2 Convergentie van E_n en F_n

Gebruik makende van de resultaten uit de vorige paragraaf is het niet moeilijk om uitdrukkingen af te leiden voor het asymptotisch gedrag van de recursiecoëfficiënten.

Stelling 4. *In de veronderstelling dat de polen wegblijven van I en dat de maat voldoet aan de voorwaarde van Erdős-Turán, geldt er dat*

$$\begin{aligned} E_n &\sim 2\frac{\sqrt{(1-\beta_{n-1}^2)(1-\beta_n^2)}(1-\beta_{n-1}\beta_n)}{(1+\beta_{n-1}^2)(1+\beta_n^2)} \;, \\ F_n &\sim -\sqrt{\frac{1-\beta_n^2}{1-\beta_{n-1}^2}}\frac{(1-\beta_{n-1}^2)(\beta_n+\beta_{n-2})+2\beta_{n-1}(1-\beta_n\beta_{n-2})}{(1+\beta_n^2)(1-\beta_{n-1}\beta_{n-2})} \;, \end{aligned}$$

met $\beta_k = J^{-1}(\alpha_k)$ *voor* $k = n, n-1, n-2$, *in die zin dat de verhouding van linker- en rechterlid naar 1 convergeert als n naar oneindig gaat. Indien de polen convergeren naar een vast punt* α *wordt dit*

$$\begin{aligned} \lim_{n\to\infty} E_n &= 2(1 - 1/\alpha^2) \;, \\ \lim_{n\to\infty} F_n &= -2/\alpha \;. \end{aligned}$$

Merk op dat de coëfficiënt E_n asymptotisch begrensd is door $0 < E_n \le 2$, terwijl F_n willekeurig groot kan worden.

3.3 Sterke convergentie

Onder de strengere Szegő-voorwaarde kunnen we ook de sterke convergentie van ORF op I bestuderen, zoals gegeven in volgende stelling.

Stelling 5. *Veronderstel dat de rij* $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ *wegblijft van I en dat* μ *voldoet aan de Szegő-voorwaarde*

$$\int_{-1}^{1} \frac{\log \mu'(x)}{\sqrt{1-x^2}}\, dx > -\infty.$$

Neem $\mathring{\mu}$ de geassocieerde maat op de eenheidscirkel en $\sigma(\mathring{\mu}', z)$ de bijhorende Szegő-functie. Dan geldt er gelijkmatig op compacten van $\overline{\mathbb{C}}^I$ dat

$$\lim_{n\to\infty} c_n B_n(z) \frac{1-\beta_n z}{\sqrt{1-\beta_n^2}} \varphi_n(x) = \frac{1}{\sqrt{2\pi}\sigma(\mathring{\mu}', z)}$$

met $z = J^{-1}(x)$, $\beta_k = J^{-1}(\alpha_k)$ en $c_n = \pm 1$ zodanig dat $E_n > 0$.

In het bijzonder geldt er dat

$$\lim_{n\to\infty} \varphi_n(x) = \infty$$

puntsgewijze voor $x \in \overline{\mathbb{C}}^I$.

3.4 Zwakke-sterconvergentie

Als laatste convergentieresultaat bekijken we de zwakke-sterconvergentie voor ORF op I. We geven alleen de belangrijkste stelling, die een klassiek resultaat van Rakhmanov voor de veeltermsituatie veralgemeent.

Stelling 6. *Veronderstel dat μ voldoet aan de Erdős-Turán-voorwaarde en dat de rij A wegblijft van I. Dan geldt er dat*

$$\frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}} \varphi_n^2(x) d\mu(x) \overset{*}{\longrightarrow} \frac{1}{\pi} \frac{dx}{\sqrt{1-x^2}}.$$

4 Kwadratuurformules

Numerieke integratie vormt een bijzonder belangrijk onderzoeksgebied binnen de toegepaste wiskunde. In dit hoofdstuk bekijken we de convergentie van gaussische kwadratuurformules gebaseerd op ORF op het interval $[-1, 1]$ en hun relatie met formules op de eenheidscirkel, alsook het verband tussen gaussische en meer algemene interpolerende formules.

4.1 Kwadratuurformules op $[-1, 1]$

Om de convergentie van rationale kwadratuurformules op I te bestuderen, hebben we informatie nodig omtrent de dichtheid van rationale functies in de L^p-ruimtes en de continue functies. Hiervoor bewezen we volgende stelling.

Stelling 7. *De ruimte $\mathcal{L} = \cup_0^\infty \mathcal{L}_n$ is dicht in elke $L^p(I)$-ruimte met $p \geq 1$ alsook in de ruimte $C(I)$ van contiue functies op I als en slechts als $\sum_{k=1}^{\infty}(1 - |\beta_k|) = \infty$, met $\beta_k = J^{-1}(\alpha_k)$.*

We beschouwen een kwadratuurformule $I_n(f) = \sum_{k=1}^{n} \lambda_{nk} f(x_{nk})$ exact voor $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$. De knooppunten zijn de nulpunten van $\varphi_n(x)$. Met behulp van vorige stelling is de convergentie van deze formules eenvoudig te bewijzen.

Stelling 8. *Onder dezelfde voorwaarden als in de vorige stelling, geldt er dat* $\lim_{n\to\infty} I_n(f) = I_\mu(f) = \int_{-1}^{1} f(x) d\mu(x)$ *voor elke* f *in* $C(I)$.

Indien $f \notin \mathcal{L}_n \cdot \mathcal{L}_{n-1}$ toonden we aan dat de kwadratuurfout $e_n(f) = I_\mu(f) - I_n(f)$ is zoals in de volgende stelling.

Stelling 9. *Veronderstel dat* f *analytisch is in een gesloten enkelvoudig samenhangend gebied* Ω *dat het interval* $[-1, 1]$ *bevat. Neem* C *een Jordancurve gelegen in* Ω *die de knooppunten* $\{x_{nk}\}_{k=1}^{n}$ *omsluit. Dan is*

$$e_n(f) = \frac{1}{2\pi\mathbf{i}} \int_C \frac{f(t)}{(1 - t/\alpha_n)\varphi_n^2(t)} \left\{ \int_{-1}^{1} \frac{\varphi_n^2(x)(1 - x/\alpha_n)}{t - x} d\mu(x) \right\} dt.$$

4.2 Een verband tussen het interval en de cirkel

In de vorige paragraaf werden alleen kwadratuurformules op I beschouwd, maar we kunnen ook gaussische formules op de complexe eenheidscirkel opstellen. Gebruik makende van de Joukowski-transformatie vinden we dan een verband tussen beide formules, zoals aangegeven in volgende stelling. De formules op de cirkel zijn exact voor $f \in \mathring{\mathcal{L}}_{n-1} \cdot \mathring{\mathcal{L}}_{(n-1)*}$ en de knooppunten zijn in dit geval de nulpunten van $\phi_n(z) + \phi_n^*(z)$.

Stelling 10. *Laat* $\varphi_n(x)$ *en* $\tilde{\phi}_{2n}(z)$ *de ORF op respectievelijk* I *en* $\mathbb{T}$ *voorstellen, gerelateerd via de Joukowski-transformatie. Neem* $\{x_{nk}\}_{k=1}^{n}$ *en* $\{\lambda_{nk}\}_{k=1}^{n}$ *de knopen en gewichten overeenkomstig* φ_n, *en* $\{z_{2n,k}\}_{k=1}^{2n}$ *en* $\{\mathring{\lambda}_{2n,k}\}_{k=1}^{2n}$ *de knopen en gewichten die horen bij* $\hat{\phi}_{2n}$. *Dan kunnen we de* $\{z_{2n,k}\}$ *zodanig ordenen dat*

$$z_{2n,n+k} = \overline{z}_{2n,k}, \quad k = 1, \ldots, n$$

en

$$x_{nk} = \Re\{z_{2n,k}\}, \quad k = 1, \ldots, n.$$

In dat geval geldt er dat

$$\lambda_{nk} = 2\pi\mathring{\lambda}_{2n,k} = 2\pi\mathring{\lambda}_{2n,n+k}, \quad k = 1, \ldots, n.$$

Een uitbreiding naar Gauss-Lobatto en Gauss-Radau kwadratuurformules ligt voor de hand, maar dit werd niet verder onderzocht.

4.3 Interpolerende kwadratuurformules

De interpolerende formules in deze paragraaf hebben als knooppunten de nulpunten van φ_n, maar integreren exact ten opzichte van een andere maat $\tilde{\mu}$. De gewichten A_{nk} worden gegeven door

$$A_{nk} = \int L_{nk}(x) d\tilde{\mu}(x), \quad k = 1, \ldots, n$$

waar $L_{nk}(x) \in \mathcal{L}_{n-1}$ de interpolerende rationale functie is door de nulpunten van $\varphi_n(x)$ (naar analogie met de Lagrangeveeltermen). De formule

$$\sum_{k=1}^{n} A_{nk} f(x_{nk}) \approx \int_{-1}^{1} f(x) d\tilde{\mu}(x)$$

is exact in $\mathcal{L}_{n-1}$. We kunnen nu een verband afleiden tussen de gaussische gewichten λ_{nk} en de gewichten A_{nk}.

Stelling 11. *Definieer* $\mathrm{k}_n(x) = \int k_n(x,t) d\tilde{\mu}(t)$*. Dan geldt er dat*

$$A_{nk} = \mathrm{k}_{n-1}(x_{nk}) \lambda_{nk}$$

voor $k = 1, \ldots, n$.

Indien zowel μ als $\tilde{\mu}$ absoluut continu zijn, vormt $\mathrm{k}_n(x)$ de n-de partieelsom in de Fourierreeksontwikkeling van $\tilde{\mu}'(x)/\mu'(x)$ in termen van de functies $\varphi_n(x)$.

5 Interpolatie-algoritmes

In dit hoofdstuk geven we een eenvoudig algoritme om de recursiecoëfficiënten te berekenen, gebaseerd op interpolatie-eigenschappen van de Riesz-Herglotz-Nevanlinna-transformatie van μ. Een foutenanalyse echter toont aan dat dit algoritme zeer onstabiel is en eigenlijk alleen maar van theoretisch belang is (o.a. omwille van een verband met kettingbreuken en Schur-algoritmes).

5.1 Een algoritme om E_n en F_n te berekenen

Definieer $\Gamma_0(z)$ als

$$\Gamma_0(z) = -\int \frac{d\mu(t)}{t - z},$$

en recursief

$$\Gamma_n(z) = E_n Z_{n-1}(z) + F_n - \frac{E_n / E_{n-1}}{\Gamma_{n-1}(z)}, \quad n \geq 1$$

(merk op dat deze formule aanleiding geeft tot een kettingbreukontwikkeling van de functie Γ_0). Stel ook $\Delta_0(z) = \Gamma_0'(z)$ en

$$\Delta_n(z) = Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)}{\Gamma_{n-1}^2(z)}, \quad n \geq 1.$$

Dan konden we aantonen dat

$$F_n = -E_n Z_{n-1}(\alpha_n) + \frac{E_n/E_{n-1}}{\Gamma_{n-1}(\alpha_n)}, \quad n \geq 1.$$

en

$$E_n = \frac{1}{|\alpha_n|}\sqrt{\frac{-1}{\Delta_n(\alpha_n)}}, \quad n \geq 1$$

op voorwaarde dat alle polen verschillend zijn van elkaar. Deze formules vormen een recursief algoritme om de coëfficiënten te berekenen, vertrekkende van de Stieltjes-transformatie en zijn afgeleide geëvalueerd in de polen. Verschillende voorbeelden echter tonen aan dat dit algoritme zeer onstabiel is. In de volgende paragraaf leggen we uit waarom.

5.2 Foutenanalyse

Veronderstellen we dat we alle coëfficiënten E_k en F_k kennen voor $k = 1, \ldots, n$ en we willen E_{n+1} en F_{n+1} berekenen. Indien we de relatieve fout op $\Gamma_n(z)$ voorstellen door $\gamma_n^r(z)$, dan kunnen we aantonen dat deze snel naar oneindig gaat met toenemende n. Voor het geval van orthogonaliteit op $[-1, 1]$ ten opzichte van een maat die voldoet aan de Szegő-voorwaarde, vinden we de volgende expliciete formule,

$$|\gamma_n^r(z)| \approx \left| \frac{\Gamma_0(t)(1 - \beta_{n-1}\beta_n)}{\pi(t^2 - 1)\sigma^2(\mathring{\mu}', z)B_n(z)B_{n-1}(z)(1 - \beta_n z)(1 - \beta_{n-1}z)} \right| \epsilon$$

waar ϵ de machineprecisie is. Deze uitdrukking moet geëvalueerd worden in α_{n+1} om een schatting te krijgen voor de relatieve fout op E_{n+1} en F_{n+1}. Aangezien de Blaschke producten naar nul convergeren, zal de fout snel naar oneindig gaan. Als voorbeeld nemen we polen die exponentieel naar oneindig gaan, $\alpha_n = a^n$ met $a > 1$. We vinden dan dat $|\gamma_n^r(\alpha_{n+1})| = O(a^{n^2})$. Dit is behoorlijk onstabiel.

5.3 Een meervoudige pool

Indien alle polen gelijk zijn aan elkaar, kunnen we een gelijkaardig algoritme geven. Nu hebben we de Stieltjes-transformatie en al zijn afgeleiden nodig in de pool α. Ook dit algoritme is zeer onstabiel en geeft alleen goede resultaten voor kleine waarden van n. In het volgende hoofdstuk zullen we zien dat alle algoritmes die gebaseerd zijn op het gebruik van de (rationale) momenten van de maat μ, onvermijdelijk zullen falen omwille van slechte conditie. Deze momenten zijn net de functiewaarden van Γ_0 en zijn afgeleiden in de polen.

6 Algoritmes gebaseerd op momenten

In het rationale geval verstaan we onder 'momenten' integralen van de vorm $\int (z-\alpha_n)^{-k} d\mu(z)$ (waarbij k niet groter is dan de meervoudigheid van de pool α_n). We hebben verschillende algoritmes ontwikkeld om, uitgaande van deze momenten, de recursiecoëfficiënten te berekenen (bijvoorbeeld de interpolatie-algoritmes uit het vorige hoofdstuk). In dit hoofdstuk tonen we aan dat deze berekeningen slecht geconditioneerd zijn.

6.1 Conditie in het geval van gewone momenten

Om de conditie van dit probleem te bestuderen, beschouwen we de afbeelding van de momenten naar de coëfficiënten als bestaande uit twee aparte afbeeldingen (van de momenten naar de kwadratuurformule en van de kwadratuurformule naar de coëfficiënten). De slecht geconditioneerde afbeelding is de eerste, die we hier noteren met $K_n^{(2)}$. We kunnen dan de volgende stelling bewijzen.

Stelling 12. *Het conditiegetal* $\operatorname{cond} K_n^{(2)}$ *voldoet aan de vergelijking*

$$\operatorname{cond} K_n^{(2)} \geq c_n \frac{\|\underline{\mu}\|}{\|\underline{q}\|} \frac{\lim_{x\to\infty} \varphi_n^2(x)}{\min_{1\leq i\leq n}\{\lambda_{ni}[\varphi_n'(x_{ni})]^2|x_{ni}-\alpha_n|\}} ,$$

waar $c_n > 0$ *een constante is die alleen van* n *en van de definitie van de matrixnorm afhangt. Indien we de* 1*-norm of de* ∞*-norm gebruiken, dan is* $c_n = 1$*. In het geval van het interval* $[-1,1]$*, met polen* A *die wegblijven van de randen en een maat* μ *die voldoet aan de Erdős-Turán-voorwaarde* $\mu' > 0$ *a.e., hebben we de asymptotische ondergrens*

$$\operatorname{cond} K_n^{(2)} \gtrsim c_n \frac{\|\underline{\mu}\|}{\|\underline{q}\|} \frac{1}{64\pi} \frac{(1-\rho)^7}{n\rho^{2n-1}} ,$$

waar $\beta_k = J^{-1}(\alpha_k)$ *en* $\rho = \sup_{1\leq k\leq n} |\beta_k|$*.*

Merk op dat de laatste formule aangeeft dat het conditiegetal exponentieel toeneemt voor grote n.

6.2 Gewijzigde momenten

Voor het veeltermgeval ontwikkelde Gautschi een methode gebaseerd op gewijzigde momenten, die niet slecht geconditioneerd is. We kunnen deze methode gedeeltelijk veralgemenen naar rationale functies, indien we veronderstellen dat alle polen gelijk zijn aan elkaar.

Veronderstel dan dat we beschikken over een stel ORF $\tilde{\varphi}_n$ met alle polen gelijk aan α en die orthogonaal zijn ten opzichte van $\tilde{\mu}$ en dat we hiermee de functies φ_n willen berekenen, orthogonaal ten opzichte van μ. Hiervoor hebben we de gewijzigde momenten $\nu_k = \int \tilde{\varphi}_k(x) d\mu(x)$ nodig. Uitgaande van deze momenten kunnen we (recursief) de matrix M opstellen, die de inwendige producten $\langle \tilde{\varphi}_i , \tilde{\varphi}_j \rangle_\mu$ bevat. Indien we de Cholesky-factorizatie van M noteren als $M = R^T R$ en $S = [s_{ij}] = R^{-1}$, dan kunnen we aantonen dat het verband tussen de recursiecoëfficiënten voor φ_n en die voor $\tilde{\varphi}_n$ gegeven wordt door de formules

$$E_n = \frac{s_{nn}}{s_{n-1,n-1}} \tilde{E}_n,$$

$$F_n = \frac{s_{n-1,n}}{s_{n-1,n-1}} + \frac{s_{nn}}{s_{n-1,n-1}} \tilde{F}_n - \frac{s_{n-2,n-1} s_{nn}}{s_{n-1,n-1}^2} \frac{\tilde{E}_n}{\tilde{E}_{n-1}}.$$

Experimenten tonen aan dat ook in dit geval het probleem niet langer slecht geconditioneerd is, maar we hebben dit niet verder geanalyseerd. Een eventueel nadeel van deze methode is dat de gewijzigde momenten (zeker voor het rationale geval) niet zomaar voorhanden zijn en in veel gevallen moeilijk uit te rekenen zijn.

7 Berekening van ORF op een interval

De algoritmes uit de vorige hoofdstukken waren niet echt bruikbaar om orthogonale rationale functies te berekenen voor hoge graad, omwille van de slechte conditie. Een andere manier om het probleem aan te pakken bestaat erin de expliciete formules voor de recursiecoëfficiënten uit te rekenen, waarbij we de integralen benaderen met behulp van één of andere kwadratuurformule. Indien we hiervoor een rationale Gauss-formule gebruiken, kunnen we zelfs nauwkeurige foutenschattingen bekomen, gegeven in volgende paragraaf.

7.1 Foutenanalyse

Veronderstellen we dat de doelfuncties φ_k polen hebben in A en orthogonaal zijn ten opzichte van μ, en de functies $\tilde{\varphi}_k$ voor de kwadratuurformule polen hebben in $\tilde{A}$. We willen m coëfficiënten berekenen, gebruik makende van een n-punts-kwadratuurformule. Om de fout te kunnen analyseren, moeten we verder nog volgende veronderstellingen maken:

- m en n zijn groot,
- A en $\tilde{A}$ blijven weg van het interval,
- μ voldoet aan Szegő's voorwaarde,
- de fout op de coëfficiënten is ongeveer gelijk aan $\Delta_{nm} = e_n(Z_m\phi_{m-1}^2)$.

We kunnen dan deze stelling bewijzen.

Stelling 13. *Stel* $\rho_1 = \min_{1\leq k\leq m}|\alpha_k|$. *Dan hebben we*

$$\Delta_{nm} \lesssim \min_{1\leq r<\rho_1} J^{-1}(r) \max_{0\leq\theta\leq\pi} \frac{(1-\beta_{m-1}^2)|1+z^2|}{|1-\beta_m z|^2|1-\beta_{m-1}z|^2} \frac{|\tilde{B}_n(z)\tilde{B}_{n-1}(z)|}{|B_m(z)B_{m-1}(z)|}$$

met $z = J^{-1}(t)$ *en* $t = re^{\mathbf{i}\theta}$. *Indien* $A = \{\alpha, \alpha, \ldots\}$, *stel dan* $\rho_2 = min_{1\leq k\leq n}|1/\tilde{\beta}_k - \beta|$. *In dit geval hebben we*

$$\Delta_{nm} \lesssim \min_{0<r<\rho_2} \frac{1-\beta^2}{r^{2m-2}} \max_{0\leq\theta\leq\pi} |1+z^2||\tilde{B}_n(z)\tilde{B}_{n-1}(z)||1-\beta z|^{2m-5}$$

met $z = \beta + re^{\mathbf{i}\theta}$.

De β's in deze stelling zijn uiteraard de Joukowski-getransformeerde polen. In praktische toepassingen zouden we deze formules graag in de andere richting kunnen gebruiken: hoeveel punten hebben we nodig in de kwadratuurformule om een gevraagde precisie te bereiken? Deze vraag wordt beantwoord in de volgende stelling.

Stelling 14. *Veronderstel dat* $\tilde{A} = \{\tilde{\alpha}, \tilde{\alpha}, \ldots\}$ *en noem de gevraagde precisie* ϵ. *Indien voor elke* n *het zadelpunt uit vorige stelling stationair is, dan hebben we*

$$n \gtrsim \min_{1\leq r<\rho_1} \max_{0\leq\theta\leq\pi} \frac{1}{2} \frac{\log\left(\frac{J^{-1}(r)(1-\beta_{m-1}^2)|1+z^2|}{\epsilon|1-\beta_m z|^2|1-\beta_{m-1}z|^2|B_m(z)B_{m-1}(z)|}\right)}{\log\left|\frac{1-\tilde{\beta}z}{z-\tilde{\beta}}\right|} + \frac{1}{2}.$$

Als bovendien $A = \{\alpha, \alpha, \ldots\}$ *dan hebben we*

$$n \gtrsim \min_{0\leq r<\rho_2} \max_{0\leq\theta\leq\pi} \frac{1}{2} \frac{\log\left(\frac{(1-\beta^2)|1+z^2||1-\beta z|^{2m-5}}{\epsilon r^{2m-2}}\right)}{\log\left|\frac{1-\tilde{\beta}z}{z-\tilde{\beta}}\right|} + \frac{1}{2}.$$

We noemen een zadelpunt stationair *indien de eerste-orde-afgeleiden in de* r- *en* θ-*richting er gelijk zijn aan nul.*

Verschillende experimenten tonen aan dat deze schattingen voldoende nauwkeurig zijn. Indien de polen A ver van het interval liggen, blijkt ook dat het gebruik van rationale kwadratuurformules niet nodig is. De klassieke Gauss-formules volstaan. Voor polen dicht bij de rand echter zouden we teveel punten nodig hebben in deze kwadratuurformules en dan is het gebruik van rationale formules wel nuttig. We bekijken dit geval apart.

7.2 Polen dicht bij de rand

Indien we veronderstellen dat $A = \{\alpha, \alpha, \ldots\}$ en $\tilde{A} = \{\tilde{\alpha}, \tilde{\alpha}, \ldots\}$, dan kunnen we een nauwkeurigere benadering vinden voor de fout Δ_{nm}. Voor het geval $\tilde{\alpha} = \infty$ (gewone Gauss-kwadratuur) krijgen we dan

$$\Delta_{nm} \approx (1 - \beta^4)\beta^{2n-2m+1} F_{m,n}(\beta)$$

waar de veelterm $F_{m,n}(\beta)$ gegeven wordt door

$$\sum_{k=0}^{2m-5} \frac{(-1)^k}{k!(2m-2-k)!} \big[(2n+1)_{2m-2-k}\beta^2 + \cdots \\ \cdots (2n-1)_{2m-2-k}\big] \beta^{2k}(2m-5)_k(1-\beta^2)^{2m-5-k}.$$

Deze formules geven duidelijk aan dat de fout toeneemt indien β van 0 naar 1 beweegt. We kunnen een gelijkaardige formule geven voor $\tilde{\alpha} \neq \infty$, maar deze is aanzienlijk ingewikkelder. Het belang van deze formules is dat ze toelaten om te schatten hoeveel coëfficiënten we kunnen berekenen tot op een gevraagde nauwkeurigheid, gegeven een bepaalde kwadratuurformule. Hiervoor bekijken we de hoogtelijnen van deze formules voor vaste n and $\tilde{\beta}$.

Hiermee is het probleem echter nog niet opgelost, want we veronderstellen dat we een stel ORF kennen om een gelijkaardig stel te berekenen. Een andere methode is het gebruik van kwadratuurformules gebaseerd op Laurent-veeltermen. Voor gewichtsfuncties van de vorm $\mu'(x) = (1-x^2)^{c-1/2}$ met $c > -1/2$ bestaan er n-punts-kwadratuurformules die exact zijn voor

$$f(x) = \frac{p_{2n-1}(x)}{(x-\alpha)^n} \frac{1}{(\alpha - x)^c}, \quad p_{2n-1} \in \mathcal{P}_{2n-1}.$$

Enigszins verrassend (omwille van de irrationale factor in de noemer) is dat deze formules ook zeer goede resultaten geven indien we rationale functies integreren. Dit wordt verklaard doordat de hoge graad van de tellerveelterm compenseert voor de factor in de noemer, zoals we konden aantonen in volgende stelling.

Stelling 15. *Noteer met* $e_n(f)$ *de kwadratuurfout in de formules gebaseerd op Laurentveeltermen, dan hebben we*

$$|e_n(f_m)| \leq \epsilon_{n-1} \|f_m\|_I \frac{2\sqrt{\pi}\,\Gamma(c+1/2)\,\delta^{2c}}{\Gamma(c+1)}$$

voor $f_m \in \mathcal{L}_m$ *en* $m \leq n$*, waar*

$$\epsilon_{n-1} = \min_{p_{n-1}\in\mathcal{P}_{n-1}} \|(\alpha-x)^c - p_{n-1}(x)\|_I\,,$$

Γ *is de Gamma-functie en* $\|\cdot\|_I$ *is de supremumnorm op* I*. De constante* δ *is gelijk aan* $\delta = \sqrt{\alpha+1} - \sqrt{\alpha-1}$.

Deze stelling laat duidelijk zien dat de kwadratuurfout kleiner zal zijn naarmate $(\alpha - x)^c$ beter kan benaderd worden door een veelterm. Experimenten bevestigen dat we met een n-punts-formule $n/2$ coëfficiënten nauwkeurig kunnen berekenen, zoals voorspeld door de stelling.

8 ORF op een halfrechte

De reden dat we tot nu toe onze aandacht bijna uitsluitend hebben gevestigd op orthogonaliteit op een interval, is dat we formules konden afleiden die de berekening van ORF op een halfrechte herleiden tot het geval van een interval.

8.1 De halfrechte transformeren naar het interval

Met behulp van de transformatie

$$\tau(x) = \frac{1-x}{1+x}, \quad x \in [0,\infty]$$

kunnen we de halfrechte $[0,\infty)$ transformeren naar $[-1,1]$. Stel dan dat we een maat $\tilde{\mu}$ hebben op $[0,\infty]$ en polen $\tilde{A}$ in $(-\infty,0)$. Dan wordt het verband tussen de oorspronkelijke recursiecoëfficiënten $\{\tilde{E}_n,\tilde{F}_n\}$ en de coëfficiënten $\{E_n,F_n\}$ van de naar het interval getransformeerde functies gegeven door de volgende formules.

Stelling 16. *De volgende relaties gelden tussen* $\{E_n,F_n\}$ *en* $\{\tilde{E}_n,\tilde{F}_n\}$ *voor* $n \geq 1$,

$$\tilde{E}_n = [2E_n - \delta_{n1}(E_1+F_1)]\left(1-\frac{1}{\alpha_{n-1}}\right)^{-1}\left(1-\frac{1}{\alpha_n}\right)^{-1},$$

$$\tilde{F}_n = -\left(1-\frac{1}{\alpha_n}\right)^{-1}\left[F_n\left(1-\frac{1}{\alpha_{n-1}}\right) + E_n - \delta_{n2}\frac{E_2}{E_1}\frac{1-1/\alpha_1}{F_1-E_1}\right].$$

Merk op dat deze formules vereenvoudigen voor $n > 2$ omwille van de Kronecker symbolen.

8.2 Asymptotisch gedrag

Het asymptotisch gedrag van ORF op een halfrechte is in het algemeen moeilijker te bestuderen dan dat van ORF op een interval. Nochtans kunnen we de transformatie uit dit hoofdstuk gebruiken om onder bepaalde voorwaarden de convergentie van ORF orthogonaal op $[0, \infty]$ af te leiden. We moeten dan veronderstellen dat de polen wegblijven van 0, maar ook van ∞ (wat het veeltermgeval uitsluit). We geven het resultaat voor het geval waar alle polen gelijk zijn aan elkaar.

Stelling 17. *Stel $\tilde{\mu}$ is een maat op $[0, \infty)$ die voldoet aan de voorwaarde $\tilde{\mu}' > 0$ a.e. en veronderstel dat alle polen gelijk zijn aan elkaar, $\tilde{A} = \{\tilde{\alpha}, \tilde{\alpha}, \ldots\}$ met $\tilde{\alpha} \in (-\infty, 0]$. Dan geldt er gelijkmatig op compacten van $\overline{\mathbb{C}} \setminus [0, \infty)$ dat*

$$\lim_{n\to\infty} \frac{\tilde{\varphi}_n(x)}{\tilde{\varphi}_{n-1}(x)} = \frac{(\sqrt{-x} + \sqrt{-\tilde{\alpha}})^2}{x - \tilde{\alpha}}$$

waar de tak van de wortel zodanig is dat de limiet reëel is voor $x < 0$. Voor de recursiecoëfficiënten hebben we

$$\lim_{n\to\infty} E_n = -\frac{4}{\tilde{\alpha}},$$
$$\lim_{n\to\infty} F_n = -2.$$

We hebben ook de zwakke-sterconvergentie

$$(x - \tilde{\alpha})\tilde{\varphi}_n^2(x) d\tilde{\mu}(x) \xrightarrow{*} \frac{\sqrt{-\tilde{\alpha}}}{\pi} \frac{dx}{(1+x)\sqrt{x}}.$$

9 Gevalstudie: Chebyshev ORF

In dit hoofdstuk bestuderen we een rationale veralgemening van de klassieke Chebyshev-veeltermen. We geven expliciete uitdrukkingen voor deze functies en de recursiecoëfficiënten en bespreken een efficiënte methode om de bijhorende kwadratuurformules op te stellen.

9.1 Chebyshev orthogonale rationale functies

We beschouwen ORF met betrekking tot de gewichtsfuncties

$$w(x) = \begin{cases} (1-x^2)^{-1/2}, \\ (1-x^2)^{1/2}, \\ \left(\frac{1-x}{1+x}\right)^{1/2} \end{cases}$$

op het interval $[-1, 1]$ en met willekeurige reële polen buiten dit interval. Gebruiken we de notatie $\varphi_n^{(i)}$ voor de ORF met betrekking tot de i-de gewichtsfunctie ($i = 1, 2, 3$), dan kunnen we volgende expliciete formules bewijzen.

Stelling 18. *De orthogonale functies* $\varphi_n^{(i)}$ *worden gegeven door*

$$\varphi_n^{(1)}(x) = \frac{1}{\sqrt{2\pi}}\sqrt{1-\beta_n^2}\left(\frac{zB_{n-1}(z)}{1-\beta_n z} + \frac{1}{(z-\beta_n)B_{n-1}(z)}\right),$$

$$\varphi_n^{(2)}(x) = \sqrt{\frac{2}{\pi}}\sqrt{1-\beta_n^2}\frac{z}{z^2-1}\left(\frac{z^2B_{n-1}(z)}{1-\beta_n z} - \frac{1}{zB_{n-1}(z)(z-\beta_n)}\right),$$

$$\varphi_n^{(3)}(x) = \frac{1}{\sqrt{\pi}}\frac{1}{z-1}\sqrt{1-\beta_n^2}\left(\frac{z^2B_{n-1}(z)}{1-\beta_n z} - \frac{1}{(z-\beta_n)B_{n-1}(z)}\right),$$

waar $x = J(z) \in \overline{\mathbb{C}}$ *en* $\alpha_k = J(\beta_k)$.

Ook voor de recursiecoëfficiënten kunnen we expliciete formules geven. Merk op dat deze formules overeenkomen met de asymptotische waarden zoals gegeven in het hoofdstuk over asymptotiek. Ook dit is een veralgemening van het veeltermgeval.

Stelling 19. *Voor* $n > 1$ *zijn de recursiecoëfficiënten voor de* $\varphi_n^{(i)}(x)$ *dezelfde in de drie gevallen en ze worden gegeven door*

$$E_n = 2\frac{\sqrt{(1-\beta_{n-1}^2)(1-\beta_n^2)}(1-\beta_{n-1}\beta_n)}{(1+\beta_{n-1}^2)(1+\beta_n^2)},$$

$$F_n = -\sqrt{\frac{1-\beta_n^2}{1-\beta_{n-1}^2}}\frac{(1-\beta_{n-1}^2)(\beta_n+\beta_{n-2}) + 2\beta_{n-1}(1-\beta_n\beta_{n-2})}{(1+\beta_n^2)(1-\beta_{n-1}\beta_{n-2})},$$

waar $\beta_k = J^{-1}(\alpha_k)$. *Voor* $n = 1$ *hebben we*

$$E_1^{(1)} = \sqrt{2}c \qquad E_1^{(2)} = 2c \qquad E_1^{(3)} = 2c$$

$$F_1^{(1)} = -\sqrt{2}\beta_1 c \qquad F_1^{(2)} = -\beta_1 c \qquad F_1^{(3)} = (1-\beta_1)c$$

waar

$$c = \frac{\sqrt{1-\beta_1^2}}{1+\beta_1^2}.$$

Voor $n = 2$ geldt de formule voor F_2 op voorwaarde dat we stellen $\beta_0 = 0$.

9.2 Kwadratuurformules

De knooppunten en gewichten in de kwadratuurformules geassocieerd aan deze functies kunnen eenvoudig en efficiënt berekend worden. De knooppunten kunnen met behulp van de methode van Newon-Raphson berekend worden uit volgende formules. We kunnen aantonen dat de functie $f_n(\theta)$ in deze stelling strikt stijgend is, zodat deze methode goed zal werken.

Stelling 20. *Noteer met $x_{nk}^{(i)}$ de nulpunten van $\varphi_n^{(i)}(x)$ en stel $x_{nk}^{(i)} = \cos\theta_{nk}^{(i)}$ dan voldoen ze aan de vergelijkingen*

$$\begin{aligned}
&f_n(\theta_{nk}^{(1)}) - (n-1)\theta_{nk}^{(1)} = \frac{\pi}{2}(2k-1),\\
&f_n(\theta_{nk}^{(2)}) - (n-2)\theta_{nk}^{(2)} = \pi k,\\
&f_n(\theta_{nk}^{(3)}) - (n-3/2)\theta_{nk}^{(3)} = \pi k,
\end{aligned}$$

voor $k = 1, 2, \ldots, n$ waar

$$f_n(\theta) = 2\sum_{j=1}^{n-1} \arctan\frac{\sin\theta}{\cos\theta - \beta_j} + \arctan\frac{\sin\theta}{\cos\theta - \beta_n}.$$

en $\arctan(y/x)$ is het argument van het complexe getal $x + \mathbf{i}y$.

De gewichten in de kwadratuurformules kunnen geschreven worden in functie van de knooppunten, zoals hierna wordt aangegeven.

Stelling 21. *De gewichten in de gaussische kwadratuurformule gebaseerd op de $\varphi_n^{(i)}$ kunnen geschreven worden in functie van de knooppunten als volgt,*

$$\begin{aligned}
&\lambda_{nk}^{(1)} = 2\pi\left(1 + g_n(x_{nk}^{(1)})\right)^{-1},\\
&\lambda_{nk}^{(2)} = 2\pi(1-(x_{nk}^{(2)})^2)\left(3 + g_n(x_{nk}^{(2)})\right)^{-1},\\
&\lambda_{nk}^{(3)} = 2\pi(1-x_{nk}^{(3)})\left(2 + g_n(x_{nk}^{(3)})\right)^{-1}
\end{aligned}$$

voor $k = 1, 2, \ldots, n$ waar

$$g_n(x) = 2\sum_{k=1}^{n-1}\frac{\sqrt{1-1/\alpha_k^2}}{1-x/\alpha_k} + \frac{\sqrt{1-1/\alpha_n^2}}{1-x/\alpha_n}.$$

Experimenten tonen aan dat deze formules zeer snel en nauwkeurig gebruikt kunnen worden om de kwadratuurformules op te stellen, zelfs voor grote waarden van n, vooral indien alle polen gelijk zijn aan elkaar.

10 Besluit

10.1 Belangrijkste bijdragen

In deze thesis hebben we verschillende nieuwe resultaten gevonden over orthogonale rationale functies, zowel theoretisch als numeriek. De meeste aandacht is gegaan naar orthogonaliteit op een eindig interval, waarvoor nog geen resultaten beschikbaar waren.

Enkele van de belangrijkste theoretische bijdragen hebben we geleverd in de studie van het asymptotisch gedrag van orthogonale rationale functies. We bestudeerden de asymptotiek van de verhoudingen en aan de hand daarvan de convergentie van de recursiecoëfficiënten. Daarnaast vonden we ook interessante resultaten in verband met sterke en zwakke-sterconvergentie.

De interpolatie-algoritmes vormen eigenlijk een overgang van theoretische naar berekeningsaspecten. Hoewel het algoritmes zijn om de recursiecoëfficiënten te berekenen, zijn ze in praktijk niet echt bruikbaar omwille van de sterke foutengroei. In deze foutenanalyse speelden de eerder afgeleide convergentieresultaten een cruciale rol.

De rest van de thesis was voornamelijk gericht op berekeningsaspecten van ORF. Hiernaar was voordien nog nauwelijks of geen aandacht gegaan, maar met het onderzoek in deze thesis kunnen we dit probleem als bijna afgehandeld beschouwen. De berekening van ORF met polen niet te dicht bij de rand kan gebeuren met klassieke kwadratuurformules uit het veeltermgeval. Gebruik makende van de asymptotische resultaten uit het eerste deel van de thesis konden we ook nauwkeurige foutenschattingen maken. Voor polen dicht bij het interval hebben we een gedeeltelijke oplossing gegeven, gebaseerd op Laurent-veeltermen, voor een aantal specifieke gewichtsfuncties en voor alle polen gelijk aan elkaar. De overblijvende gevallen dienen nog verder onderzocht te worden.

Ook hebben we de bekende methode van de gewijzigde momenten voor de berekening van orthogonale veeltermen veralgemeend naar het rationale geval, indien alle polen gelijk zijn aan elkaar. Het meer algemene geval lijkt veel ingewikkelder te zijn. Bovendien kunnen we ook functies op een halfrechte berekenen omdat we deze via een transformatie terugbrengen tot functies op een interval.

Het berekenen van ORF op de eenheidscirkel werd niet bestudeerd, maar de bijhorende kwadratuurformules kunnen we berekenen uitgaande van de formules voor het interval, zoals uitgelegd in het hoofdstuk over kwadratuurformules.

In het laatste hoofdstuk introduceerden we een rationale veralgemening van de klassieke Chebyshev-veeltermen. We gaven expliciete formules voor deze functies en hun recursiecoëfficiënten en legden uit hoe we efficiënt de kwadratuurformules kunnen opstellen. Dit hoofdstuk vormt een zeer belangrijke stap in het vinden van expliciete voorbeelden van ORF.

10.2 Verder onderzoek

We vermelden heel kort enkele onderwerpen voor mogelijk toekomstig onderzoek. Eerst en vooral is er op het vlak van asymptotisch gedrag nog zeer veel te bestuderen. Zowel convergentie op de drager van de maat, exponentiële gewichten (vooral van belang voor de halfrechte), voor polen die niet wegblijven van de rand, relatieve convergentie, convergentie van de kernfunctie enz. kan nog onderzocht worden.

Op het vlak van kwadratuurformules is het vooral belangrijk om formules te vinden die snel en eenvoudig uit te rekenen zijn, zoals in de gevalstudie van het laatste hoofdstuk. Rationale kwadratuurformules zijn vaak nog heel rekenintensief en dat wordt niet altijd gecompenseerd door de kleinere kwadratuurfout voor bepaalde integranden.

Nauw verwant hiermee is het zoeken naar expliciete voorbeelden van ORF, of tenminste functies die eenvoudig kunnen worden berekend. Dit is een van de meest fundamentele verschillen met het veeltermgeval, waar een grote diversiteit van expliciet gekende voorbeelden bestaat. Ook het berekenen van willekeurige ORF met polen zeer dicht bij de rand verdient nog verdere aandacht.

Een onderwerp dat helemaal niet aan bod is gekomen in deze thesis, maar dat dicht aanleunt bij convergentie van kwadratuurformules en dichtheidsproblemen, is dat van de momentenproblemen. ORF geven aanleiding tot zogenaamde *uitgebreide* momentenproblemen, waar de momenten gegeven zijn in verschillende punten. Voor het geval van de gehele reële rechte is dit reeds bestudeerd, maar er zijn nog geen resultaten op het interval. Dit zou echter een voor de hand liggend gevolg zijn van ons onderzoek.

