On the convergence of quasi-Random Sampling Importance Resampling

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Outline

- 1 Introduction
- 2 Quasi-Monte Carlo tools
- 3 The SIR and QSIR algorithm
- 4 Numerical Example
- 5 Conclusions

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The problem

The problem we study is ...

- ... the generation of samples from a given probability density function (PDF)

$$f(\boldsymbol{\theta}) = \frac{h(\boldsymbol{\theta})}{\int_{\mathbb{R}^s} h(\boldsymbol{\theta}) d\boldsymbol{\theta}}.$$

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$$f(\boldsymbol{\theta}) = \frac{h(\boldsymbol{\theta})}{\int_{\mathbb{R}^s} h(\boldsymbol{\theta}) d\boldsymbol{\theta}}.$$

- However, we do not know the normalizing constant:

$$\int_{\mathbb{R}^s} h(\boldsymbol{\theta}) d\boldsymbol{\theta} = ?$$

Generation of samples: normalized PDF

If the normalizing constant is known, one can use for example the inverse CDF method ...

Generation of samples: normalized PDF

...or other well-known methods from the literature. See for example

Generation of samples: normalizing constant unknown

Things become more complicated if the normalizing constant is not known:

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How can we do this?

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How can we do this?

- Sampling Importance Resampling (SIR)
[Rubin, D. B., 1988]

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- Sampling Importance Resampling (SIR)
[Rubin, D. B., 1988]
- **Quasi-Random** Sampling Importance Resampling (QSIR)
[Pérez et al., 2005]

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[Rubin, D. B., 1988]
- **Quasi-Random** Sampling Importance Resampling (QSIR)
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⇒ We will take a closer look at QSIR...

But let's not rush and start with the start. . .

We need some quasi-Monte Carlo ideas and concepts.

Let's take a look at them. . .

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Koksma-Hlawka inequality

Theorem (Koksma-Hlawka)

$$\left| \frac{1}{N} \sum_{n=1}^N f(\mathbf{x}_n) - \int_{[0,1]^s} f(\mathbf{x}) d\mathbf{x} \right| \leq V_{HK}(f) D_N^*(\mathcal{P})$$

- Well-known among MC and QMC-people.
- No further explanation needed here.

Discrepancy

Definition (Star-discrepancy of a point set $\mathcal{P}$)

$$D_N^*(\mathcal{P}) := \sup_{\mathbf{x} \in [0,1]^s} \left| \frac{1}{N} \sum_{n=1}^N I_{[0,\mathbf{x})}(\mathbf{x}_n) - \text{Vol}(\mathbf{x}) \right|$$

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Discrepancy in one-dimension

Theorem

For a *one-dimensional ordered* point set $\mathcal{P}$, we have

$$D_N^*(\mathcal{P}) = \frac{1}{2N} + \max_{1 \leq n \leq N} \left| x_n - \frac{2n-1}{2N} \right|.$$

- This is for *one-dimensional* point sets.
- The point set must be *ordered*.

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Corollary

In *one dimension*, the point set

$$x_i = \frac{2i-1}{2N}, \quad i = 1, \dots, N$$

has the lowest possible discrepancy of $\frac{1}{2N}$.

Our goal

So far our first QMC-steps...

Let us now try to formalize what we are trying to accomplish:

- We are given ...

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Let us now try to formalize what we are trying to accomplish:

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 - ... where each point can have an *associated weight*.

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- We ask ourselves the questions:

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So far our first QMC-steps...

Let us now try to formalize what we are trying to accomplish:

- We are given ...
 - ... a *multidimensional* point set,
 - ... where each point can have an *associated weight*.
- We ask ourselves the questions:
 - How representative is this point set for a certain cumulative distribution function (CDF)?

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So far our first QMC-steps. . .

Let us now try to formalize what we are trying to accomplish:

- We are given . . .
 - . . . a *multidimensional* point set,
 - . . . where each point can have an *associated weight*.
- We ask ourselves the questions:
 - How representative is this point set for a certain cumulative distribution function (CDF)?
 - How do we measure ‘representativeness’ of a point set?

Measuring 'representativeness'

We use the following definition for the Empirical Cumulative Distribution Function (ECDF):

- If **weights** are specified:

$$F_N(\mathbf{x}) := \sum_{i=1}^N q_i I_{(-\infty, \mathbf{x}]}(\mathbf{x}_i) \quad \text{with } q_i > 0 \text{ and } \sum_{i=1}^N q_i = 1.$$

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- If **no weights** are specified, assume all weights **uniform**:

$$F_N(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N l_{(-\infty, \mathbf{x}]}(\mathbf{x}_i).$$

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We speak of F -discrepancy. . .