Contents

Notations

List of symbols

A	sequence of poles in $\overline{\mathbb{R}} \setminus \{0\}$, $A = \{\alpha_1, \alpha_2, \ldots\}$
A_{nk}	interpolatory quadrature weight
α_k	real number in $\overline{\mathbb{R}} \setminus \{0\}$, outside $\operatorname{supp}(\mu)$
$b_n(z)$	basis function, $b_n(z) = Z_1(z) \ldots Z_n(z)$
B	sequence in $\mathbb{D}$, $B = \{\beta_1, \beta_2, \ldots\}$
$B_n(z)$	Blaschke product, $B_n(z) = \zeta_1(z) \ldots \zeta_n(z)$
β_k	complex number in $\mathbb{D}$
$\mathbb{C}$	set of complex numbers
$\overline{\mathbb{C}}$	Riemann sphere, $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$
$\mathbb{D}$	open unit disc, $\mathbb{D} = \{z : \lvert z\rvert < 1\}$
$D(t,z)$	kernel for the real line, $D(t,z) = -\mathbf{i}(1+tz)/(t-z)$
$\mathbb{E}$	exterior of closed unit disc, $\mathbb{E} = \{z : \lvert z\rvert > 1\}$
E_n, F_n	recurrence coefficients for φ_n
η_n	unimodular constant, $\eta_n = \prod_{k=1}^{n}(-\overline{\beta}_k/\lvert\beta_k\rvert)$
$\varphi_n(z)$	ORF of degree n associated with (A, μ)
$\varphi_n^{(i)}(z)$	Chebyshev ORF of type i
$\phi_n(z)$	ORF of degree n associated with $(B, \mathring{\mu})$
$\phi_{n,m}(z)$	OP of degree m with respect to varying measure $d\mathring{\mu}(\theta)/\lvert w_n(z)\rvert^2$ on $\mathbb{T}$
$\Gamma_n(z), \Delta_n(z)$	recursively defined functions in interpolation algorithm
$H_{ni}(z), \tilde{H}_{ni}(z)$	Hermite interpolating rational functions
$\mathbf{i}$	imaginary unit, $\mathbf{i}^2 = -1$
I	interval $[-1, 1]$
$J(z)$	Joukowski transform, $J(z) = \frac{1}{2}(z + z^{-1})$
κ_n	leading coefficient of φ_n in canonical basis
$\mathring{\kappa}_n$	leading coefficient of ϕ_n in canonical basis
$k_n(z,w)$	reproducing kernel for $\mathcal{L}_n$
$\mathring{k}_n(z,w)$	reproducing kernel for $\mathring{\mathcal{L}}_n$
$\mathrm{k}_n(x)$	rational function relating gaussian and interpolatory

	weights, $\mathrm{k}_n(x) = \int k_n(x,t)d\tilde{\mu}(t)$
$l_{ni}(z)$	fundamental Lagrange interpolating polynomial
$L_{ni}(z)$	Lagrange interpolating rational function
$\mathcal{L}_n$	space of rational functions of degree n on $X \subset \overline{\mathbb{R}}$, $\mathcal{L}_n = \{p_n/\pi_n : p_n \in \mathcal{P}_n\}$
$\mathring{\mathcal{L}}_n$	space of rational functions of degree n on $\mathbb{T}$, $\mathring{\mathcal{L}}_n = \{p_n/w_n^* : p_n \in \mathcal{P}_n\}$
$L^p(\mu)$	space of all measurable f such that $\|f\|_p < \infty$
λ_{nk}	quadrature weight corresponding to x_{nk}
$\mathring{\lambda}_{nk}$	quadrature weight corresponding to z_{nk}
μ	positive bounded Borel measure on $X \subset \overline{\mathbb{R}}$
μ_0	total mass of μ, $\mu_0 = \mu(\overline{\mathbb{R}})$
$\mathring{\mu}$	positive bounded Borel measure on $\mathbb{T}$
μ', $\mathring{\mu}'$	Radon-Nikodym derivative of μ and $\mathring{\mu}$ respectively
$\mathbb{N}$	set of natural numbers
$\nu_{n,m}$	leading coefficient of $\phi_{n,m}$ in canonical basis
$\Omega_\mu(z)$	transform of μ, $\Omega_\mu(z) = \int D(t,z)d\mu(t)$
$P(z,t)$	Poisson kernel, $P(z,t) = (1-\|t\|^2)/\|z-t\|^2$ for $z \in \mathbb{T}$
$\mathcal{P}_n$	space of polynomials of degree n
$\pi_n(z)$	polynomial $\pi_n(z) = (1 - z/\alpha_1)\ldots(1 - z/\alpha_n)$
$\psi_n(z)$	functions of the second kind, $\psi_n(z) = \int D(t,z)[\varphi_n(t) - \varphi_n(z)]d\mu(t)$
$Q_n(z,\tau)$	para-orthogonal rational function, $Q_n = \phi_n + \tau\phi_n^*$
$\mathbb{R}$	set of real numbers
$\overline{\mathbb{R}}$	extended real numbers, $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$
$R_n(z)$	remainder function in interpolation algorithm
$\sigma(h,z)$	Szegő function associated with h
$\mathrm{supp}(\mu)$	support of μ
$\mathbb{T}$	complex unit circle, $\mathbb{T} = \{z : \|z\| = 1\}$
$T_n(x)$	Chebyshev polynomial of degree n
$w_n(z)$	polynomial $w_n(z) = (z - \beta_1)\ldots(z - \beta_n)$
x_{nk}	zeros of $\varphi_n(x)$
X^I	complement of $I = [-1,1]$ with respect to X
z_{nk}	zeros of $Q_n(z,\tau)$
$\mathbb{Z}$	set of integers
$Z_n(z)$	basis factor, $Z_n(z) = z/(1 - z/\alpha_n)$
$\zeta_n(z)$	Blaschke factor, $\zeta_n(z) = -\overline{\beta}_n/\|\beta_n\| \cdot (z-\beta_n)/(1-\overline{\beta}_n z)$
$a_n \sim b_n$	$\lim_{n\to\infty} a_n/b_n = 1$
$f_*(z)$	substar conjugate, $f_*(z) = \overline{f(1/\overline{z})}$
$f_n^*(z)$	$f_n^*(z) = z^n f_{n*}(z)$ if $f_n \in \mathcal{P}_n$, $f_n^*(z) = B_n(z) f_{n*}(z)$ if $f_n \in \mathring{\mathcal{L}}_n$

$\|f\|_p$	L^p-norm of f, $\|f\|_p = (\int \|f\|^p d\mu)^{1/p}$
$\langle f\,, g\rangle$	inner product of f and g with respect to μ
$\mu_n \xrightarrow{*} \mu$	weak star convergence

Abbreviations

GEP	generalized eigenvalue problem
OP	orthogonal polynomial(s)
ORF	orthogonal rational function(s)

Chapter 1

Introduction

1.1 Some history

Probably the easiest way to orthogonal rational functions (ORF) is through orthogonal polynomials (OP). The branch of mathematics dealing with orthogonal polynomials has a long history and applications in such diverse topics as numerical integration, quantum physics, system theory etc. One of the major events in this field was the publication of Szegő's book [52] in 1939. Apart from a very thorough survey of the classical polynomials on (a subset of) the real line, such as the Jacobi, Laguerre and Hermite polynomials, a large part of the book deals with polynomials orthogonal on the complex unit circle, usually referred to as Szegő polynomials. Using these polynomials and the theory of positive functions, Szegő was able to study the strong asymptotic behaviour of general orthogonal polynomials $p_n(x)$ on an interval of the real line, under certain conditions on the weight function (the so-called Szegő condition). Strong (or power) asymptotics for orthogonal polynomials on the interval $[-1, 1]$ give expressions for $\lim_{n\to\infty} p_n(x)/[J^{-1}(x)]^n$, where $J(z)$ is the Joukowski transform defined in the next chapter.

When the weight (or measure) does not satisfy Szegő's condition, but the weaker Erdős-Turán condition instead, ratio asymptotics are typically obtained, where limits of the form $\lim_{n\to\infty} p_{n+1}(x)/p_n(x)$ are studied. There is a close connection between ratio asymptotics and the three term recurrence relation satisfied by the polynomials $p_n(x)$, since the asymptotic behaviour of the recurrence coefficients can be obtained from the ratio asymptotics. Among the many contributions to this theory we mention Rakhmanov [47, 48] for the case of polynomials orthogonal on an interval, and López Lagomasino [32, 34] for the case of varying orthogonal polynomials on the unit circle.

These orthogonal polynomials with respect to varying measures introduced by López Lagomasino are only one example of the many possible cases where the orthogonality measure is different for each degree n, but we mention them here because they are important in the theory of orthogonal rational functions, as we will explain later on in this thesis. Several properties of orthogonal polynomials have been generalized to this case of varying measures, such as the recurrence relations, asymptotic behaviour etc.

But of course there is more to orthogonal polynomials than theory, and there has always been a very vivid interest in more applied topics such as numerical integration or computational aspects of orthogonal polynomials. We would especially like to mention the work of Gautschi, who has dedicated several decades to the study of efficiently computing orthogonal polynomials on the real line and Gauss integration formulas derived from them, see e.g. [18, 19, 20] and the survey article [21].

Gauss formulas are numerical integration formulas based on orthogonal polynomials, with the property that, for a given number of nodes, they integrate a maximal space of polynomials exactly. Several generalizations have been made, such as gaussian formulas based on Laurent polynomials, see e.g. [5, 15, 16]. In spite of many theoretical results, the fast and accurate construction of such rules is still a difficult problem.

Now how do orthogonal rational functions fit in with everything which was said before? Orthogonal rational functions are a natural generalization of orthogonal polynomials, in the sense that we can always recover the polynomials by placing all the poles of the rational functions at infinity. Therefore, it is not surprising that many properties of general orthogonal polynomials on the unit circle or the real line can be extended to the case of rational functions. Most of these results have been gathered in [10], where recurrence relations, quadrature formulas, asymptotic behaviour, moment problems etc. are treated for rational functions orthogonal on the unit circle and the whole real line. In the next section we give a brief overview of the existing results.

1.2 Current state of affairs

We limit our attention to the results which are relevant for this thesis. For an extensive treatment of orthogonal rational functions we refer to [10] and to [8, 9] for some recent developments. It is also worth mentioning that Li and Pan have several articles dealing with orthogonal rational functions on the unit circle, such as [30, 31, 42, 43, 44, 45, 46]. Many of their results have been used in [10]. The article [53] contains some information about zero distribution, quadrature formulas and other topics for rational functions orthogonal on the interval $[-1, 1]$.

The book [10] deals with orthogonal rational functions on the unit circle and (through a conformal mapping) on the whole extended real line. The case of the interval is nowhere treated, although some results are valid for the interval as well, such as the recurrence relation from chapter 11. Asymptotic behaviour of orthogonal rational functions is treated in chapter 9 of [10], but the results in this chapter do not include the case of the interval. However, using the Joukowski transform, many results from the circle case can be translated to the interval, as we will show later on in this thesis. Among the relevant results for the unit circle are ratio asymptotics (which, in their most explicit form, are obtained under the condition that the poles stay away from the boundary), strong asymptotics and some weak-star convergence results. Root asymptotics are also studied, but we shall make no further reference to them.

The quadrature formulas studied in [10] are all of gaussian type, more general interpolatory quadrature formulas are not given. Several expressions for the gaussian weights are obtained, analogous to the polynomial case. Among these expressions is the formula which gives the weights as functions of the nodes (using the reproducing kernel), which is relatively interesting from a computational point of view, although computational aspects of ORF and their related quadrature formulas are not treated in the book. In [11] a generalized eigenvalue problem (GEP) is presented to compute the nodes and weights from the recurrence coefficients, analogous to the eigenvalue problem with the Jacobi matrix for the polynomial case. Algorithms to compute these recurrence coefficients themselves are not given, although the book [10] contains some information about the Nevanlinna-Pick algorithm, which can be used to compute the reflection coefficients in the coupled recurrence formulas for ORF on the unit circle.

In fact, to our knowledge, computational aspects of orthogonal rational functions have not been studied thus far. Much of the theory of orthogonal polynomials has been generalized to the rational case and several applications of ORF in system theory are being studied, see e.g. [64, 65], but the accurate and efficient computation of ORF in its general form for non-discrete measures has not been a subject of investigation. There is however an important numerical side to the theory of orthogonal rational functions through its connection with semiseparable matrices, which was discovered only very recently [54], but we will not deal with it.

As for explicit examples of ORF, the Malmquist basis on the unit circle (see the conclusion to chapter 9) is one of the few cases where the ORF are explicitly known, and probably the only one for an arbitrary pole sequence. Classical cases such as the Chebyshev or Legendre polynomials are not known in the rational situation. The case study in chapter 9 is a first attempt to overcome this problem. Generating functions and differential equations for ORF are also not known to exist at this moment.

1.3 Outline of the thesis

This thesis is roughly divided into two parts: a theoretical (chapters 3 - 4) and a computational (chapters 5 - 8) part. Most of the results from the first part will be used in the second part, e.g. in accuracy estimation or error analyses. Chapter 9 combines both theory and practice in a case study about Chebyshev rational functions.

Chapter 2 starts with some basic definitions that we will use throughout the text. The spaces of rational functions are introduced and some simple lemmas are proved for further reference. The chapter concludes with an important relation between orthogonal rational functions on the unit circle and the interval $[-1, 1]$.

That relation will be very important in chapter 3, which contains some results about the asymptotic behaviour of orthogonal rational functions on an interval. After studying ratio asymptotics and the convergence of the recurrence coefficients, we also give strong and weak-star convergence results. Some open problems in asymptotic behaviour are given in the appendix.

In chapter 4 we look at gaussian quadrature formulas based on orthogonal rational functions. The convergence of these formulas is studied for the case of an interval and some relations between quadrature formulas on the unit circle and the interval are derived. Finally we briefly look at interpolatory rules as well.

Studying the computation of the recurrence coefficients for ORF on (a subset of) the real line forms a major part of this thesis. Chapter 5 gives an elegant algorithm based on interpolation properties of the Riesz-Herglotz-Nevanlinna transform of the orthogonality measure, which, however, suffers from extreme instability. Its interest is therefore mainly theoretical, dealing with a somewhat neglected aspect of the theory of orthogonal rational functions.

The interpolation algorithm is essentially based on using the (rational) moments of the measure to compute the recurrence coefficients. In chapter 6 we show that this can never work well, but generalizing the method of modified moments from the polynomial case to the rational case, we are able to provide an algorithm which, in certain special cases, can be of more use.

The most general way, however, of constructing orthogonal rational functions on an interval, is described in chapter 7, together with a detailed error analysis. It turns out that the case where poles are close to the boundary has to be treated separately, because the polynomial-based approach for the general case fails. Using results from the theory of Laurent polynomials we can give a partial solution to the problem.

The reason why we limit our attention to the case of a finite interval, is that the case of a halfline can easily be transformed to the case of an interval, so that, at least from a computational point of view, there is no need to regard the halfline as a special case. This is explained in chapter 8.

The last chapter contains a detailed case study of a class of orthogonal rational functions which, for an arbitrary pole sequence, can be given explicitly. They are rational generalizations of the Chebyshev polynomials and share several of their properties. We provide explicit formulas for the rational functions and their recurrence coefficients, as well as efficient algorithms to compute the nodes and weights in the associated quadrature formulas. We also look at a rational version of Fejér's rule. Several examples serve as illustration.

Chapter 2

Preliminaries

2.1 Introduction

In this chapter we recall some basic facts about orthogonal polynomials (OP) and orthogonal rational functions (ORF) on the unit circle and on (a subset of) the real line. We introduce the function spaces we will be dealing with and present some important tools and concepts for later use. But first let us give some notation which will be used throughout this thesis.

2.2 Subsets of the Riemann sphere

We will only be concerned with orthogonality on the complex unit circle and on the real line (or a subset thereof). The field of complex numbers will be denoted by $\mathbb{C}$ and the Riemann sphere by $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. For the real line we use the symbol $\mathbb{R}$ and for the *extended* real line, $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. The unit circle, the open unit disc and the exterior of the closed unit disc are denoted respectively by

$$\mathbb{T} = \{z : |z| = 1\}, \quad \mathbb{D} = \{z : |z| < 1\}, \quad \mathbb{E} = \{z : |z| > 1\}.$$

A large part of this thesis will be devoted to the study of orthogonal rational functions on the real interval $I = [-1, 1]$. The complement of this interval with respect to a set X will be given by X^I, e.g.

$$\overline{\mathbb{C}}^I = \overline{\mathbb{C}} \setminus I.$$

Finally, we will use the blackboard $\mathbb{N}$ to denote the set of natural numbers and $\mathbb{Z}$ for the integers.

2.3 Theoretical background and definitions

In what follows, the word *measure* will always mean a positive bounded Borel measure whose support is an infinite set (unless stated otherwise). The support of a measure μ is defined here as the smallest closed set whose complement with respect to $\overline{\mathbb{C}}$ has μ-measure zero.

The spaces $L^p(\mu)$, $1 \leq p \leq \infty$ are well known, see e.g. [50, Chap. 3]. Introducing the inner product

$$\langle f\,, g\rangle = \int f\overline{g}d\mu$$

turns $L^2(\mu)$ into a Hilbert space. In the case of orthogonality on the unit circle, there is usually a factor $1/(2\pi)$ in front of the integral. We will follow this convention. When all functions involved are real, we occasionally omit the complex conjugate bar from this definition. Recall that $L^p(\mu)$ should be regarded as a space of equivalence classes of functions. Two functions f and g are equivalent if they are equal almost everywhere (a.e.) with respect to μ.

Let H be a Hilbert space and $\{\phi_k\}_{k\in\Gamma}$ an orthonormal set in H, where Γ is some index set. The *Fourier* coefficients of a function f are then defined as

$$f_k = \langle f\,, \phi_k\rangle\,, \quad k \in \Gamma$$

and Bessel's inequality says that

$$\sum_{k\in\Gamma} |f_k|^2 \leq \|f\|^2\,.$$

Equality holds only if the orthonormal set is *complete* in H. In this case it is often called an orthonormal basis. The unique reproducing kernel $k(z,w)$ for a separable Hilbert space with orthonormal basis $\{\phi_k\}_{k\in\Gamma}$ is given by

$$k(z,w) = \sum_{k\in\Gamma} \phi_k(z)\overline{\phi_k(w)}$$

whenever this sum converges. It has the property that $\langle f\,, k(\cdot,w)\rangle = f(w)$ for every $f \in H$. These reproducing kernels will play an important role when studying the asymptotic behaviour of orthogonal polynomials and rational functions.

The substar or para-hermitian conjugate of a function f is defined as

$$f_*(z) = \overline{f(1/\overline{z})}.$$

Note that for $z \in \mathbb{T}$ this reduces to taking the complex conjugate of $f(z)$.

The last concept we introduce in this paragraph is that of weak star convergence. A sequence of measures μ_n is said to converge in the weak star topology to a measure μ, if for every continuous and bounded function f it holds that

$$\lim_{n\to\infty} \int f d\mu_n = \int f d\mu.$$

This is usually written $\mu_n \xrightarrow{*} \mu$. The definition is also valid for complex Borel measures of bounded variation.

2.4 Orthogonality on the unit circle

In this section we assume that the orthogonality measure is supported on the unit circle and we denote it by $\mathring{\mu}$. Given a sequence of complex numbers $B = \{\beta_1, \beta_2, \ldots\}$ all in $\mathbb{D}$, we can construct orthonormal polynomials $\phi_{n,m}(z) = \nu_{n,m} z^m + \ldots$ with respect to the varying measure $d\mathring{\mu}/|w_n(z)|^2$ with $w_n(z) = (z-\beta_1)\ldots(z-\beta_n)$ that are uniquely determined by the conditions

$$\frac{1}{2\pi}\int_0^{2\pi} \phi_{n,m}(z)\overline{z}^j \frac{d\mathring{\mu}(\theta)}{|w_n(z)|^2} = 0, \quad j = 0, \ldots, m-1,$$
$$\frac{1}{2\pi}\int_0^{2\pi} |\phi_{n,m}(z)|^2 \frac{d\mathring{\mu}(\theta)}{|w_n(z)|^2} = 1, \quad \nu_{n,m} > 0, \quad z = e^{\mathbf{i}\theta}.$$

These polynomials were introduced by López Lagomasino, who has generalized many properties of (ordinary) Szegő polynomials to the case of varying measures on the unit circle, see e.g. [14, 26, 27, 32, 33, 34].

For each polynomial p_n of strict degree n we define the superstar transformation as $p_n^*(z) = z^n p_{n*}$. It follows that $|p_n^*(z)| = |p_n(z)|$ for $|z| = 1$.

With the sequence B and the measure $\mathring{\mu}$ we can also associate a set of orthonormal rational functions as follows. Define the Blaschke factors

$$\zeta_n(z) = -\frac{\overline{\beta}_n}{|\beta_n|}\frac{z-\beta_n}{1-\overline{\beta}_n z}, \quad n = 1, 2, \ldots$$

(for $\beta_n = 0$ the constant factor in front is taken equal to 1) and the Blaschke products

$$B_0 = 1, \quad B_n(z) = \zeta_n(z) B_{n-1}(z), \quad n = 1, 2, \ldots$$

It is well known that with $z \in \mathbb{D}$ a Blaschke product converges to a nonzero value if and only if

$$\sum_{n=1}^{\infty} (1 - |\beta_n|) < \infty.$$

This condition is often referred to as the Blaschke condition. If it is not satisfied, the Blaschke product will converge to zero in $\mathbb{D}$. Curiously, in this case it is often said that the product *diverges*. These Blaschke products $B_n(z)$ can roughly be seen as rational generalizations of the monomials z^n in the polynomial case.

Now the space $\mathring{\mathcal{L}}_n$ of rational functions associated with $(B, \mathring{\mu})$ is defined as

$$\mathring{\mathcal{L}}_n = \text{span}\{B_0, \dots, B_n\}.$$

Orthonormalizing this basis we obtain the orthonormal rational functions $\{\phi_n\}$ where we take the leading coefficient $\mathring{\kappa}_n$ in the expansion $\phi_n(z) = \mathring{\kappa}_n B_n(z) + \dots$ to be positive. Note that we obtain the orthonormal Szegő polynomials if $\beta_k = 0$ for all k.

If we write $\phi_n(z) = g_n(z)/w_n^*(z)$ then we have the following relation between the orthogonal rational functions and the orthogonal polynomials with respect to the varying measures. For the proof we refer to [31] or for a more general formulation to [10].

Lemma 2.4.1. *Let $\phi_{n,m}$ and ϕ_n be as defined above. Then the following relation holds,*

$$g_n(z) = \frac{1}{z - \beta_n} \frac{\tau_n}{\nu_{n,n}} \left(z\phi_{n,n}(z) - \beta_n \frac{\phi_{n,n}(\beta_n)}{\phi_{n,n}^*(\beta_n)} \phi_{n,n}^*(z) \right)$$

where $g_n = \tau_n z^n + \dots$ is the numerator polynomial of $\phi_n(z) = g_n(z)/w_n^*(z)$.

We also define a superstar transformation for the rational functions as follows. If f_n is a function in $\mathring{\mathcal{L}}_n$ then $f_n^*(z) = B_n(z) f_{n*}$. Again we have $|f_n^*(z)| = |f_n(z)|$ for $|z| = 1$. It should be clear from the context whether the superstar refers to the polynomial superstar transformation or the rational superstar transformation. If all $\beta_k = 0$ then both transformations are the same. Note that for any $f = p_n/w_n^* \in \mathring{\mathcal{L}}_n$ we have

$$f^*(z) = \eta_n \frac{p_n^*(z)}{w_n^*(z)}, \tag{2.1}$$

where $\eta_n = \prod_{k=1}^n (-\overline{\beta}_k/|\beta_k|)$.

The reproducing kernel for the space $\mathring{\mathcal{L}}_n$ will be denoted by $\mathring{k}_n(z, w)$ and is obviously given by

$$\mathring{k}_n(z, w) = \sum_{k=0}^n \phi_k(z)\overline{\phi_k(w)}.$$

It is not difficult to see that the functions $\{\phi_{n,k}(z)/w_n^*(z)\}_{k=0}^n$ also form an orthonormal basis for $\mathring{\mathcal{L}}_n$, [10, p. 194] and since the reproducing kernel is unique, we therefore also have

$$\mathring{k}_n(z,w) = \left[\sum_{k=0}^{n} \phi_{n,k}(z)\overline{\phi_{n,k}(w)}\right] (w_n^*(z)\overline{w_n^*(w)})^{-1}.$$

Concerning this kernel function, we have the following Christoffel-Darboux relations from [10, Chap. 3 and 9].

Theorem 2.4.2. *The following relations hold between reproducing kernel and orthonormal basis functions of* $\mathring{\mathcal{L}}_n$*:*

$$\begin{aligned}\mathring{k}_n(z,w) &= \frac{\phi_n^*(z)\overline{\phi_n^*(w)} - \zeta_n(z)\overline{\zeta_n(w)}\phi_n(z)\overline{\phi_n(w)}}{1-\zeta_n(z)\overline{\zeta_n(w)}}, \\ &= \frac{\phi_{n,n}^*(z)\overline{\phi_{n,n}^*(w)} - z\overline{w}\phi_{n,n}(z)\overline{\phi_{n,n}(w)}}{(1-z\overline{w})(w_n^*(z)\overline{w_n^*(w)})}.\end{aligned}$$

Finally, for any nonnegative measurable function h on $[0,2\pi)$ such that $\log h \in L^1[0,2\pi]$ we define the Szegő function $\sigma(h,z)$ as

$$\sigma(h,z) = \exp\left(\frac{1}{4\pi}\int_0^{2\pi} \frac{u+z}{u-z}\log h(\theta)d\theta\right), \quad u = e^{\mathbf{i}\theta}, z \in \mathbb{D}.$$

It is well known that σ has a nontangential limit from inside the unit circle that satisfies

$$h(\theta) = |\sigma(h, e^{\mathbf{i}\theta})|^2 \quad \text{a.e. on } \mathbb{T},$$

see e.g. [50, p. 343]. Furthermore, we can easily prove the following lemma which gives an explicit representation of the Szegő function for a large class of functions.

Lemma 2.4.3. *Assume that f is a bounded analytic function in a region Ω such that $\mathbb{D}\cup\mathbb{T} \in \Omega$ and that f has no zeros in $\mathbb{D}$. Denote by $\tilde{f}$ the restriction of f to $\mathbb{T}$, i.e. $\tilde{f}(\theta) = f(e^{\mathbf{i}\theta})$. Then we have*

$$\sigma(|\tilde{f}|, z) = c\sqrt{f(z)}, \quad z \in \mathbb{D}$$

where c is a unimodular constant such that $\sigma(|\tilde{f}|, 0) > 0$.

Proof. According to [50, p. 249], $\log|f|$ is harmonic in $\mathbb{D}$. Because f is bounded it is not difficult to see that the integrals

$$\int_0^{2\pi} \left|\log|f(re^{\mathbf{i}\theta})|\right|^p d\theta$$

are bounded as $r \to 1$ for every $1 \leq p < \infty$. Then according to the second corollary on p. 38 of [28], $\log|f|$ is the Poisson integral of $\log|\tilde{f}|$, which means that in $\mathbb{D}$ it is the real part of the analytic function

$$g(z) = \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{\mathbf{i}\theta}+z}{e^{\mathbf{i}\theta}-z}\log|f(e^{\mathbf{i}\theta})|d\theta.$$

This means that we must have $g(z) = \log(f(z)) + \mathbf{i}\gamma$ where γ is an arbitrary real constant. The lemma now follows from the observation that

$$\sigma(|\tilde{f}|, z) = \exp\frac{1}{2}g(z)$$

and $\sigma(|\tilde{f}|, 0) > 0$ according to the definition of a Szegő function. □

2.5 Orthogonality on a subset of the real line

Here we assume that $\text{supp}(\mu) \subset \overline{\mathbb{R}}$, where $\text{supp}(\mu)$ is the support of the measure μ. Let a sequence of poles $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}} \setminus \{0\}$ be given such that $A \cap \text{supp}(\mu) = \emptyset$ (so all the poles are outside the support of the measure). As a consequence we cannot have $\text{supp}(\mu) = \overline{\mathbb{R}}$. Note that we may have poles at infinity. Define factors

$$Z_n(z) = \frac{z}{1 - z/\alpha_n}, \quad n = 1, 2, \ldots$$

and basis functions

$$b_0 = 1, \quad b_n(z) = b_{n-1}(z)Z_n(z), \quad n = 1, 2, \ldots$$

Then the space of rational functions with poles in A is defined as

$$\mathcal{L}_n = \text{span}\{b_0, \ldots, b_n\}.$$

Let $\mathcal{P}_n$ denote the space of polynomials of degree n (a polynomial of strict degree less than n is also a polynomial of degree n) and define

$$\pi_n(z) = \prod_{k=1}^{n}(1 - z/\alpha_k),$$

then we may write equivalently

$$\mathcal{L}_n = \{p_n/\pi_n, p_n \in \mathcal{P}_n\}.$$

Orthonormalising the basis $\{b_0, \ldots, b_n\}$ with respect to μ we obtain orthogonal rational functions $\{\varphi_0, \ldots, \varphi_n\}$ where we choose the leading coefficient κ_n in the expansion $\varphi_n(z) = \kappa_n b_n(z) + \ldots$ to be real. The φ_n will be uniquely determined once the sign of κ_n is fixed. We will get back to this later on. The following lemma from [10] will be useful.

Lemma 2.5.1. *The orthonormal functions φ_n have real coefficients with respect to the basis $\{b_k\}$.*

It follows in particular that $\varphi_n(z)$ is real for real z and for any inner product $\langle f, \varphi_n\rangle$ we may omit the complex conjugate bar.

The orthogonal rational function φ_n is called *regular* if its numerator polynomial p_n satisfies $p_n(\alpha_{n-1}) \neq 0$. The system $\{\varphi_n\}$ is regular if φ_n is regular for every n. We now mention an important theorem in the theory of orthogonal rational functions on the real line, which states that they satisfy a three term recurrence relation, analogous to the one for the polynomial case. For the proof of the theorem we refer to [10].

Theorem 2.5.2. *Put by convention $\alpha_{-1} = \alpha_0 = \infty$. Then for $n = 1, 2, \ldots$ the orthonormal rational functions φ_n satisfy the following three term recurrence relation if and only if φ_n and φ_{n-1} are regular:*

$$\varphi_n(z) = \left(E_n Z_n(z) + F_n \frac{Z_n(z)}{Z_{n-1}(z)}\right) \varphi_{n-1}(z) - \frac{E_n}{E_{n-1}} \frac{Z_n(z)}{Z_{n-2}(z)} \varphi_{n-2}(z). \quad (2.2)$$

The initial conditions are $\varphi_{-1}(z) \equiv 0$, $\varphi_0(z) \equiv 1/\sqrt{\mu_0}$ with $\mu_0 = \mu(\overline{\mathbb{R}})$. The coefficients E_n are nonzero.

Note that the coefficient E_0 is not used and can be arbitrarily chosen. We take it equal to $E_0 = 1$. If we take the coefficient E_n to be positive, then the functions φ_n will be uniquely determined. This amounts to fixing the sign of κ_n. Unless stated otherwise, this will be the normalization convention used throughout this thesis.

If we take all poles outside the convex hull of supp(μ), then the system $\{\varphi_n\}$ will be regular and thus the recurrence relation will hold for every n. This follows from the fact that in this case the zeros of φ_n are inside the convex hull of supp(μ). Therefore, if supp(μ) is connected then $\{\varphi_n\}$ will be regular (because of the assumptions we made on the location of the poles). This is the case for example when we consider orthogonality on an interval or on a halfline.

Explicit expressions for the recurrence coefficients can easily be found, as shown in the following lemma.

Lemma 2.5.3. *The coefficients in the recurrence relation* (2.2) *have the following explicit representation in terms of inner products,*

$$F_n = -E_n \frac{\langle Z_n \varphi_{n-1}, \varphi_k\rangle - \frac{1}{E_{n-1}} \left\langle \frac{Z_n}{Z_{n-2}} \varphi_{n-2}, \varphi_k \right\rangle}{\left\langle \frac{Z_n}{Z_{n-1}} \varphi_{n-1}, \varphi_k \right\rangle} = -E_n \hat{F}_n,$$

$$E_n = \frac{1}{\|\hat{\varphi}_n\|},$$

where

$$\hat{\varphi}_n(x) = \left(Z_n(x) - \hat{F}_n \frac{Z_n(x)}{Z_{n-1}(x)} \right) \varphi_{n-1}(x) - \frac{1}{E_{n-1}} \frac{Z_n(x)}{Z_{n-2}(x)} \varphi_{n-2}(x)$$

and $k < n$.

Proof. Taking the inner product on both sides of (2.2) with φ_k for $k < n$ and solving for F_n yields the first equation. Substituting this back into the recurrence relation and using the fact that $\|\varphi_n\| = 1$ completes the proof. □

The reproducing kernel for the space $\mathcal{L}_n$ will be denoted by $k_n(x, y)$ and the orthogonal rational functions φ_n also satisfy a Christoffel-Darboux relation, which we will only need in its confluent form as given in the next theorem from [10, Chap. 11].

Theorem 2.5.4. *The following relation holds between reproducing kernel and orthonormal basis functions of* $\mathcal{L}_n$*:*

$$f'_n(z) f_{n-1}(z) - f_n(z) f'_{n-1}(z) = E_n k_{n-1}(z, z),$$

where

$$f_k(z) = \left(1 - \frac{z}{\alpha_k} \right) \varphi_k(z)$$

and the prime means derivative.

Later on in this thesis, we will need interpolating rational functions analogous to the Lagrange interpolating polynomials. Assume that n numbers $\{x_{nk}\}_{k=1}^n \subset \mathbb{R}$ are given, all different from each other and such that none of them coincides with any of the poles in A. Only the case where $\{x_{nk}\}_{k=1}^n$ are the zeros of $\varphi_n(z)$ will be of interest to us. Let $l_{ni}(z)$ denote the Lagrange interpolating polynomial

$$l_{ni}(z) = \prod_{\substack{k=1 \\ k \neq i}}^{n} \frac{z - x_{nk}}{x_{ni} - x_{nk}}$$

satisfying $l_{ni}(x_{nk}) = \delta_{ik}$, then the following lemma is easily checked and we omit the proof.

Lemma 2.5.5. *Let* $\{x_{nk}\}_{k=1}^n$ *denote the zeros of* $\varphi_n(z)$ *then the unique rational function* $L_{ni} \in \mathcal{L}_{n-1}$ *which satisfies* $L_{ni}(x_{nk}) = \delta_{ik}$ *is given by*

$$L_{ni}(z) = \frac{\varphi_n(z)}{(z - x_{ni}) \varphi'_n(x_{ni})} \frac{1 - z/\alpha_n}{1 - x_{ni}/\alpha_n} .$$

The unique Hermite interpolating rational functions $H_{ni}, \tilde{H}_{ni} \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$ satisfying

$$H_{ni}(x_{nk}) = \delta_{ik}, \qquad \tilde{H}_{ni}(x_{nk}) = 0,$$
$$H'_{ni}(x_{nk}) = 0, \qquad \tilde{H}'_{ni}(x_{nk}) = \delta_{ik}$$

are given by

$$H_{ni}(z) = L^2_{ni}(z)\left[1 - 2L'_{ni}(x_{ni})(z - x_{ni})\frac{1 - x_{ni}/\alpha_n}{1 - z/\alpha_n}\right],$$
$$\tilde{H}_{ni}(z) = L^2_{ni}(z)(z - x_{ni})\frac{1 - x_{ni}/\alpha_n}{1 - z/\alpha_n}$$

Finally we give a simple lemma which will be useful for future reference.

Lemma 2.5.6. *Let a, b and x be given all in $\mathbb{C}$. Then for any f such that (as a function of t) $(at + b)/(t - x)[f(t) - f(x)] \in \mathcal{L}_{n-1}$ we have*

$$\int \frac{at + b}{t - x}\varphi_n(t)f(t)d\mu(t) = f(x)\int \frac{at + b}{t - x}\varphi_n(t)d\mu(t).$$

This holds in particular if $f \in \mathcal{L}_{n-1}$.

Proof. It follows from $\varphi_n \perp \mathcal{L}_{n-1}$ that

$$\int \varphi_n(t)\frac{at + b}{t - x}[f(t) - f(x)]d\mu(t) = 0.$$

The result is now immediate. □

2.6 Relating the interval to the unit circle

When the measure μ is supported on the interval $[-1, 1]$, we can relate the orthogonal rational functions φ_n on I to the ϕ_n on $\mathbb{T}$ using the Joukowski transformation. These relations are very similar to the ones for the polynomial case as given in [52] and were derived in [63].

We denote the Joukowski transform $x = \frac{1}{2}(z + z^{-1})$ by $x = J(z)$, mapping the open unit disc $\mathbb{D}$ to the cut Riemann sphere $\overline{\mathbb{C}}^I$ and the unit circle $\mathbb{T}$ to the interval I. The inverse mapping is denoted by $z = J^{-1}(x)$ and is chosen so that $z \in \mathbb{D}$ if $x \in \overline{\mathbb{C}}^I$. To the sequence $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ we associate a sequence $B = \{\beta_1, \beta_2, \ldots\} \subset I$ such that $\beta_k = J^{-1}(\alpha_k)$, and a sequence $\hat{B} = \{\hat{\beta}_1, \hat{\beta}_2, \ldots\}$ such that $\hat{\beta}_{2k} = \hat{\beta}_{2k-1} = \beta_k$. The corresponding Blaschke products and orthogonal functions are denoted by a hat. Obviously $\hat{B}_{2k}(z) = (B_k(z))^2$.

Next define the measure[1] $\mathring{\mu}$ on $\mathbb{T}$ as

$$\mathring{\mu}(E) = \mu(\{\cos\theta, \theta \in E \cap [0,\pi)\}) + \mu(\{\cos\theta, \theta \in E \cap [\pi, 2\pi)\}). \quad (2.3)$$

for every Borel measurable set E. This is sometimes written $\mathring{\mu}(E) = \int_E |d\mu(\cos\theta)|$, but we prefer the less ambiguous notation. Using the Lebesgue decomposition of μ and the change-of-variables theorem (see e.g. [50, p. 153]) it is not difficult to see that

$$\mathring{\mu}'(\theta) = \mu'(\cos\theta)|\sin\theta| \quad (2.4)$$

where $\mathring{\mu}'$ and μ' are the Radon-Nikodym derivatives of $\mathring{\mu}$ and μ respectively. Equation (2.3) implies that for every $d\mu$-measurable function f we have

$$\int_{-1}^{1} f(x)d\mu(x) = \frac{1}{2}\int_0^{2\pi} f(\cos\theta)d\mathring{\mu}(\theta). \quad (2.5)$$

Then if $\{\hat{\phi}_n\}$ is the orthonormal set associated with $(\hat{B}, \mathring{\mu})$, we have the following theorem from [63] (note that we have to double the multiplicity of every pole).

Theorem 2.6.1. *Let $\{\varphi_n\}$ be a set of orthonormal rational functions on I and $\{\hat{\phi}_n\}$ the corresponding set of functions orthogonal on $\mathbb{T}$ with poles and measure as defined above, then they are related by*

$$\varphi_n(x) = \delta_n(2\pi)^{-\frac{1}{2}} \left\{1 + \frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}^*_{2n}(\beta_n)}\right\}^{-\frac{1}{2}} \frac{\hat{\phi}_{2n}(z) + \hat{\phi}^*_{2n}(z)}{B_n(z)}$$

where $x = J(z)$ and $\delta_n = \pm 1$ is such that the normalization $E_n > 0$ holds.

[1] In [63] the measure μ was assumed to be absolutely continuous, but this can easily be extended to arbitrary positive Borel measures whose support is an infinite set. See also [17, p. 190] for the polynomial case

Chapter 3

Asymptotic behaviour

3.1 Introduction

The convergence of orthogonal polynomials as the degree n tends to infinity is one of the topics which has attracted most attention throughout the history of this particular field of mathematics. A substantial part of the theory was developed by Szegő in his famous book [52] and has been extended by various authors beyond Szegő's condition and to the theory of OP with respect to varying measures and ORF. In this chapter we wish to present some new results concerning asymptotic behaviour of ORF on the unit circle and on the interval $[-1, 1]$. We will look at ratio asymptotics, i.e. the convergence of φ_n/φ_{n-1}, and use this to derive asymptotic expressions for the recurrence coefficients. Next we look at strong convergence and finally we give a weak-star convergence result. Before we can state and prove our theorems, we need several auxiliary results which will be given in the next section.

3.2 Auxiliary results

When studying the asymptotic behaviour of orthogonal polynomials, there are two different conditions which are often imposed on the measure. The first (and more restrictive) condition is usually referred to as Szegő's condition and for the circle case it takes the form

$$\int_0^{2\pi} \log \mathring{\mu}'(\theta) d\theta > -\infty.$$

It basically says that the weight cannot tend to zero too quickly. An important class of weight functions not satisfying Szegő's condition are the *expo-*

nential weights, for more information we refer to [29]. Using the Joukowski transformation gives Szegő's condition for the interval $[-1,1]$,

$$\int_{-1}^{1} \frac{\log \mu'(x)}{\sqrt{1-x^2}} dx > -\infty.$$

Szegő's condition is typically used to derive strong asymptotics, i.e. to find the limit function of the orthogonal polynomials or rational functions themselves, as opposed to, for example, ratio asymptotics.

For the latter kind of asymptotic behaviour it is more common to impose the so-called Erdős-Turán condition

$$\mathring{\mu}' > 0 \text{ a.e.}$$

(which is of course the same for the interval). The 'almost everywhere' is with respect to the Lebesgue measure.

Working with orthogonal rational functions, we not only need conditions on the measure, but also on the location of the poles. Many results, especially in the theory of the varying orthogonal polynomials discussed in section 2.4, are derived under the condition

$$\sum_{n=1}^{\infty} (1-|\beta_n|) = \infty$$

(i.e. the divergence to zero of the Blaschke product). This means that the poles can converge to the boundary $\mathbb{T}$, but not too quickly. For example in the case where $|\beta_n| = 1 - n^{-p}$, the condition will only be satisfied for $p \leq 1$. However, for the rational case this condition is often too loose to obtain general results and instead it is required that the sequence B be compactly included in $\mathbb{D}$, which means the β_n remain at a positive distance from the boundary as n tends to infinity. This implies that there exists a ρ such that $|\beta_k| \leq \rho < 1$ for all k. In the rest of this chapter, ρ will have this meaning.

After these introductory comments we are ready to present the convergence results needed in the following sections. They are all about convergence in the unit disc, since it is usually not difficult to deduce the interval case from the circle case using the Joukowski transform.

In what follows, locally uniform convergence in a region Ω will mean uniform convergence on compact subsets of Ω.

The first theorem is about the convergence of varying orthogonal polynomials and can be found in [32].

Theorem 3.2.1. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is such that*

$$\sum_{n=1}^{\infty} (1-|\beta_n|) = \infty.$$

Then for every integer k we have

$$\lim_{n\to\infty} \frac{\phi_{n,n+k}(z)}{\phi^*_{n,n+k}(z)} = 0,$$

locally uniformly in $\mathbb{D}$.

The same theorem, but under a stricter condition on the location of the poles, can be proved for the rational case, as was done in chapter 9 of [10].

Theorem 3.2.2. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is compactly included in $\mathbb{D}$. Then we have*

$$\lim_{n\to\infty} \frac{\phi_n(z)}{\phi^*_n(z)} = 0,$$

locally uniformly in $\mathbb{D}$.

In the same chapter we find the following result regarding ratio asymptotics of orthogonal rational functions. Note that the assumptions are the same as in the previous theorem.

Theorem 3.2.3. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is compactly included in $\mathbb{D}$. Then we have*

$$\lim_{n\to\infty} \frac{\epsilon_{n+1}\phi^*_{n+1}(z)(1-\overline{\beta}_{n+1}z)\sqrt{1-|\beta_n|^2}}{\epsilon_n\phi^*_n(z)(1-\overline{\beta}_n z)\sqrt{1-|\beta_{n+1}|^2}} = 1,$$

where ϵ_n is a unimodular normalization constant such that $\epsilon_n\phi^*_n(0) > 0$, i.e. $\epsilon_n = |\phi^*_n(0)|/\phi^*_n(0)$. Again convergence is locally uniform in $\mathbb{D}$.

As mentioned before, strong convergence results are usually obtained when the measure satisfies Szegő's condition. The following theorem can also be found in chapter 9 of [10].

Theorem 3.2.4. *Let $\mathring{\mu}$ satisfy Szegő's condition $\log\mathring{\mu}' \in L^1[0,2\pi]$ and assume that the sequence B is compactly included in $\mathbb{D}$. Then locally uniformly in $\mathbb{D}$*

$$\lim_{n\to\infty} \epsilon_n \frac{\phi^*_n(z)(1-\overline{\beta}_n z)}{\sqrt{1-|\beta_n|^2}} = \frac{1}{\sigma(\mathring{\mu}', z)},$$

where ϵ_n is as in theorem 3.2.3 and σ is the Szegő function defined in section 2.4.

Finally we give a weak-star convergence result for orthogonal rational functions on the unit circle. Again we refer to [10, Chapter 9] for the proof.

Theorem 3.2.5. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is compactly included in $\mathbb{D}$. Let $P(z,t)$ denote the Poisson kernel,*

$$P(z,t) = \frac{1-|t|^2}{|z-t|^2}, \quad z = e^{\mathbf{i}\theta}.$$

Then we have

$$\frac{|\phi_n(z)|^2}{P(z,\beta_n)}\mathring{\mu}'(\theta)d\theta \overset{*}{\longrightarrow} d\theta.$$

With the aid of the previous theorems, we can prove the convergence results in the following sections.

3.3 Ratio asymptotics

We will now prove our main result about the convergence of the ratio of orthogonal rational functions on I. Of course more restrictive conditions on the location of the poles lead to more specific convergence results. In the sequel we will use the concept of aymptotic periodicity, which we define as follows.

Definition 3.3.1. A sequence $\{\alpha_1, \alpha_2, \ldots\}$ is asymptotically periodic with period m if there exists a periodic sequence $\{\alpha_1^0, \alpha_2^0, \ldots\}$,

$$\alpha_{n+m}^0 = \alpha_n^0, \quad n = 1, 2, \ldots$$

such that

$$\lim_{n\to\infty} |\alpha_n - \alpha_n^0| = 0.$$

Now we shall state our first and most general result, where no other assumptions are made on the location of the poles than that they stay away from the boundary.

Theorem 3.3.2. *Assume the sequence $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ is bounded away from I and let μ satisfy the Erdős-Turán condition $\mu' > 0$ a.e. Then locally uniformly in $\overline{\mathbb{C}}^I$ we have*

$$\lim_{n\to\infty} \frac{z-\beta_{n+1}}{1-\beta_n z}\sqrt{\frac{1-\beta_n^2}{1-\beta_{n+1}^2}}\frac{\varphi_{n+1}(x)}{\varphi_n(x)} = 1$$

where $z = J^{-1}(x)$ and $\beta_k = J^{-1}(\alpha_k)$ for $k = n, n+1$.

Proof. Define the measure $\mathring{\mu}$ on $\mathbb{T}$ by (2.3) and then use theorem 2.6.1 to write

$$\frac{\varphi_{n+1}(x)}{\varphi_n(x)} = \frac{\delta_{n+1}}{\delta_n}\frac{1}{\zeta_{n+1}(z)}\frac{\hat{\phi}^*_{2n+2}(z)}{\hat{\phi}^*_{2n}(z)}\sqrt{\frac{1+\frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}^*_{2n}(\beta_n)}}{1+\frac{\hat{\phi}_{2n+2}(\beta_{n+1})}{\hat{\phi}^*_{2n+2}(\beta_{n+1})}}\frac{\frac{\hat{\phi}_{2n+2}(z)}{\hat{\phi}^*_{2n+2}(z)}+1}{\frac{\hat{\phi}_{2n}(z)}{\hat{\phi}^*_{2n}(z)}+1}}\ .$$

Using theorems 3.2.2 and 3.2.3 we obtain

$$\lim_{n\to\infty} -\frac{\beta_{n+1}}{|\beta_{n+1}|}\frac{\hat{\epsilon}_{2n+2}}{\hat{\epsilon}_{2n}}\frac{\delta_n}{\delta_{n+1}}\frac{z-\beta_{n+1}}{1-\beta_n z}\sqrt{\frac{1-\beta_n^2}{1-\beta_{n+1}^2}}\frac{\varphi_{n+1}(x)}{\varphi_n(x)} = 1$$

locally uniformly in $\overline{\mathbb{C}}^I$.

The asymptotic behaviour of the unimodular constant in front of this expression can be found as follows. From the recurrence relation (2.2) we obtain the following expression,

$$E_{n+1} = \lim_{x\to\alpha_n}\frac{\varphi_{n+1}(x)}{\varphi_n(x)Z_{n+1}(x)}\ .$$

Then using the normalization $E_{n+1} > 0$ and the fact that convergence is uniform we find

$$\lim_{n\to\infty} -\frac{\beta_{n+1}}{|\beta_{n+1}|}\frac{\hat{\epsilon}_{2n+2}}{\hat{\epsilon}_{2n}}\frac{\delta_n}{\delta_{n+1}} = 1$$

(remember that all α_k and β_k are real, $|\alpha_k| > 1$, $|\beta_k| < 1$ and $\alpha_k\beta_k > 0$). This proves the theorem. □

If all poles are at infinity, then all $\beta_k = 0$ and we recover a well known result about the asymptotic behaviour of the ratio of orthogonal polynomials on $[-1, 1]$, see e.g. [47].

As a corollary to our main theorem we consider the case of an asymptotically periodic pole sequence.

Corollary 3.3.3. *Assume the sequence $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ is asymptotically m-periodic with limiting values $\{\alpha_i^0\}_{i=1}^m \subset \overline{\mathbb{R}}^I$ and assume the measure μ satisfies the Erdős-Turán condition. Then we have*

$$\lim_{n\to\infty}\frac{\varphi_{nm+i}(x)}{\varphi_{nm+i-1}(x)} = \frac{1-\beta_{i-1}^0 z}{z-\beta_i^0}\sqrt{\frac{1-(\beta_i^0)^2}{1-(\beta_{i-1}^0)^2}},\quad i = 1,\ldots,m$$

locally uniformly in $\overline{\mathbb{C}}^I \setminus \{\alpha_i^0\}$ where $z = J^{-1}(x)$, $\beta_k^0 = J^{-1}(\alpha_k^0)$ for $k = i, i-1$ and $\alpha_0^0 = \alpha_m^0$.

If $m = 1$ we can easily obtain a more explicit expression for the limit function. We state the following result without proof, since this is a matter of simple algebra.

Corollary 3.3.4. *Assume the sequence* $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ *is such that* $\lim_{n\to\infty} \alpha_n = \alpha \in \overline{\mathbb{R}}^I$ *and assume the measure* μ *satisfies the Erdős-Turán condition. Then we have for* $|\alpha| < \infty$

$$\lim_{n\to\infty} \frac{\varphi_{n+1}(x)}{\varphi_n(x)} = \frac{1-\alpha x}{x-\alpha} - \frac{\sqrt{(x^2-1)(\alpha^2-1)}}{x-\alpha}$$

locally uniformly in $\overline{\mathbb{C}}^I \setminus \{\alpha\}$ *where the branch of the square root is chosen so that the expression on the right hand side is greater than 1 in modulus for* $x \in \overline{\mathbb{C}}^I$.

If $|\alpha| = \infty$ *then we have*

$$\lim_{n\to\infty} \frac{\varphi_{n+1}(x)}{\varphi_n(x)} = x + \sqrt{x^2-1}$$

locally uniformly in $\overline{\mathbb{C}}^I$, *with the same convention for the branch of the square root.*

3.4 Asymptotics for E_n and F_n

In this section we wish to derive asymptotic formulas for the recurrence coefficients E_n and F_n. First we note that explicit formulas for the coefficients in terms of the orthogonal functions φ_n are given by

$$\begin{aligned} E_n &= \lim_{x\to\alpha_{n-1}} \frac{\varphi_n(x)}{\varphi_{n-1}(x) Z_n(x)}, \\ F_n &= \lim_{x\to\alpha_{n-2}} \left(\frac{\varphi_n(x)}{\varphi_{n-1}(x)} \frac{Z_{n-1}(x)}{Z_n(x)} - E_n Z_{n-1}(x) \right). \end{aligned}$$

These formulas are readily obtained from the recurrence formula (2.2). Now we can use theorem 3.3.2 to find the asymptotic formulas for E_n and F_n. The computations are cumbersome but straightforward and we omit the proof.

Theorem 3.4.1. *Under the assumptions of theorem 3.3.2, the following relations hold in the sense that the ratio of the left hand side and the right* *hand side tends to 1 as n tends to infinity,*

$$
\begin{aligned}
E_n &\sim 2\frac{\sqrt{(1-\beta_{n-1}^2)(1-\beta_n^2)}(1-\beta_{n-1}\beta_n)}{(1+\beta_{n-1}^2)(1+\beta_n^2)}\ , \\
F_n &\sim -\sqrt{\frac{1-\beta_n^2}{1-\beta_{n-1}^2}}\frac{(1-\beta_{n-1}^2)(\beta_n+\beta_{n-2})+2\beta_{n-1}(1-\beta_n\beta_{n-2})}{(1+\beta_n^2)(1-\beta_{n-1}\beta_{n-2})}\ ,
\end{aligned}
$$

where $\beta_k = J^{-1}(\alpha_k)$ *for* $k = n, n-1, n-2$.

It is interesting to note that for n large enough the coefficients E_n and F_n will only depend on respectively the last two or three poles. Another conclusion we can draw from this theorem is that E_n is bounded by $0 < E_n \leq 2$ for large enough n, while F_n can become arbitrarily large, depending on how close the poles come to the boundary of the interval. Take for example $\beta_n = \beta_{n-2} = 0$ and $\beta_{n-1} = \pm(1-\epsilon)$ (where ϵ is a small positive number), then for large n we will have $F_n \approx \mp\sqrt{2/\epsilon}$.

Of course we can write down explicit limits for the case of an asymptotically periodic pole sequence. If the period is equal to m, then both sequences $\{E_n\}_{n=1}^{\infty}$ and $\{F_n\}_{n=1}^{\infty}$ will have m accumulation points, which are given by the expressions from theorem 3.4.1 with n replaced by i for $i = 1, \ldots, m$. In the special case $m = 1$ where all poles tend to a fixed pole $\alpha \in \overline{\mathbb{R}}^I$ these expressions are simplified considerably and are given in the following corollary.

Corollary 3.4.2. *Under the assumptions of corollary 3.3.4 we have the following convergence results for the recurrence coefficients,*

$$
\begin{aligned}
\lim_{n\to\infty} E_n &= 2(1-1/\alpha^2)\ , \\
\lim_{n\to\infty} F_n &= -2/\alpha\ .
\end{aligned}
$$

Again we note the correspondence with the polynomial case. If α equals infinity, the recurrence coefficients will behave asymptotically as the recurrence coefficients in the well known recurrence formula for orthogonal polynomials on I, see e.g. [52, p. 310] for the case of an absolutely continuous measure satisfying Szegő's condition, and [47, p. 212] for the general situation.

3.5 Strong convergence

Strong asymptotics for φ_n can be given using theorem 3.2.4, as we will prove now.

Theorem 3.5.1. *Assume the sequence* $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ *is bounded away from* I *and assume* μ *satisfies the Szegő condition*

$$\int_{-1}^{1} \frac{\log \mu'(x)}{\sqrt{1-x^2}}\, dx > -\infty.$$

Let $\mathring{\mu}$ *be defined by* (2.3) *and let* $\sigma(\mathring{\mu}', z)$ *be the associated Szegő function as defined in section 2.4. Then locally uniformly in* $\overline{\mathbb{C}}^I$ *we have*

$$\lim_{n\to\infty} c_n B_n(z) \frac{1-\beta_n z}{\sqrt{1-\beta_n^2}} \varphi_n(x) = \frac{1}{\sqrt{2\pi}\sigma(\mathring{\mu}', z)}$$

where $z = J^{-1}(x)$, $\beta_k = J^{-1}(\alpha_k)$ *and* $c_n = \pm 1$ *according to the normalization* $E_n > 0$.

In particular we have

$$\lim_{n\to\infty} \varphi_n(x) = \infty$$

pointwise for $x \in \overline{\mathbb{C}}^I$.

Proof. As in the proof of theorem 3.3.2, $\varphi_n(x)$ can be written as

$$\varphi_n(x) = \delta_n \frac{\hat{\phi}_{2n}^*(z)}{B_n(z)} (2\pi)^{-\frac{1}{2}} \left\{ 1 + \frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}_{2n}^*(\beta_n)} \right\}^{-\frac{1}{2}} \{\hat{\phi}_{2n}(z)/\hat{\phi}_{2n}^*(z) + 1\}.$$

Using theorem 3.2.2 and 3.2.4 this yields

$$\lim_{n\to\infty} \frac{\tilde{\epsilon}_{2n}}{\delta_n} B_n(z) \frac{1-\beta_n z}{\sqrt{1-\beta_n^2}} \varphi_n(x) = \frac{1}{\sqrt{2\pi}\sigma(\mathring{\mu}', z)}$$

locally uniformly in $\overline{\mathbb{C}}^I$.

It follows from [63] that the function $\hat{\phi}_{2n}(z)$ is real for real z. This implies that also $\hat{\epsilon}_{2n}$ is real, so we must have

$$\frac{\hat{\epsilon}_{2n}}{\delta_n} = \pm 1.$$

The last statement in the theorem follows from the fact that the Blaschke product $B_n(z)$ diverges to zero for $z \in \mathbb{D}$. □

Remark. If we take the normalization $\kappa_n > 0$ instead of $E_n > 0$ for the functions $\varphi_n(x)$ then using $\kappa_n = \lim_{x\to\alpha_n} \varphi_n(x)/b_n(x)$ and the fact that $\sigma(\mathring{\mu}', z)$ is real and positive for real z (because $\mathring{\mu}'(\theta)$ as defined by (2.4) is an even function), it is not difficult to show that c_n in the previous theorem tends to 1 with n so we can omit it from the statement.

3.6 Weak-star convergence

In this section we derive a weak-star convergence result for the φ_n, which generalizes a result by Rakhmanov [47]. We will need several lemmas about ORF on the unit circle before we can prove our main theorem.

The next lemma will be useful when we make the transition from the unit circle to the interval $[-1, 1]$. It is completely analogous to the one for the case of a fixed measure as described in [47].

Lemma 3.6.1. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is such that*

$$\sum_{n=1}^{\infty}(1 - |\beta_n|) = \infty.$$

Then for every integer k we have

$$\frac{\phi^2_{n,n+k}(z)}{z^{n+k}} \frac{d\mathring{\mu}(\theta)}{|w_n(z)|^2} \xrightarrow{*} 0, \quad z = e^{\mathbf{i}\theta}.$$

Proof. We only briefly outline the proof, since it is exactly the same as in [47], apart from the obvious modifications for the case of a varying measure.

Use the first statement in theorem 3.2.1 and the Poisson representation for harmonic functions to find that

$$\frac{\phi_{n,n+k}(z)}{\phi^*_{n,n+k}(z)} d\theta \xrightarrow{*} 0, \quad z = e^{\mathbf{i}\theta}$$

for every integer k.

Then write

$$\frac{\phi_{n,n+k}(z)}{\phi^*_{n,n+k}(z)} = \frac{\phi^2_{n,n+k}(z)}{z^{n+k}|\phi_{n,n+k}(z)|^2}, \quad z = e^{\mathbf{i}\theta}$$

and use

$$\lim_{n\to\infty} \left| \frac{\phi_{n,n+k+m}(z)}{\phi_{n,n+k}(z)} \right|^2 = 1, \quad z = e^{\mathbf{i}\theta}$$

for every integer k and for every $m \in \mathbb{N}$ and

$$\int_0^{2\pi} z^j |\phi_{n,m}(z)|^{-2} d\theta = \int_0^{2\pi} z^j \frac{d\mathring{\mu}(\theta)}{|w_n(z)|^2}, \quad j = 0, \pm 1, \ldots, \pm m, \quad z = e^{\mathbf{i}\theta}. \tag{3.1}$$

Both statements can be found in [34]. Combining all the previous formulas we can prove the lemma. □

The following result is a simple consequence of theorems 2.4.2 and 3.2.2 and we give it without proof.

Lemma 3.6.2. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}' > 0$ a.e. and assume that the sequence B is compactly included in $\mathbb{D}$. Then we have*

$$\left|\frac{\phi_n^*(0)}{\phi_{n,n}^*(0)}\right| \sim \sqrt{1-|\beta_n|^2}$$

in the sense that the ratio of the left hand side and the right hand side tends to 1 as n tends to infinity.

Now we state and prove a weak-star convergence result for the unit circle, which is analogous to the main theorem for the interval at the end of this section and which we will need to prove the latter theorem. It extends the result of theorem 3.2.5.

Theorem 3.6.3. *Under the assumptions and with the definitions of theorem 3.2.5 we have*

$$\frac{|\phi_n(z)|^2}{P(z,\beta_n)} d\mathring{\mu}(\theta) \xrightarrow{*} d\theta.$$

Proof. We begin by proving that

$$\lim_{n\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \frac{|\phi_n(z)|^2}{P(z,\beta_n)} d\mathring{\mu}(\theta) = 1, \quad z = e^{\mathbf{i}\theta}. \tag{3.2}$$

Define $K_n(z) = \mathring{k}_n(z,0)/\sqrt{\mathring{k}_n(0,0)}$ then it follows from the orthogonality of the ϕ_k that

$$\frac{1}{2\pi} \int_0^{2\pi} |K_n(z)|^2 d\mathring{\mu}(\theta) = 1. \tag{3.3}$$

Using theorem 2.4.2 together with the definition of $K_n(z)$ we obtain after some computations

$$|K_n(z)| = \frac{\left|1 - |\beta_n| \overline{\frac{\phi_n(0)}{\phi_n^*(0)}} \frac{\phi_n(z)}{\phi_n^*(z)} \zeta_n(z)\right|}{\sqrt{1-|\beta_n|^2 \left|\frac{\phi_n(0)}{\phi_n^*(0)}\right|^2}} \frac{|1-\overline{\beta}_n z|}{\sqrt{1-|\beta_n|^2}} |\phi_n^*(z)|$$

so if $z \in \mathbb{T}$ we get

$$\frac{|\phi_n^*(z)|^2}{P(z,\beta_n)} = |K_n(z)|^2 \frac{1-|\beta_n|^2 \left|\frac{\phi_n(0)}{\phi_n^*(0)}\right|^2}{\left|1-|\beta_n| \overline{\frac{\phi_n(0)}{\phi_n^*(0)}} \frac{\phi_n(z)}{\phi_n^*(z)} \zeta_n(z)\right|^2}.$$

Integrating both sides this yields using (3.3)

$$\frac{1}{2\pi}\int_0^{2\pi}\frac{|\phi_n(z)|^2}{P(z,\beta_n)}d\mathring{\mu}(\theta) \le \max_{z\in\mathbb{T}} \frac{1-|\beta_n|^2\left|\frac{\phi_n(0)}{\phi_n^*(0)}\right|^2}{\left|1-|\beta_n|\overline{\frac{\phi_n(0)}{\phi_n^*(0)}}\frac{\phi_n(z)}{\phi_n^*(z)}\zeta_n(z)\right|^2}.$$

Because B is compactly included in $\mathbb{D}$ and $|\phi_n(z)/\phi_n^*(z)|<1$ for $z\in\mathbb{D}$ (this follows from corollary 3.1.4 in [10]), the maximum in the right hand side will be finite. Using theorem 3.2.2 we obtain

$$\limsup_{n\to\infty}\frac{1}{2\pi}\int_0^{2\pi}\frac{|\phi_n(z)|^2}{P(z,\beta_n)}d\mathring{\mu}(\theta)\le 1$$

but because of theorem 3.2.5 we also have

$$\liminf_{n\to\infty}\frac{1}{2\pi}\int_0^{2\pi}\frac{|\phi_n(z)|^2}{P(z,\beta_n)}d\mathring{\mu}(\theta)\ge 1$$

so that (3.2) follows.

Because the unit sphere in the dual space of the space of 2π-periodic continuous functions on $[0,2\pi)$ is compact in the weak star topology we can extract from any sequence of natural numbers a subsequence $\Gamma\subset\mathbb{N}$ such that $|\phi_n(z)|^2/P(z,\beta_n)d\mathring{\mu}(\theta)\stackrel{*}{\longrightarrow} dg(\theta)$ as $n\to\infty, n\in\Gamma$, where $dg(\theta)$ is a positive Borel measure and $\int dg = 2\pi$ (the last statement follows from equation (3.2) which we just proved). The rest of the proof is now exactly as in the proof of lemma 2 in [47] and since it is rather technical, we do not repeat it. The key element is that we also have

$$\frac{P(z,\beta_n)}{|\phi_n(z)|^2}d\theta \stackrel{*}{\longrightarrow} d\mathring{\mu}(\theta), \quad z=e^{\mathbf{i}\theta}.$$

This is theorem 9.7.1 in [10]. Using this formula we can prove that dg is the Lebesgue measure on $[0,2\pi)$. We refer to [47] for more details. □

Now let us prove the last lemma before we move to the interval.

Lemma 3.6.4. *Let $\mathring{\mu}$ satisfy the Erdős-Turán condition $\mathring{\mu}'>0$ a.e. and assume that the sequence B is compactly included in $\mathbb{D}$. Then we have*

$$\frac{\phi_n^2(z)}{P(z,\beta_n)B_n(z)}d\mathring{\mu}(\theta)\stackrel{*}{\longrightarrow} 0, \quad z=e^{\mathbf{i}\theta}.$$

Proof. Take $z=e^{\mathbf{i}\theta}$ and let $\phi_n=g_n/w_n^*$, then from the definition of $B_n(z)$ and $P(z,\beta_n)$ we have

$$\frac{\phi_n^2(z)}{P(z,\beta_n)B_n(z)}=\frac{g_n^2(z)(1-\overline{\beta}_n z)(z-\beta_n)}{\eta_n z^{n+1}(1-|\beta_n|^2)|w_n^*(z)|^2}.$$

With lemma 2.4.1 and some calculations we obtain

$$\frac{\phi_n^2(z)}{P(z,\beta_n)B_n(z)} = \frac{1}{1-|\beta_n|^2}\frac{\tau_n^2}{\nu_{n,n}^2}\frac{1-\overline{\beta}_n z}{z-\beta_n}\frac{1}{\eta_n|w_n^*(z)|^2}\left(\frac{\phi_{n,n}^2(z)}{z^{n-1}}\right.$$
$$\left. -2\frac{\phi_{n,n}(\beta_n)}{\phi_{n,n}^*(\beta_n)}\beta_n|\phi_{n,n}(z)|^2 + \left(\frac{\phi_{n,n}(\beta_n)}{\phi_{n,n}^*(\beta_n)}\beta_n\right)^2 z^{n-1}\overline{\phi_{n,n}^2(z)}\right).$$

Because of theorem 3.2.1 it suffices to show that

$$\frac{1}{1-|\beta_n|^2}\frac{\tau_n^2}{\nu_{n,n}^2}\frac{1}{\eta_n}\frac{z(1-\overline{\beta}_n z)}{z-\beta_n}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2} \xrightarrow{*} 0$$

but since it follows from lemma 3.6.2 that the constant factor in this expression is bounded (it tends to 1 in modulus), we can ignore it. It thus remains to prove that

$$\frac{z(1-\overline{\beta}_n z)}{z-\beta_n}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2} \xrightarrow{*} 0.$$

First expand $z(1-\overline{\beta}_n z)/(z-\beta_n)$ in a Taylor series as follows

$$\frac{z(1-\overline{\beta}_n z)}{z-\beta_n} = 1-|\beta_n|^2-\overline{\beta}_n z + (1-|\beta_n|^2)\beta_n\sum_{l=0}^{\infty}\frac{\beta_n^l}{z^{l+1}}.$$

This series will converge because $|z|=1$ and $|\beta_k|\le\rho<1$ for all k.

Because the trigonometric polynomials are dense in the space of 2π-periodic continuous functions on $[0,2\pi)$, the theorem will be proved if we can show that

$$\lim_{n\to\infty}\int_0^{2\pi} z^k\frac{z(1-\overline{\beta}_n z)}{z-\beta_n}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}=0$$

for every integer k. Using the Taylor series expansion we may write

$$\left|\int_0^{2\pi} z^k\frac{z(1-\overline{\beta}_n z)}{z-\beta_n}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right| \le (1-|\beta_n|^2)\left|\int_0^{2\pi} z^k\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right|$$
$$+|\beta_n|\left|\int_0^{2\pi} z^{k+1}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right|$$
$$+(1-|\beta_n|^2)\sum_{l=0}^{\infty}|\beta_n|^{l+1}\left|\int_0^{2\pi} z^{k-l-1}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right|,$$
$$\le \left|\int_0^{2\pi} z^k\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right| + \rho\left|\int_0^{2\pi} z^{k+1}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right|$$
$$+\sum_{l=0}^{\infty}\rho^{l+1}\left|\int_0^{2\pi} z^{k-l-1}\frac{\phi_{n,n}^2(z)}{z^n}\frac{d\mathring{\mu}(\theta)}{|w_n^*(z)|^2}\right|.$$

Taking limits on both sides and using lemma 3.6.1 then proves the lemma (note that each integral in the series is less than one in modulus). □

Now we are ready to state and prove the main theorem in this section.

Theorem 3.6.5. *Assume that μ satisfies the Erdős-Turán condition and that the sequence A is bounded away from I. Then we have*

$$\frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}}\, \varphi_n^2(x) d\mu(x) \xrightarrow{\ *\ } \frac{1}{\pi} \frac{dx}{\sqrt{1 - x^2}}.$$

Proof. First note that

$$\frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}} = P(z, \beta_n)^{-1}$$

where $P(z,t)$ is the Poisson kernel, $x = J(z)$ and $\alpha_n = J(\beta_n)$.

The sequence of norms of the measures

$$d\mu_n(x) = \frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}}\, \varphi_n^2(x) d\mu(x)$$

is bounded because A is bounded away from I and $\int_{-1}^{1} \varphi_n^2(x) d\mu(x) = 1$ by definition. Therefore it suffices to show that for each nonnegative integer k we have

$$\lim_{n\to\infty} \int_{-1}^{1} x^k \frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}}\, \varphi_n^2(x) d\mu(x) = \frac{1}{\pi} \int_{-1}^{1} \frac{x^k}{\sqrt{1 - x^2}} dx.$$

Using equation (2.5) and theorem 2.6.1 we obtain

$$\int_{-1}^{1} x^k \frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}}\, \varphi_n^2(x) d\mu(x) =$$

$$\frac{1}{4\pi} \left\{ 1 + \frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}^*_{2n}(\beta_n)} \right\}^{-1} \int_0^{2\pi} \frac{\cos^k \theta}{P(z, \beta_n)} \left(\frac{\hat{\phi}_{2n}(z) + \hat{\phi}^*_{2n}(z)}{B_n(z)} \right)^2 d\mathring{\mu}(\theta) =$$

$$\frac{1}{2\pi} \left\{ 1 + \frac{\hat{\phi}_{2n}(\beta_n)}{\hat{\phi}^*_{2n}(\beta_n)} \right\}^{-1} \int_0^{2\pi} \frac{\cos^k \theta}{P(z, \beta_n)} \left(|\hat{\phi}_{2n}(z)|^2 + \Re \left\{ \frac{\hat{\phi}^2_{2n}(z)}{\hat{B}_{2n}(z)} \right\} \right) d\mathring{\mu}(\theta).$$

Taking limits and using theorem 3.2.2, theorem 3.6.3 and lemma 3.6.4 this yields

$$\lim_{n\to\infty} \int_{-1}^{1} x^k \frac{1 - x/\alpha_n}{\sqrt{1 - 1/\alpha_n^2}}\, \varphi_n^2(x) d\mu(x) = \frac{1}{2\pi} \int_0^{2\pi} \cos^k \theta d\theta,$$

which proves the theorem. □

Example 3.6.6. Later on in this thesis we discuss gaussian quadrature formulas based on orthogonal rational functions. For analytical integrands, the expression for the quadrature error involves the following function,

$$H(t) = \int_{-1}^{1} \frac{\varphi_n^2(x)(1 - x/\alpha_n)}{t - x} d\mu(x), \quad t \in \overline{\mathbb{C}}^I.$$

We will use these quadrature formulas in the computation of orthogonal rational functions on $[-1, 1]$ and in order to estimate the accuracy we need to evaluate the function $H(t)$ at different points in the complex plane. The exact evaluation of $H(t)$ can be very difficult, but since we are only interested in the order of magnitude, we may use theorem 3.6.5 to approximate this function. First note that

$$\int_{-1}^{1} \frac{dx}{(t - x)\sqrt{1 - x^2}} = \frac{1}{2}\int_{0}^{2\pi} \frac{d\theta}{t - \cos\theta} = \frac{z}{\mathbf{i}} \oint_{\mathbb{T}} \frac{du}{(u - z)(1 - zu)} = \frac{2\pi z}{1 - z^2}$$

where the last equality follows from the residue theorem and $t = J(z)$. Using this formula, theorem 3.6.5 and some algebra then gives

$$H(t) \approx \frac{2z}{1 - z^2} \frac{1 - \beta_n^2}{1 + \beta_n^2}$$

where $\beta_n = J^{-1}(\alpha_n)$. This expression can of course easily be evaluated. Also note that the approximation is exact for $t = \infty$ and $t = \alpha_n$. Numerical experiments indicate that, as long as the poles do not get too close to the boundary, convergence takes place rather quickly, yielding about 4 or 5 correct digits for $n = 20$.

3.7 Conclusion

All results from this chapter can be seen as rational generalizations of known theorems about orthogonal polynomials, as we have indicated throughout our discussion. The connection between orthogonal polynomials with respect to varying measures and orthogonal rational functions has proved to be very useful, as was already apparent in [10], chapter 9. However, as we mentioned earlier on in this chapter, many results for varying orthogonal polynomials have been deduced under weaker conditions on the poles (they do not have to be compactly included in $\mathbb{D}$) and it would be interesting to find out if this condition is also sufficient for the theorems in the rational case. Looking closely at the proofs of theorems 3.2.2 - 3.2.5 and using lemma 2.4.1, it can be seen that this problem reduces to the question whether

$$\lim_{n\to\infty} \frac{\phi_{n,n}(\beta_n)}{\phi_{n,n}^*(\beta_n)} = 0 \tag{3.4}$$

if the β_n satisfy

$$\sum_{n=1}^{\infty}(1-|\beta_n|)=\infty.$$

This is a far from trivial problem, which is still open for investigation. For the case where $\mathring{\mu}$ is the Lebesgue measure on $\mathbb{T}$, it is easy to check that we have

$$\phi_{n,n}(z)=w_n(z)$$

and thus equation (3.4) is clearly satisfied. The Lebesgue measure, however, is in many ways not the most representative example, consider e.g. the zero distribution of Szegő polynomials as described in [36].

In the appendix we present two more open problems concerning asymptotic behaviour of orthogonal rational functions and give some partial results already obtained. The first problem deals with the relative convergence of two systems of ORF on the unit circle, and the second one is about the convergence of $nk_n(x,x)^{-1}$ for $x \in I$. This is the only time in this thesis we study convergence *on* the support of the measure.

Chapter 4

Quadrature formulas

4.1 Introduction

Numerical quadrature is a very important topic in applied mathematics. The so-called Gauss quadrature formulas, based on orthogonal polynomials, form a special case in this field. They are in a certain sense optimal: for a fixed number of nodes, they will integrate a maximal space of polynomials exactly. Furthermore, Gauss quadrature formulas are also used in the study of moment problems, since the discrete measure defined by the quadrature sum will converge (under certain conditions) to a solution of the moment problem. Since the development of this type of formulas, many generalizations have been studied, e.g. formulas integrating exactly in spaces of Laurent polynomials, see [5, 15, 16] or formulas based on orthogonal rational functions. In this chapter we derive some new results concerning the latter quadrature formulas. We mainly look at formulas on $[-1, 1]$, but also study their relation to formulas on the unit circle and very briefly we touch upon interpolatory quadrature rules.

4.2 Preliminaries

Although the quadrature formulas introduced in this section can be given for more general measures, we limit our attention to the circle and interval cases. So as in the previous chapter, $\mathring{\mu}$ will be a measure on $\mathbb{T}$ and μ on I.

To study quadrature formulas on the unit circle, we need the concept of para-orthogonal functions. Let $\tau \in \mathbb{T}$ be given and define

$$Q_n(z, \tau) = \phi_n(z) + \tau\phi_n^*(z) \in \mathring{\mathcal{L}}_n$$

then Q_n is called para-orthogonal because it is only orthogonal to a subspace of $\mathring{\mathcal{L}}_{n-1}$. It is easily checked that

$$Q_n(z,\tau) \perp (\mathring{\mathcal{L}}_{n-1} \cap \zeta_n \mathring{\mathcal{L}}_{n-1}).$$

Concerning these para-orthogonal functions we have the following theorem from [10].

Theorem 4.2.1. *Let $\tau \in \mathbb{T}$ be given, then all the zeros $Q_n(z,\tau)$ are on $\mathbb{T}$ and they are simple.*

This theorem is the reason why para-orthogonal functions are studied. The zeros of ϕ_n are in $\mathbb{D}$ and thus not on $\mathbb{T}$ (this is corollary 3.2.2. in [10]), which means they are not very suitable to be used as the nodes in a quadrature formula. Now we can present the gaussian quadrature formulas based on orthogonal rational functions on the unit circle. For the proof of the following theorem we refer to chapter 5 in [10].

Theorem 4.2.2. *Let $\tau \in \mathbb{T}$ be given and let $\{z_{nk}\}_{k=1}^{n}$ denote the zeros of $Q_n(z,\tau)$. Define the weights $\mathring{\lambda}_{nk}$ by*

$$\mathring{\lambda}_{nk} = \left[\sum_{j=0}^{n-1} |\phi_j(z_{nk})|^2 \right]^{-1}.$$

Then the quadrature formula

$$\frac{1}{2\pi} \int_0^{2\pi} f(e^{\mathbf{i}\theta}) d\mathring{\mu}(\theta) \approx \sum_{k=1}^{n} \mathring{\lambda}_{nk} f(z_{nk})$$

is exact for $f \in \mathring{\mathcal{L}}_{n-1} \cdot \mathring{\mathcal{L}}_{(n-1)*}$.

For the case of orthogonality on the interval $[-1,1]$ the formulas are very similar. In [10] so-called quasi-orthogonal functions are introduced, analogous to the para-orthogonal functions in the circle case. However, in this thesis we do not need quasi-orthogonal functions. The next theorem is a special case of [10, Theorem 11.6.2.].

Theorem 4.2.3. *Let $\{x_{nk}\}_{k=1}^{n}$ be the zeros of the n-th orthogonal rational function φ_n and let λ_{nk} be defined by*

$$\lambda_{nk} = \left[\sum_{j=0}^{n-1} (\varphi_j(x_{nk}))^2 \right]^{-1}.$$

Then the quadrature formula

$$\int_{-1}^{1} f(x)d\mu(x) \approx \sum_{k=1}^{n} \lambda_{nk} f(x_{nk})$$

is exact for $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$*.*

These formulas reduce to the classical Gauss formulas taking $\alpha_k = \infty$ for all k. Note that we have $\lambda_{nk} = k_{n-1}(x_{nk}, x_{nk})^{-1} = k_n(x_{nk}, x_{nk})^{-1}$. The same is true in the circle case. Another expression for the weights λ_{nk} as given in [10, p. 287] is

$$\lambda_{nk} = \int_{-1}^{1} L_{nk}(x)d\mu(x) \tag{4.1}$$

where L_{nk} is as in lemma 2.5.5. This is only saying that gaussian quadrature formulas are a special kind of interpolatory quadrature formulas.

The nodes and weights in this quadrature formula can be computed from the recurrence coefficients by solving a generalized eigenvalue problem (GEP), as given in the following theorem from [11].

Theorem 4.2.4. *For* $n = 0, 1, \dots$ *define the numbers* a_n *and* b_n *as*

$$a_n = -\frac{F_{n+1}}{E_{n+1}}, \quad b_n = \frac{1}{E_{n+1}}$$

and the matrices

$$J_n = \begin{bmatrix} a_0 & b_0 & & & \\ b_0 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b_{n-1} \\ & & & b_{n-1} & a_n \end{bmatrix}, \quad D_n = \begin{bmatrix} 0 & & & & \\ & \alpha_1^{-1} & & & \\ & & \alpha_2^{-1} & & \\ & & & \ddots & \\ & & & & \alpha_n^{-1} \end{bmatrix}.$$

Then the eigenvalues z *of the generalized eigenvalue problem*

$$J_n \underline{v} = (J_n D_n + I_n)\underline{v} z$$

(where I_n *is the* n*-dimensional unit matrix) are equal to the nodes* $x_{n+1,k}$ *and the weights are given by* $\lambda_{n+1,k} = \mu_0 \underline{v}_1^2$*, where* $\underline{v}_1$ *denotes the first component of the eigenvector* $\underline{v}$ *(which we assume normalized to have Euclidean norm 1).*

Note that this reduces to the classical eigenvalue problem in the polynomial case.

4.3 Quadrature formulas on $[-1, 1]$

First let us introduce some notation. The quadrature formula on I will be denoted by

$$I_n(f) = \sum_{k=1}^{n} \lambda_{nk} f(x_{nk})$$

and the linear functional defined by μ will be written

$$I_\mu(f) = \int_{-1}^{1} f(x) d\mu(x).$$

To study the convergence of this quadrature formula, we need some results about the density of the rational functions. First we give the following lemma, which is a special case of the more general result in [1, p. 250].