- . . . of a **point set**,
- . . . with respect to F .

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In one dimension: Kolmogorov-Smirnov statistic

cdf-rep-points

What set of points is the best representation for $F(\mathbf{x})$?

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Definition (cdf-rep-points, [Wang & Fang, 1990])

A point set $\mathcal{P}^* = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ for which

$$D_N^*(\mathcal{P}^*, F) = \min_{\mathcal{P}} D_N^*(\mathcal{P}, F),$$

is called a set of *cdf-rep-points* of $F(\mathbf{x})$.

Koksma-Hlawka: a variant

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Koksma-Hlawka: a variant

- Note that the Koksma-Hlawka inequality is traditionally given over the unit s -dimensional hypercube.
- The following variant is over $\mathbb{R}^s$ [Chelson, 1976]:

$$\left| \frac{1}{N} \sum_{n=1}^N f(\mathbf{x}_n) - \int_{\mathbb{R}^s} f(\mathbf{x}) dG(\mathbf{x}) \right| \leq V_{HK}(f) D_N^*(\mathcal{P}, G).$$

$\Rightarrow$ This variant seems less cited and used by MC and QMC-people!

Discrepancy-preserving transformation

- Let $\mathcal{A} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ be a point set in $[0, 1]^s$.
- Let G be a multivariate CDF having independent marginals:

$$G(\mathbf{x}) = G(x_1, \dots, x_s) = \prod_{i=1}^s G_i(x_i).$$

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Lemma

If we take $\mathcal{B} = \{\mathbf{y}_1, \dots, \mathbf{y}_N\}$ as

$$\mathbf{y}_k = (G_1^{-1}(x_{k,1}), \dots, G_s^{-1}(x_{k,s})), \quad k = 1, \dots, N,$$

then $D_N^*(\mathcal{B}, G) = D_N^*(\mathcal{A})$.

Discrepancy-preserving transformation

Corollary

Let $F(x)$ be a *univariate continuous* CDF. Then the set

$$\mathcal{Z} = \{z_i = F^{-1}\left(\frac{2i-1}{2N}\right), i = 1, \dots, N\},$$

contains the cdf-rep-points of size N of $F(x)$ with $D_N^*(\mathcal{Z}, F)$ optimal and equal to $\frac{1}{2N}$.

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Let $F(x)$ be a *univariate continuous* CDF. Then the set

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contains the cdf-rep-points of size N of $F(x)$ with $D_N^*(\mathcal{Z}, F)$ optimal and equal to $\frac{1}{2N}$.

- How about the *discrete* case?
- Let's first review *multinomial resampling*...

Multinomial Resampling

What do we have?

An ECDF $F_N(\theta)$ formed by the samples $\theta_1, \dots, \theta_N$ and their respective weights $q_1, \dots, q_N$.

Multinomial Resampling

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What do we want?

n new samples from this distribution (with weights $\frac{1}{n}$).

Multinomial Resampling: 1 dimension

In one dimension, this is easy:

Multinomial Resampling: more than 1 dimension

In more than one dimension, work with the **indices**:

Multinomial resampling

Note that

- we start from **one-dimensional points** in $[0, 1]$.
- the new samples are all given the same weight $\frac{1}{n}$.
- the new samples of course also have an ECDF.

$\Rightarrow$ Denote this new ECDF by $F_{N,n}(\theta)$.

Multinomial resampling

What about

$$\sup_{\theta \in \mathbb{R}^s} |F_N(\theta) - F_{N,n}(\theta)|?$$

$\Rightarrow$ need to make distinction between 'ordered' and 'unordered' points.

Ordered vs. unordered points

The points:

(a) Ordered

(b) Unordered

Ordered vs. unordered points

The ECDF's:

(c) Ordered

(d) Unordered

Ordered vs. unordered points

Having noticed the difference between

ordered vs. unordered

multidimensional point sets, what can we then say about

$$\sup_{\boldsymbol{\theta} \in \mathbb{R}^s} |F_N(\boldsymbol{\theta}) - F_{N,n}(\boldsymbol{\theta})|$$

if we use the *one-dimensional* point set

$$\mathcal{Z} = \left\{ z_i = \frac{2i-1}{2n}, i = 1, \dots, n \right\}$$

for the multinomial resampling?

Ordered points

Let $F_N(\boldsymbol{\theta})$ be the ECDF of the **ordered** s -dimensional points $\mathbf{x}_1 \leq \mathbf{x}_2 \leq \cdots \leq \mathbf{x}_N$ with their respective weights q_i .