Lemma 4.3.1. *Let the polynomial*

$$\pi_n(x) = \prod_{k=1}^{n} \left(1 - \frac{x}{\alpha_k}\right)$$

be given with real zeros α_k such that $|\alpha_k| > 1$ (α_k may equal infinity) and take $\beta_k = J^{-1}(\alpha_k)$ then we have for $m > n$ and $p = 1$ or $p = \infty$

$$\min_{A_k} \left\| \frac{x^m + A_1 x^{m-1} + \ldots + A_m}{\pi_n(x)} \right\|_p = \frac{1}{2^{m-1}} \prod_{k=1}^{n} (1 + \beta_k^2).$$

Using this lemma it is not difficult to obtain conditions under which the rational functions are dense in the space $C(I)$ of continuous functions on I or in the $L^p(I)$ spaces. The following theorem is very similar to a theorem in [1], but we do not require that all the poles be different from each other.

Theorem 4.3.2. *The space $\mathcal{L} = \cup_0^\infty \mathcal{L}_n$ is dense in any $L^p(I)$ space with $p \geq 1$ as well as in the class $C(I)$ of continuous functions on I if and only if $\sum_{k=1}^{\infty}(1 - |\beta_k|) = \infty$, where $\beta_k = J^{-1}(\alpha_k)$.*

Proof. The proof is very much like the one of theorem 7.1.2 in [10], but we give it for the sake of completeness.

It suffices to show that divergence of the sum implies the completeness of the system $\{b_k\}_{k=0}^{\infty}$ in the space $C(I)$ and that it is necessary for completeness in the space $L^1(I)$.

First note that if there are infinitely many poles at infinity, then there is nothing to prove because in that case the system contains all the polynomials and these are known to be complete while the sum certainly diverges.

So assume (without loss of generality) that the first q poles are at infinity ($q < \infty$) and that the sum diverges. Then we have to show that all x^k with $k > q$ can be approximated arbitrarily close (according to the Chebyshev norm) by elements of $\mathcal{L}_n$ for n sufficiently large. This follows from the following observation (using the previous lemma):

$$\min_{f\in\mathcal{L}_n, A_i} \left\| x^{m+q} + A_1 x^{m+q-1} + \ldots + A_{m-1}x^{q+1} + f(x) \right\|_\infty =$$
$$\frac{1}{|\alpha_{q+1}\alpha_{q+2}\ldots\alpha_n|} \min_{p\in\mathcal{P}_{n+m-1}} \left\| \frac{x^{n+m}+p(x)}{\pi_n(x)} \right\|_\infty = \frac{1}{2^{m+q-1}} \prod_{k=q+1}^{n} |\beta_k|.$$

Since the sum diverges to infinity, we must have that $\prod_{q+1}^n |\beta_k| \to 0$. The rest of the proof is then by induction.

To prove that divergence of the sum is necessary for completeness in $L^1(I)$, we proceed as follows. By the previous lemma for $p = 1$ we have that

$$\min_{f\in\mathcal{L}_n} \|x^{q+1} - f(x)\|_1 =$$
$$\frac{1}{|\alpha_{q+1}\alpha_{q+2}\ldots\alpha_n|} \min_{p\in\mathcal{P}_n} \left\| \frac{x^{n+1}+p(x)}{\pi_n(x)} \right\|_1 = \frac{1}{2^q} \prod_{k=q+1}^{n} |\beta_k|.$$

Since the system is supposed to be complete in $L^1(I)$, the previous expression should tend to zero as $n \to \infty$. Whence $\sum(1 - |\beta_k|) = \infty$. □

As a direct consequence of this theorem and the fact that the weights in the quadrature formula are positive, we have the following theorem which we give without proof.

Theorem 4.3.3. *Under the same conditions as in theorem 4.3.2, it holds that*

$$\lim_{n\to\infty} I_n(f) = I_\mu(f) = \int_{-1}^{1} f(x)d\mu(x)$$

for any function f in $C(I)$.

If $f \notin \mathcal{L}_n \cdot \mathcal{L}_{n-1}$ then we can derive an expression for the quadrature error

$$e_n(f) = I_\mu(f) - I_n(f).$$

This will be done in the following theorem.

Theorem 4.3.4. *Let f be analytic in a closed simply connected region Ω containing the interval $[-1,1]$. Let C be a Jordan curve that lies in Ω and surrounds the quadrature nodes $\{x_{nk}\}_{k=1}^n$. Then*

$$e_n(f) = \frac{1}{2\pi\mathbf{i}}\int_C \frac{f(t)}{(1-t/\alpha_n)\varphi_n^2(t)}\left\{\int_{-1}^1 \frac{\varphi_n^2(x)(1-x/\alpha_n)}{t-x}d\mu(x)\right\}dt.$$

Proof. Let $R_{2n-1}(f,x)$ denote the (unique) element of $\mathcal{L}_n\cdot\mathcal{L}_{n-1}$ satisfying the interpolation conditions

$$R_{2n-1}(f,x_{nj}) = f(x_{nj})$$
$$R'_{2n-1}(f,x_{nj}) = f'(x_{nj})$$

for $j=1,\dots,n$. Then it can easily be seen that

$$R_{2n-1}(f,x) = \sum_{k=1}^n H_{nk}(x)f(x_{nk}) + \sum_{k=1}^n \tilde{H}_{nk}(x)f'(x_{nk})$$

where $H_{nk}(x)$ and $\tilde{H}_{nk}(x)$ are the fundamental Hermite interpolating rational functions defined in chapter 2. Integrating with respect to μ we obtain

$$I_\mu(R_{2n-1}(f,\cdot)) = \sum_{k=1}^n A_{nk}f(x_{nk}) + \sum_{k=1}^n \tilde{A}_{nk}f'(x_{nk})$$

with $A_{nk} = I_\mu(H_{nk})$ and $\tilde{A}_{nk} = I_\mu(\tilde{H}_{nk})$. Now it follows from lemma 2.5.5 that $\tilde{H}_{nk}(x) = c_{nk}\varphi_n(x)g_{n-1}(x)$ where c_{nk} is a constant and $g_{n-1}\in\mathcal{L}_{n-1}$. Therefore $\tilde{A}_{nk}=0$. From the same lemma and from lemma 2.5.6 it follows that $A_{nk} = I_\mu(L_{nk})$. Putting everything together we conclude that $e_n(f) = I_\mu(f - R_{2n-1}(f,\cdot))$.

Writing $R_{2n-1}(f,x) = p_{2n-1}(f,x)/(\pi_n(x)\pi_{n-1}(x))$ it is not difficult to see that $p_{2n-1}(f,x)$ is the unique Hermite interpolating polynomial for the function $\pi_n(x)\pi_{n-1}(x)f(x)$. From theorem 3.6.1 in [13] the interpolation error is given by

$$\pi_n(x)\pi_{n-1}(x)f(x) - p_{2n-1}(f,x) =$$
$$\frac{1}{2\pi\mathbf{i}}\int_C \frac{(x-x_{n1})^2\dots(x-x_{nn})^2}{(t-x_{n1})^2\dots(t-x_{nn})^2}\frac{\pi_n(t)\pi_{n-1}(t)f(t)}{t-x}dt$$

where C is as in the statement of this theorem. Dividing by $\pi_n(x)\pi_{n-1}(x)$ this yields

$$f(x) - R_{2n-1}(f,x) = \frac{1}{2\pi\mathbf{i}}\int_C \frac{(1-x/\alpha_n)\varphi_n^2(x)}{(1-t/\alpha_n)\varphi_n^2(t)}\frac{f(t)}{t-x}dt.$$

Integrating over I with respect to $d\mu(x)$ now proves the theorem. □

4.4 Relating the interval to the unit circle

In this section we derive relations between quadrature formulas on the unit circle and quadrature formulas on the interval. The approach we take is very similar to the one in [3] for the polynomial case, although we do not restrict our attention to absolutely continuous measures.

The following definition will be needed in the sequel. It is the measure theoretic equivalent of an even (or symmetric) weight function on $[0, 2\pi)$.

Definition 4.4.1. A measure $\mathring{\mu}$ on $[0, 2\pi)$ will be called *symmetric* if it satisfies

$$\mathring{\mu}(E) = \mathring{\mu}(\{\theta : 2\pi - \theta \in E\})$$

for every Borel measurable set $E \in [0, 2\pi)$.

We will also use a lemma from [63]. It was proved for the case of absolutely continuous measures and a sequence B where each β_k has even multiplicity, but it extends without changes in the proof to our more general case.

Lemma 4.4.2. *Let $\mathring{\mu}$ be symmetric and assume that $B \subset I$. Then ϕ_n has real coefficients with respect to the basis $\{B_0, B_1, \ldots, B_n\}$.*

The following theorem relates the quadrature formulas on $\mathbb{T}$ to those on the interval $[-1, 1]$.

Theorem 4.4.3. *Let $\varphi_n(x)$ and $\tilde{\phi}_{2n}(z)$ be the ORF on I and $\mathbb{T}$ respectively, related by theorem 2.6.1. Denote by $\{x_{nk}\}_{k=1}^{n}$ and $\{\lambda_{nk}\}_{k=1}^{n}$ the nodes and weights corresponding to φ_n, and by $\{z_{2n,k}\}_{k=1}^{2n}$ and $\{\mathring{\lambda}_{2n,k}\}_{k=1}^{2n}$ the nodes and weights corresponding to $\hat{\phi}_{2n}$ with $\tau = 1$. Then we can arrange the $\{z_{2n,k}\}$ such that*

$$z_{2n,n+k} = \overline{z}_{2n,k}, \quad k = 1, \ldots, n \tag{4.2}$$

and

$$x_{nk} = \Re\{z_{2n,k}\}, \quad k = 1, \ldots, n. \tag{4.3}$$

Assuming that this has been done, we have

$$\lambda_{nk} = 2\pi\mathring{\lambda}_{2n,k} = 2\pi\mathring{\lambda}_{2n,n+k}, \quad k = 1, \ldots, n. \tag{4.4}$$

Proof. It follows from the fact that $\mathring{\mu}$ as defined by (2.3) is a symmetric measure and from lemma 4.4.2 that the coefficients of $\hat{\phi}_{2n}(z)$ are real with respect to the basis $\{\hat{B}_0, \hat{B}_1, \ldots, \hat{B}_{2n}\}$. Since the β_k are also real, the numerator polynomial of both $\hat{\phi}_{2n}(z)$ and $\hat{\phi}^*_{2n}(z)$ have real coefficients with respect to the canonical basis $\{1, z, \ldots, z^{2n}\}$. Thus, the zeros of $\hat{\phi}_{2n}(z) + \hat{\phi}^*_{2n}(z)$ appear in complex conjugate pairs, which proves (4.2). Equation (4.3) now follows from theorem 2.6.1. From these remarks and the expression for $\mathring{\lambda}_{2n,k}$ in theorem 4.2.2, we also conclude that

$$\mathring{\lambda}_{2n,n+k} = \mathring{\lambda}_{2n,k}, \quad k = 1, \ldots, n.$$

To prove (4.4), we either have to prove that

$$\frac{1}{2\pi}\sum_{k=1}^{n} \lambda_{nk}[f(z_{nk}) + f(\overline{z}_{nk})] = \frac{1}{2\pi}\int_0^{2\pi} f(e^{\mathbf{i}\theta})d\mathring{\mu}(\theta)$$

for every $f \in \mathring{\mathcal{L}}_{2n-1} \cdot \mathring{\mathcal{L}}_{(2n-1)*}$, or that

$$2\pi \sum_{k=1}^{n} \mathring{\lambda}_{2n,k} f(x_{nk}) = \int_{-1}^{1} f(x)d\mu(x)$$

for every $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$. We choose to prove the second relation. First note that

$$\pi_n(x) = \frac{w_n(z)w_n^*(z)}{z^n \prod_{k=1}^{n}(1+\beta_k^2)}$$

and that for every $p_n \in \mathcal{P}_n$ there is a $q_n \in \mathcal{P}_n$ such that $p_n(x) = q_n(z) + q_n(1/z)$, where $x = J(z)$. Combining these two statements shows that $f \circ J \in \mathring{\mathcal{L}}_{2n-1} \cdot \mathring{\mathcal{L}}_{(2n-1)*}$ whenever $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$. So taking such an f, we have

$$\begin{aligned}
\sum_{k=1}^{n} \mathring{\lambda}_{2n,k} f(x_{nk}) &= \sum_{k=1}^{n} \mathring{\lambda}_{2n,k}(f \circ J)(z_{2n,k}) \\
&= \frac{1}{2}\sum_{k=1}^{n} \mathring{\lambda}_{2n,k}[(f \circ J)(z_{2n,k}) + (f \circ J)(1/z_{2n,k})] \\
&= \frac{1}{2}\sum_{k=1}^{2n} \mathring{\lambda}_{2n,k}(f \circ J)(z_{2n,k}) \\
&= \frac{1}{4\pi}\int_0^{2\pi} (f \circ J)(z)d\mathring{\mu}(\theta) \\
&= \frac{1}{2\pi}\int_{-1}^{1} f(x)d\mu(x)
\end{aligned}$$

which proves the theorem. □

4.5 Interpolatory quadrature formulas

The name 'interpolatory quadrature formulas' usually refers to quadrature formulas where the weights are obtained by integrating some kind of interpolating function in the nodes (in our case an interpolating rational function). It therefore also covers the gaussian quadrature formulas we discussed in the previous sections. However, in this section we will only be concerned with formulas which have nodes at the zeros of $\varphi_n(x)$, but which integrate exactly with respect to a different measure $\tilde{\mu}$. Contrary to the previous section, we do not limit our attention to the interval $[-1, 1]$.

So as before let $\varphi_n(x)$ be orthogonal with respect to μ and denote its zeros by $\{x_{nk}\}_{k=1}^{n}$. Then assume we are given a measure $\tilde{\mu}$ and define the weights

$$A_{nk} = \int L_{nk}(x) d\tilde{\mu}(x), \quad k = 1, \ldots, n \tag{4.5}$$

where $L_{nk}(x)$ is the interpolating rational function from lemma 2.5.5. It is not difficult to see that the formula

$$\sum_{k=1}^{n} A_{nk} f(x_{nk}) \approx \int_{-1}^{1} f(x) d\tilde{\mu}(x)$$

is exact for every $f \in \mathcal{L}_{n-1}$. Now we would like to know in what way these weights are related to the gaussian weights λ_{nk}. We introduce the function $\mathrm{k}_n(x)$ defined as

$$\mathrm{k}_n(x) = \int k_n(x,t) d\tilde{\mu}(t).$$

Note that this is a function in $\mathcal{L}_n$. We can now prove the following simple lemma.

Lemma 4.5.1. *Let $\mathrm{k}_n(x)$ be as defined above. Then we have*

$$\int \mathrm{k}_n(x) f(x) d\mu(x) = \int f(x) d\tilde{\mu}(x)$$

for every $f \in \mathcal{L}_n$.

Proof. By the definition of $\mathrm{k}_n(x)$ we have

$$\int \mathrm{k}_n(x) f(x) d\mu(x) = \int \left[\int k_n(x,t) d\tilde{\mu}(t) \right] f(x) d\mu(x).$$

Because of Fubini's theorem, this may be written

$$\int \mathrm{k}_n(x) f(x) d\mu(x) = \int \left[\int k_n(x,t) f(x) d\mu(x) \right] d\tilde{\mu}(x).$$

The lemma now follows from the fact that $f \in \mathcal{L}_n$ and $k_n(x,t)$ is the reproducing kernel for $\mathcal{L}_n$. □

With the aid of this lemma, it is not difficult to find the relation between A_{nk} and λ_{nk}, as given in the next theorem.

Theorem 4.5.2. *With the definitions of this section we have*

$$A_{nk} = \mathrm{k}_{n-1}(x_{nk})\lambda_{nk}$$

for $k = 1, \ldots, n$.

Proof. The weights A_{nk} were defined as

$$A_{nk} = \int L_{nk}(x)d\tilde{\mu}(x)$$

which by the previous lemma may be written as

$$A_{nk} = \int \mathrm{k}_{n-1}(x)L_{nk}(x)d\mu(x).$$

Applying lemma 2.5.6 then gives

$$A_{nk} = \mathrm{k}_{n-1}(x_{nk}) \int L_{nk}(x)d\mu(x)$$

which, according to equation (4.1), proves the theorem. □

The previous theorem shows that the interpolatory weights can be computed from the gaussian weights as soon as we have obtained the function $\mathrm{k}_n(x)$. In the case study of the last chapter we look at an example for this theorem. The function $\mathrm{k}_n(x)$ is related to the modified moments from section 6.3. For more information we refer to that section and to section 9.8.

Before concluding this chapter, we note that in the case where both μ and $\tilde{\mu}$ are absolutely continuous, $\mathrm{k}_n(x)$ is the n-th partial sum of the expansion of $\tilde{\mu}'(x)/\mu'(x)$ in terms of the functions $\varphi_n(x)$. This can be seen as follows. The Fourier coefficients c_n of $\tilde{\mu}'/\mu$ with respect to the system $\{\varphi_n\}$ are given by

$$c_n = \int \frac{\tilde{\mu}'(x)}{\mu'(x)}\varphi_n(x)d\mu(x).$$

If both μ and $\tilde{\mu}$ are absolutely continuous (with respect to the Lebesgue measure), this becomes

$$c_n = \int \varphi_n(x)d\tilde{\mu}(x).$$

Now we have

$$\begin{aligned}
\mathrm{k}_n(x) &= \int k_n(x,t)d\tilde{\mu}(t) \\
&= \sum_{k=0}^{n} \int \varphi_k(t)d\tilde{\mu}(t)\varphi_k(x) \\
&= \sum_{k=0}^{n} c_k\varphi_k(x)
\end{aligned}$$

which proves our statement. If the φ_n are dense in $L^2(\mu)$ then this means that

$$\lim_{n\to\infty} \left\| \frac{\tilde{\mu}'}{\mu'} - \mathrm{k}_n \right\|_\mu^2 = 0.$$

Pointwise convergence presents a more delicate problem. Without further study, we can only say that there exists a subsequence $\{n_i\}_{i=0}^{\infty}$ such that

$$\lim_{i\to\infty} \mathrm{k}_{n_i}(x) = \frac{\tilde{\mu}'(x)}{\mu'(x)} \text{ a.e. } [\mu]$$

but since μ is absolutely continuous, this is the same as convergence a.e. with respect to the Lebesgue measure.

4.6 Conclusion

This chapter presents some theoretical considerations about gaussian quadrature formulas based on orthogonal rational functions. Most of the results here will be used later on in this thesis. For example, the expression for the quadrature error appears in the accuracy estimate of the main algorithm in chapter 7 and the theorem about interpolatory quadrature is used in an example in chapter 9. It is worth mentioning that the relation between formulas on I and $\mathbb{T}$ can probably also yield information about Gauss-Lobatto and Gauss-Radau quadrature formulas, as was done for the polynomial case in [3], but this is still open for future research. It is expected, however, that generalization to the rational case will not present many fundamental problems.

Chapter 5

Interpolation algorithms

5.1 Introduction

In the rest of this thesis we will mainly be concerned with the computation of orthogonal rational functions on a subset of the real line. This chapter presents some algorithms to compute the recurrence coefficients based on certain interpolation properties of the Riesz-Herglotz-Nevanlinna transform of the orthogonality measure. A detailed error analysis will show that these algorithms are not practically useful because of the unbounded error growth. For research purposes however (when one can work in multiprecision) they are still of interest. Furthermore, there are some relations with multipoint Padé approximants, continued fractions and Schur algorithms, as we will point out in the text.

5.2 Preliminaries

We will assume that μ and A are as in section 2.5, which means we do not limit our attention to the case of orthogonality on an interval. However, it will be convenient to assume that the measure is normalized, i.e. $\mu_0 = 1$.

The Riesz-Herglotz-Nevanlinna kernel $D(t, z)$ for the real line is defined as

$$D(t, z) = -\mathbf{i}\frac{1 + tz}{t - z}$$

and the Riesz-Herglotz-Nevanlinna transform of the measure μ as

$$\Omega_\mu(z) = \int D(t, z) d\mu(t).$$

As in the polynomial case we introduce functions of the second kind,

$$\psi_n(z) = \int D(t,z)[\varphi_n(t) - \varphi_n(z)]d\mu(t)$$

for $n \geq 1$ and $\psi_0(z) = \mathbf{i}z$. From lemma 2.5.1 it follows that $\psi_n(z)$ is purely imaginary for real z, i.e. $\psi_n(z) \in \mathbf{i}\overline{\mathbb{R}}$ if $z \in \overline{\mathbb{R}}$. Concerning these functions of the second kind, we have the following theorem from [10, p. 267].

Theorem 5.2.1. *Suppose that the system of orthogonal rational functions φ_n is regular and let ψ_n be the functions of the second kind associated with them. Then for $n \geq 2$ these ψ_n satisfy the same recurrence relation* (2.2) *as the φ_n, but with different initial values.*

If we want to start the recursion from $n = 1$ we will need an expression for $\psi_{-1}(z)$, which will be given in the following lemma.

Lemma 5.2.2. *In order to satisfy the recurrence relation* (2.2) *for $n = 1$, $\psi_{-1}(z)$ has to be defined as*

$$\psi_{-1}(z) = \mathbf{i}(1 + z^2).$$

Proof. This is a matter of straightforward calculation. Compute ψ_1 using the definition and compare it with the expression obtained using the recurrence relation. □

So the initial values in the recurrence relation for the ψ_n are $\psi_0(z) = \mathbf{i}z$ and $\psi_{-1}(z) = \mathbf{i}(1 + z^2)$.

5.3 Interpolation properties for Ω_μ

In this section we will derive certain interpolation properties for the Riesz-Herglotz-Nevanlinna transform $\Omega_\mu(z)$ which will be used to provide an algorithm to compute the recursion coefficients E_n and F_n. It may seem more natural to use the Stieltjes transform instead of the Riesz-Herglotz-Nevanlinna transform, but then the functions of the second kind would have to be defined in a different way as well and we prefer to be consistent with the definitions and notation of [10] and related articles.

Using lemma 2.5.6 we can easily prove the following interpolation result for Ω_μ. The same result could also be obtained using interpolating polynomials, as in [10, p. 328-334], but then the argument is a lot more involved.

Theorem 5.3.1. *Let Ω_μ be the Riesz-Herglotz-Nevanlinna transform of the measure μ. Let φ_n be the orthonormal functions and ψ_n the associated functions of the second kind. Then we have*

$$\psi_n(z) + \varphi_n(z)\Omega_\mu(z) = \frac{R_n(z)}{b_{n-1}(z)}, \quad n \geq 1 \tag{5.1}$$

with $R_n(z)$ defined by

$$R_n(z) = \int D(t,z) b_{n-1}(t)\varphi_n(t) d\mu(t)$$

and $R_n(z)$ is finite for $z \in \overline{\mathbb{C}} \setminus \operatorname{supp}(\mu)$. Equivalently

$$\psi_n(z) + \varphi_n(z)\Omega_\mu(z) = -\mathbf{i}\frac{1+z^2}{b_{n-1}(z)} \int \frac{\varphi_n(t) b_{n-1}(t)}{t-z} d\mu(t). \tag{5.2}$$

If all poles are outside the convex hull of supp(μ) *then $-\psi_n/\varphi_n$ interpolates Ω_μ in Hermite sense at the points $\{\mathbf{i}, -\mathbf{i}, \alpha_1, \alpha_1, \ldots, \alpha_{n-1}, \alpha_{n-1}, \alpha_n\}$.*

Proof. Use the definition of ψ_n and Ω_μ to write

$$\psi_n(z) + \varphi_n(z)\Omega_\mu(z) = \int D(t,z)\varphi_n(t) d\mu(t). \tag{5.3}$$

The first result then follows from Lemma 2.5.6 with $f = b_{n-1}$. To obtain the second equation, write

$$D(t,z) = -\mathbf{i}\left(z + \frac{1+z^2}{t-z}\right)$$

and use the orthogonality of φ_n. This yields (5.2). Dividing by $\varphi_n(z)$ we obtain

$$\frac{\psi_n(z)}{\varphi_n(z)} + \Omega_\mu(z) = -\mathbf{i}(1+z^2)\frac{\pi_{n-1}(z)}{z^{n-1}} \frac{\pi_n(z)}{p_n(z)} \int \frac{\varphi_n(t) b_{n-1}(t)}{(t-z)} d\mu(t),$$

where p_n is the numerator of φ_n. If all poles are outside the convex hull of supp(μ), then none of the zeros of p_n will coincide with any of the poles, hence the Hermite interpolation. □

It follows from (5.3) that $\psi_n(z) + \varphi_n(z)\Omega_\mu(z)$ is the n-th Fourier coefficient of $D(t,z)$ as a function of t, relative to the orthonormal system $\{\varphi_k\}$. Therefore

$$\lim_{n\to\infty} \frac{R_n(z)}{b_{n-1}(z)} = 0, \quad z \in \overline{\mathbb{C}} \setminus \operatorname{supp}(\mu). \tag{5.4}$$

This is an easy consequence of Bessel's inequality, see e.g. [50, p. 85]. Without further assumptions on the measure nothing can be said for $z \in \operatorname{supp}(\mu)$, since $D(t,z)$ may not be in $L^2(\mu)$.

5.4 An algorithm to compute E_n and F_n

In the rest of this paper we assume that the system $\{\varphi_n\}$ is regular. Then since both φ_n and ψ_n satisfy the recurrence relation (2.2), so does $\psi_n + \varphi_n \Omega_\mu$. Therefore we have from (5.1) for $n \geq 3$

$$\frac{R_n}{b_{n-1}Z_n} = (E_n Z_{n-1} + F_n)\frac{R_{n-1}}{b_{n-2}Z_{n-1}} - \frac{E_n}{E_{n-1}}\frac{R_{n-2}}{b_{n-3}Z_{n-2}}.$$

We formally define $R_{-1}(z)$ and $R_0(z)$ using (5.1) so that the recursion also holds for $n = 1, 2$ as follows

$$R_{-1}(z) = \mathbf{i}(1 + z^2), \quad R_0(z) = \mathbf{i}z + \Omega_\mu(z). \tag{5.5}$$

Putting

$$\Gamma_n(z) = \frac{b_{n-2}(z)}{b_{n-1}(z)}\frac{Z_{n-1}(z)}{Z_n(z)}\frac{R_n(z)}{R_{n-1}(z)}, \quad n \geq 0 \tag{5.6}$$

where $b_k(z) \equiv 1$ if $k \leq 0$, we get the following recurrence relation

$$\Gamma_n(z) = E_n Z_{n-1}(z) + F_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}, \quad n \geq 1. \tag{5.7}$$

Note that for $n \geq 2$ the expression for Γ_n reduces to

$$\Gamma_n(z) = \frac{1 - z/\alpha_n}{z}\frac{R_n(z)}{R_{n-1}(z)}, \quad n \geq 2$$

and for $n = 1$ we have

$$\Gamma_1(z) = (1 - z/\alpha_1)\frac{R_1(z)}{R_0(z)}.$$

Since $R_n(z)$ is finite for any z outside $\mathrm{supp}(\mu)$ and because none of the poles is in $\mathrm{supp}(\mu)$, it follows that $\Gamma_n(\alpha_n) = 0$ for $n \geq 1$. The initial condition for the recurrence relation follows from (5.5) and (5.6),

$$\Gamma_0(z) = \frac{\mathbf{i}z + \Omega_\mu(z)}{\mathbf{i}(1 + z^2)}.$$

With the definition of Ω_μ this can be rewritten as

$$\Gamma_0(z) = -\int \frac{d\mu(t)}{t - z}. \tag{5.8}$$

It follows that $-\Gamma_0(z)$ is the Stieltjes transform of the measure μ, see e.g. [25].

The functions $\Gamma_n(z)$ are closely related to certain functions arising in a modified Schur algorithm, as described in [41]. For the case of cyclicly repeated poles $\{\alpha_1, \ldots, \alpha_p, \alpha_1, \ldots, \alpha_p, \ldots\}$, the author defines Nevanlinna functions $F_n(z)$ which after careful consideration turn out to be equal to the Γ_n functions (up to a multiplicative constant only depending on n). For more information we refer to his article.

Equation (5.7) obviously gives rise to a continued fraction expansion for the function $-\Gamma_0(z)$. The approximants of this continued fraction are multipoint Padé approximants for the Stieltjes transform of μ. A detailed description can be found in [7].

Using the recursion formula (5.7) it is possible to compute the recursion coefficients E_n and F_n in (2.2). In the rest of this section we assume that all poles are different from each other. We will get back to this at the end of the section. Using the fact that $\Gamma_n(\alpha_n) = 0$ we easily find that

$$F_n = -E_n Z_{n-1}(\alpha_n) + \frac{E_n/E_{n-1}}{\Gamma_{n-1}(\alpha_n)}\ , \quad n \geq 1.$$

To find an expression for E_n we multiply (5.7) by $\Gamma_{n-1}(z)$ and take the limit for $z \to \alpha_{n-1}$, which gives, using l'Hôpital's rule (and increasing the index $n-1$ to n in the final result)

$$E_n = \frac{-1}{\alpha_n^2 \Gamma_n'(\alpha_n)}\ .$$

This is of course not a very useful expression, because it still involves (the derivative of) Γ_n to compute E_n. Differentiating (5.7) however gives

$$\Gamma_n'(z)/E_n = Z_{n-1}'(z) + \frac{\Gamma_{n-1}'(z)/E_{n-1}}{\Gamma_{n-1}^2(z)}$$

or defining $\Delta_n(z) = \Gamma_n'(z)/E_n$ we may write

$$\Delta_n(z) = Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)}{\Gamma_{n-1}^2(z)}\ , \quad n \geq 1 \tag{5.9}$$

and $\Delta_0(z) = \Gamma_0'(z)$. We finally substitute this into the expression for E_n to find

$$E_n = \frac{1}{|\alpha_n|}\sqrt{\frac{-1}{\Delta_n(\alpha_n)}}, \quad n \geq 1.$$

This concludes our discussion. To compute E_n and F_n we will need Γ_0 and its derivative at the poles $\{\alpha_1, \ldots, \alpha_n\}$.

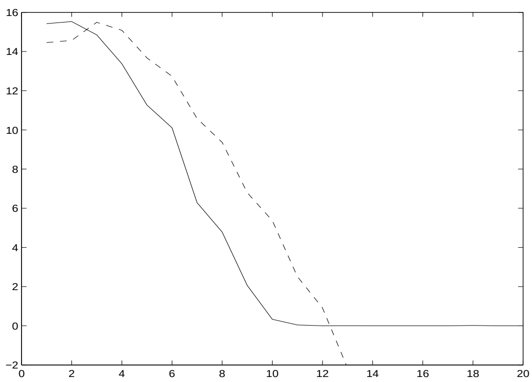

Figure 5.1: Number of correct digits of E_n against n, example 5.5.1 (solid line) and the estimate from example 5.7.1 (dashed line)

In the case of repeated poles, we will need higher order derivatives of $\Gamma_0(z)$. Consider for example the case where for a certain value of n we would have $\alpha_n = \alpha_{n-1}$. To compute F_n we cannot simply substitute α_n for z in (5.7) since α_n is also a zero of $Z_{n-1}(z)$ and $\Gamma_{n-1}(z)$. This is only another formulation of theorem 11.10.3 in [10], which states that for a pole α with multiplicity $\alpha^{\#}$ the first $2\alpha^{\#} - 1$ derivatives of Ω_μ (and thus of Γ_0) are needed to characterise the inner product. Indeed if all poles are different from each other, we only need Γ_0 and its derivative.

5.5 Examples

Before we go into a numerical analysis of the error propagation in the algorithm derived in the previous section, we look at some examples. In all examples supp(μ) is connected and the poles are simple, so we can use the algorithm to compute the recursion coefficients.

Example 5.5.1. First consider the sequence of poles $\{\omega, -\omega, 2\omega, -2\omega, \ldots\}$ where $\omega = 1.1$. We use the normalised Lebesgue measure on the interval $[-1, 1]$, so we have $d\mu(z) = 1/2dz$. For this case some computations yield

$$\Gamma_0(z) = \frac{1}{2} \ln \frac{z+1}{z-1}, \quad z \in \overline{\mathbb{C}} \setminus [-1, 1].$$

In figure 5.1 the number of correct digits in double precision for the coefficient E_n is plotted against n. All computations were done in Maple, using 16 digits for double precision and 80 for the ‘exact’ values. It seems that for $n = 10$ we have already lost *all* correct digits.

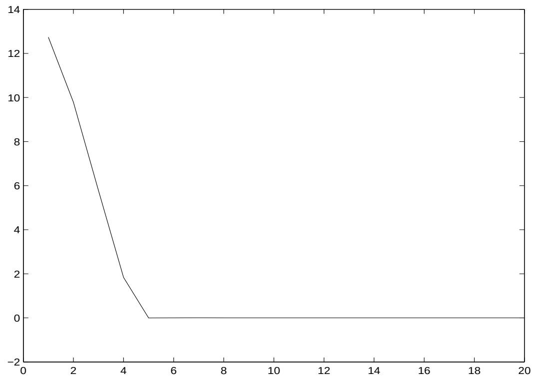

Figure 5.2: Number of correct digits of E_n against n, example 5.5.2

Example 5.5.2. In this example the poles are at $\alpha_i = -10+5/i, i = 1, 2, \ldots$ and the weight function is e^{-z} on the halfline $[0, \infty)$. In this case we have

$$\Gamma_0(z) = \mathrm{Ei}(z)e^{-z}, \quad z \in \overline{\mathbb{C}} \setminus [0, \infty),$$

where $\mathrm{Ei}(z)$ is the exponential integral, defined for real $z < 0$ as $\int_{-\infty}^{z} e^t/t\,dt$. Again we plotted the number of correct digits for E_n against n (figure 5.2). Here the situation is even worse than in the previous example. We have lost all correct digits for $n = 5$.

Example 5.5.3. Now we wish to look at how the location of the poles influences the computations. In figure 5.3 we compare the number of correct digits for different poles. As in the last example we have the weight function e^{-z} on the halfline $[0, \infty)$. In solid line is the number of correct digits for poles located at $\alpha_i = -10^{i-1}, i = 1, 2, \ldots$ and tending to infinity very fast, while for the dashed line the poles are at $\alpha_i = -1/2^{i-1}, i = 1, 2, \ldots$ and tend to zero. In this case we still have 6 correct digits for $n = 20$, while for the poles tending to infinity we have lost all digits for $n = 5$.

5.6 Properties of Δ_n

The following theorem can be found in [10], chapter 11, section 3.

Theorem 5.6.1. *Let φ_n be the orthonormal functions and let ψ_n be the functions of the second kind. Define*

$$\chi_n(z; s) = \psi_n + s\varphi_n(z)$$

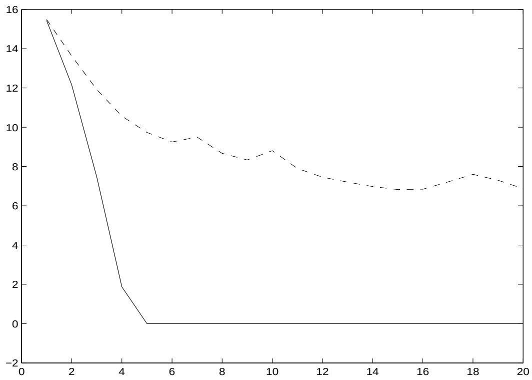

Figure 5.3: Number of correct digits of E_n against n, poles tending to infinity (solid line) and poles tending to zero (dashed line)

Then for arbitrary complex s and t,

$$\frac{\chi_n(w;t)\chi_{n-1}(z;s)}{Z_n(w)Z_{n-1}(z)} - \frac{\chi_n(z;s)\chi_{n-1}(w;t)}{Z_n(z)Z_{n-1}(w)} \\ = -\frac{z-w}{zw}E_n\left[\sum_{k=1}^{n-1}\chi_k(z;s)\chi_k(w;t) + [st-1+D(z,w)(t-s)\right],$$

with E_n the recursion coefficient and $D(z,w)$ the Riesz-Herglotz-Nevanlinna kernel.

With the aid of this theorem we are able to prove that the functions $\Delta_n(z)$ are nonpositive for real z outside $\text{supp}(\mu)$.

Theorem 5.6.2. *With $\Delta_n(z)$ as defined above we have,*

$$\Delta_n(z) \leq 0, \quad z \in \mathbb{R} \setminus \text{supp}(\mu).$$

The inequality is strict for $z \notin \{\alpha_1, \alpha_2, \ldots, \alpha_{n-1}\}$.

Proof. First note that for real z the functions χ_n, Ω_μ and Ω'_μ (prime denotes derivative) are purely imaginary, so we may write for example $|\Omega_\mu(z)|^2 = -(\Omega_\mu(z))^2$.

It follows from the definition of $\Gamma_n(z)$ that

$$\Gamma_n(z) = \frac{\chi_n(z)}{Z_n(z)} / \frac{\chi_{n-1}(z)}{Z_{n-1}(z)}$$

where $\chi_n(z) = \psi_n(z) + \varphi_n(z)\Omega_\mu(z)$. Taking derivatives and dividing by E_n we obtain

$$\Delta_n(z) = \frac{1}{E_n}\left[\left(\frac{\chi_n(z)}{Z_n(z)}\right)' \frac{\chi_{n-1}(z)}{Z_{n-1}(z)} - \frac{\chi_n(z)}{Z_n(z)}\left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)}\right)'\right] \Big/ \left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)}\right)^2.$$

Now use theorem 5.6.1 with $s = \Omega_\mu(z)$ and $t = \Omega_\mu(w)$, where z and w are in $\mathbb{R} \setminus \operatorname{supp}(\mu)$. If we divide by $(z - w)$ and let w tend to z, some calculations yield

$$\frac{1}{E_n}\left[\left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)}\right)' \frac{\chi_n(z)}{Z_n(z)} - \frac{\chi_{n-1}(z)}{Z_{n-1}(z)}\left(\frac{\chi_n(z)}{Z_n(z)}\right)'\right]$$
$$= -\frac{1}{z^2}\left[\sum_{k=1}^{n-1} \chi_k^2(z) + \Omega_\mu^2(z) - 1 + \mathbf{i}(1+z^2)\Omega_\mu'(z)\right]$$

which, using the definition of Ω_μ and the fact that $z \in \mathbb{R}$, may be written as

$$\frac{1}{E_n}\left[\left(\frac{\chi_n(z)}{Z_n(z)}\right)' \frac{\chi_{n-1}(z)}{Z_{n-1}(z)} - \frac{\chi_n(z)}{Z_n(z)}\left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)}\right)'\right]$$
$$= -\frac{1}{z^2}\left[\sum_{k=1}^{n-1} |\chi_k(z)|^2 + |\Omega_\mu(z)|^2 + 1 - (1+z^2)|\Omega_\mu'(z)|\right].$$

Recall that $\chi_n(z)$ is the n-th Fourier coefficient of $D(t,z)$ as a function of t, relative to the orthonormal system $\{\varphi_k\}$ and note that we have

$$1 - (1+z^2)|\Omega_\mu'(z)| = -\int |D(t,z)|^2 d\mu(t).$$

This is a matter of straightforward computation.

Putting all the previous results together we have the following expression for the function $\Delta_n(z)$ when $z \in \mathbb{R} \setminus \operatorname{supp}(\mu)$,

$$\Delta_n(z) = \frac{1}{z^2}\left|\frac{Z_{n-1}(z)}{\chi_{n-1}(z)}\right|^2 \left[\sum_{k=0}^{n-1}\left|\int D(t,z)\varphi_k(t)d\mu(t)\right|^2 - \int |D(t,z)|^2 d\mu(t)\right]. \tag{5.10}$$

It follows from Bessel's inequality that

$$\sum_{k=0}^{n-1}\left|\int D(t,z)\varphi_k(t)d\mu(t)\right|^2 \leq \int |D(t,z)|^2 d\mu(t)$$

with equality only when $D(t,z)$ (as a function of t) is an element of $\mathcal{L}_{n-1}$. This happens only for $z \in \{\alpha_1, \alpha_2, \ldots, \alpha_{n-1}\}$. Note that

$$\int D(t,z)\varphi_k(t)d\mu(t) = R_k(z)/b_{k-1}(z)$$

and that $Z_{n-1}(z)b_{n-2}(z) = b_{n-1}(z)$. Using this and again Bessel's inequality we may write

$$\Delta_n(z) \leq -\frac{1}{z^2}\left|\frac{b_{n-1}(z)}{R_{n-1}(z)}\right|^2 \sum_{k=n}^{\infty}\left|\frac{R_k(z)}{b_{k-1}(z)}\right|^2 \leq 0.$$

The first inequality becomes an equality if the system $\{\varphi_k\}$ is dense in $L^2(\mu)$ (this is theorem 4.18 in [50]) and the second inequality is an equality for $z = \alpha_k$, $1 \leq k \leq n-1$ only when α_k is a zero of $R_m(z)$ for every $m \geq n$ and is not a zero of $R_{n-1}(z)$. This proves the theorem. □

From the proof of this theorem we have the following corollary.

Corollary 5.6.3. *Assume that* $\operatorname{supp}(\mu)$ *is bounded from at least one side. Then it follows that*

$$\lim_{z\to\infty} \Delta_n(z) = 0$$

with z tending to infinity in the unbounded component of $\overline{\mathbb{R}} \setminus \operatorname{supp}(\mu)$.

Proof. The proof is immediate from formula (5.10) and the definition of $D(t,z)$. □

5.7 Error analysis

Let us assume that we know all the coefficients E_k and F_k exactly for $k = 1, \ldots, n$ and we wish to compute E_{n+1} and F_{n+1}. The only errors in this case would be initial errors on our data (Γ_n and Δ_n evaluated in the poles) that become large with increasing n through formula (5.7). If we denote the computed Γ_n-function by $\tilde{\Gamma}_n(z)$ then the relative error $\gamma_n^r(z)$ equals $(\tilde{\Gamma}_n(z) - \Gamma_n(z))/\Gamma_n(z)$. Furthermore we also assume that the error on $Z_n(z)$ is negligible compared to $\gamma_n^r(z)$. From the recurrence relation for

$\Gamma_n(z)$ we find

$$\begin{aligned}\tilde{\Gamma}_n(z) &= E_n Z_{n-1}(z) + F_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)(1+\gamma_{n-1}^r(z))} \\ &\approx E_n Z_{n-1}(z) + F_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}(1-\gamma_{n-1}^r(z)) \\ &\approx \Gamma_n(z) + \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}\gamma_{n-1}^r(z)\end{aligned}$$

so we find for the relative error $\gamma_n^r(z)$ that

$$\gamma_n^r(z) \approx \frac{E_n/E_{n-1}}{\Gamma_n(z)\Gamma_{n-1}(z)}\gamma_{n-1}^r(z)\ .$$

Writing this recursion explicitly and using the defining relation (5.6) we obtain after some calculations

$$\gamma_n^r(z) \approx \mathbf{i}\frac{E_n b_n(z) b_{n-1}(z)(1+1/z^2)R_0(z)}{R_n(z)R_{n-1}(z)}\gamma_0^r(z)$$

and if we assume that the errors $\gamma_0^r(z)$ on the data are approximately equal to the machine precision ϵ, then we obtain the following estimate,

$$|\gamma_n^r(z)| \approx \left|\frac{E_n b_n(z) b_{n-1}(z)(1+1/z^2)R_0(z)}{R_n(z)R_{n-1}(z)}\right|\epsilon$$

or using the definition of b_n,

$$\begin{aligned}|\gamma_n^r(z)| \approx \Bigg| &\frac{R_n(z)}{b_{n-1}(z)}\frac{R_{n-1}(z)}{b_{n-2}(z)}\left(\frac{1}{z}-\frac{1}{\alpha_n}\right)\cdots \\ &\cdots\left(\frac{1}{z}-\frac{1}{\alpha_{n-1}}\right)\frac{1}{E_n R_0(z)(1+1/z^2)}\Bigg|^{-1}\epsilon. \qquad (5.11)\end{aligned}$$

To compute F_n we need the function $\Gamma_{n-1}(z)$ evaluated at the pole α_n. It follows from equation (5.4) that the error will become unbounded as long as α_n and E_n do not tend to zero. This may explain why in figure 5.3 we obtain better results for the poles tending to zero. The asymptotic behaviour of E_n obviously depends on the measure μ and the location of the poles. For a measure supported on the interval $[-1, 1]$ and satisfying the condition $\mu' > 0$ a.e. (where μ' is the Radon-Nikodym derivative of the measure μ with respect to the Lebesgue measure), we can use the results from section 3.4. It follows that E_n is bounded away from zero if the poles are bounded away from the interval. Using the conformal mapping

$$\tau(z) = \frac{1-z}{1+z}, \quad z \in [-1, 1]$$

we can obtain similar results for measures supported on the halfline $[0,\infty)$. We will discuss this in more detail in chapter 8. In this case the error will become unbounded if the poles stay away from infinity and from zero. This explains the behaviour of the first two examples in section 5.5.

Next we will look at the relative error $\delta_n^r(z)$ on $\Delta_n(z)$. We assume that the error on $Z_n'(z)$ is negligible compared to $\delta_n^r(z)$. From (5.9) we obtain

$$\begin{aligned}\tilde{\Delta}_n(z) &= Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)(1+\delta_{n-1}^r(z))}{(\Gamma_{n-1}(z)(1+\gamma_{n-1}^r(z)))^2}\\ &\approx Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)}{\Gamma_{n-1}^2(z)}(1+\delta_{n-1}^r(z)-2\gamma_{n-1}^r(z))\\ &\approx \Delta_n(z) + (\Delta_n(z)-Z_{n-1}'(z))(\delta_{n-1}^r(z)-2\gamma_{n-1}^r(z))\ .\end{aligned}$$

The relative error $\delta_n^r(z)$ thus equals

$$\delta_n^r(z) \approx \left(1-\frac{Z_{n-1}'(z)}{\Delta_n(z)}\right)(\delta_{n-1}^r(z)-2\gamma_{n-1}^r(z))$$

and a bound is given by

$$|\delta_n^r(z)| \le \left|1-\frac{Z_{n-1}'(z)}{\Delta_n(z)}\right|\left(|\delta_{n-1}^r(z)|+2|\gamma_{n-1}^r(z)|\right)\ . \tag{5.12}$$

It is difficult to write this error bound in an explicit form like the one for γ_n^r. To compute the coefficient E_n we need $\Delta_n(\alpha_n)$. For the poles tending to infinity in figure 5.3, we can use corollary 5.6.3 and formula (5.12) to explain why the error becomes unbounded.

Sometimes we require computable error bounds, for example to decide how many digits to use in a multiprecision calculation to obtain a certain precision. For the case of orthogonality on $[-1,1]$ with respect to a measure satisfying Szegő's condition, we can use the asymptotic results from chapter 3 to estimate the error (5.11).

From equation (5.3) and lemma 2.5.6 we get after some computations that

$$\frac{R_n(t)}{b_{n-1}(t)} = \frac{\mathbf{i}H(t)(1+t^2)}{\varphi_n(t)(1-t/\alpha_n)}$$

where $H(t)$ is as in example 3.6.6. Using the approximation of that example and the strong convergence of φ_n yields the estimate

$$\left|\frac{R_n(t)}{b_{n-1}(t)}\left(\frac{1}{t}-\frac{1}{\alpha_n}\right)\right| \approx \left|\frac{2z}{1-z^2}\frac{1-\beta_n^2}{1+\beta_n^2}\frac{1+t^2}{t}\frac{1-\beta_n z}{\sqrt{1-\beta_n^2}}B_n(z)\sqrt{2\pi}\sigma(\mathring{\mu}',z)\right|$$

where we have used the notation of chapter 3. Combining this with the asymptotic estimate of E_n and the definition of $R_0(z)$ we finally get

$$|\gamma_n^r(z)| \approx \left| \frac{\Gamma_0(t)(1-\beta_{n-1}\beta_n)}{\pi(t^2-1)\sigma^2(\mathring{\mu}', z)B_n(z)B_{n-1}(z)(1-\beta_n z)(1-\beta_{n-1}z)} \right| \epsilon.$$

All quantities in this expression can be computed once the measure and poles are known.

Example 5.7.1. We estimate the error in the first example of section 5.5 using the above formula. The derivative of the measure $\mathring{\mu}$ corresponding to the normalized Lebesgue measure is equal to $\mathring{\mu}'(\theta) = |\sin\theta|/2$, which can be written as

$$\mathring{\mu}'(\theta) = \frac{1}{4}|1-z^2|, \quad z = e^{\mathbf{i}\theta}.$$

The function $f(z) = (1-z^2)/4$ obviously satisfies the conditions of lemma 2.4.3, so we get

$$\sigma^2(\mathring{\mu}', z) = \frac{1}{4}(1-z^2).$$

An expression for $\Gamma_0(t)$ has already been given in section 5.5. Together with the previous expression we can compute the estimate for $\gamma_{n-1}^r(\alpha_n)$. The dashed line in figure 5.1 shows the estimated $-\log_{10}|\gamma_{n-1}^r(\alpha_n)|$ as a function of n. For ϵ we used the Matlab constant `eps`.

Example 5.7.2. In this example we take $\alpha_n = a^n$ where $a > 1$ and μ an arbitrary measure satisfying Szegő's condition. For large n we have that

$$\beta_n = J^{-1}(\alpha_n) \approx \frac{1}{2}a^{-n}$$

and

$$|\zeta_k(\beta_{n+1})| \approx \frac{1}{2}a^{-n-1}|1-a^{n-k+1}|$$

which gives

$$\begin{aligned} |B_n(\beta_{n+1})| &\approx \frac{\prod_{k=1}^n |1-a^{n-k+1}|}{2^n a^{n(n+1)}} \\ &\lesssim \frac{\prod_{k=1}^n a^{n-k+1}}{2^n a^{n(n+1)}} = 2^{-n}a^{-\frac{1}{2}n(n+1)} \end{aligned}$$

where the symbol $\lesssim$ means that the inequality holds only asymptotically. A similar computation for $B_{n-1}(\beta_{n+1})$ leads to

$$|B_n(\beta_{n+1})B_{n-1}(\beta_{n+1})|^{-1} \gtrsim 2^{2n-1}a^{n^2}.$$

We also have $\Gamma_0(\alpha_{n+1}) \approx \mu(I)/a^{n+1}$ and $\sigma(\mathring{\mu}', \beta_{n+1}) \approx \sigma(\mathring{\mu}', 0)$, which is finite because μ satisfies Szegő's condition. Putting things together gives the estimate

$$|\gamma_n^r(\alpha_{n+1})| \gtrsim \left| \frac{\mu(I) 2^{2n-1} a^{n^2}}{\sigma^2(\mathring{\mu}', 0) \pi a^{3n+2}} \right| \epsilon$$

which shows that $|\gamma_n^r(\alpha_{n+1})| = O(a^{n^2})$.

5.8 One multiple pole

If all poles are equal to each other, we can give a similar algorithm, based on the same interpolation properties. However, the approach to follow is a little bit different. In this case, assume that $A = \{\alpha, \alpha, \alpha, \ldots\}$ where $0 \neq \alpha \in \mathbb{R}$ (so α is not equal to infinity), and that the support of μ is connected. The functions $R_n, n \geq 1$ are analytic outside the support of μ and it can easily be seen that $R_n(\alpha) \neq 0$ (because φ_n cannot be orthogonal to a function $f \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$). Then it follows from equation (5.6) that Γ_n is analytic in a neighbourhood of α and $\Gamma_n(\alpha) = 0$. This means we may write

$$\Gamma_n(z) = \sum_{k=1}^{\infty} c_k^{(n)} (z-\alpha)^k, \quad \frac{1}{\Gamma_n(z)} = \sum_{k=-1}^{\infty} d_k^{(n)} (z-\alpha)^k.$$

Plugging these sums into (5.7) and equating powers of $(z - \alpha)$ gives

$$F_n = E_n \left(\alpha + \frac{d_0^{(n-1)}}{E_{n-1}} \right)$$

and

$$E_n = -\frac{d_{-1}^{(n)}}{\alpha^2}, \quad c_k^{(n)} = -\frac{E_n}{E_{n-1}} d_k^{(n-1)}, \quad k = 1, 2, \ldots$$

but since $c_1^{(n)} d_{-1}^{(n)} = 1$ we may combine these last two equations to get

$$E_n = \frac{1}{|\alpha|} \sqrt{\frac{E_{n-1}}{d_1^{(n-1)}}}.$$

The relations between $c_k^{(n)}$ and $d_k^{(n)}$ can be obtained through power series inversion, see e.g. [24, p. 12]. The previous formulas have to be modified for $n = 1$, because $\Gamma_0(\alpha) \neq 0$ and $Z_0(z) = z$. The computations are straightforward and we only give the results:

$$\begin{aligned} E_1 &= \frac{1}{|\alpha|\sqrt{d_1^{(0)} - 1}}, \\ F_1 &= E_1(d_0^{(0)} - \alpha), \\ c_1^{(1)} &= E_1(1 - d_1^{(0)}), \\ c_k^{(1)} &= -E_1 d_k^{(0)}, \quad k = 2, 3, \ldots \end{aligned}$$

We now have a very simple algorithm to compute the recurrence coefficients given a series expansion of $\Gamma_0(z)$ around $z = \alpha$. Of course, like the previous algorithm, it will not be very useful when working in (ordinary) double precision. However, in this case we do not actually use the recurrence relation (5.7), so the error analysis of the previous section is no longer valid. But as we will see later on, the underlying and more fundamental problem in both algorithms is that we are using (rational) moments of the orthogonality measure to compute the recurrence coefficients, which is an ill-conditioned problem. For more details we refer to chapter 6.

Remark. We could probably use the techniques of this section to give a more general algorithm for arbitrary poles, given a series expansion of Γ_0 around each of the different poles, but we will not do this. The computations become rather cumbersome and we do not feel there would be much use. The main purpose of this section was to present a different approach based on the functions Γ_n.

5.9 Conclusion

The interpolation algorithms discussed in this chapter are real line analogues of the Nevanlinna-Pick algorithm for the circle case, as described in chapter 6 of [10]. As we mentioned before, their interest is mainly theoretical (connections with a modified Schur algorithm and continued fractions) because of the unbounded error growth, which makes them of little use when working in double precision. In the next chapter we explain why all moment-based algorithms to compute orthogonal rational functions must inevitably fail and in chapter 7 we discuss another type of algorithm which will provide satisfactory results in most cases.

Chapter 6

Moment-based algorithms

6.1 Introduction

In a series of articles [18, 19, 20] about the numerical computation of orthogonal polynomials on a subset of the real line, Gautschi shows that computing orthogonal polynomials starting from the moments $\mu_k = \int x^k d\mu(x)$ of the measure is an ill-conditioned problem. However, in [19] an alternative approach is presented, based on so-called *modified* moments, which works better in certain situations. For a survey of computational aspects of orthogonal polynomials we refer to [21]. In this chapter we generalize some results to the rational case.

6.2 Ordinary moments

First let us define what is meant by *moments* in the case of orthogonal rational functions. This chapter will only deal with orthogonality on a subset of the real line. Most of the notation is as usual, but it will be convenient to make repetitions among the poles explicit.

In the rest of this chapter we assume that there are no poles at infinity. Let there be m distinct numbers in the sequence of the first n poles

$$A_n = \{\alpha_1, \alpha_2, \ldots, \alpha_n\}$$

and denote these by $\{\tilde{\alpha}_k\}_{k=1}^m$. Assume that the multiplicity of $\tilde{\alpha}_k$ in A_n is m_k (this implies $\sum_{k=1}^m m_k = n$). Then the sequence

$$\tilde{A}_n = \{\underbrace{\tilde{\alpha}_1, \ldots, \tilde{\alpha}_1}_{m_1}, \underbrace{\tilde{\alpha}_2, \ldots, \tilde{\alpha}_2}_{m_2}, \ldots, \underbrace{\tilde{\alpha}_m, \ldots, \tilde{\alpha}_m}_{m_m}\}$$

will generate the same space $\mathcal{L}_n$ as A_n. If we order the $\tilde{\alpha}_k$ such that $\alpha_n = \tilde{\alpha}_m$, then A_{n-1} will also generate the same $\mathcal{L}_{n-1}$ as $\tilde{A}_{n-1}$. Assume that this has been done. A basis for $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$ can then be given by

$$\begin{cases} 1, \\ \dfrac{1}{z-\tilde{\alpha}_1}, \dfrac{1}{(z-\tilde{\alpha}_1)^2}, \ldots, \dfrac{1}{(z-\tilde{\alpha}_1)^{2m_1}}, \\ \dfrac{1}{z-\tilde{\alpha}_2}, \dfrac{1}{(z-\tilde{\alpha}_2)^2}, \ldots, \dfrac{1}{(z-\tilde{\alpha}_2)^{2m_2}}, \\ \vdots \\ \dfrac{1}{z-\tilde{\alpha}_{m-1}}, \dfrac{1}{(z-\tilde{\alpha}_{m-1})^2}, \ldots, \dfrac{1}{(z-\tilde{\alpha}_{m-1})^{2m_{m-1}}}, \\ \dfrac{1}{z-\tilde{\alpha}_m}, \dfrac{1}{(z-\tilde{\alpha}_m)^2}, \ldots, \dfrac{1}{(z-\tilde{\alpha}_m)^{2m_m-1}}. \end{cases}$$

There are obviously $2n$ functions in this basis, which we denote by $\{p_k\}_{k=0}^{2n-1}$. So we have

$$p_0(z) \equiv 1,$$
$$p_i(z) = (z-\tilde{\alpha}_k)^{-l}, \quad i = 2\sum_{j=1}^{k-1} m_j + l.$$

Now the moments μ_k of the orthogonality measure μ are defined as

$$\mu_k = \int p_k(z)d\mu(z), \quad k = 0, \ldots, 2n-1 \tag{6.1}$$

As Gautschi does for the polynomial case, we take the position that the fundamental quantities in the computation of orthogonal rational functions are the recurrence coefficients. Once these are known, the accurate evaluation of the functions is straightforward. Furthermore, as explained in chapter 4, these coefficients can be gathered in a tridiagonal matrix to obtain a generalized eigenvalue problem whose solutions are the zeros of φ_n, i.e. the nodes in the quadrature formulas. The weights are defined by the first components of the corresponding eigenvectors.

Once the moments (6.1) are known, the recurrence coefficients E_n and F_n can be computed by moment-based algorithms. One such algorithm was presented in the previous chapter: when all poles are different from each other, the moments (6.1) are (up to constant factors) equal to the functions Γ_n and Δ_n evaluated at the poles. Another algorithm based on the moments would be to evaluate the inner products from lemma 2.5.3 by a partial fraction decomposition and integrating term by term.

However, as we will see in this section, computing the coefficients from the moments is usually an ill-conditioned problem. We assume here that the support of the measure is connected (which means we are in the case of an interval or a halfline). First we define the vectors

$$\underline{\mu}^T = [\mu_0, \mu_1, \ldots, \mu_{2n-1}], \quad \underline{c}^T = [E_1, \ldots, E_n, F_1, \ldots, F_n].$$

Now we are interested in the condition of the map $K_n : \underline{\mu} \to \underline{c}$.

It is a consequence of the fact that the support of μ is connected and of theorem 11.6.2 in [10] that the quadrature formula

$$\int f(x) d\mu(x) \approx \sum_{k=1}^{n} \lambda_{nk} f(x_{nk})$$

exists and is exact for $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}$, where $\{x_{nk}\}_{k=1}^n$ are the zeros of φ_n and $\{\lambda_{nk}\}_{k=1}^n$ the corresponding weights. It is convenient to think of K_n as the composition of two maps,

$$K_n = K_n^{(1)} \circ K_n^{(2)},$$

where $K_n^{(2)}$ is the map from the moments to the quadrature formula,,

$$K_n^{(2)} : \underline{\mu} \to \underline{q}, \quad \underline{q}^T = [x_{n1}, \ldots, x_{nn}, \lambda_{n1}, \ldots, \lambda_{nn}],$$

and $K_n^{(1)}$ the map from the quadrature formula to the coefficients,

$$K_n^{(1)} : \underline{q} \to \underline{c}.$$

The latter map is usually not very sensitive and we do not study it. We focus on the map $K_n^{(2)}$, which is the ill-conditioned one. As condition number of a map $M : x \to y$ from one finite-dimensional space into another we generally adopt the quantity

$$(\operatorname{cond} M)(x) = \frac{\|x\| \, \|J_M(x)\|}{\|Mx\|}$$

where J_M is the Jacobian matrix of M, and $\|\cdot\|$ a suitable vector norm and subordinate matrix norm. The map $K_n^{(2)}$ amounts to solving the nonlinear system of equations,

$$\sum_{i=1}^{n} \lambda_{ni} p_k(x_{ni}) = \mu_k, \quad k = 0, 1, 2, \ldots, 2n-1. \tag{6.2}$$

The Jacobian of the map defined by (6.2) can easily be computed and equals

$$J^{-1}_{K_n^{(2)}} = T\Lambda,$$

where

$$\Lambda = \operatorname{diag}(1,\ldots,1,\lambda_{n1},\ldots,\lambda_{nn}),$$

$$T = \begin{bmatrix} p_0(x_{n1}) & \cdots & p_0(x_{nn}) & p_0'(x_{n1}) & \cdots & p_0'(x_{nn}) \\ p_1(x_{n1}) & \cdots & p_1(x_{nn}) & p_1'(x_{n1}) & \cdots & p_1'(x_{nn}) \\ \vdots & & \vdots & \vdots & & \vdots \\ p_{2n-1}(x_{n1}) & \cdots & p_{2n-1}(x_{nn}) & p_{2n-1}'(x_{n1}) & \cdots & p_{2n-1}'(x_{nn}) \end{bmatrix}.$$

It follows that

$$(\operatorname{cond} K_n^{(2)})(\underline{\mu}) = \frac{\|\underline{\mu}\|\,\|\Lambda^{-1}T^{-1}\|}{\|\underline{q}\|}.$$

To compute T^{-1} we note that it may be written as

$$T^{-1} = \begin{bmatrix} T^{(1)} \\ T^{(2)} \end{bmatrix}$$

with

$$T^{(1)} = [t_{ij}^{(1)}], \quad i = 1,\ldots,n, \quad j = 0,\ldots,2n-1,$$
$$T^{(2)} = [t_{ij}^{(2)}], \quad i = 1,\ldots,n, \quad j = 0,\ldots,2n-1$$

and the entries $t_{ij}^{(1)}$ and $t_{ij}^{(2)}$ can be computed from the equation $TT^{-1} = I_{2n}$ (where I_{2n} is the identity matrix of order $2n$). This yields the equations

$$\sum_{j=0}^{2n-1} t_{ij}^{(1)} p_j(x_{nk}) = \delta_{ik}, \qquad \sum_{j=0}^{2n-1} t_{ij}^{(2)} p_j(x_{nk}) = 0,$$
$$\sum_{j=0}^{2n-1} t_{ij}^{(1)} p_j'(x_{nk}) = 0, \qquad \sum_{j=0}^{2n-1} t_{ij}^{(2)} p_j'(x_{nk}) = \delta_{ik},$$

which is equivalent to saying that

$$\sum_{j=0}^{2n-1} t_{ij}^{(1)} p_j(z) = H_{ni}(z),$$
$$\sum_{j=0}^{2n-1} t_{ij}^{(2)} p_j(z) = \tilde{H}_{ni}(z),$$

where H_{ni} and $\tilde{H}_{ni}$ are the Hermite interpolating rational functions from lemma 2.5.5. As in the polynomial case, we can give a lower bound for the condition number, involving orthogonal polynomials, as shown in the following theorem.

Theorem 6.2.1. *The condition number* $\operatorname{cond} K_n^{(2)}$ *satisfies*

$$\operatorname{cond} K_n^{(2)} \geq c_n \frac{\|\underline{\mu}\|}{\|\underline{q}\|} \frac{\lim_{x\to\infty} \varphi_n^2(x)}{\min_{1\leq i\leq n}\{\lambda_{ni}[\varphi_n'(x_{ni})]^2|x_{ni}-\alpha_n|\}} ,$$

where $c_n > 0$ *is a constant only depending on* n *and the definition of the matrix norm. If we use the* 1*-norm (maximum column sum) or the* ∞*-norm (maximum row sum), then* $c_n = 1$*. In the case of the interval* $[-1, 1]$*, with poles* A *staying away from the boundary and the measure* μ *satisfying the Erdős-Turán condition* $\mu' > 0$ *a.e., we get the asymptotic lower bound*

$$\operatorname{cond} K_n^{(2)} \gtrsim c_n \frac{\|\underline{\mu}\|}{\|\underline{q}\|} \frac{1}{64\pi} \frac{(1-\rho)^7}{n\rho^{2n-1}} ,$$

where $\beta_k = J^{-1}(\alpha_k)$ *and* $\rho = \sup_{1\leq k\leq n} |\beta_k|$*.*

Proof. It follows from the equivalence of norms in a finite-dimensional vector space that for every matrix norm (not necessarily induced by a vector norm)

$$\|\cdot\| : \mathbb{C}^{2n\times 2n} \to \mathbb{R}^+ : A \to \|A\|$$

there exists a constant $c_n > 0$ such that for all $A \in \mathbb{C}^{2n\times 2n}$ we have

$$\|A\| \geq c_n \max_{1\leq i,j\leq 2n} |a_{ij}| \tag{6.3}$$

(where a_{ij} are the elements of A).

Note that for every $1 \leq i \leq n$ we have $t_{i0}^{(2)} = \lim_{x\to\infty} \tilde{H}_{ni}(x)$. The first statement in the theorem now follows from the definition of Λ, equation (6.3) and lemma 2.5.5.

To obtain the second statement, note that it follows from the Christoffel-Darboux relation 2.4.2 and the definition of $\mathring{k}_n(z, w)$ that

$$|\phi_n^*(0)|^2 \geq 1 - \beta_n^2.$$

Using theorems 2.6.1 and 3.2.2 then yields

$$\lim_{x\to\infty} \varphi_n^2(x) \approx \frac{1}{2\pi} \frac{1-\beta_n^2}{\prod_{k=1}^n \beta_k^2}.$$

Bounding the denominator (with the derivative of φ_n) is a bit more complicated, but we can use the confluent Christoffel-Darboux relation from theorem 2.5.4 and the fact that $k_{n-1}(x_{ni}, x_{ni}) = \lambda_{ni}^{-1}$ to obtain

$$\lambda_{ni}[\varphi_n'(x_{ni})]^2|x_{ni}-\alpha_n| = \frac{E_n^2\alpha_n^2\alpha_{n-1}^2}{\lambda_{ni}|x_{ni}-\alpha_{n-1}|^2\varphi_{n-1}^2(x_{ni})|x_{ni}-\alpha_n|}.$$

Because the quadrature formula is exact in $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$, we know that

$$\int_{-1}^{1} \varphi_{n-1}^2(x) d\mu(x) = \sum_{k=1}^{n} \lambda_{nk} \varphi_{n-1}^2(x_{nk}) = 1$$

from which it follows that

$$\max_{1 \le i \le n} \lambda_{ni} \varphi_{n-1}^2(x_{ni}) > \frac{1}{n}.$$

The quadrature nodes are all contained in I, so we also have

$$|x_{ni} - \alpha_k| > |\alpha_k| - 1, \quad 1 \le i \le n, \quad k = 1, 2, \ldots$$

From theorem 3.4.1 it follows that $E_n \le 2$ for large n. Combining all the previous results and using the definition of the Joukowski transformation gives after some computations that

$$\operatorname{cond} K_n^{(2)} \gtrsim c_n \frac{\|\underline{\mu}\|}{\|\underline{q}\|} \frac{1}{2\pi} \frac{1 - \beta_n^2}{\prod_{k=1}^{n-1} \beta_k^2 \beta_n} \frac{(1 - |\beta_{n-1}|)^4}{(1 + \beta_{n-1}^2)^2} \frac{(1 - |\beta_n|)^2}{(1 + \beta_n^2)^2} \frac{1}{2n}.$$

Using the fact that $|\beta_k| \le \rho$ and $1/(1 + \rho^2) \ge 1/2$ finishes the proof. □

Note that the statement we just proved shows that the condition number grows exponentially for large n.

Example 6.2.2. Let us look at the case where we have an exponential weight on I and where all poles are equal to each other. We take

$$d\mu(x) = \exp\left(-\frac{a}{1+x}\right) dx$$

with $a > 0$ a parameter, and

$$A = \{\alpha, \alpha, \alpha, \ldots\}$$

where $|\alpha| > 1$. We need expressions for the moments

$$\mu_k = \int_{-1}^{1} \frac{\exp\left(-\frac{a}{1+x}\right)}{(x - \alpha)^k} dx, \quad k = 0, 1, \ldots$$

which can be obtained as follows. Integrating by parts twice gives

$$\begin{aligned} \mu_n &= \frac{1}{(1-\alpha)^n} \left[2e^{-a/2} + a \operatorname{Ei}(-a/2) \right] + n\mu_n \\ &\quad + n(1+\alpha)\mu_{n+1} + an \int_{-1}^{1} \frac{\operatorname{Ei}\left(-\frac{a}{1+x}\right)}{(x-\alpha)^{n+1}} dx \\ &= \frac{2e^{-a/2}}{(1-\alpha)^n} + n\mu_n + n(1+\alpha)\mu_{n+1} - a \int_{-1}^{1} \frac{\exp\left(-\frac{a}{1+x}\right)}{(1+x)(x-\alpha)^n} dx \end{aligned}$$

n	cond $K_n^{(2)}$	err. growth
2	$8.1316e+00$	$3.0805e+03$
5	$8.2203e+02$	$2.5416e+05$
8	$2.0054e+04$	$1.4776e+08$
11	$1.8818e+06$	$8.9086e+10$
14	$3.9708e+08$	$8.8312e+13$
17	$1.3211e+11$	$3.5909e+15$
20	$6.7577e+13$	$8.0136e+16$

Table 6.1: Condition of the map $K_n^{(2)}$

where $\mathrm{Ei}(z)$ is the exponential integral, as defined in section 5.5. Although the second integration by parts is only valid for $n \geq 1$, it is easily checked that the final formula also holds for $n = 0$. Putting

$$\nu_n = \int_{-1}^{1} \frac{\exp\left(-\frac{a}{1+x}\right)}{(1+x)(x-\alpha)^n} dx$$

it can be verified that $\nu_n = (\mu_n - \nu_{n-1})/(1+\alpha)$. Substituting back and eliminating ν_n and ν_{n-1} then yields the recurrence relation

$$-n(1+\alpha)^2 \mu_{n+1} = \frac{4e^{-a/2}}{(1-\alpha)^n} + [2(n-1)(1+\alpha) - a]\mu_n + (n-2)\mu_{n-1}.$$

for $n \geq 1$. The initial values have to be computed explicitly and are

$$\begin{aligned} \mu_0 &= 2e^{-a/2} + a\,\mathrm{Ei}(-a/2), \\ \mu_1 &= -\mathrm{Ei}(-a/2) + \mathrm{Ei}\left(-\frac{a}{2}\frac{\alpha-1}{\alpha+1}\right)\exp\left(-\frac{a}{1+\alpha}\right). \end{aligned}$$

With the previous formulas all the moments can be computed and used in the algorithm of section 5.8. As an example we take $a = 4$ and $\alpha = -1.01$. Table 6.1 gives the observed error growth (the largest relative error on the recurrence coefficients divided by the machine precision) and the lower bound for the condition number computed using the first formula of the previous theorem. Note that this bound underestimates the actual error growth.

6.3 Modified moments

As shown in the previous section, computing the recurrence coefficients from the moments is generally an ill-conditioned problem. To overcome this problem in the polynomial case, so-called *modified* moments were introduced. In this section we study the possibility of using modified moments in the construction of orthogonal rational functions. The procedure is analogous to the one for the polynomial case as described in [19]. However, for reasons explained later on, it is required that all poles be equal to each other.

Assume that we are given a set of rational functions $\{\tilde{\varphi}_n\}$ orthogonal with respect to a measure $\tilde{\mu}$ and with one multiple pole in α. The functions we wish to compute are (as usual) denoted by φ_n and orthogonal with respect to μ. They have the same multiple pole α as the $\tilde{\varphi}_n$. Furthermore assume that we have at our disposition all the *modified* moments

$$\nu_k = \int \tilde{\varphi}_k(x) d\mu(x).$$

Consider then the Gram matrix $M = [m_{ij}]$ of order $n+1$ where

$$m_{ij} = \int \tilde{\varphi}_i(x)\tilde{\varphi}_j(x) d\mu(x), \quad i,j = 0,1,\ldots,n$$

and let $M = R^T R$ be the Cholesky decomposition of M. Putting $S = [s_{ij}] = R^{-1}$ it follows from [37] that

$$\varphi_j(x) = \sum_{i=0}^{j} s_{ij}\tilde{\varphi}_i(x), \quad j = 0,1,\ldots,n.$$

Substituting this equation into the recurrence relation for the φ_n, we get

$$\frac{x}{1-x/\alpha}\sum_{i=0}^{n-1} s_{i,n-1}\tilde{\varphi}_i(x) = \frac{1}{E_n}\sum_{i=0}^{n} s_{in}\tilde{\varphi}_i(x) - \frac{F_n}{E_n}\sum_{i=0}^{n-1} s_{i,n-1}\tilde{\varphi}_i(x) + \frac{1}{E_{n-1}}\sum_{i=0}^{n-2} s_{i,n-2}\tilde{\varphi}_i(x) \tag{6.4}$$

for $n \geq 3$. Because $Z_{-1}(x) = Z_0(x) = x$ is different from $Z_n(x)$ for $n \geq 1$, we have to modify the above relation when $n < 3$, but we leave the details to the reader. The left hand side of (6.4) can also be written as a linear combination of the $\tilde{\varphi}_i$, using the recurrence for these functions backwards. We have

$$\frac{x}{1-x/\alpha}\tilde{\varphi}_i(x) = \frac{1}{\tilde{E}_{i+1}}\tilde{\varphi}_{i+1}(x) - \frac{\tilde{F}_{i+1}}{\tilde{E}_{i+1}}\tilde{\varphi}_i(x) + \frac{1}{\tilde{E}_i}\tilde{\varphi}_{i-1}(x)$$

Note that this can only be done if all poles are equal to each other. Otherwise we would have to find the coefficients in an expression of the form

$$\frac{1}{1-x/\alpha_n}\tilde{\varphi}_i(x) = \sum_{k=0}^{n} c_k^{(i)}\tilde{\varphi}_k(x)$$

which is much more complicated.

Now coefficients of equal $\tilde{\varphi}_i$ must agree on both sides of (6.4) because of the linear independence. For $\tilde{\varphi}_n$ and $\tilde{\varphi}_{n-1}$ this yields after some computations

$$E_n = \frac{s_{nn}}{s_{n-1,n-1}}\tilde{E}_n,$$
$$F_n = \frac{s_{n-1,n}}{s_{n-1,n-1}} + \frac{s_{nn}}{s_{n-1,n-1}}\tilde{F}_n - \frac{s_{n-2,n-1}s_{nn}}{s^2_{n-1,n-1}}\frac{\tilde{E}_n}{\tilde{E}_{n-1}}$$

for $n \geq 3$. These relations can be written in terms of the elements of R using $s_{jj} = 1/r_{jj}$ and $s_{j,j+1} = -r_{j,j+1}/(r_{jj}r_{j+1,j+1})$. This means that, once the Gram matrix M is known, we can easily compute the recurrence coefficients for φ_n from the coefficients for $\tilde{\varphi}_n$. The Gram matrix can be constructed from the modified moments by applying the recursion twice as follows.

$$\begin{aligned}
m_{ij} &= \langle\tilde{\varphi}_i\,,\tilde{\varphi}_j\rangle \\
&= \tilde{E}_i\left\langle\frac{x}{1-x/\alpha}\tilde{\varphi}_{i-1}\,,\tilde{\varphi}_j\right\rangle + \tilde{F}_i\,\langle\tilde{\varphi}_{i-1}\,,\tilde{\varphi}_j\rangle - \frac{\tilde{E}_i}{\tilde{E}_{i-1}}\,\langle\tilde{\varphi}_{i-2}\,,\tilde{\varphi}_j\rangle \\
&= \tilde{E}_i\left\langle\tilde{\varphi}_{i-1}\,,\frac{1}{\tilde{E}_{j+1}}\tilde{\varphi}_{j+1} - \frac{\tilde{F}_{j+1}}{\tilde{E}_{j+1}}\tilde{\varphi}_j + \frac{1}{\tilde{E}_j}\tilde{\varphi}_{j-1}\right\rangle \\
&\quad + \tilde{F}_i\,\langle\tilde{\varphi}_{i-1}\,,\tilde{\varphi}_j\rangle - \frac{\tilde{E}_1}{\tilde{E}_{i-1}}\,\langle\tilde{\varphi}_{i-2}\,,\tilde{\varphi}_j\rangle
\end{aligned}$$

which finally gives us

$$m_{ij} = \frac{\tilde{E}_i}{\tilde{E}_{j+1}}m_{i-1,j+1} + \frac{\tilde{E}_i}{\tilde{E}_j}m_{i-1,j-1} + \left(\tilde{F}_i - \frac{\tilde{E}_i\tilde{F}_{j+1}}{\tilde{E}_{j+1}}\right)m_{i-1,j} - \frac{\tilde{E}_i}{\tilde{E}_{i-1}}m_{i-2,j}.$$

This formula has to be modified for $i, j < 3$, but again we omit the details. Since $m_{0j} = \nu_j$ this gives us a recursive scheme to construct the matrix M. Again note that the derivation would become more complicated if all poles were not equal to each other.

The main reason why modified moments are used in the polynomial case is that the problem is no longer ill-conditioned. Experiments have indicated that this remains so for the rational case, with no significant loss of accuracy even for high degrees. However, we do not go into an analysis of the condition. Of course, as in the polynomial case this method only works well if the modified moments are available or can easily be computed. In chapter 9 we give an example. In general however, it may be very difficult to obtain these modified moments.

6.4 Conclusion

The main purpose of this rather short chapter was to discuss the computation of orthogonal rational functions based on ordinary and modified moments, using more or less the same methods which Gautschi presents in his articles on the computation of orthogonal polynomials. We did not intend to give a detailed analysis with sharp error bounds as in the polynomial case, but only to show the analogy between polynomial and rational case and the additional difficulties that arise by using rational functions. We note here that the computation of the moments (ordinary or modified) is often difficult in the rational case (e.g. try to compute the moments of example 6.2.2 for an arbitrary pole sequence).

Chapter 7

Computing ORF on an interval

7.1 Introduction

In this chapter we study an algorithm to compute orthogonal rational functions on the interval $[-1, 1]$ which does not suffer from progressive ill-conditioning with increasing degree n. It is basically a rational version of what Gautschi calls the *discretized Stieltjes procedure* and amounts to approximating the inner products in the formulas from lemma 2.5.3 using some kind of quadrature rule. It would make sense to demand that this rule can easily be generated (also for a large number of nodes), like e.g. Fejér's rule. However, we will first focus upon the use of gaussian rules, because then we can give a detailed error estimate which will allow us to predict how many nodes we need to obtain a certain precision. When the poles are very close to the boundary, polynomial-based quadrature rules become of little use and we will treat that case separately. It turns out that quadrature rules based on orthogonal Laurent polynomials can solve some problems here.

7.2 Error bounds

Let us recapitulate the problem under consideration. Given a set of poles A and a measure μ we want to compute the recurrence coefficients associated with them (up to arbitrarily high degree) and estimate how accurate the computed coefficients are, i.e. estimate how much the numerical values differ from the theoretical value. To compute the coefficients we use the formulas from lemma 2.5.3 where we approximate the inner products using the quadrature rules from chapter 4 based on a different set of orthogonal rational functions, which we assume known.

In this section we will estimate the accuracy of the computed recurrence coefficients, based on certain assumptions. First let us fix some notation. The functions whose recurrence coefficients we wish to compute are $\{\varphi_k\}$. They have poles in A and are orthogonal with respect to μ. The functions used in the quadrature formulas are $\{\tilde{\varphi}_k\}$, with poles in $\tilde{A}$. The number of coefficients we wish to compute is m, the number of nodes in the quadrature formula is n. The quadrature error for the function f is denoted by $e_n(f)$ and the Blaschke products associated with A and $\tilde{A}$ are $\{B_k(z)\}$ and $\{\tilde{B}_k(z)\}$ respectively. The assumptions we make in our analysis are the following:

- m and n are large (theoretically infinite),
- A and $\tilde{A}$ are bounded away from I,
- the measure μ satifies Szegő's condition
- the quadrature error for each of the inner products in lemma 2.5.3 is roughly the same (i.e. of the same order of magnitude); to justify this assumption note that for any p, q we have $Z_p(x)/Z_q(x) = 1 + Z_p(x)/Z_q(\alpha_p)$ and if $\alpha_p \neq \alpha_q$ and they are not both equal to infinity, then $Z_p(x)Z_q(x) = Z_q(\alpha_p)Z_p(x) + Z_p(\alpha_q)Z_q(x)$,
- the absolute errors on E_m and F_m are of the same order of magnitude and approximately equal to $e_n(Z_m\phi_{m-1}^2)$; this is justified by taking $k = m-1$ in lemma 2.5.3 and by the previous assumption; we denote this error by Δ_{nm}.

Now we can prove the following theorem.

Theorem 7.2.1. *Put $\rho_1 = \min_{1\leq k\leq m} |\alpha_k|$. Then under the assumptions made in the introduction to this section we have the following error bound,*

$$\Delta_{nm} \lesssim \min_{1\leq r<\rho_1} J^{-1}(r) \max_{0\leq\theta\leq\pi} \frac{(1-\beta_{m-1}^2)|1+z^2|}{|1-\beta_m z|^2|1-\beta_{m-1}z|^2} \frac{|\tilde{B}_n(z)\tilde{B}_{n-1}(z)|}{|B_m(z)B_{m-1}(z)|} \quad (7.1)$$

where $z = J^{-1}(t)$ and $t = re^{\mathbf{i}\theta}$. If $A = \{\alpha, \alpha, \ldots\}$ however, then put $\rho_2 = min_{1\leq k\leq n}|1/\tilde{\beta}_k - \beta|$. In this case an alternative estimate is given by

$$\Delta_{nm} \lesssim \min_{0<r<\rho_2} \frac{1-\beta^2}{r^{2m-2}} \max_{0\leq\theta\leq\pi} |1+z^2||\tilde{B}_n(z)\tilde{B}_{n-1}(z)||1-\beta z|^{2m-5} \quad (7.2)$$

where $z = \beta + re^{\mathbf{i}\theta}$. We use the symbol $\lesssim$ to denote that the inequality only holds if n and m tend to infinity.