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Theorem

If we use the point set

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for the multinomial resampling, then

$$\sup_{\boldsymbol{\theta} \in \mathbb{R}^s} |F_N(\boldsymbol{\theta}) - F_{N,n}(\boldsymbol{\theta})| < \frac{1}{2n}.$$

Ordered points

One-dimensional example: always ordered!

Unordered points

Let $F_N(\boldsymbol{\theta})$ be the ECDF of the **unordered** s -dimensional points $\mathbf{x}_1 \leq \mathbf{x}_2 \leq \cdots \leq \mathbf{x}_N$ with their respective weights q_i .

Unordered points

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If we use the point set

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for the multinomial resampling, then

$$\sup_{\boldsymbol{\theta} \in \mathbb{R}^s} |F_N(\boldsymbol{\theta}) - F_{N,n}(\boldsymbol{\theta})| < \frac{N}{n}.$$

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SIR

Remember the problem:

$$f(\boldsymbol{\theta}) = \frac{h(\boldsymbol{\theta})}{\int_{\mathbb{R}^s} h(\boldsymbol{\theta}) d\boldsymbol{\theta}}$$

A possible solution:

- SIR = Sampling Importance Resampling [Rubin, D. B., 1988].
- Also sometimes called 'Importance Resampling' or 'weighted bootstrap'.

SIR-Algorithm

Algorithm (SIR-Algorithm)

- 1 Choose a proposal distribution with density g .

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$$\omega_i = \frac{h(\theta_i)}{g(\theta_i)} \xrightarrow{\text{normalize}} q_i = \frac{\omega_i}{\sum_{i=1}^N \omega_i}, \quad \text{for } i = 1, \dots, N.$$

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- 4 generate n samples θ^* from the ECDF of $\{\theta_1, \dots, \theta_N\}$ with mass q_i at θ_i .

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We then have

$$\theta^* \sim f(\theta).$$

Restriction

For the rest of the talk, G is a multivariate CDF having independent marginals:

$$G(\mathbf{x}) = G(x_1, \dots, x_s) = \prod_{i=1}^s G_i(x_i),$$

QSIR

QSIR = Quasi-random Sampling Importance Resampling
[Pérez et al., 2005]

- *Two* modifications of the original SIR
- Based on Quasi-Monte Carlo ideas
- Empirically verified to be better:
 - samples have smaller F -discrepancy
 - samples are thus 'more representative'

QSIR: Algorithm 1

The first modification:

Algorithm (QSIR 1)

- 1 Generate a *quasi-random* sample $\theta_1, \dots, \theta_N$ from the density g .

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⇒ quasi-randomness in the first (sample) step.

⇒ randomness in the last (resample) step.

QSIR: Algorithm 2

The second modification:

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- 4 Use $\{u_1, \dots, u_n\}$ to obtain a sample of size n from the the ECDF which places mass q_i at θ_i .

⇒ quasi-randomness in both *sample* and *resample* step.

⇒ completely deterministic!

Algorithm 1 and 2: convergence after first step

For the **first step** of both algorithms,

- we start from a QMC-point set $\mathcal{L}$ on $[0, 1]^s$ of size N with star discrepancy $D_N^*(\mathcal{L})$.
- G is assumed to define a discrepancy-preserving transformation.

Therefore...

Algorithm 1 and 2: convergence after first step

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Therefore...

Theorem (G -discrepancy after step 1)

The G -discrepancy of the samples $\mathcal{P} = \{\theta_1, \dots, \theta_N\}$ has the value $D_N^(\mathcal{L})$.*

Algorithm 1 and 2: convergence after first step (1D)

In **one** dimension, since both algorithms start from

$$\mathcal{L} = \left\{ \frac{2i-1}{2N}, i = 1, \dots, N \right\}$$

with best possible discrepancy $\frac{1}{2N}$, we have...

Algorithm 1 and 2: convergence after first step (1D)

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with best possible discrepancy $\frac{1}{2N}$, we have...

Corollary (G-discrepancy after step 1 in one dimension)

The G-discrepancy of the samples θ_i will have the optimal value $\frac{1}{2N}$.