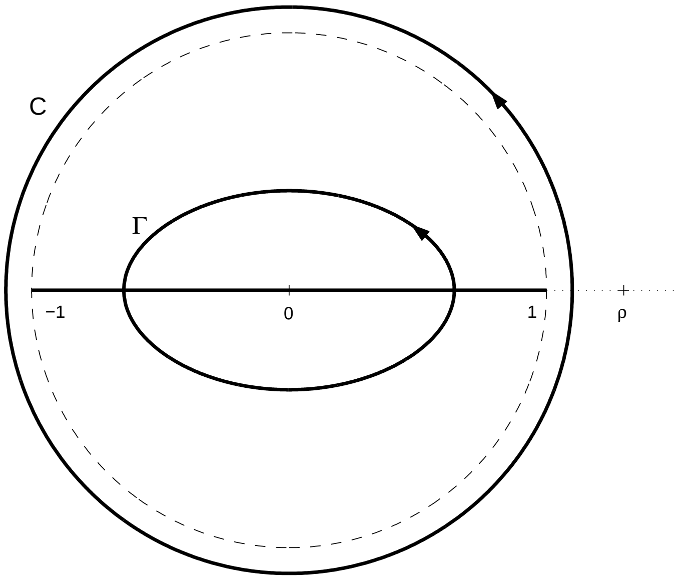

Figure 7.1: Curves used in the proof of theorem 7.2.1.

Proof. To prove (7.1) write

$$\Delta_{nm} = |e_n(Z_m\phi_{m-1}^2)| = \left|\frac{1}{2\pi\mathbf{i}}\int_C \frac{Z_m(t)\phi_{m-1}^2(t)}{(1-t/\tilde{\alpha}_n)\tilde{\phi}_n^2(t)}H(t)dt\right|$$

using theorem 4.3.4, where C is a circle with center 0 and radius $1 \le r < \rho_1$ (so that the integrand is analytic inside the disc with boundary C and I is contained in it), and $H(t)$ is as in example 3.6.6. Use the transformation $t = J(z)$ to convert this into

$$\Delta_{nm} = \left|\frac{1}{4\pi\mathbf{i}}\int_\Gamma \frac{Z_m(J(z))\phi_{m-1}^2(J(z))}{(1-J(z)/J(\tilde{\beta}_n))\tilde{\phi}_n^2(J(z))}H(J(z))\left(\frac{1}{z^2}-1\right)dz\right| \quad (7.3)$$

where $\Gamma = J^{-1}(C)$ is as shown in figure 7.1. Next use theorem 3.5.1 to obtain that

$$\frac{\phi_{m-1}^2(J(z))}{\tilde{\phi}_n^2(J(z))} \approx \frac{\tilde{B}_n^2(z)}{B_{m-1}^2(z)}\frac{(1-\tilde{\beta}_n z)^2}{(1-\beta_{m-1}z)^2}\frac{(1-\beta_{m-1}^2)}{(1-\tilde{\beta}_n^2)} \quad (7.4)$$

if n and m tend to infinity and use the definition of $Z_m(x)$ to get after some calculations

$$Z_m(J(z)) = \frac{1}{2}\frac{(1+\beta_m^2)(1+z^2)}{(z-\beta_m)(1-\beta_m z)}, \quad 1-\frac{J(z)}{J(\tilde{\beta}_n)} = \frac{(z-\tilde{\beta}_n)(1-\tilde{\beta}_n z)}{z(1+\tilde{\beta}_n^2)}\ . \quad (7.5)$$

Combining formulas (7.3) - (7.5) with the approximation from example 3.6.6 and canceling terms yields

$$\Delta_{nm} \approx \left| \frac{1}{4\pi \mathbf{i}} \int_\Gamma \frac{(1+\beta_m^2)(1-\beta_{m-1}^2)(1+z^2)}{(1-\beta_m z)^2(1-\beta_{m-1}z)^2} \frac{\tilde{B}_n(z)\tilde{B}_{n-1}(z)}{B_m(z)B_{m-1}(z)} dz \right|. \quad (7.6)$$

To estimate an upper bound for the integral we take the length of Γ times the maximum of the absolute value of the integrand. An upper bound for length(Γ) is given by $2\pi J^{-1}(r)$ (the circumference of the smallest disc which contains Γ in its interior)[1]. Because all poles are real the absolute value of the integrand is symmetric with respect to $\theta = \pi$ so that we may limit our search for the maximum value to the range $0 \le \theta \le \pi$. Also note that $1 \le 1 + \beta_m^2 < 2$. This gives

$$\Delta_{nm} \lesssim J^{-1}(r) \max_{0 \le \theta \le \pi} \frac{(1-\beta_{m-1}^2)|1+z^2|}{|1-\beta_m z|^2 |1-\beta_{m-1}z|^2} \frac{|\tilde{B}_n(z)\tilde{B}_{n-1}(z)|}{|B_m(z)B_{m-1}(z)|}$$

Taking the minimum over all possible curves gives (7.1).

In the case where $A = \{\alpha, \alpha, \ldots, \}$ we can obtain a more accurate approximation to the integral in (7.6). Now the integrand is a meromorphic function with a pole of order $2m-1$ at $z = \beta$. The poles in $\tilde{B}_n(z)\tilde{B}_{n-1}(z)$ are not important because they are outside of Γ. Using the residue theorem we get that

$$\Delta_{nm} \approx \frac{1}{2}(1+\beta^2)(1-\beta^2)|\operatorname{Res}(F;\beta)|$$

where the function F equals

$$F(z) = \frac{(1+z^2)(1-\beta z)^{2m-5}}{(z-\beta)^{2m-1}} \tilde{B}_n(z)\tilde{B}_{n-1}(z).$$

If we put $G(z) = F(z)(z-\beta)^{2m-1}$ then we have that

$$\operatorname{Res}(F;\beta) = \frac{G^{(2m-2)}(\beta)}{(2m-2)!} .$$

The accurate numerical calculation of the high order derivative is very difficult, but we can approximate it using a Cauchy estimate, as given by theorem 10.26 in [50, p. 213]. This then yields

$$|G^{(2m-2)}(\beta)| \le \frac{(2m-2)! \max_C |G(z)|}{r^{2m-2}}$$

[1] In practice we will approximate $J^{-1}(r) = r - \sqrt{r^2-1}$ by $1/(2r)$ (even for r close to 1). Since we are only interested in the number of correct digits of the recurrence coefficients (i.e. the order of magnitude of the error), this approximation is good enough and the formulas become a bit simpler (one could even drop the factor 1/2).

where C is a circle with center at β and radius r and such that $G(z)$ is analytic inside C. Obviously, the maximum radius for C is $\min_{1\le k\le n}|1/\bar{\beta}_k-\beta|$. Putting everything together and taking the minimum over all possible circles then finally gives (7.2). □

Remark. Theoretically we could also have used the residue theorem to estimate the error in the first case. However, in practice this will usually be impossible. The numerical computation of the residues is very difficult and even if we can compute them, they tend to be very large (especially for large m and n) and it is a well known fact that summing large numbers (not all positive or negative) to obtain a very small number is a numerical disaster.

The previous theorem provides us with an easy way to estimate the accuracy of the computed recurrence coefficients. However, it would be more useful if we could use the formulas in the opposite direction: suppose we want to compute the recurence coefficients with a given precision, then how many nodes would we need in the quadrature formula? If we regard Δ_{nm} as a function of n, then this amounts to finding the inverse function $n=\Delta_{nm}^{-1}(\epsilon)$, where ϵ is the required precision. In general this will be very difficult, but if we make some additional assumptions, then we can obtain useful results. First we need the following lemma.

Lemma 7.2.2. *Let $F(r,\theta,n)$ be a real continuous function defined on the box $[r_1,r_2]\times[\theta_1,\theta_2]\times[0,\infty)$, which has continuous partial derivatives up to second order with respect to r and θ and such that $\partial F/\partial n<0$ on the domain of F. We will call a point (r^*,θ^*)* stationary *if it satisfies $\frac{\partial F}{\partial r}(r^*,\theta^*,n)=\frac{\partial F}{\partial \theta}(r^*,\theta^*,n)=0$. Then put*

$$\epsilon=f(n)=\min_{r_1\le r\le r_2}\max_{\theta_1\le\theta\le\theta_2}F(r,\theta,n)$$

and assume that for each n there is a unique stationary point (r_n,θ_n) such that $f(n)=F(r_n,\theta_n,n)$. Then it holds that

$$n=f^{-1}(\epsilon)=\min_{r_1\le r\le r_2}\max_{\theta_1\le\theta\le\theta_2}F^{-1}(r,\theta,\epsilon)=F^{-1}(r_n,\theta_n,\epsilon)$$

where F^{-1} is the inverse function with respect to n, i.e. $F^{-1}(r,\theta,\epsilon)=n$ implies $F(r,\theta,n)=\epsilon$.

Proof. First define the function $G(r,n)=\max_{\theta_1\le\theta\le\theta_2}F(r,\theta,n)$. Since we assumed that the saddle point (r_n,θ_n) is stationary, we may write down the following equations,

$$\frac{\partial F}{\partial\theta}(r_n,\theta_n,n)=0,\qquad \frac{\partial^2 F}{\partial\theta^2}(r_n,\theta_n,n)\le 0,\tag{7.7}$$

$$\frac{\partial G}{\partial r}(r_n,n)=0,\qquad \frac{\partial^2 G}{\partial r^2}(r_n,n)\ge 0.\tag{7.8}$$

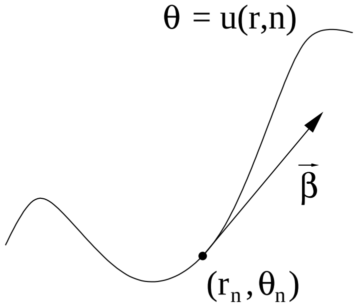

Figure 7.2: Illustration for the proof of lemma 7.2.2.

Because F is continuous with continuous derivatives and (r_n, θ_n) is unique for each n, the equation $\partial F/\partial\theta = 0$ defines $\theta = u(r, n)$ as a function of r and n in a neighbourhood of (r_n, θ_n), such that $G(r, n) = F(r, u(r, n), n)$. The function u corresponds to a ridge on the surface $\epsilon = F(r, \theta, n)$. Figure 7.2 may serve as illustration. Using the chain rule and (7.7), we may rewrite the last equation of (7.8) as

$$\frac{\partial^2 F}{\partial r^2}(r_n, \theta_n, n) + 2\frac{\partial^2 F}{\partial r \partial\theta}(r_n, \theta_n, n)\frac{\partial u}{\partial r}(r_n, n) + \frac{\partial^2 F}{\partial\theta^2}(r_n, \theta_n, n)\left(\frac{\partial u}{\partial r}(r_n, n)\right)^2 \geq 0 \quad (7.9)$$

which is the same as saying that the second order directional derivative of F in the direction $\vec{\beta} = (1, \frac{\partial u}{\partial r}(r_n, n))$ is nonnegative, i.e.

$$\frac{\partial^2 F}{\partial\vec{\beta}^2}(r_n, \theta_n, n) \geq 0.$$

The relation $F(r, \theta, n) = \epsilon$ defines $n = F^{-1}(r, \theta, \epsilon)$ as a function of r, θ and ϵ. Differentiating this expression for fixed ϵ with respect to r gives

$$\frac{\partial F}{\partial r}(r, \theta, n) + \frac{\partial F}{\partial n}(r, \theta, n)\frac{\partial F^{-1}}{\partial r}(r, \theta, \epsilon) = 0$$

and substituting (r_n, θ_n) for (r, θ) we get

$$\frac{\partial F^{-1}}{\partial r}(r_n, \theta_n, \epsilon) = 0.$$

In the same way we obtain the relations

$$\frac{\partial^2 F}{\partial r^2}(r_n,\theta_n,n) + \frac{\partial F}{\partial n}(r_n,\theta_n,n)\frac{\partial^2 F^{-1}}{\partial r^2}(r_n,\theta_n,\epsilon) = 0,$$
$$\frac{\partial^2 F}{\partial r\partial\theta}(r_n,\theta_n,n) + \frac{\partial F}{\partial n}(r_n,\theta_n,n)\frac{\partial^2 F^{-1}}{\partial r\partial\theta}(r_n,\theta_n,\epsilon) = 0,$$
$$\frac{\partial^2 F}{\partial \theta^2}(r_n,\theta_n,n) + \frac{\partial F}{\partial n}(r_n,\theta_n,n)\frac{\partial^2 F^{-1}}{\partial \theta^2}(r_n,\theta_n,\epsilon) = 0.$$

Substituting this into equation (7.9) yields

$$-\frac{\partial F}{\partial n}(r_n,\theta_n,n)\frac{\partial^2 F^{-1}}{\partial \vec{\beta}^2}(r_n,\theta_n,\epsilon) \geq 0$$

and because $\partial F/\partial n < 0$ we get

$$\frac{\partial^2 F^{-1}}{\partial \vec{\beta}^2}(r_n,\theta_n,\epsilon) \geq 0.$$

Using the same procedure we obtain the conditions

$$\frac{\partial F^{-1}}{\partial \theta}(r_n,\theta_n,\epsilon) = 0, \quad \frac{\partial^2 F^{-1}}{\partial \theta^2}(r_n,\theta_n,\epsilon) \leq 0.$$

Together these relations show that (r_n,θ_n) is a stationary saddle point for the function F^{-1}, thus proving the theorem. □

Using this lemma it is not difficult to invert the formulas from theorem 7.2.1, if we make the additional assumptions that all the poles in the quadrature formula are equal to each other as given in the following theorem.

Theorem 7.2.3. *Assume that $\tilde{A} = \{\tilde{\alpha},\tilde{\alpha},\ldots\}$ and let ϵ denote the required precision. If for each n the saddle point (r_n,θ_n) in (7.1) is stationary, then under the assumptions and with the notation of theorem 7.2.1 we have the following estimate for the number of nodes n needed in the quadrature formula,*

$$n \gtrsim \min_{1\leq r<\rho_1}\max_{0\leq\theta\leq\pi}\frac{1}{2}\frac{\log\left(\frac{J^{-1}(r)(1-\beta_{m-1}^2)|1+z^2|}{\epsilon|1-\beta_m z|^2|1-\beta_{m-1}z|^2|B_m(z)B_{m-1}(z)|}\right)}{\log\left|\frac{1-\tilde{\beta}z}{z-\tilde{\beta}}\right|} + \frac{1}{2}. \quad (7.10)$$

If furthermore $A = \{\alpha,\alpha,\ldots\}$ then under the same assumptions we have

$$n \gtrsim \min_{0\leq r<\rho_2}\max_{0\leq\theta\leq\pi}\frac{1}{2}\frac{\log\left(\frac{(1-\beta^2)|1+z^2||1-\beta z|^{2m-5}}{\epsilon r^{2m-2}}\right)}{\log\left|\frac{1-\tilde{\beta}z}{z-\tilde{\beta}}\right|} + \frac{1}{2}. \quad (7.11)$$

Proof. The inequality (7.1) may be written

$$\Delta_{nm} \lesssim \min_{1 \le r < \rho_1} \max_{0 \le \theta \le \pi} F(r, \theta, n)$$

where it is not difficult to see that F is certainly twice continuously differentiable with respect to r and θ and also $\partial F / \partial n < 0$. The rest of the proof is a simple application of the previous lemma. Since $F(r_n, \theta_n, n)$ is an upper bound for the actual error, $F^{-1}(r_n, \theta_n, \epsilon)$ will of course be a lower bound for the required number of nodes. This gives (7.10). The proof of (7.11) is completely analogous. □

Note that the proof of this theorem depends on the assumption that for each n the saddle point (r_n, θ_n) satisfies the conditions (7.7) and (7.8). This assumption is very difficult to analyze theoretically, but the examples in the next section show that in practice it seems to be satisfied, in the sense that the formulas in this theorem provide reasonable estimates for the required number of nodes.

7.3 Numerical examples

The examples in this section serve as illustration for theorems 7.2.1 and 7.2.3. The figures show the number of correct digits for the coefficient E_m. Computations were done in double precision. In solid line is the exact number of correct digits. To compute the exact values of E_m needed here, we used the Fortran multiprecision package `mpfun` by David H. Bailey [2].

The dashed lines show the estimated number of correct digits. To estimate this number for each coefficient, we used the formulas from theorem 7.2.1 (implemented in Matlab with a nested call to the function `fminbnd`). These formulas yield an estimate for the absolute error on E_m. To obtain an estimate for the relative error (and thus for the number of correct digits), we approximated the real value of E_m using the asymptotic formula from section 3.4.

In all four examples μ is equal to the normalized Lebesgue measure on $[-1, 1]$. The number of nodes in the quadrature formula equals $n = 150$.

Example 7.3.1. Let us start with the case where

$$A = \{2, 4, 6, \ldots\},$$
$$\tilde{A} = \{\omega, -\omega, 2\omega, -2\omega, \ldots\}, \quad \omega = 1.1 \,.$$

The results are as shown in figure 7.3. The oscillatory behaviour in the beginning is of course due to machine limitations: working in IEEE double precision, no more than approximately 16 correct digits can be reached.

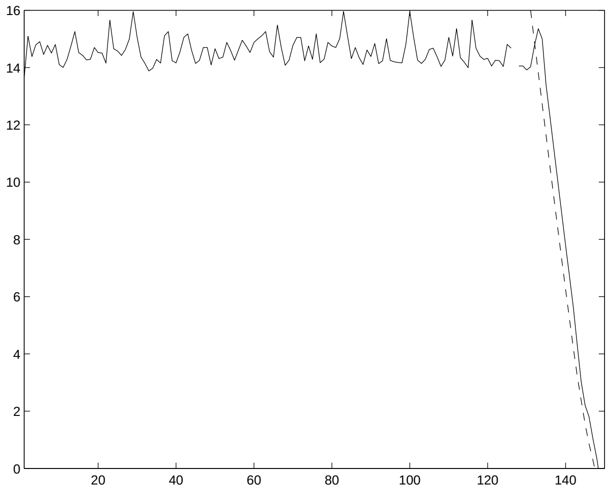

Figure 7.3: Example 7.3.1. Estimated and actual number of correct digits for the recurrence coefficient E_m.

Using 150 nodes in the quadrature formula, it is possible to compute over 130 coefficients up to machine precision. It is also clear from the figure that the estimated number of correct digits is very close to the actual number of correct digits.

Example 7.3.2. In the previous example the poles in the computed functions are at a reasonable distance from the boundary. In that case, one might as well use Gauss-Legendre quadrature formulas to compute the inner products. This is shown in the following example, where we thus have

$$A = \{2, 4, 6, \ldots\},$$
$$\tilde{A} = \{\infty, \infty, \infty, \ldots\}.$$

Figure 7.4 gives the results. It is clear that the use of a quadrature formula based on rational functions was not necessary in example 7.3.1; ordinary Gauss-Legendre quadrature gives the same results. In this case all poles in $\tilde{A}$ are equal and we can use theorem 7.2.3 to predict the number of nodes needed to compute $m = 132$ coefficients up to a precision of $\epsilon = 10^{-15}$. This yields $n = 152$, which is a good approximation to the actual number of nodes used.

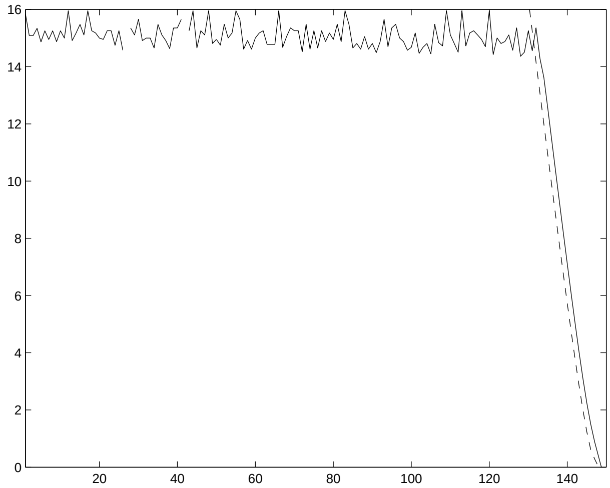

Figure 7.4: Example 7.3.2. Estimated and actual number of correct digits for the recurrence coefficient E_m.

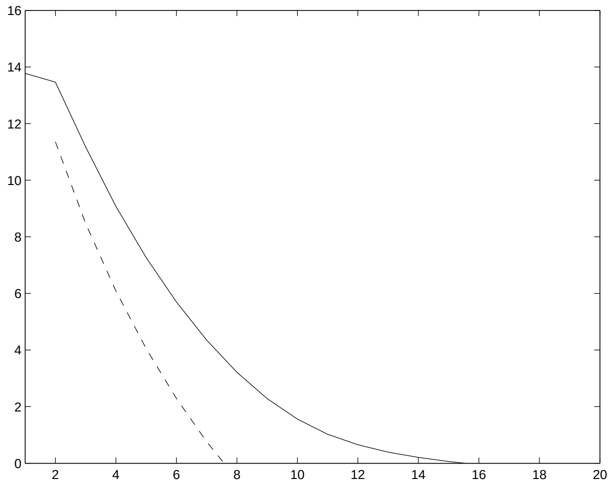

Figure 7.5: Example 7.3.3. Estimated and actual number of correct digits for the recurrence coefficient E_m.

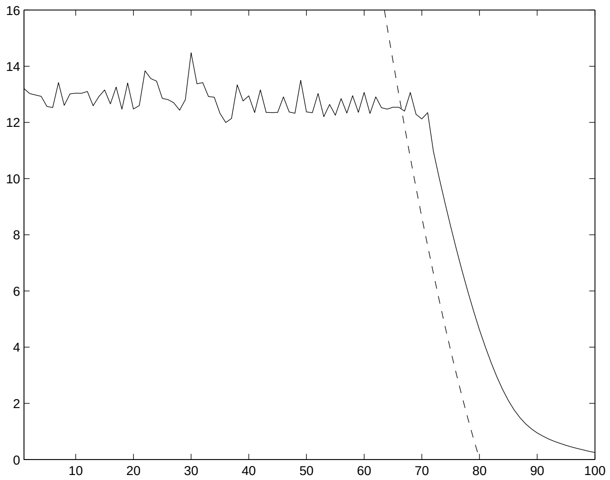

Figure 7.6: Example 7.3.4. Estimated and actual number of correct digits for the recurrence coefficient E_m.

Example 7.3.3. The advantage of using rational quadrature formulas only becomes apparent in the case where the poles in the computed functions are close to the boundary. In this example we take

$$A = \{1.01, 1.01, 1.01, \ldots\},$$
$$\tilde{A} = \{\infty, \infty, \infty, \ldots\},$$

so there is a multiple pole very close to 1. The Gauss-Legendre quadrature formulas fail completely, as is shown in figure 7.5. Only 2 or 3 coefficients can be computed 'exactly'. In this case we have used the second formula in theorem 7.2.1 to estimate the number of correct digits. If we use the first formula, we get an estimate of only 1 correct digit even when $m = 2$, which is far from the actual number of correct digits. According to theorem 7.2.3, we would need approximately $n = 2600$ nodes in the quadrature formula to compute $m = 150$ coefficients up to machine precision.

Example 7.3.4. However, if we take

$$A = \{1.01, 1.01, 1.01, \ldots\},$$
$$\tilde{A} = \{1.03, 1.03, 1.03, \ldots\},$$

then we are able to compute approximately 70 coefficients up to machine precision, as shown in figure 7.6. The second formula in theorem 7.2.3

predicts that we would need $n = 157$ nodes to compute $m = 71$ coefficients up to a precision of $\epsilon = 10^{-13}$. This is a reasonable estimate.

7.4 Poles close to the boundary

As shown by the previous examples, the computation of orthogonal rational functions with poles close to the interval of integration is a complicated matter. In this section we analyze the problem and indicate some possible solutions. First let us look in more detail at the error Δ_{nm} of the previous section. We assume that the poles α_k in the target functions are all equal to $\alpha > 1$ (this is not an essential restriction) and that the poles $\tilde{\alpha}_k$ in the functions which yield the quadrature formula are all equal to $\tilde{\alpha} > 1$. In this case, instead of estimating the integral in (7.6), we can compute it explicitly using the residue theorem. If we denote the integral by

$$\Delta(m, n, \beta, \tilde{\beta}) = \frac{1}{2}(1-\beta^4)\frac{1}{2\pi\mathbf{i}}\int_\Gamma \frac{(1+z^2)(z-\tilde{\beta})^{2n-1}(1-\beta z)^{2m-5}}{(1-\tilde{\beta}z)^{2n-1}(z-\beta)^{2m-1}}dz$$

then with the previous notation we have $\Delta_{nm} \approx |\Delta(m, n, \beta, \tilde{\beta})|$ (we have omitted the unimodular constants in $B_n(z)$ because they do not contribute to the error).

First we will look at the simpler situation where $\tilde{\beta} = 0$ (this corresponds to ordinary Gauss quadrature). Using the residue theorem and Leibniz' formula for the high order derivative of a product of two functions, we can obtain an explicit expression for the function Δ. Some computations yield

$$\begin{aligned}\Delta(m, n, \beta, 0) = \frac{1}{2}(1-\beta^4)\beta^{2n-2m+1}\sum_{k=0}^{2m-5}\frac{(-1)^k}{k!(2m-2-k)!}\cdots \\ \cdots\left[(2n+1)_{2m-2-k}\beta^2 + (2n-1)_{2m-2-k}\right]\cdots \\ \cdots\beta^{2k}(2m-5)_k(1-\beta^2)^{2m-5-k}\end{aligned}$$

where we have used the symbol $(a)_n = a(a-1)(a-2)\ldots(a-n+1)$. This formula clearly shows that for fixed m and β and for large enough n, the function Δ will be decreasing with increasing n, which corresponds to saying that the quadrature error decreases when the number of nodes increases. More interesting, however, is the fact that for large n the function Δ will be increasing if β increases from 0 to 1, since for large n the behaviour of Δ is dominated by the exponential term in front of the summation.

For the general situation $\tilde{\beta} \neq 0$ it is also possible to give an explicit representation of $\Delta(m, n, \beta, \tilde{\beta})$, using Leibniz' rule twice. The formula, however, is quite complicated and it is difficult to deduce the behaviour of Δ

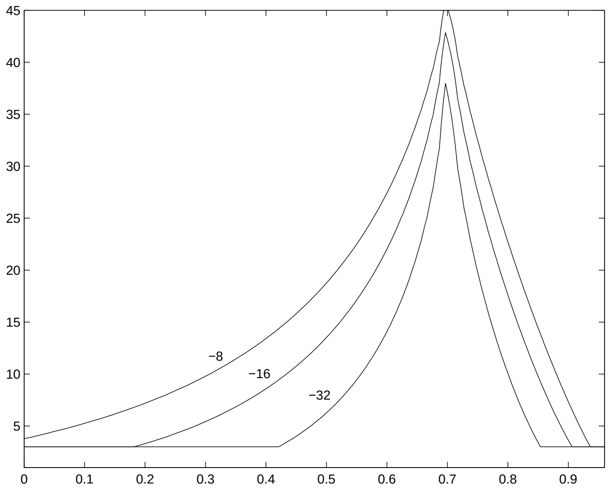

Figure 7.7: Contour plot of $\log_{10}|\Delta(m, 50, \beta, 0.7)|$

by simple inspection of the expression. But it is an explicit expression which allows a direct computation. We give it only for the sake of completeness:

$$\Delta(m, n, \beta, \tilde{\beta}) = \frac{1}{2}(1-\beta^4)\frac{1}{(2m-2)!}\Big[F^{(2m-2)}(\beta)(1+\beta^2) \\ +4(m-1)\beta F^{(2m-3)}(\beta) + 2(m-1)(2m-3)F^{(2m-4)}(\beta)\Big]$$

where the k-th derivative of the function $F(z)$ is given by

$$F^{(k)}(z) = \sum_{i=0}^{k}\binom{k}{i}\sum_{j=0}^{k-i}\binom{k-i}{j}(2n-1)_{k-i-j}(2n-1)^{(j)}\tilde{\beta}^j \\ \frac{(z-\tilde{\beta})^{2n-1-k+i+j}}{(1-\tilde{\beta}z)^{2n-1+j}}(2m-5)_i(1-\beta z)^{2m-5-i}(-\beta)^i$$

and we have used the symbol $(a)^{(n)} = a(a+1)(a+2)\dots(a+n-1)$. One conclusion we can draw from this formula, is that the quadrature error will be small if β is close to $\tilde{\beta}$ (which is of course not very surprising).

A practical application of the function $\Delta(m, n, \beta, \tilde{\beta})$ is explained below. Assume we have at our disposition a quadrature formula (i.e. n different nodes and weights) based on a set of orthogonal rational functions (with respect to μ) with a multiple pole in $\tilde{\beta}$, and we wish to use this quadrature formula to compute the recurrence coefficients for rational functions orthogonal with respect to the same measure, but with a multiple pole in β. A contourplot of the function Δ with n and $\tilde{\beta}$ fixed will tell us how many (m) coefficients we can compute, as a function of β and given a certain precision level (contour) ϵ. Figure 7.7 shows a contourplot of $\log_{10}|\Delta(m, 50, \beta, 0.7)|$. The contours shown correspond to the machine precision when working in single, double and quadruple precision. For example, if $\beta = 0.58$ ($\alpha = 1.15$) and when working in double precision, we can compute more or less 20 coefficients up to machine precision ($\epsilon \approx 10^{-16}$).

The obvious weakness in the previous approach is that we need to know a set of orthogonal rational functions with poles close to the boundary to compute a similar set of functions. In the ideal situation, we want to be able to compute rational functions orthogonal with respect to an arbitrary measure, using a quadrature formula which is easily generated. The solution to this problem is still under investigation, but we have been able to solve it for a certain class of weight functions, using a connection with orthogonal Laurent polynomials. In [49] a quadrature formula is presented to approximate integrals of the form

$$I(g, \lambda, r) = \int_{-1}^{1} \frac{g(u)}{(u+\lambda)^r} \frac{1}{\sqrt{1-u^2}} du,$$

where g is a continuous function in $[-1, 1]$, λ is any real number such that $|\lambda| > 1$, and r is an integer. The nodes and weights in this quadrature formula can be computed explicitly from the nodes and weights for Gauss-Chebyshev quadrature. In [16] this type of formulas has been extended to more general weight functions and the following theorem is an immediate consequence of that article.

Theorem 7.4.1. *Let μ be absolutely continuous with weight*

$$\mu'(x) = (1-x^2)^{c-1/2}, \quad c > -1/2$$

and let t_{nk} and A_{nk} denote respectively the nodes and weights for the (polynomial) Gauss quadrature formula associated with μ. For $\alpha > 1$ define

$$\xi_{nk} = \alpha - x_{nk}, \quad \Lambda_{nk} = \lambda_{nk}\sqrt{x_{nk}}$$

where

$$x_{nk} = \left(\frac{\delta t_{nk} + \sqrt{(\delta t_{nk})^2 + 4\gamma}}{2} \right)^2$$

$$\lambda_{nk} = \frac{2\delta}{1 + \gamma / x_{nk}} A_{nk}$$

with

$$\delta = \sqrt{\alpha+1} - \sqrt{\alpha-1}, \quad \gamma = \sqrt{\alpha^2-1}.$$

Then the formula

$$\int_{-1}^{1} f(x)d\mu(x) \approx \frac{1}{\delta}\left(\frac{4}{\delta^2+4\gamma}\right)^c \sum_{k=1}^{n} \Lambda_{nk} f(\xi_{nk}) \tag{7.12}$$

is exact for every f of the form

$$f(x) = \frac{p_{2n-1}(x)}{(x-\alpha)^n}\frac{1}{(\alpha-x)^c}, \quad p_{2n-1} \in \mathcal{P}_{2n-1}.$$

It is clear that for integer c these formulas become extremely interesting, integrating exactly rational functions with a multiple pole in α. However, for the case where $c = 0$ or $c = 1$, the orthogonal rational functions are known explicitly and treated in the case study of the last chapter. It may seem that if c is not an integer, then these quadrature formulas are not very useful, because of the factor $(\alpha - x)^c$ in the denominator of the integrand. It will turn out that this is not really a problem, because the high degree of the numerator can compensate for the irrational term in the denominator (in a sense we explain below). First let us look at an example.

Example 7.4.2. As in some of the previous examples, assume we wish to compute orthogonal rational functions on I with a multiple pole in $\alpha = 1.01$ and with respect to the Lebesgue measure. Now we use the quadrature formula from theorem 7.4.1 to compute the recurrence coefficients. To get the Lebesgue measure, we have to take $c = 1/2$ in this theorem and then the constant factor in front of the summation in (7.12) will be equal to 1. The nodes and weights are computed from the nodes and weights for the Gauss-Legendre quadrature, which we assume known. We used $n = 150$ nodes, the relative error for the coefficients E_m and F_m for $m = 74, \ldots, 81$ is as shown in table 7.1. For $m < 74$ the error was of the order of machine precision. Note that we can compute approximately $m = n/2$ coefficients 'exactly', while for $m > n/2$ the error increases rapidly. In spite of the factor $\sqrt{\alpha - x}$, this quadrature formula seems to work very well and the computational effort is minimal. Of course, one might argue that computing the Gauss-Legendre nodes and weights requires a considerable effort, since they are not explicitly known. However, recent techniques allow the fast and stable computation of these values (especially for large n), based on Fourier-Newton methods and not solving the tridiagonal eigenvalue problem. For more information we refer to [51].

m	rel. err. E_m	rel. err. F_m
74	$5.9868e-15$	$1.5699e-14$
75	$3.9636e-13$	$4.0155e-13$
76	$2.8428e-09$	$2.8096e-09$
77	$1.2139e-06$	$1.1353e-06$
78	$9.8147e-05$	$8.5249e-05$
79	$2.6482e-03$	$2.0655e-03$
80	$2.8900e-02$	$1.8914e-02$
81	$1.4754e-01$	$7.1077e-02$

Table 7.1: Example 7.4.2. Relative error for E_m and F_m.

As the example already indicated, the quadrature formulas from theorem 7.4.1 seem to work very well as long as $m \leq n/2$ (or equivalently, as long as the degree of the rational functions we are integrating does not exceed the number of nodes; remember that to compute E_m we have to integrate a function of degree $2m-1$). In the following theorem we try to explain why this is so.

Theorem 7.4.3. *Let $e_n(f)$ denote the quadrature error for a function f in the formula of theorem 7.4.1. Then with the notation of that theorem we have*

$$|e_n(f_m)| \leq \epsilon_{n-1} \|f_m\|_I \frac{2\sqrt{\pi}\,\Gamma(c+1/2)\,\delta^{2c}}{\Gamma(c+1)}$$

for $f_m \in \mathcal{L}_m$ and $m \leq n$, where

$$\epsilon_{n-1} = \min_{p_{n-1}\in\mathcal{P}_{n-1}} \|(\alpha-x)^c - p_{n-1}(x)\|_I\,, \tag{7.13}$$

Γ is the Gamma function and $\|\cdot\|_I$ denotes the supremum norm on I.

Proof. Let p_{n-1} denote the polynomial which minimizes (7.13) and define $r_{n-1}(x)$ as

$$r_{n-1}(x) = (\alpha-x)^c - p_{n-1}(x)$$

(it follows that $\epsilon_{n-1} = \|r_{n-1}(x)\|_I$). Then write

$$f_m(x) = f_m(x)\frac{r_{n-1}(x)+p_{n-1}(x)}{(\alpha-x)^c}$$

and note that $e_n(f_m(x)p_{n-1}(x)/(\alpha-x)^c) = 0$ because of theorem 7.4.1. We then have

$$\begin{aligned}|e_n(f_m)| &= \left| e_n\left(f_m(x)\frac{r_{n-1}(x)}{(\alpha-x)^c}\right)\right| \\ &= \left| I_\mu\left(f_m(x)\frac{r_{n-1}(x)}{(\alpha-x)^c}\right) - I_n\left(f_m(x)\frac{r_{n-1}(x)}{(\alpha-x)^c}\right)\right| \\ &\le \epsilon_{n-1}\,\|f_m\|_I\,\left[I_\mu((\alpha-x)^{-c}) + I_n((\alpha-x)^{-c})\right]\end{aligned}$$

where $I_\mu(f) = \int f d\mu$ and $I_n(f)$ denotes the quadrature sum of theorem 7.4.1. Since the quadrature formula is exact for $(\alpha-x)^{-c}$, this last expression gives

$$|e_n(f_m)| \le \epsilon_{n-1}\,\|f_m\|_I\,2I_\mu((\alpha-x)^{-c}).$$

Some computations show that

$$\int_{-1}^{1}\frac{(1-x^2)^{c-1/2}}{(\alpha-x)^c}dx = \frac{\sqrt{\pi}\,\Gamma(c+1/2)\,\delta^{2c}}{\Gamma(c+1)}$$

proving the theorem. □

Remark. This theorem shows that for integer $c < n$ the quadrature formula is exact when integrating $f_m \in \mathcal{L}_m$ and $m \le n$, which also follows immediately from theorem 7.4.1. For other values of c the quadrature error will depend on how well $(\alpha - x)^c$ can be approximated by a polynomial. To compute ϵ_{n-1} we could use Remes' algorithm to find the minimax polynomial, but a good estimate is usually given by the coefficient of the first neglected term in a Chebyshev approximation, which is much simpler to compute. Using this estimate in example 7.4.2 we find

$$\epsilon_{n-1} \approx 8.6311\ 10^{-14}$$

for $n = 150$. The function f_m would in this case equal $Z_m\varphi_{m-1}^2$ (if we want to estimate the accuracy of E_m). For $m = 74$ this gives

$$\left\|Z_m\varphi_{m-1}^2\right\|_I = 2.9465\ 10^6.$$

Combining these numbers gives an estimate of 10^{-7} which is quite pessimistic compared to the actual error. This is probably due to taking the function f_m outside the integral in the proof of theorem 7.4.3. For poles close to the boundary, $\|f_m\|_I$ will be large, while the quadrature error remains small. It is not clear, however, how we could get a more accurate estimate.

7.5 Conclusion

In this chapter we presented a method for computing orthogonal rational functions on an interval. A detailed analysis shows that for the case where the poles stay away from the boundary, this can be done using polynomial-based quadrature formulas. This is essentially due to the fact that the ORF look very much like polynomials when the poles are far from the interval. We focused on the use of gaussian quadrature rules, because they allow a more detailed analysis, but it should be clear that in practice it is often better to use quadrature formulas which require less computational effort to generate, such as Fejér's rule. However, since gaussian rules are in a certain sense optimal (they have a maximal domain of validity for a fixed number of nodes), we can think of the analysis in this chapter as a 'best-case scenario'.

For the case where there are poles close to the interval of integration, it becomes unfeasible to use quadrature rules based on polynomials, because of the enormous number of nodes we would need. A recent development, based on orthogonal Laurent polynomials has given a partial solution to this problem, providing a way to compute the ORF with poles close to the boundary for a number of special weight functions, under the assumption that all poles are equal to each other. For more general measures, the problem is still under investigation.

Chapter 8

ORF on a halfline

8.1 Introduction

Uptill now most of our attention has gone to orthogonality on the interval $[-1, 1]$. From a computational point of view, there is a good reason for this. As described in this chapter, we can map the halfline $[0, \infty)$ to the interval and find a relation between the respective orthogonal rational functions (or more precisely, between their recurrence coefficients). This mapping can also be used to obtain some asymptotic results for ORF on a halfline. We will first derive the relations between ORF on I and on $[0, \infty)$ and then use them to obtain some asymptotic results. Some examples will serve as illustration.

8.2 Mapping the halfline to the interval

Suppose we are given a measure $\tilde{\mu}$ on the halfline $[0, \infty]$ and a set of poles $\tilde{A} = \{\tilde{\alpha}_1, \tilde{\alpha}_2, \ldots\} \subset (-\infty, 0)$. With this measure and poles we associate a set of orthonormal rational functions $\{\tilde{\varphi}_n\}$. Since $\mathrm{supp}(\tilde{\mu})$ is connected, the recurrence relation holds for every n. We will denote the recurrence coefficients by $\{\tilde{E}_n, \tilde{F}_n\}_{n=1}^{\infty}$. According to the conventions from chapter 2, we cannot have poles at infinity, because this is in the support of the measure.

We map the halfline to the interval $[-1, 1]$ using the transformation

$$\tau(x) = \frac{1-x}{1+x}, \quad x \in [0, \infty]. \tag{8.1}$$

Note that $y = \tau(x)$ implies $x = \tau(y)$. Then associate to $\tilde{\mu}$ and $\tilde{A}$ a measure μ on I and a set of poles $A = \{\alpha_1, \alpha_2, \ldots\} \subset \overline{\mathbb{R}}^I$ in the following way. For every Borel measurable set $E \subset [-1,1]$ set

$$\mu(E) = \tilde{\mu}(\{\tau(y), y \in E\}) \tag{8.2}$$

and for the poles A set

$$\alpha_n = \tau(\tilde{\alpha}_n), \quad n = 1, 2, \ldots \tag{8.3}$$

From (8.2) we have $\mu' = |\tau'|(\tilde{\mu}' \circ \tau)$, where the prime means derivative (in case of a measure this is of course the Radon-Nikodym derivative with respect to the Lebesgue measure). More explicitly this yields

$$\mu'(y) = \frac{2}{(1+y)^2}\tilde{\mu}'\left(\frac{1-y}{1+y}\right) .$$

We will need several simple lemmas before we can prove the main theorem. Let $\tilde{\mathcal{L}}_n$ denote the space of rational functions of degree n with poles in $\{\tilde{\alpha}_1, \ldots, \tilde{\alpha}_n\}$ and $\tilde{b}_n(z) = \prod_{k=1}^n \tilde{Z}_k(z)$ the corresponding basis functions. As before, the symbols without a tilde refer to the interval. The proof of the following lemma is a matter of straightforward computation and we omit it.

Lemma 8.2.1. *Put $y = \tau(x)$ then we have*

$$\tilde{Z}_n(x) = -\frac{1}{2}\left(1 - \frac{1}{\alpha_n}\right)\left[\left(1 - \frac{1}{\alpha_n}\right) Z_n(y) - 1\right], \quad n \geq 1$$
$$\frac{\tilde{Z}_n(x)}{\tilde{Z}_m(x)} = \frac{1-1/\alpha_n}{1-1/\alpha_m}\frac{Z_n(y)}{Z_m(y)}, \quad n, m \geq 1$$

and for every pair of complex numbers (a, b) we have

$$aZ_n(y) + b = \left(a - \frac{b}{Z_{n-1}(\alpha_n)}\right) Z_n(y) + b\frac{Z_n(y)}{Z_{n-1}(y)}, \quad n \geq 1$$

Next we derive a relation between the rational functions in $\mathcal{L}_n$ orthonormal with respect to μ and those in $\tilde{\mathcal{L}}_n$ orthonormal with respect to $\tilde{\mu}$.

Lemma 8.2.2. *Let $\{\tilde{\varphi}_n\}_{n=1}^\infty$ denote the set of orthonormal rational functions associated with $(\tilde{A}, \tilde{\mu})$ and $\{\varphi_n\}_{n=1}^\infty$ those associated with (A, μ). Then we have*

$$\tilde{\varphi}_n \circ \tau = \pm\varphi_n, \quad n \geq 1$$

where the sign is determined by the normalization $\tilde{E}_n > 0$ for $\tilde{\varphi}_n$ and $E_n > 0$ for φ_n.

Proof. It is clear that $\tilde{\varphi}_n \circ \tau \in \mathcal{L}_n$. Because $\tilde{\alpha}_k \neq 0$ for all k we have $\alpha_k \neq 1$ and then it follows from lemma 8.2.1 that the basis functions b_k and $\tilde{b}_k$ satisfy the following relation,

$$\tilde{b}_k = \sum_{j=0}^{k} c_j^{(k)} (b_j \circ \tau), \quad c_k^{(k)} \neq 0$$

for some constants $\{c_j^{(k)}\}$. Next expand $\tilde{\varphi}_n$ in the basis $\{\tilde{b}_0, \ldots \tilde{b}_n\}$,

$$\tilde{\varphi}_n = \sum_{k=0}^{n} d_k^{(n)} \tilde{b}_k$$

where $d_n^{(n)} \neq 0$ because $\tilde{\varphi}_n \in \tilde{\mathcal{L}}_n$ and $\tilde{\varphi}_n \perp \tilde{\mathcal{L}}_{n-1}$. Then with the previous relation and the fact that $\tilde{b}_k \circ \tau \circ \tau = \tilde{b}_k$ it follows that

$$\begin{aligned}
\tilde{\varphi}_n \circ \tau &= \sum_{k=0}^{n} d_k^{(n)} (\tilde{b}_k \circ \tau) \\
&= \sum_{k=0}^{n} d_k^{(n)} \sum_{j=0}^{k} c_j^{(k)} b_j \\
&= \sum_{k=0}^{n} \tilde{d}_k^{(n)} b_k
\end{aligned}$$

and $\tilde{d}_n^{(n)} = d_n^{(n)} c_n^{(n)} \neq 0$. This shows that $\tilde{\varphi}_n \circ \tau \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$ and thus $\{\tilde{\varphi}_0 \circ \tau, \ldots, \tilde{\varphi}_n \circ \tau\}$ forms a basis for $\mathcal{L}_n$.

Because of orthogonality we have

$$\int \tilde{\varphi}_n \tilde{\varphi}_m d\tilde{\mu} = \delta_{nm}, \quad n, m \geq 0$$

where δ_{nm} is the Kronecker symbol. Using the definition of τ this becomes

$$\int (\tilde{\varphi}_n \circ \tau)(\tilde{\varphi}_m \circ \tau) d\mu = \delta_{nm}, \quad n, m \geq 0.$$

This means that $\tilde{\varphi}_n \circ \tau \perp \mathcal{L}_{n-1}$ and $\|\tilde{\varphi}_n \circ \tau\| = 1$. But we also have $\varphi_n \perp \mathcal{L}_{n-1}$ and $\|\varphi_n\| = 1$ so it follows that $\tilde{\varphi}_n \circ \tau = \gamma_n \varphi_n$ with $|\gamma_n| = 1$. Using lemma 2.5.1 we then get

$$\tilde{\varphi}_n \circ \tau = \pm \varphi_n$$

which proves the lemma. □

Using the previous two lemmas we can express the recurrence coefficients $\{\tilde{E}_n, \tilde{F}_n\}$ for $\{\tilde{\varphi}_n\}$ in terms of the recurrence coefficients $\{E_n, F_n\}$ for $\{\varphi_n\}$. We will need one more lemma before we can prove our main theorem.

Lemma 8.2.3. *If $n = 1$ then the recurrence coefficients for φ_1 satisfy*

$$E_1 > F_1.$$

Proof. From the recurrence relation, taking the inner product with $\varphi_0 = 1$ on both sides, we obtain,

$$-F_1 = E_1 \frac{\int_{-1}^{1} Z_1(x) d\mu(x)}{\int_{-1}^{1} \frac{Z_1(x)}{x} d\mu(x)}$$

or writing Z_1 explicitly

$$E_1 - F_1 = E_1 \frac{\int_{-1}^{1} \frac{x+1}{1-x/\alpha_1} d\mu(x)}{\int_{-1}^{1} \frac{1}{1-x/\alpha_1} d\mu(x)} .$$

Both integrands are positive on $[-1, 1]$ and so is E_1. Therefore also $E_1 - F_1 > 0$, proving the lemma. □

We now state and prove our main theorem.

Theorem 8.2.4. *With the definitions of this section we obtain the following relations between $\{E_n, F_n\}$ and $\{\tilde{E}_n, \tilde{F}_n\}$ for $n \geq 1$,*

$$\tilde{E}_n = [2E_n - \delta_{n1}(E_1 + F_1)] \left(1 - \frac{1}{\alpha_{n-1}}\right)^{-1} \left(1 - \frac{1}{\alpha_n}\right)^{-1},$$

$$\tilde{F}_n = -\left(1 - \frac{1}{\alpha_n}\right)^{-1} \left[F_n \left(1 - \frac{1}{\alpha_{n-1}}\right) + E_n - \delta_{n2} \frac{E_2}{E_1} \frac{1 - 1/\alpha_1}{F_1 - E_1}\right].$$

Note that the formulas simplify for $n > 2$ because of the Kronecker symbols.

Proof. First we will prove the theorem for the cases $n = 1$ and $n = 2$ and then for general $n > 2$. The first two cases are special because by convention we have $\alpha_{-1} = \alpha_0 = \infty$ but also $\tilde{\alpha}_{-1} = \tilde{\alpha}_0 = \infty$ which shows that $\alpha_k \neq \tau(\tilde{\alpha}_k)$ for $k = -1, 0$.

For $n = 1$ use lemma 8.2.2 to write $(\tilde{\varphi}_1 \circ \tau)(x) = c\varphi_1(x)$ where $c = \pm 1$. Then write down the recurrence relations for $\tilde{\varphi}_1$ and φ_1, use the definition of τ and equate the coefficients of like powers of x to obtain (recall that $\tilde{\varphi}_0 = \varphi_0 = 1$)

$$\left(1 - \frac{1}{\alpha_1}\right) \tilde{E}_1 = c(F_1 - E_1),$$

$$\left(1 - \frac{1}{\alpha_1}\right) \tilde{F}_1 = c(F_1 + E_1),$$

Now it follows from $|\alpha_1| > 1$, $\tilde{E}_1 > 0$ and lemma 8.2.3 that $c = -1$, proving the theorem for $n = 1$.

For $n = 2$ we proceed in the same way. Write down the recurrence relation for $\tilde{\varphi}_2 \circ \tau$, using the fact that we already know that $\tilde{\varphi}_1 \circ \tau = -\varphi_1$ and of course $\tilde{\varphi}_0 \circ \tau = \varphi_0$. Then use the relation

$$E_2 = \left. \frac{\varphi_2(x)}{\varphi_1(x) Z_2(x)} \right|_{x=\alpha_1}$$

and $E_2 > 0$ to find

$$E_2 = \frac{\tilde{E}_2}{2} \left(1 - \frac{1}{\alpha_2}\right) \left(1 - \frac{1}{\alpha_1}\right) .$$

To find the relation for $\tilde{F}_2$ use $\varphi_2(0) = F_2 \varphi_1(0) - E_2/E_1$ and $\varphi_1(0) = F_1$, again comparing the recurrence relations for $\tilde{\varphi}_2 \circ \tau$ and φ_2 and using all the previous results.

The general case $n > 2$ is the easiest to prove. Write down the recurrence relation for φ_n and for $\tilde{\varphi}_n \circ \tau$ using $\tilde{\varphi}_k \circ \tau = c_k \varphi_k$ for $k = n, n-1, n-2$ and $c_k = \pm 1$ and the formulas from lemma 8.2.1. Comparing the factors in front of φ_{n-1} and φ_{n-2} and using $E_n > 0$ immediately yields the result, thus proving the theorem. □

Remark. If we take all poles $\tilde{\alpha}_k = -1$ then transforming to the interval we obtain the orthogonal polynomials on $[-1, 1]$ with respect to μ. For the case of Legendre polynomials we would have to take $\tilde{\mu}$ absolutely continuous with weight $\tilde{\mu}'(x) = (1 + x)^{-2}$. See [23] for an application of this special case.

We could also transform orthogonal polynomials on $[0, \infty)$ to get orthogonal rational functions on $[-1, 1]$. In this case the poles $\tilde{\alpha}_n$ are in the support of the measure (polynomials have poles at infinity) and thus far we have always excluded this case. However, most of the theory remains valid for poles in the support of the measure, as long as all the moments μ_k exist and are finite. Asymptotic results are much more difficult to obtain now, but the recurrence relation remains valid whenever the $\tilde{\varphi}_n$ are regular, and so do the transformation formulas from theorem 8.2.4. Next we look at an example of this case.

Example 8.2.5. The Laguerre polynomials $L_n(x)$ are orthonormal on $[0, \infty)$ with respect to the weight function e^{-x} and usually normalized such that the coefficient of x^n has sign $(-1)^n$, see e.g. [52, p. 100]. In that case they satisfy the recurrence formula

$$n L_n(x) = (-x + 2n - 1) L_{n-1}(x) - (n-1) L_{n-2}(x).$$

n	E_n	F_n
1	$\frac{10}{3}$	$-\frac{2}{3}$
2	1	$\frac{37}{40}$
$n > 2$	$\frac{2}{n}$	$2\left(1 - \frac{1}{n}\right)$

Table 8.1: Recurrence coefficients for φ_n

with initial values $L_{-1}(x) = 0$ and $L_0(x) = 1$. If we regard them as orthogonal rational functions on the halfline and normalize them according to our convention $\tilde{E}_n > 0$, then it follows from the above recurrence relation that

$$\tilde{E}_n = \frac{1}{n}, \quad \tilde{F}_n = \frac{1}{n} - 2, \quad n = 1, 2, \ldots$$

Because of the remark following theorem 8.2.4, we may still use the transformation formulas from that theorem to obtain ORF on $[-1, 1]$. Of course now we have to use them in the opposite direction to obtain $\{E_n, F_n\}$ from $\{\tilde{E}_n, \tilde{F}_n\}$. We then get rational functions $\varphi_n(x)$ on $[-1, 1]$ with all poles in -1 and orthogonal with respect to the absolutely continuous measure

$$d\mu(x) = \frac{2}{(1+x)^2} \exp\left\{\frac{x-1}{x+1}\right\}.$$

Some computations then yield the recurrence coefficients as given in table 8.1.

8.3 Asymptotic behaviour

Using lemma 8.2.2 and theorem 8.2.4 it is very easy to obtain convergence results for orthogonal rational functions on the halfline $[0, \infty)$ when the poles stay away from infinity (this excludes the polynomial case). In fact, because of lemma 8.2.2 and the remark following (8.1) we know that $\tilde{\varphi}_n = \pm\varphi_n \circ \tau$, so we can rephrase most of the theorems from chapter 3, putting $\tau(x)$ in place of x, writing $\tau(\tilde{\alpha}_n)$ for α_n, etc. Instead of repeating all the formulas in their general form, we feel it is more informative to look at the special case where all poles are equal to each other, because then we can rewrite the expressions to obtain explicit representations for the limit functions. The computations are very straightforward and we only give the result in the following theorem.

Theorem 8.3.1. *Let $\tilde{\mu}$ be a measure on $[0,\infty)$ satisfying the condition $\tilde{\mu}' > 0$ a.e. and assume that all poles are equal to each other, $\tilde{A} = \{\tilde{\alpha}, \tilde{\alpha}, \ldots\}$ where $\tilde{\alpha} \in (-\infty, 0]$ (so the pole is finite). Then locally uniformly in $\overline{\mathbb{C}} \backslash [0,\infty)$ we have*

$$\lim_{n\to\infty} \frac{\tilde{\varphi}_n(x)}{\tilde{\varphi}_{n-1}(x)} = \frac{(\sqrt{-x} + \sqrt{-\tilde{\alpha}})^2}{x - \tilde{\alpha}}$$

where the branch of the square root is such that the limit is real for $x < 0$. For the recurrence coefficients we have the limits

$$\lim_{n\to\infty} E_n = -\frac{4}{\tilde{\alpha}},$$
$$\lim_{n\to\infty} F_n = -2.$$

We also have the weak-star convergence result

$$(x - \tilde{\alpha})\tilde{\varphi}_n^2(x) d\tilde{\mu}(x) \xrightarrow{*} \frac{\sqrt{-\tilde{\alpha}}}{\pi} \frac{dx}{(1+x)\sqrt{x}}.$$

8.4 Conclusion

In this chapter we presented some formulas to transform orthogonal rational functions on $[0,\infty)$ to $[-1,1]$. The main reason for studying these formulas is that they allow us to limit our attention to the interval case. Especially from a computational point of view, there no longer exists a fundamental difference between orthogonal rational functions on a halfline and on an interval. However, the asymptotic results obtained through this transformation suffer from the limitation that the poles cannot tend to infinity. As in the conclusion to chapter 3, we mention that the asymptotic behaviour for rational functions orthogonal on the unit circle with poles tending to the boundary not too quickly (Blaschke's condition), is still open to investigation. But even if we could generalize the theorems to that case, it would still be impossible to include the polynomial case in the asymptotic behaviour of orthogonal rational functions on $[0,\infty)$. As is well known, the study of convergence for polynomials orthogonal on a halfline (or on the whole real line), is much more complicated than the case of the interval, see e.g. [29] and the references therein.

Chapter 9

Case study: Chebyshev ORF

9.1 Introduction

The Chebyshev polynomials $T_m(x)$ are very well-known among the classical orthogonal polynomials. They are orthogonal with respect to the weight function $1/\sqrt{1-x^2}$ and are explicitly given by $T_m(x) = \cos(m \arccos x)$. There are very simple expressions for the nodes and weights in Gauss-Chebyshev quadrature and in Fejér's rule (interpolatory quadrature in the Chebyshev nodes with respect to the Lebesgue measure). In many ways the Chebyshev polynomials are 'typical' orthogonal polynomials, e.g. it can be shown that under very broad conditions on the measure the recurrence coefficients of orthogonal polynomials on I behave asymptotically as the recurrence coefficients of the Chebyshev polynomials. In this chapter we wish to study a rational generalization of these polynomials. We give explicit representations of these functions and their recurrence coefficients and provide an efficient way to compute the quadrature nodes and weights. We look at the convergence of the kernel function inside the support of the measure and finally we have a brief look at a rational Fejér rule (and the difficulties involved).

9.2 Bernstein-Szegő polynomials

The key to most results in this chapter is a theorem which can be found in Szegő's book [52, p. 31]. Let $\rho(x)$ be a polynomial of strict degree l and positive in $[-1, 1]$, then this theorem gives explicit representations for polynomials $p_n(x)$ orthogonal with respect to the weight functions

$$w(x) = \begin{cases} (1-x^2)^{-1/2}\{\rho(x)\}^{-1}, \\ (1-x^2)^{1/2}\{\rho(x)\}^{-1}, \\ \left(\frac{1-x}{1+x}\right)^{1/2}\{\rho(x)\}^{-1} \end{cases}$$

These orthogonal polynomials $p_n(x)$ are called Bernstein-Szegő polynomials and can be given explicitly provided that $l < 2n$ in the first case, $l < 2(n+1)$ in the second case and $l < 2n+1$ in the third. We give the theorem without proof.

Theorem 9.2.1. *Let $\rho(x)$ be a polynomial of strict degree l and positive in $[-1,1]$. Let $\rho(\cos\theta) = |h(e^{\mathbf{i}\theta})|^2$ be the normalized representation of $\rho(\cos\theta)$ such that $h(z)$ is a polynomial of degree l, with $h(z) \neq 0$ in $\mathbb{D}$ and $h(0) > 0$. Writing $h(e^{\mathbf{i}\theta}) = c(\theta) + \mathbf{i}s(\theta)$, $c(\theta)$ and $s(\theta)$ real, we have the following formulas for the orthonormal polynomials $p_n(x)$:*

$$\begin{aligned} p_n(\cos\theta) &= (2/\pi)^{1/2}\Re\{e^{\mathbf{i}n\theta}\overline{h(e^{\mathbf{i}\theta})}\} \\ w(x) &= (1-x^2)^{-1/2}\{\rho(x)\}^{-1}, && l < 2n; \\ p_n(\cos\theta) &= (2/\pi)^{1/2}(\sin\theta)^{-1}\Im\{e^{\mathbf{i}(n+1)\theta}\overline{h(e^{\mathbf{i}\theta})}\}, \\ w(x) &= (1-x^2)^{1/2}\{\rho(x)\}^{-1}, && l < 2(n+1); \\ p_n(\cos\theta) &= \pi^{-1/2}(\sin(\theta/2))^{-1}\Im\{e^{\mathbf{i}(n+1/2)\theta}\overline{h(e^{\mathbf{i}\theta})}\}, \\ w(x) &= \left(\frac{1-x}{1+x}\right)^{1/2}\{\rho(x)\}^{-1}, && l < 2n+1. \end{aligned}$$

The connection with orthogonal rational functions is as follows. If we denote as usual the orthonormal rational functions with respect to μ by $\varphi_n(x)$, then writing $\varphi_n(x) = p_n(x)/\pi_n(x)$ it follows that $p_n(x)$ is a polynomial orthogonal (*not* orthonormal) to the varying measure $d\mu(x)/(\pi_n(x)\pi_{n-1}(x))$. As pointed out already by Van Assche in [53], when the measure is absolutely continuous and the weight is one of

$$w(x) = \begin{cases} (1-x^2)^{-1/2}, \\ (1-x^2)^{1/2}, \\ \left(\frac{1-x}{1+x}\right)^{1/2} \end{cases} \tag{9.1}$$

then we can use the previous theorem to compute the polynomials p_n (and thus also the rational functions φ_n).

Before we can proceed with our discussion, some lemmas are needed which simplify the computations. In the rest of this chapter we will use a simpler definition for the Blaschke factors $\zeta_k(z)$ and the corresponding Blaschke product $B_n(z)$, omitting the normalization constants. First of all we assume that all the numbers $B = \{\beta_1, \beta_2, \ldots\}$ are real (and thus in I). Then define

$$\zeta_k(z) = \frac{z - \beta_k}{1 - \beta_k z}, \quad k = 1, 2, \ldots,$$
$$B_n(z) = B_{n-1}(z)\zeta_n(z), \quad B_0(z) = 1, \quad n = 1, 2, \ldots$$

The first lemma computes an integral we will encounter later on.

Lemma 9.2.2. *With the previous definition of the Blaschke product $B_n(z)$ we have*

$$\int_0^{2\pi} \frac{[z^k B_n(z) B_{n-1}(z) \pm 1]^2}{(z - \beta_n)^2 B_{n-1}^2(z) z^{k-1}} d\theta = \pm \frac{4\pi}{1 - \beta_n^2}$$

for every $k = 1, 2, \ldots$

Proof. First expand the square in the numerator to get

$$\int_0^{2\pi} \frac{[z^k B_n(z) B_{n-1}(z) \pm 1]^2}{(z - \beta_n)^2 B_{n-1}^2(z) z^{k-1}} d\theta = \int_0^{2\pi} \frac{z^{k+1} B_n^2(z)}{(z - \beta_n)^2} d\theta$$
$$\pm 2 \int_0^{2\pi} \frac{z}{(z - \beta_n)(1 - \beta_n z)} d\theta + \int_0^{2\pi} \frac{1}{(z - \beta_n)^2 B_{n-1}^2(z) z^{k-1}} d\theta.$$

Note that the last integral in this expression is the complex conjugate of the first one, so we may write

$$\int_0^{2\pi} \frac{[z^k B_n(z) B_{n-1}(z) \pm 1]^2}{(z - \beta_n)^2 B_{n-1}^2(z) z^{k-1}} d\theta$$
$$= 2\Re \left\{ \frac{1}{\mathbf{i}} \oint_{\mathbb{T}} \frac{z^k B_n^2(z)}{(z - \beta_n)^2} dz \right\} \pm \frac{2}{\mathbf{i}} \oint_{\mathbb{T}} \frac{1}{(z - \beta_n)(1 - \beta_n z)} dz.$$

The first integrand is analytic in $\mathbb{D} \cup \mathbb{T}$ and the second one has a simple pole in $z = \beta_n$. The result now follows from the residue theorem. □

As indicated by this lemma, Blaschke products have a peculiar behaviour when z is on the unit circle. For example, in the proof we used the fact that $\overline{B_n(z)} = 1/B_n(z)$ when $z \in \mathbb{T}$. The next lemma gives an interesting expression for the derivative of a Blaschke product on the unit circle.

Lemma 9.2.3. *With the definition of the Poisson kernel*

$$P(z, t) = \frac{1 - |t|^2}{|z - t|^2}, \quad z \in \mathbb{T}$$

the derivative $B_n'(z)$ *can be written*

$$B_n'(z) = \frac{1}{z} B_n(z) \sum_{k=1}^{n} P(z, \beta_n)$$

whenever $z \in \mathbb{T}$.

Proof. Note that with $z \in \mathbb{T}$ we have

$$\zeta_n'(z) = \frac{1}{z} \zeta_n(z) P(z, \beta_n).$$

The result is now immediate using the definition of the Blaschke product. □

Now we are ready to give explicit expressions for orthogonal rational functions with respect to the weights in (9.1).

9.3 Chebyshev orthogonal rational functions

Assume as before that we have arbitrary real poles outside I. We use the notation $\varphi_n^{(i)}$, $i = 1, 2, 3$ to denote the orthogonal rational functions with respect to the i-th weight in (9.1), so e.g. $\varphi_n^{(1)}$ denotes the rational generalization of the classical Chebyshev polynomials. However, we will use the name 'Chebyshev orthogonal rational functions' for all three cases. They are given in the next theorem.

Theorem 9.3.1. *The orthonormal functions* $\varphi_n^{(i)}$ *are given by*

$$\begin{aligned}
\varphi_n^{(1)}(x) &= \frac{1}{\sqrt{2\pi}} \sqrt{1-\beta_n^2} \left(\frac{z B_{n-1}(z)}{1-\beta_n z} + \frac{1}{(z-\beta_n) B_{n-1}(z)} \right), \\
\varphi_n^{(2)}(x) &= \sqrt{\frac{2}{\pi}} \sqrt{1-\beta_n^2} \frac{z}{z^2-1} \left(\frac{z^2 B_{n-1}(z)}{1-\beta_n z} - \frac{1}{z B_{n-1}(z)(z-\beta_n)} \right), \\
\varphi_n^{(3)}(x) &= \frac{1}{\sqrt{\pi}} \frac{1}{z-1} \sqrt{1-\beta_n^2} \left(\frac{z^2 B_{n-1}(z)}{1-\beta_n z} - \frac{1}{(z-\beta_n) B_{n-1}(z)} \right),
\end{aligned}$$

where $x = J(z) \in \overline{\mathbb{C}}$ *and* $\alpha_k = J(\beta_k)$.

Proof. It is not difficult to see that

$$\pi_n(\cos\theta) = \left| \prod_{k=1}^{n} \frac{1-\beta_k z}{\sqrt{1+\beta_k^2}} \right|, \quad z = e^{\mathrm{i}\theta}. \tag{9.2}$$

The polynomial between the absolute value signs obviously satisfies the conditions for the normalized representation of π_n as mentioned in theorem 9.2.1. Using that theorem and the remark following it, we then find

$$p_n^{(1)}(x) = c\sqrt{\frac{2}{\pi}}\Re\left\{z^n \prod_{k=1}^{n-1} \frac{(z-\beta_k)^2}{1+\beta_k^2} \frac{(z-\beta_n)}{\sqrt{1+\beta_n^2}}\right\}$$

where $\varphi_n^{(1)}(x) = p_n^{(1)}(x)/\pi_n(x)$ and c is a normalization constant such that

$$\int_{-1}^{1} \frac{(\varphi_n^{(1)}(x))^2}{\sqrt{1-x^2}} dx = 1. \tag{9.3}$$

Dividing by $\pi_n(x)$ as given in (9.2) and using the definition of the Blaschke products yields

$$\begin{aligned}\varphi_n^{(1)}(x) &= c\sqrt{\frac{2}{\pi}}\Re\left\{\frac{zB_{n-1}(z)}{1-\beta_n z}\sqrt{1+\beta_n^2}\right\} \\ &= c\frac{1}{\sqrt{2\pi}}\sqrt{1+\beta_n^2}\left(\frac{zB_{n-1}(z)}{1-\beta_n z} + \frac{1}{(z-\beta_n)B_{n-1}(z)}\right).\end{aligned}$$

The second equation holds for x anywhere in the complex plane and not just on I. To find the constant c use equations (9.3) and (2.5) and lemma 9.2.2. This completes the proof for $\varphi_n^{(1)}(x)$. The other two cases are proved in a completely analogous way. □

Using the explicit expressions we can derive many other formulas, e.g. for the nodes and weights in the quadrature formulas. This will be done in the next sections. First we look at the recurrence coefficients.

9.4 Recurrence coefficients

With the explicit expressions for the Chebyshev ORF we can easily compute the coefficients in the three term recurrence relation. The following theorem shows that these recurrence coefficients are exactly the asymptotic values as given by theorem 3.4.1.

Theorem 9.4.1. *For $n > 1$ the recurrence coefficients for the $\varphi_n^{(i)}(x)$ are the same for the three different cases and are given by*

$$E_n = 2\frac{\sqrt{(1-\beta_{n-1}^2)(1-\beta_n^2)}(1-\beta_{n-1}\beta_n)}{(1+\beta_{n-1}^2)(1+\beta_n^2)}, \tag{9.4}$$

$$F_n = -\sqrt{\frac{1-\beta_n^2}{1-\beta_{n-1}^2}}\frac{(1-\beta_{n-1}^2)(\beta_n+\beta_{n-2})+2\beta_{n-1}(1-\beta_n\beta_{n-2})}{(1+\beta_n^2)(1-\beta_{n-1}\beta_{n-2})}, \tag{9.5}$$

where $\beta_k = J^{-1}(\alpha_k)$. *For* $n = 1$ *we have*

$$E_1^{(1)} = \sqrt{2}c \qquad E_1^{(2)} = 2c \qquad E_1^{(3)} = 2c$$
$$F_1^{(1)} = -\sqrt{2}\beta_1 c \qquad F_1^{(2)} = -\beta_1 c \qquad F_1^{(3)} = (1-\beta_1)c$$

where

$$c = \frac{\sqrt{1-\beta_1^2}}{1+\beta_1^2}.$$

For $n = 2$ *the formula for* F_2 *holds with the convention that* $\beta_0 = 0$.

Proof. The coefficients can be computed using the formulas

$$E_n = \lim_{x\to\alpha_{n-1}} \frac{\varphi_n(x)}{\varphi_{n-1}(x)Z_n(x)},$$
$$F_n = \lim_{x\to\alpha_{n-2}} \left(\frac{\varphi_n(x)}{\varphi_{n-1}(x)}\frac{Z_{n-1}(x)}{Z_n(x)} - E_n Z_{n-1}(x)\right).$$

These formulas are valid for $n \geq 1$ (with the usual convention that $\alpha_{-1} = \alpha_0 = \infty$), but the case $n = 1$ has to be treated separately because the expressions for $\varphi_n^{(i)}(x)$ as given by theorem 9.3.1 do not include $\varphi_0^{(i)}$. For the case $n > 1$ equations (9.4) and (9.5) can easily be verified. If $n = 1$ then use the fact that $\varphi_0^{(i)} = 1/\sqrt{\mu_i(I)}$ where μ_i refers to the three different weight functions. To compute $F_1^{(i)}$ the simpler formula

$$F_1^{(i)} = \frac{\varphi_1^{(i)}(0)}{\varphi_0^{(i)}}$$

can be used. Some computations now finish the proof. □

Once the recurrence coefficients are known, we can use the generalized eigenvalue problem from chapter 4 to compute the nodes and weights in the gaussian quadrature formulas. However, in the next sections we derive alternative expressions to compute these values, which are far more efficient, especially for very large values of n. Some examples at the end of this chapter will illustrate this.

9.5 Zeros

The zeros of Chebyshev polynomials can easily be expressed in closed form as

$$x_{nk} = \cos\left(\pi\frac{2k-1}{2n}\right), \quad k = 1, 2, \dots, n.$$

It is difficult (or even impossible) to given similar explicit representations for the zeros of Chebyshev ORF, but we can derive formulas which allow an efficient computation of these zeros, as shown in the next theorem.

Theorem 9.5.1. *Let $x_{nk}^{(i)}$ denote the zeros of $\varphi_n^{(i)}(x)$ and put $x_{nk}^{(i)} = \cos\theta_{nk}^{(i)}$ then they satisfy the following equations,*

$$\begin{aligned} f_n(\theta_{nk}^{(1)}) - (n-1)\theta_{nk}^{(1)} &= \frac{\pi}{2}(2k-1), \\ f_n(\theta_{nk}^{(2)}) - (n-2)\theta_{nk}^{(2)} &= \pi k, \\ f_n(\theta_{nk}^{(3)}) - (n-3/2)\theta_{nk}^{(3)} &= \pi k, \end{aligned}$$

for $k = 1, 2, \ldots, n$ where

$$f_n(\theta) = 2\sum_{j=1}^{n-1} \arctan\frac{\sin\theta}{\cos\theta - \beta_j} + \arctan\frac{\sin\theta}{\cos\theta - \beta_n}.$$

and $\arctan(y/x)$ *refers to the argument of the complex number $x + \mathbf{i}y$.*

Proof. Again we only prove the theorem for the first case. From the expression for $\varphi_{nk}^{(1)}(x)$ we get that the zeros satisfy

$$z_{nk}^{(1)} B_n(z_{nk}^{(1)}) B_{n-1}(z_{nk}^{(1)}) = -1 = e^{\mathbf{i}\pi(2k-1)}, \quad k \in \mathbb{Z}$$

where $z_{nk}^{(1)} = J^{-1}(x_{nk}^{(1)})$. The function $zB_n(z)B_{n-1}(z)+1$ has $2n$ zeros which are pairwise complex conjugate. Taking the real parts gives us the n zeros of $\varphi_n^{(1)}(x)$. Note that $\zeta_n(z)$ may be written as

$$\zeta_n(z) = \exp\left\{2\arctan\frac{\sin\theta}{\cos\theta - \beta_n}\right\}, \quad z = e^{\mathbf{i}\theta}.$$

Some computations complete the proof. Note that for the second case the function $z^3 B_n(z)B_{n-1}(z) - 1$ has zeros at -1 and 1 which cancel against the same zeros in the denominator of $\varphi_n^{(2)}(x)$ and which therefore have to be ignored. The same occurs in the third case for $z = 1$. □

As we mentioned before, in a later section we give some examples to show that the zeros can be computed very efficiently for arbitrarily large n from these formulas. This is important because they can be used as the nodes in quadrature formulas. In the next section we show how the weights in these quadrature formulas can be given as functions of the nodes.

9.6 Quadrature weights

Once the nodes have been computed, the weights can be found by evaluating the kernel function as explained in chapter 4. Since we have explicit formulas for the orthogonal functions, this is a straightforward task. However, it is possible to give much simpler expressions for the weights, as shown in this section's theorem.

Theorem 9.6.1. *The weights in the gaussian quadrature formulas based on the $\varphi_n^{(i)}$ can be given as functions of the nodes in the following way,*

$$\lambda_{nk}^{(1)} = 2\pi \left(1 + g_n(x_{nk}^{(1)})\right)^{-1},$$

$$\lambda_{nk}^{(2)} = 2\pi(1 - (x_{nk}^{(2)})^2) \left(3 + g_n(x_{nk}^{(2)})\right)^{-1},$$

$$\lambda_{nk}^{(3)} = 2\pi(1 - x_{nk}^{(3)}) \left(2 + g_n(x_{nk}^{(3)})\right)^{-1}$$

for $k = 1, 2, \ldots, n$ where

$$g_n(x) = 2 \sum_{k=1}^{n-1} \frac{\sqrt{1 - 1/\alpha_k^2}}{1 - x/\alpha_k} + \frac{\sqrt{1 - 1/\alpha_n^2}}{1 - x/\alpha_n}.$$

Proof. We give the proof for the first case. To simplify the notation, we omit the superscripts, so we write φ_n instead of $\varphi_n^{(1)}$ and also we write x_k instead of $x_{nk}^{(1)}$ etc. The proof is based on the confluent Christoffel-Darboux formula from theorem 2.5.4. It follows from this theorem and the formula for the weights in the quadrature formula that

$$\left(1 - \frac{x_k}{\alpha_n}\right) \varphi_n'(x_k)\varphi_{n-1}(x_k) \left(1 - \frac{x_k}{\alpha_{n-1}}\right) = \frac{E_n}{\lambda_k}. \tag{9.6}$$

First note that for any $x \in I$,

$$\left(1 - \frac{x}{\alpha_n}\right) \left(1 - \frac{x}{\alpha_{n-1}}\right) = \frac{|1 - \beta_n z|^2}{1 + \beta_n^2} \frac{|1 - \beta_{n-1} z|^2}{1 + \beta_{n-1}^2}, \tag{9.7}$$

where $x = J(z)$. Using the formula for φ_n from theorem 9.3.1 and the chain rule for differentiation gives

$$\varphi_n'(x) = \frac{1}{\sqrt{2\pi}} \sqrt{1 - \beta_n^2} \left[\frac{zB_n(z)B_{n-1}(z) + 1}{(z - \beta_n)B_{n-1}(z)}\right]' \frac{2z^2}{z^2 - 1}$$

which, using lemma 9.2.3 and the fact that x_k is a zero of φ_n, can be written as

$$\varphi_n'(x_k) = \frac{1}{2\pi} \sqrt{1 - \beta_n^2} \frac{B_n(z_k)}{(z_k - \beta_n)} \left[1 + 2 \sum_{j=1}^{n-1} P(z_k, \beta_j) + P(z_k, \beta_n)\right] \frac{2z_k^2}{z_k^2 - 1}.$$

(9.8)

It follows from the fact that $z_k B_n(z_k) B_{n-1}(z_k) + 1 = 0$ that

$$\frac{B_n(z_k)}{(z_k - \beta_n)} \left[\frac{z_k B_{n-2}(z_k)}{1 - \beta_{n-1} z_k} + \frac{1}{(z_k - \beta_{n-1}) B_{n-2}(z_k)} \right] = \frac{(z_k^2 - 1)(1 - \beta_n \beta_{n-1})}{z_k^2 |1 - \beta_n z_k|^2 |1 - \beta_{n-1} z_k|^2}$$

which gives

$$\varphi_{n-1}(x_k) \frac{B_n(z_k)}{(z_k - \beta_n)} = \frac{1}{\sqrt{2\pi}} \sqrt{1 - \beta_{n-1}^2} \frac{(z_k^2 - 1)(1 - \beta_n \beta_{n-1})}{z_k^2 |1 - \beta_n z_k|^2 |1 - \beta_{n-1} z_k|^2}.$$

Combining this formula with equations (9.6) - (9.8) and the formula for E_n gives after cancelling terms

$$\lambda_k = 2\pi \left[1 + 2 \sum_{j=1}^{n-1} P(z_k, \beta_j) + P(z_k, \beta_n) \right]^{-1}.$$

Transforming back to x_k and α_j then proves the theorem for the first case. The other two cases are proved in the same way. □

9.7 Convergence of $nk_n(x,x)^{-1}$

In the appendix we discuss the convergence of $nk_n(x,x)^{-1}$ when x is in the support of the measure. We are only able to give a partial solution to the problem for general measures. However, here we show that conjecture A.2.6 is certainly true for the measures discussed in this chapter. For more information on this convergence problem we refer to the appendix. The following theorem is an easy consequence of theorems 9.6.1 and A.2.4.

Theorem 9.7.1. *Assume that μ is an absolutely continuous measure and that the weight function is one of the three cases in* (9.1)*. Furthermore assume that the asymptotic distribution of the poles A is given by a measure ν satisfying the conditions of theorem A.2.4. Then we have*

$$\lim_{n\to\infty} nk_n(x,x)^{-1} = \pi\mu'(x)\sqrt{1-x^2} \left[\int_{\mathbb{R}\setminus I} \frac{\sqrt{1-1/t^2}}{1-x/t} d\nu(t) \right]^{-1}$$

for $x \in [-1,1]$.

Proof. It follows from theorem 9.6.1 that for all three cases the quadrature weights λ_{nk} can be written as (we omit the superscript)

$$\lambda_{nk} = 2\pi\mu'(x_{nk})\sqrt{1-x_{nk}^2}\,(c+g_n(x_{nk}))^{-1} \tag{9.9}$$

where c is a different constant in each case. Putting

$$\lambda_n(x) = n2\pi\mu'(x)\sqrt{1-x^2}\,(c+g_n(x))^{-1}$$

we get from the assumptions of this theorem that

$$\lim_{n\to\infty} \lambda_n(x) = \pi\mu'(x)\sqrt{1-x^2}\left[\int_{\mathbb{R}\setminus I} \frac{\sqrt{1-1/t^2}}{1-x/t} d\nu(t)\right]^{-1}.$$

However, it follows from equation (9.9) that $\lambda_n(x)$ interpolates the function $nk_n(x,x)^{-1}$ in the points $\{x_{nk}\}_{k=1}^n$. Since theorem A.2.4 shows that these points are dense in I and because the functions $\lambda_n(x)$ and $nk_n(x,x)^{-1}$ are continuous on I, this concludes the proof. □

9.8 A rational Fejér rule

Before we move to the examples section, we look at a rational generalization of Fejér's quadrature rule. This is an interpolatory rule with nodes at the Chebyshev points $x_{nk} = \cos((2k-1)\pi/2n)$ which integrates exactly polynomials of degree $n-1$ with respect to the Lebesgue measure. The weights are expressible in closed form, see e.g. [18].

In the rest of this section we assume that all poles are equal to $\alpha > 1$. Our aim is to construct a quadrature formula

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=1}^{n} A_{nk} f(x_{nk})$$

where x_{nk} are the zeros of $\varphi_n^{(1)}(x)$ and which is exact for $f \in \mathcal{L}_{n-1}$. As shown by theorem 4.5.2, there is a close connection between modified moments and interpolatory quadrature formulas, since the weights A_{nk} satisfy

$$A_{nk} = \mathrm{k}_{n-1}(x_{nk})\lambda_{nk}$$

where λ_{nk} are the gaussian weights associated with the nodes x_{nk} and

$$\mathrm{k}_{n-1}(x) = \int_{-1}^{1} k_{n-1}(x,w)dw, \quad k_{n-1}(x,w) = \sum_{k=0}^{n-1} \varphi_k^{(1)}(x)\varphi_k^{(1)}(w).$$

If we denote the modified moments by

$$\nu_k = \int_{-1}^{1} \varphi_k^{(1)}(x)dx, \quad k = 0, 1, \ldots \tag{9.10}$$

then the formula for $\mathrm{k}_{n-1}(x)$ becomes

$$\mathrm{k}_{n-1}(x) = \sum_{k=0}^{n-1} \nu_k \varphi_k^{(1)}(x).$$

Thus, if we can compute the modified moments, we can also compute the interpolatory quadrature rule.

We need the following lemma.

Lemma 9.8.1. *Let $T_k(x)$ denote the k-th Chebyshev polynomial, $T_k(x) = \cos(k \arccos x)$ and fix $\alpha > 1$. Denote by I_{kn} the integrals*

$$I_{kn} = \int_{-1}^{1} \frac{T_k(x)}{(x-\alpha)^n}, \quad k = 0, 1, \ldots, n, \quad n = 0, 1, \ldots$$

then they satisfy the recurrence relation

$$I_{kn} = \frac{2k}{n-1} I_{k-1,n-1} + \frac{k}{k-2} I_{k-2,n} - \frac{2}{(n-1)(k-2)} \left[\frac{(-1)^k}{(-1-\alpha)^{n-1}} - \frac{1}{(1-\alpha)^{n-1}} \right]$$

for $k > 2$. If $k = 0$ we have

$$I_{00} = 2, \quad I_{01} = \log \frac{\alpha - 1}{\alpha + 1}$$
$$I_{0n} = \frac{1}{n-1} \left[\frac{1}{(-1-\alpha)^{n-1}} - \frac{1}{(1-\alpha)^{n-1}} \right], \quad n > 1.$$

For $k = 1$ we have

$$I_{1n} = I_{0,n-1} + \alpha I_{0n}, \quad n \geq 1$$

and for $k = 2$ we have

$$I_{2n} = 2I_{0,n-2} + 4\alpha I_{0,n-1} + (2\alpha^2 - 1)I_{0n}, \quad n \geq 2.$$

Proof. The cases $k = 0, 1, 2$ can easily be verified by direct computation. Therefore, we will only prove the recurrence relation for the case $k > 2$. The proof is based on the observation that the antiderivative of $T_k(x)$ satisfies

$$\int T_k(x)dx = \frac{1}{2} \left(\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1} \right)$$

for $k \geq 2$. Using this relation and integrating by parts gives

$$\begin{aligned} I_{kn} &= \frac{1}{2(x-\alpha)^n}\left(\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1}\right)_{-1}^{1} \\ &\quad + \frac{n}{2}\int_{-1}^{1} \frac{1}{(x-\alpha)^{n+1}}\left(\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1}\right) dx, \quad k \geq 2. \end{aligned}$$

Using the fact that $T_k(1) = 1$ and $T_k(-1) = (-1)^k$ this yields after some computations

$$\begin{aligned} I_{kn} &= \frac{1}{k^2-1}\left[\frac{(-1)^{k+1}}{(-1-\alpha)^n} - \frac{1}{(1-\alpha)^n}\right] \\ &\qquad + \frac{n}{2(k+1)} I_{k+1,n+1} - \frac{n}{2(k-1)} I_{k-1,n+1}, \quad k \geq 2. \end{aligned}$$

Changing the indices from $k+1$ to k and $n+1$ to n then proves the lemma.

□

The next step is to write $\varphi_n^{(1)}(x)$ in a more explicit form. From theorem 9.3.1 we get that

$$\varphi_n^{(1)}(x) = \frac{1}{\sqrt{2\pi}}\sqrt{1-\beta^2}\,\frac{z^{-(n-1)}(z-\beta)^{2n-1} + z^{-n}(1-\beta z)^{2n-1}}{(-2\beta)^n (x-\alpha)^n}. \quad (9.11)$$

If we put

$$z^{-(n-1)}(z-\beta)^{2n-1} = \sum_{k=-(n-1)}^{n} c_k^{(n)} z^k, \quad c_n^{(n)} = 1,$$

then the numerator equals

$$\begin{aligned} z^{-(n-1)}(z-\beta)^{2n-1} + z^{-n}(1-\beta z)^{2n-1} &= \sum_{k=-(n-1)}^{n} c_k^{(n)}(z^k + z^{-k}) \\ &= 2\sum_{k=1}^{n-1}(c_k^{(n)} + c_{-k}^{(n)})T_k(x) + 2(T_n(x) + c_0^{(n)}). \quad (9.12) \end{aligned}$$

To find the coefficients $c_k^{(n)}$ write

$$\begin{aligned} z^{-n}(z-\beta)^{2n+1} &= z^{-1}z^{-(n-1)}(z-\beta)^{2n-1}(z-\beta)^2 \\ &= \sum_{k=-(n-1)}^{n} c_k^{(n)} z^{k-1}(z-\beta)^2 \\ &= \sum_{k=-n}^{n+1} [c_{k-1}^{(n)} - 2\beta c_k^{(n)} + \beta^2 c_{k+1}^{(n)}] z^k \end{aligned}$$

n	$\alpha = 10$	$\alpha = 1.01$
1	$1.2181e-13$	$2.5213e-12$
2	$4.4607e-14$	$1.9261e-12$
3	$1.0193e-11$	$3.2761e-11$
4	$9.3484e-11$	$2.2006e-09$
5	$2.5182e-08$	$4.3359e-07$
6	$1.3044e-07$	$5.0330e-05$
7	$2.8850e-05$	$4.8073e-03$
8	$1.2455e-04$	$2.0750e-01$
9	$2.4680e-02$	$6.4897e+00$
10	$9.7337e-02$	$2.0453e+04$

Table 9.1: Example 9.8.2. Relative error for ν_n.

if we take the convention that $c_k^{(n)} = 0$ for $k \leq -n$ or $k > n$. This yields the recurrence relation

$$c_k^{(n+1)} = c_{k-1}^{(n)} - 2\beta c_k^{(n)} + \beta^2 c_{k+1}^{(n)} \tag{9.13}$$

with the initial conditions $c_0^{(1)} = -\beta$ and $c_1^{(1)} = 1$ (from which it also follows that $c_n^{(n)} = 1$ for all n).

Equations (9.11) - (9.13) together with lemma 9.8.1 provide a method to compute the modified moments ν_k as defined by (9.10). This means that we can compute the rational Fejér rule from the rational Gauss-Chebyshev quadrature formula.

Example 9.8.2. First let us look at the case where α is not close to the boundary. We take $\alpha = 10$ and compute ν_k for $k = 1, \ldots, 10$ with the formulas from this section. Table 9.1 gives the relative error on the modified moments ν_k when working in double precision (the exact values were computed by integrating $\varphi_n^{(i)}(x)$ using a Gauss-Legendre quadrature formula). Note that the error increases rapidly with n.

In the same table we give the relative error for the case where $\alpha = 1.01$. Here the error growth is even worse. It seems that our procedure for computing a rational Fejér rule, although elegant in theory, is not of much practical use. This is just another illustration of the difficulties involved in using modified moments for rational functions.

9.9 Examples

In this last section we look at the numerical computation of the quadrature nodes using the formulas from theorem 9.5.1. Once the nodes are known, the weights are easily computed using the formulas from theorem 9.6.1. First let us show that the functions $f_n(\theta) - (n-c)\theta$ from theorem 9.5.1 are strictly increasing for $0 \leq \theta \leq \pi$. This follows from the fact that

$$\frac{d}{d\theta}\left(\arctan\frac{\sin\theta}{\cos\theta-\beta}\right) = \frac{1-\beta\cos\theta}{1-2\beta\cos\theta+\beta^2} \geq \frac{1}{1+|\beta|} > \frac{1}{2}$$

for $|\beta| < 1$. This means that $f_n'(\theta) - (n-c) > c - 1/2$, which is strictly positive for all three cases. Newton's method for finding zeros works particularly well for monotonous functions, especially if the initial values are not too far from the exact solutions. For the case where the poles tend to a fixed limit with increasing n, we can obtain very accurate initial values (especially for large n), using the asymptotic zero distribution as given by theorem A.2.4. It follows from this theorem that when $\lim_{n\to\infty}\alpha_n = \alpha$ then the zero distribution is given by a measure λ whose derivative is equal to

$$\lambda'(x) = \frac{1}{\pi}\frac{1}{\sqrt{1-x^2}}\frac{\sqrt{1-1/\alpha^2}}{1-x/\alpha}.$$

The zero density on the interval $[-1, x]$ equals

$$t = \int_{-1}^{x}\lambda'(u)du = \frac{1}{\pi}\arcsin\frac{\alpha x-1}{\alpha-x} + \frac{1}{2}.$$

Solving for x gives

$$x = \frac{\alpha\cos(\pi t)+1}{\cos(\pi t)+\alpha} \tag{9.14}$$

so if we take n equally distributed numbers $t_{kn} \in [0,1]$ as

$$t_{kn} = \frac{2k-1}{2n}, \quad k = 1, \ldots, n$$

then we can estimate the zeros x_{kn} by plugging the values t_{kn} into equation (9.14). Note that for $\alpha = \infty$ this gives us exactly the zeros of the Chebyshev polynomial $T_n(x)$. If we use these estimates as initial values in Newton's method, it may be expected that convergence to the exact values takes only a few iterations.

Example 9.9.1. Since the procedure is exactly the same in all three cases, we limit our attention to the first case. In this example we take all poles equal to $\alpha = 1.01$. All computations were done in Matlab. Table 9.2 gives some relevant timings for computing the nodes and weights in an n-point quadrature formula, using Newton's method as explained in this section and solving the generalized eigenvalue problem (GEP) of chapter 4. Note that

n	Newton	GEP
100	$5.64e-03$	$5.77e-01$
200	$3.82e-03$	$2.46e+00$
400	$4.72e-03$	$2.40e+01$
800	$7.76e-03$	$3.10e+02$
1600	$1.14e-02$	$3.05e+03$
3200	$2.19e-02$	-
6400	$7.84e-02$	-
12800	$2.23e-01$	-

Table 9.2: Example 9.9.1. Time (in seconds) to compute nodes and weights.

the first approach is far more efficient than the second one. This can be explained as follows. Because all poles are equal to each other, we can avoid the sums in the formulas from theorems 9.5.1 and 9.6.1. Taking advantage of Matlab's ability for vector operations we can apply Newton's method to all zeros at the same time, which makes this method of order $O(n)$. To solve the GEP, we used Matlab's `polyeig` function, which seems to be of order $O(n^3)$. Taking advantage of the special structure of the GEP in our case, we should probably be able to reduce this to $O(n^2)$ using a suitable implementation. For $n > 1600$ we did not solve the GEP, because this was taking too long.

Example 9.9.2. In this example we take the poles at the even integers, $\alpha_k = 2k$, so they tend to infinity with increasing n. This means that we will take the Chebyshev nodes as initial values in Newton's method. Table 9.3 gives some timings for this example. Now the first procedure is (more or less) of order $O(n^2)$, because we cannot avoid using at least one loop (either to sum over the different α_k's, or to apply Newton's method to each zero separately). If we want to avoid this loop, the storage requirements would become too large (we would have to store an $(n \times n)$-matrix). Of course the complexity of the GEP does not change.

9.10 Conclusion

In this chapter we presented several formulas concerning a rational generalization of the well-known Chebyshev polynomials. These are among the very few orthogonal rational functions that are explicitly known. The main interest lies in the quadrature formulas associated with these ORF, which can be constructed very efficiently (even for large n) in the case where all poles are equal to each other.

n	Newton	GEP
100	$2.24e-01$	$4.85e-01$
200	$3.84e-01$	$3.27e+00$
400	$8.99e-01$	$3.04e+01$
800	$3.93e+00$	$3.34e+02$
1600	$1.47e+01$	$2.91e+03$
3200	$6.08e+01$	-
6400	$2.42e+02$	-
12800	$6.91e+02$	-

Table 9.3: Example 9.9.2. Time (in seconds) to compute nodes and weights.

We note that all the results for $\varphi_n^{(1)}(x)$ could also be deduced in another way. The so-called Malmquist basis is a basis of rational functions orthogonal on the unit circle with respect to the Lebesgue measure. In our notation we would have

$$\phi_n(x) = \frac{zB_{n-1}(z)}{1-\overline{\beta}_n z}\sqrt{1-|\beta_n|^2}$$

for a sequence $B = \{\beta_1, \beta_2, \dots\} \subset \mathbb{D}$. This basis is of particular interest in system theorey, see e.g. [38, 39, 40].

Transforming this basis to the interval $[-1,1]$ using theorem 2.6.1 then immediately gives the first Chebyshev ORF $\varphi_n^{(1)}(x)$. Using the relation between quadrature formulas on I and on $\mathbb{T}$ from chapter 4 we can also obtain the first formula from theorem 9.6.1. However, the other two cases cannot be obtained in this way, which is why we chose to use the approach based on Bernstein-Szegő polynomials.

Chapter 10

Conclusion

10.1 Main contributions

Compared to the polynomial case, the study of orthogonal rational functions is still in a very early stage. In this thesis we have obtained several new results in this field, both theoretical and numerical. Special attention has gone to the case of orthogonality on a finite interval, which is not really covered in the monograph [10]. Some earlier work, preceding this thesis, was reported in [57].

Some of the major theoretical contributions are about the asymptotic behaviour of orthogonal rational functions. Starting from known results about convergence on the unit disc, we were able to find expressions for the limit of the ratio of two succesive orthogonal rational functions, which we used to derive the asymptotic behaviour of the recurrence coefficients. This yielded the rather surprising result that these coefficients asymptotically only depend on the last two or three poles. Strong and weak-star asymptotics were next, where in the latter case we obtained some results about convergence on the unit disc along the way. All the results for the interval reduce to the polynomial situation if we take the poles at infinity, which shows that orthogonal rational functions are indeed a natural generalization of orthogonal polynomials. The results from this chapter appeared in [58] and [59].

Another theoretical contribution is the interpolation algorithm from chapter 5. Although we only hinted at this connection, they are closely related to the Nevanlinna-Pick algorithm for the circle case [10] and to a modified Schur algorithm as described in [41], as well as to continued fractions and multipoint Padé approximants. Although these interpolation algorithms are particularly elegant and simple, they cannot be used to compute the recurrence coefficients in a stable way, as we clearly showed by a detailed error analysis, where we used the asymptotic results obtained before. The research about interpolation algorithms reported in chapter 5 was published in [60] (apart from the last section about a multiple pole, which is from a later date).

The computational aspects of orthogonal rational functions form the other major part of this thesis. Before we started our research, hardly any attention had gone to the accurate and efficient computation of these functions. With the results from chapters 6 and 7 we can consider this problem almost solved. For the case of the interval, the algorithm from chapter 7 works very well for poles not too close to the boundary and combining the asymptotic results from chapter 3 and the quadrature error derived in chapter 4 with our analysis, we were able to provide accurate error estimates. When the poles are close to the boundary, we have solved the problem for some special weight functions, assuming that all poles are equal to each other, using the quadrature formula based on Laurent polynomials. For different weight functions and for poles not all equal to each other, further research needs to be done. Our investigations about the computational aspects of ORF have led to [56], which contains the material from section 4.3 and the first three sections of chapter 7, and to [62], which contains the results from the last section of chapter 7. The latter results were obtained in collaboration with Pablo González Vera during my stay at the Universidad de La Laguna in Tenerife.

We also generalized the well-known method of modified moments from the polynomial case to the rational case, at least when the poles are all equal to each other. The general situation seems to be much more complicated. Furthermore, using the formulas from chapter 8 we can use all the previous methods for the interval case to compute orthogonal rational functions on a halfline as well, so they do not have to be treated as a special case (at least from a computational point of view). The results from this chapter were derived in [55].

The computation of orthogonal rational functions on the unit circle was not studied in this thesis, but in the case where they are needed only to derive quadrature formulas, one can use the relation between formulas on I and on $\mathbb{T}$ as derived in chapter 4.

In the last chapter we introduced a rational generalization of the classical Chebyshev polynomials. Explicit representations were given for the rational functions and their recurrence coefficients (for an arbitrary pole sequence) and we provided a fast and stable way to compute the quadrature formulas associated with them. This chapter is of both theoretical and practical interest. We are preparing a publication to present these results [61].

Finally we would like to mention that all the proofs given in this thesis are ours. Known theorems which we used are given without proof and with clear reference to their source. Some of our own results are also given without proof, when the proof is trivial. This has been indicated in the text.

10.2 Further research

The field of orthogonal rational functions is relatively young and many questions are still open for investigation. Here we recall some of the open problems hinted at throughout the text and we give some new research directions which were not explored in this thesis.

Convergence

The convergence results from chapter 3 only represent a very small fraction of asymptotic behaviour that can be studied. As we mentioned in the conclusion to that chapter, we give two more problems in the appendix which are partially solved. The first one deals with the relative convergence of ORF on the unit circle and on the interval and relies on an erroneously proved theorem of Pan. The second problem is about the convergence of $nk_n(x,x)^{-1}$ for x in the support of the measure. We already studied this in the case study of chapter 9.

In chapter 3 we also mentioned that the question whether convergence results remain valid under looser conditions on the poles depends on the convergence of $\phi_{n,n}(\beta_n)/\phi^*_{n,n}(\beta_n)$. Solving this problem is also important to study the convergence on a halfline, as pointed out in chapter 8. However, asymptotic behaviour on a halfline in its most general form will probably require a very different approach, as for the polynomial case.

Furthermore, little is known about boundary asymptotics. There are some results in [12] but much more can be done. Also the convergence for exponential weights is still open to investigation (which is particularly interesting for the halfline, since most common weights on the halfline are exponential), as are so many other convergence problems which we did not mention here.

Quadrature formulas

The relation between quadrature formulas on the unit circle and on the interval can probably also be used to study rational Gauss-Lobatto and Gauss-Radau formulas, as well as interpolatory rules as in [3, 4]. This could be a straightforward generalization from the polynomial case, but it has not been studied yet.

More important is the study of quadrature formulas which can easily be calculated, like the ones from the last chapter, or which are explicitly known. At the moment, most rational quadrature formulas still require a great computational effort, which is not always compensated by their superior performance for specific integrands. It remains a challenge to find more 'classical' cases, like the Chebyshev and Fejér rule for polynomials.

Also, it would be interesting to see if our quadrature formulas can be used to compute Cauchy principal value integrals, as the formulas presented by Gautschi in [22].

Computational aspects

The computation of ORF with arbitrary measure and poles very close to the boundary has not been solved completely. The last part of chapter 7 suggests that this will probably depend on the discovery of easily generated quadrature formulas for integrands with poles close to the interval of integration.

Another problem is the computation of the modified moments from chapter 6. As for the polynomial case, this technique can only be used when the moments are explicitly known or when they can easily be generated. However, much more explicit examples are known for the polynomial case than for the rational case. In fact this is one of the most poignant problems in the field of orthogonal rational functions: the need for more 'classical' cases. We believe that the case study in chapter 9 is an important step in this direction.

Moment problems

The problem of moments is a subject which was not discussed in this thesis, but which is closely related to the convergence of quadrature formulas and density problems. Orthogonal rational functions naturally give rise to so-called *extended* moment problems, where the moments of the measure are given in distinct points (the poles), as in chapter 6. Solutions of these extended moment problems have been studied for several cases, such as the extended Hamburger moment problem in [41]. However, extended Hausdorff moment problems (on an interval) have thus far not been studied, but this would be a natural consequence of our investigations in rational functions orthogonal on an interval.

10.3 Acknowledgements

The results from the last section of chapter 7 were obtained in collaboration with Pablo González Vera during my stay at the Universidad de La Laguna in Tenerife, as well as the results in the last two sections of chapter 4, most of chapter 9 and section A.2.

Appendix A

Open problems in asymptotic behaviour

A.1 Relative convergence

In this section we prove some theorems about the relative convergence of orthogonal polynomials with respect to varying measures and orthogonal rational functions. The proofs are based on a theorem by Pan [42, Theorem 2.1.]. However, as pointed out to us by G. López Lagomasino, there is an error in the proof of this theorem. On page 338, the second inequality following “Then, from (3.5), we have” is based on a variant of Fatou's lemma for the lim sup of a sequence of functions (the original lemma is for the lim inf). This application is not justified here, because for this variant of Fatou's lemma one needs domination by an integrable function (as for Lebesgue's dominated convergence theorem). So far, the error has not been fixed and no valid proof has been found, but it is suspected that the theorem remains true. Therefore, we will present it here as a conjecture.

Conjecture A.1.1. *Let p_n denote the orthonormal Szegő-polynomials with respect to $\mathring{\mu}$, i.e. $\langle p_n , p_m \rangle_{\mathring{\mu}} = \delta_{nm}$ where δ_{nm} is the Kronecker delta. Assume that $\mathring{\mu}' > 0$ a.e. and that B is compactly included in $\mathbb{D}$. Then we have*

$$\lim_{n\to\infty} \frac{p_n^*(z)w_m^*(z)}{\phi_{m,n+m}^*(z)} = 1$$

locally uniformly in $z \in \mathbb{D}$ and uniformly in $m \in \mathbb{N}$.

Following exactly the same reasoning as Pan did and with the aid of [32, Lemma 1] and [14, Theorem 2] we can “prove” the following result.

Of course, the proof suffers from the same problem we mentioned before (illegitimate use of a variant of Fatou's lemma), so we can merely present it as a conjecture. However, since the reasoning is exactly the same in both conjectures, proving one would most likely also prove the other.

Conjecture A.1.2. *Assume that $\mathring{\mu}' > 0$ a.e. and that the sequence B is compactly included in $\mathbb{D}$. Then we have for every integer k*

$$\lim_{n\to\infty} \frac{\phi^*_{n,n+k}(z)}{\phi^*_{n,n+k+m}(z)} = 1,$$

locally uniformly in $z \in \mathbb{D}$ and uniformly in $m \in \mathbb{N}$.

Using these two conjectures we can obtain relative convergence results for the varying orthogonal polynomials and the orthogonal rational functions. We will also use the following theorem which can be found in [26].

Theorem A.1.3. *Assume that $\mathring{\mu}' > 0$ a.e. and that B is compactly included in $\mathbb{D}$. Let h be a nonnegative $d\mathring{\mu}/|w_n|^2$-integrable function for each $n \in \mathbb{N}$ and assume that there exists a polynomial Q such that $Q(e^{\mathbf{i}\theta})h(\theta)$ and $Q(e^{\mathbf{i}\theta})h^{-1}(\theta)$ are Riemann-integrable. Let $\phi_{n,n+k}$ denote the orthogonal polynomials with respect to $d\mathring{\mu}/|w_n|^2$ and $\psi_{n,n+k}$ the orthogonal polynomials with respect to $hd\mathring{\mu}/|w_n|^2$. Then we have*

$$\lim_{n\to\infty} \frac{\psi^*_{n,n+k}(z)}{\phi^*_{n,n+k}(z)} = \sigma(h^{-1}, z)$$

locally uniformly in $\mathbb{D}$.

We now give the most important theorem based on the previous conjectures. It is an extension to the case $\mu' > 0$ a.e. of a well known result from [33].

Theorem A.1.4. *Assume that both conjectures A.1.1 and A.1.2 are true and that $\mathring{\mu}' > 0$ a.e. Let $B = \{\beta_1, \beta_2, \ldots\}$ and $\tilde{B} = \{\tilde{\beta}_1, \tilde{\beta}_2, \ldots\}$ be two sequences of complex numbers, both compactly included in $\mathbb{D}$ and let w_n and $\tilde{w}_n$ be the associated polynomials. Let h be a function satisfying the conditions of theorem A.1.3 with $\tilde{B}$. Then if $\phi_{n,n+k}$ and $\tilde{\phi}_{n,n+k}$ denote the orthogonal polynomials with respect to $d\mathring{\mu}/|w_n|^2$ and $hd\mathring{\mu}/|\tilde{w}_n|^2$ respectively, we have for every integer k*

$$\lim_{n\to\infty} \frac{\tilde{\phi}^*_{n,n+k}(z)/\tilde{w}^*_n(z)}{\phi^*_{n,n+k}(z)/w^*_n(z)} = \sigma(h^{-1}, z)$$

locally uniformly in $\mathbb{D}$.

Proof. Let $\psi_{n,n+k}$ denote the polynomials orthogonal with respect to the measure $d\mathring{\mu}/|\tilde{w}_n|^2$ and p_n as before the orthogonal polynomials with respect to $d\mathring{\mu}$. Then write

$$\begin{aligned}\frac{\tilde{\phi}^*_{n,n+k}(z)/\tilde{w}^*_n(z)}{\phi^*_{n,n+k}(z)/w^*_n(z)} &= \frac{\tilde{\phi}^*_{n,n+k}(z)}{\psi^*_{n,n+k}(z)} \times \frac{\psi^*_{n,n+k}(z)}{\psi^*_{n,2n+k}(z)} \times \frac{\psi^*_{n,2n+k}(z)}{p^*_{n+k}(z)\tilde{w}^*_n(z)} \\ &\times \frac{p^*_{n+k}(z)w^*_n(z)}{\phi^*_{n,2n+k}(z)} \times \frac{\phi^*_{n,2n+k}(z)}{\phi^*_{n,n+k}(z)}.\end{aligned}$$

Taking limits on both sides and using A.1.1, A.1.2 and A.1.3 we find that the first factor in the right hand side tends to $\sigma(h^{-1}, z)$ with n while the other factors tend to one. This proves the theorem. □

Using this theorem and lemma 2.4.1 we can study the relative convergence of rational functions orthogonal on the unit circle.

Theorem A.1.5. *Assume that both conjectures A.1.1 and A.1.2 are true and that $\mathring{\mu}' > 0$ a.e. Let B, $\tilde{B}$ and h be as in theorem A.1.4. Denote by $\{\phi_n\}$ the orthogonal rational functions associated with $(B, d\mathring{\mu})$ and by $\{\tilde{\phi}_n\}$ those associated with $(\tilde{B}, hd\mathring{\mu})$. Then locally uniformly in $\mathbb{D}$*

$$\lim_{n\to\infty} \frac{\tilde{\epsilon}_n \tilde{\phi}^*_n(z)(1-\overline{\tilde{\beta}}_n z)\sqrt{1-|\beta_n|^2}}{\epsilon_n \phi^*_n(z)(1-\overline{\beta}_n z)\sqrt{1-|\tilde{\beta}_n|^2}} = \sigma(h^{-1}, z)$$

where $\epsilon_n = |\phi^*_n(0)|/\phi^*_n(0)$ (an analogous definition holds for $\tilde{\epsilon}_n$).

Proof. First use lemma 2.4.1 and the definition of the superstar transform for polynomials to write

$$g^*_n(z) = \frac{\phi^*_{n,n}(z)}{1-\overline{\beta}_n z}\frac{\overline{\tau}_n}{\nu_{n,n}}\left(1-\overline{\beta}_n z\frac{\overline{\phi_{n,n}(\beta_n)}}{\phi^*_{n,n}(\beta_n)}\frac{\phi_{n,n}(z)}{\phi^*_{n,n}(z)}\right)$$

where g_n is the numerator of $\phi_n = g_n/w^*_n$ (recall that $\nu_{n,n} > 0$). Using (2.1), theorem 3.2.1 and the fact that $\phi^*_n(0) = \eta_n \overline{\tau}_n$ this can be transformed into

$$\phi^*_n(z) \sim \overline{\epsilon}_n \left|\frac{\phi^*_n(0)}{\phi^*_{n,n}(0)}\right| \frac{\phi^*_{n,n}(z)}{w^*_n(z)} \frac{1}{1-\overline{\beta}_n z}$$

(in the sense that the ratio of left hand side and right hand side tends to one as n tends to infinity). The result now follows from theorem A.1.4 and lemma 3.6.2. □

Using the relations from section 2.6 we easily obtain the relative convergence for orthogonal rational functions on I, as given in the last theorem in this section.

Theorem A.1.6. *Assume that both conjectures A.1.1 and A.1.2 are true and that* $\mu' > 0$ *a.e. Let* $A \subset \overline{\mathbb{R}}^I$ *and* $\tilde{A} \subset \overline{\mathbb{R}}^I$ *be two sequences bounded away from* I*. Let* h *be a nonnegative* $d\mu/\pi_n$*-integrable function for each* $n \in \mathbb{N}$ *and assume there exists a polynomial* Q *such that* $Q(e^{\mathbf{i}\theta})h(\cos\theta)$ *and* $Q(e^{\mathbf{i}\theta})h^{-1}(\cos\theta)$ *are Riemann-integrable on* $[0, 2\pi)$*. Denote by* $\{\varphi_n\}$ *the orthogonal rational functions associated with* (A, μ) *and by* $\{\tilde{\varphi}_n\}$ *those associated with* $(\tilde{A}, hd\mu)$*. Then locally uniformly in* $\overline{\mathbb{C}}^I$

$$\lim_{n\to\infty} \frac{\tilde{c}_n \tilde{\varphi}_n(x) \tilde{B}_n(z)(1 - \tilde{\beta}_n z)\sqrt{1 - \beta_n^2}}{c_n \varphi_n(x) B_n(z)(1 - \beta_n z)\sqrt{1 - \tilde{\beta}_n^2}} = \sigma(\tilde{h}^{-1}, z)$$

where $\tilde{h}(\theta) = h(\cos\theta)$*,* $z = J^{-1}(x)$*,* $\beta_k = J^{-1}(\alpha_k)$ *for all* k*,* $B_n(z)$ *is the Blaschke product associated with* $\{\beta_1, \ldots, \beta_n\}$ *and* $c_n = \pm 1$ *is such that the normalization* $E_n > 0$ *holds. Similar definitions hold for the expressions with a tilde.*

Proof. If $x \in I$ and $z = J^{-1}(x)$ then $(1 - x/\tilde{\alpha}_k) = |1 - \tilde{\beta}_k z|^2/(1 + \tilde{\beta}_k^2)$. This means that

$$\pi_n(x) = a_n |\tilde{w}_n(z)|^2$$

where $\tilde{w}_n$ is as in theorem A.1.4 and a_n is a constant depending on n. Using equation (2.5) it then follows that $\tilde{h}$ is $d\mathring{\mu}/|\tilde{w}_n|^2$-integrable. Then use theorems 3.2.2, A.1.5 and 2.6.1 to find that

$$\lim_{n\to\infty} \frac{\tilde{\epsilon}_{2n} \tilde{\delta}_n \tilde{\varphi}_n(x) \tilde{B}_n(z)(1 - \tilde{\beta}_n z)\sqrt{1 - \beta_n^2}}{\epsilon_{2n} \delta_n \varphi_n(x) B_n(z)(1 - \beta_n z)\sqrt{1 - \tilde{\beta}_n^2}} = \sigma(\tilde{h}^{-1}, z).$$

The unimodular constants are all real, which proves the theorem. □

A.2 Convergence of $nk_n(x,x)^{-1}$

In a celebrated article of Máté, Nevai and Totik [35], the authors show (among other things) that the kernel function for orthogonal polynomials on the interval $[-1, 1]$ satisfies

$$\lim_{n\to\infty} nk_n(x,x)^{-1} = \pi\mu'(x)\sqrt{1 - x^2}, \quad x \text{ a.e. in } I \tag{A.1}$$

under the condition that μ satisfies Szegő's condition. This property has not yet been generalized to the rational case, but in [6] the authors conjecture that equation (A.1) still holds true if k_n is the kernel function for orthogonal rational functions on I,

$$k_n(x,y) = \sum_{k=0}^{n} \varphi_k(x)\overline{\varphi_k(y)}.$$

It is our aim to show that this cannot be so without some modifications and we give a partial solution to the problem. Before we proceed, several measure theoretic results are needed. The following theorem can be found in [50, p. 55]. It says basically that, under certain conditions, measurable functions can be approximated arbitrarily close by continuous functions. We rephrase it according to our discussion.

Theorem A.2.1 (Lusin's Theorem). *Suppose f is a complex measurable function on I, μ a positive bounded Borel measure on I and $\epsilon > 0$. Then there exists a $g \in C(I)$ such that*

$$\mu(\{x : f(x) \neq g(x)\}) < \epsilon,$$

where $C(I)$ denotes the class of continuous functions on I. Furthermore, we may arrange it so that

$$\sup_{x\in I} |g(x)| \leq \sup_{x\in I} |f(x)|. \tag{A.2}$$

We will also use a theorem about absolute continuity of measures. Again we refer to [50, p. 124] for the proof. In the rest of this section it will be convenient to write $\lambda \ll \mu$ to mean that λ is absolutely continuous with respect to μ.

Theorem A.2.2. *Suppose μ and λ are measures on a σ-algebra $\mathfrak{M}$, μ is positive, and λ is complex. Then the following two conditions are equivalent:*

(a) $\lambda \ll \mu$

(b) To every $\epsilon > 0$ corresponds a $\delta > 0$ such that $|\lambda(E)| < \epsilon$ for all $E \in \mathfrak{M}$ with $\mu(E) < \delta$.

Using these two theorems we can prove a lemma which will be needed in the sequel.

Lemma A.2.3. *Let μ_1, μ_2 and m be positive bounded Borel measures on I such that $\mu_1 \ll m$ and $\mu_2 \ll m$, satisfying*

$$\int_I f d\mu_1 = \int_I f d\mu_2$$

for every $f \in C(I)$. Then we have

$$\mu_1 = \mu_2$$

from which it also follows that $\mu_1' = \mu_2'$ a.e. $[m]$.

Proof. Take $\epsilon_1 > 0$ arbitrarily small and let $\delta_1 > 0$ be as in theorem A.2.2 applied to μ_1 and m. Do the same for μ_2, yielding ϵ_2 and δ_2. Then take $\epsilon_3 > 0$ such that $\epsilon_3 < \min\{\delta_1, \delta_2\}$.

Now let $E \subset I$ be an arbitrary Borel measurable set in I. Then its characteristic function χ_E is obviously a measurable function. Take a function $f \in C(I)$ such that

$$m(\{x : \chi_E(x) \neq f(x)\}) = m(A) < \epsilon_3$$

(this can always be done according to theorem A.2.1).

Then we have

$$\begin{aligned}\mu_1(E) &= \int_I \chi_E d\mu_1 \\ &= \int_A \chi_E d\mu_1 + \int_{I \setminus A} f d\mu_1\end{aligned}$$

and this gives, using the fact that $\int_I f d\mu_1 = \int_I f d\mu_2$,

$$\begin{aligned}\mu_1(E) &= \int_I f d\mu_2 + \int_A (\chi_E - f) d\mu_1 \\ &= \mu_2(E) + \int_A (\chi_E - f) d\mu_1 - \int_A (\chi_E - f) d\mu_2.\end{aligned}$$

Because of (A.2) we know that $|f| \leq 1$ so that we may write

$$\mu_1(E) \leq \mu_2(E) + 2\mu_1(A) + 2\mu_2(A)$$

and because $\epsilon_3 < \min\{\delta_1, \delta_2\}$ this can be written as

$$\mu_1(E) < \mu_2(E) + 2\epsilon_1 + 2\epsilon_2$$

and since ϵ_1 and ϵ_2 are arbitrarily small, this gives $\mu_1(E) \leq \mu_2(E)$. In the same way we obtain $\mu_2(E) \leq \mu_1(E)$, proving that $\mu_1(E) = \mu_2(E)$. Because E was an arbitrary Borel measurable subset of I, this proves the lemma. □

To prove the main result in this section, we also need a theorem from [53] about the zero distribution of the φ_n, which in our notation translates as follows.

Theorem A.2.4. *Let μ be absolutely continuous, satisfying the Erdős-Turán condition $\mu' > 0$ a.e. and suppose that the asymptotic distribution of the poles A is given by a measure ν on $\overline{\mathbb{R}} \setminus I$, i.e. for every continuous function f on $\overline{\mathbb{R}} \setminus I$ which vanishes at infinity we have*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} f(\alpha_j) = \int_{\overline{\mathbb{R}}\setminus I} f(x) d\nu(x).$$

If $\nu = p\delta_\infty + (1-p)\nu_0$, where δ_∞ is a unit measure with all its mass concentrated at infinity and $0 \le p \le 1$, and

$$\int_{\mathbb{R}\setminus I} \log|t| d\nu_0(t) < \infty, \tag{A.3}$$

then the asymptotic distribution of the zeros of φ_n is given by the measure

$$\lambda = p\lambda_0 + (1-p)\lambda_b,$$

where λ_0 is the arcsin measure on I with weight function

$$\lambda_0'(x) = \frac{1}{\pi} \frac{1}{\sqrt{1-x^2}}$$

and λ_b is an absolutely continuous measure on I with weight function

$$\lambda_b'(x) = \frac{1}{\pi} \frac{1}{\sqrt{1-x^2}} \int_{\mathbb{R}\setminus I} \frac{\sqrt{1-1/t^2}}{1-x/t} d\nu_0(t).$$

Remark. Note that condition (A.3) is always satisfied for an asymptotically periodic pole sequence, since in this case ν is a discrete measure whose support is a finite set.

We are now in a position to prove a partial result, concerning the convergence of $nk_n(x,x)^{-1}$ for $x \in I$, as given in the following theorem.

Theorem A.2.5. *Let μ be absolutely continuous (with respect to the Lebesgue measure on I), satisfying $\mu' > 0$ a.e. and assume that A is bounded away from I and satisfies condition* (A.3). *Assume furthermore that*

$$\lim_{n\to\infty} nk_n(x,x)^{-1} = k(x)$$

uniformly on I. Then we must have

$$k(x) = \pi\mu'(x)\sqrt{1-x^2} \left[\int_{\mathbb{R}\setminus I} \frac{\sqrt{1-1/t^2}}{1-x/t} d\nu(t) \right]^{-1}, \quad x \text{ a.e. in } I$$

where the notation is as in A.2.4.

Proof. As before, let $\{x_{nk}\}_{k=1}^n$ denote the zeros of $\varphi_n(x)$ and λ the corresponding zero distribution. Then we have for every continuous function f on I

$$\lim_{n\to\infty} \frac{1}{n}\sum_{k=1}^{n} f(x_{nk}) = \int_{-1}^{1} f(x)d\lambda(x). \tag{A.4}$$

Since A is bounded away from I, the poles certainly satisfy the conditions of theorem 4.3.3, so if λ_{nk} are the weights in the quadrature formula discussed in chapter 4, we also have for every $f \in C(I)$,

$$\lim_{n\to\infty} \sum_{k=1}^{n} \lambda_{nk} f(x_{nk}) = \int_{-1}^{1} f(x)d\mu(x). \tag{A.5}$$

It follows from the formulas in chapter 4 that

$$\lambda_{nk} = k_n(x_{nk}, x_{nk})^{-1}$$

so we may rewrite (A.5) as

$$\lim_{n\to\infty} \frac{1}{n}\sum_{k=1}^{n} [nk_n(x_{nk}, x_{nk})^{-1}] f(x_{nk}) = \int_{-1}^{1} f(x)d\mu(x).$$

Because of (A.4) and using the fact that the k_n converge uniformly on I, we then have

$$\int_{-1}^{1} f(x)d\mu(x) = \int_{-1}^{1} k(x)f(x)d\lambda(x)$$

for every continuous f on I. It follows from lemma A.2.3 that

$$\mu'(x) = k(x)\lambda'(x), \quad x \text{ a.e. in } I.$$

because $nk_n(x,x)^{-1}$ is positive for every n. We may use theorem A.2.4 to complete the proof (note that the two terms in λ' can be combined into one expression). □

Of course, this is only a partial result: we have obtained an expression for the limit function $k(x)$ *whenever* $nk_n(x,x)^{-1}$ *converges*. The actual convergence still has to be proven. Looking at the polynomial situation, it is reasonable to assume that uniform convergence is not necessary and that μ does not have to be absolutely continuous. However, the polynomial theorem is proved for measures satisfying Szegő's condition (although some remarks are given in [35] for measures satisfying a weaker condition). There is no reason to assume that the rational case is different in this respect, which leads us to the following conjecture.

Conjecture A.2.6. *Assume that μ satisfies Szegő's condition and that A is bounded away from I and satisfies condition* (A.3)*. Then we have*

$$\lim_{n\to\infty} nk_n(x,x)^{-1} = \pi\mu'(x)\sqrt{1-x^2}\left[\int_{\mathbb{R}\setminus I} \frac{\sqrt{1-1/t^2}}{1-x/t}d\nu(t)\right]^{-1}, \quad x \text{ a.e. in } I$$

As in the polynomial case, the proof will probably proceed along very different lines than the proof of theorem A.2.5. It may very well be that condition (A.3) is not necessary, since in the polynomial case, no reference is made to the zero distribution of the orthogonal polynomials to prove the theorem. Further research needs to be done here, but a straightforward generalization of the proof from [35] seems to be impossible.

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Curriculum Vitae

Onderwijs- en onderzoeksloopbaan

- 30/06/2000
  Burgerlijk Ingenieur in de Computerwetenschappen, K.U.Leuven
  geslaagd met grote onderscheiding

- 01/09/2000-31/12/2000
  Assistentenmandaat K.U.Leuven
  Numerieke Approximatie en Lineaire Algebra Groep, K.U.Leuven

- 01/01/2001-31/12/2004
  Onderzoeksbursaal IWT
  Numerieke Approximatie en Lineaire Algebra Groep, K.U.Leuven

Buitenlandse verblijven

- 06/09/1998 - 02/07/1999
  Erasmusverblijf aan de Universidad del País Vasco, San Sebastián, Spanje

- 07/09/2003 - 19/12/2003
  Studieverblijf aan het Departamento de Análisis Matemático, Universidad de La Laguna, Tenerife, Spanje

Publicaties

- J. Van Deun en A. Bultheel, Orthogonal Rational Functions on an Interval, Department of Computer Science, K.U.Leuven, Report TW322, Leuven, Belgium, 2001.

- J. Van Deun en A. Bultheel, Ratio Asymptotics for Orthogonal Rational Functions on the Interval $[-1, 1]$, Department of Computer Science, K.U.Leuven, Report TW332, Leuven, Belgium, 2001.
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