Algorithm 1: convergence after second step

After the second step (the multinomial **random** resampling) we have

Theorem (Algorithm 1)

$$\sup_{\boldsymbol{\theta} \in \mathbb{R}^s} |F(\boldsymbol{\theta}) - F_{N,n}(\boldsymbol{\theta})| \in \mathcal{O} \left(\max \left(\kappa(N), \frac{1}{\sqrt{n}} \right) \right).$$

with

$$\kappa(N) = \begin{cases} \frac{1}{N} & \text{if } s = 1, \\ \frac{(\log(N))^s}{N} & \text{if } s > 1. \end{cases}$$

Algorithm 2: convergence after second step

After the second step (the multinomial **deterministic** resampling) we have

Theorem (Algorithm 2)

$$\sup_{\theta \in \mathbb{R}^s} |F_{N,n}(\theta) - F(\theta)| \leq \tau(N, n) + \mathcal{O}(\kappa(N)).$$

with

$$\tau(N, n) = \begin{cases} \frac{1}{2n} & \text{if } s = 1, \\ \frac{N}{n} & \text{if } s > 1. \end{cases}$$

and

$$\kappa(N) = \begin{cases} \frac{1}{N} & \text{if } s = 1, \\ \frac{(\log(N))^s}{N} & \text{if } s > 1. \end{cases}$$

Convergence summarized

Summarized:

		$s = 1$	$s > 1$
Alg. 1	ordered	$\mathcal{O}\left(\max\left(\frac{1}{N}, \frac{1}{\sqrt{n}}\right)\right)$	$\mathcal{O}\left(\max\left(\frac{(\log N)^s}{N}, \frac{1}{\sqrt{n}}\right)\right)$
	unordered	/	$\mathcal{O}\left(\max\left(\frac{(\log N)^s}{N}, \frac{1}{\sqrt{n}}\right)\right)$
Alg. 2	ordered	$\frac{1}{2n} + \mathcal{O}\left(\frac{1}{N}\right)$	$\frac{1}{2n} + \mathcal{O}\left(\frac{(\log N)^s}{N}\right)$
	unordered	/	$\frac{N}{n} + \mathcal{O}\left(\frac{(\log N)^s}{N}\right)$

$\Rightarrow$ relative sizes of n and N matter!

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Numerical example

Take g as the standard Cauchy distribution

$$g(x) = \frac{1}{\pi(1+x^2)}$$

and f the t -distribution with two degrees of freedom

$$f(x) = \frac{\Gamma(3/2)}{\sqrt{2\pi}\Gamma(1)} \left(1 + \frac{x^2}{2}\right)^{-3/2}.$$

Numerical example

f is already normalized, so $f = h$ and we have

$$\frac{h(x)}{g(x)} = \frac{\pi}{2\sqrt{2}}(1+x^2) \left(1 + \frac{x^2}{2}\right)^{-3/2}$$

Numerical example: Algorithm 1

$$\sup_{\theta \in \mathbb{R}^s} |F_{N,n}(\theta) - F(\theta)| \in \mathcal{O} \left(\max \left(\frac{1}{N}, \frac{1}{\sqrt{n}} \right) \right)$$

(e) fixed N

(f) fixed n

Numerical example: Algorithm 2

$$\sup_{\theta \in \mathbb{R}^s} |F_{N,n}(\theta) - F(\theta)| \leq \mathcal{O}\left(\frac{1}{N}\right) + \frac{1}{2n}$$

(g) fixed N

(h) fixed n

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- Our analysis explains empirical results from [Pérez et al., 2005].
- Asymptotic error convergence results for QSIR.
- In **one** dimension, if $N = n$, then Algorithm 1 is $\mathcal{O}(1/\sqrt{N})$ and Algorithm 2 is $\mathcal{O}(1/N)$.
- The order of convergence depends on s , N , and n and their relative sizes influence the usefulness of the bounds (F -discrepancy is never larger than 1).

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- Instead of a QMC-point set for step 1, one could use $\{u_i = \frac{2i-1}{2n}\}$ for each dimension...

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- The order of convergence depends on s , N , and n and their relative sizes influence the usefulness of the bounds (F -discrepancy is never larger than 1).
- Instead of a QMC-point set for step 1, one could use $\{u_i = \frac{2i-1}{2n}\}$ for each dimension...
 - Disadvantage: the term $\mathcal{O}\left(\frac{(\log N)^s}{N}\right)$ becomes worse.

Conclusions

- Our analysis explains empirical results from [Pérez et al., 2005].
- Asymptotic error convergence results for QSIR.
- In **one** dimension, if $N = n$, then Algorithm 1 is $\mathcal{O}(1/\sqrt{N})$ and Algorithm 2 is $\mathcal{O}(1/N)$.
- The order of convergence depends on s , N , and n and their relative sizes influence the usefulness of the bounds (F -discrepancy is never larger than 1).
- Instead of a QMC-point set for step 1, one could use $\{u_i = \frac{2i-1}{2n}\}$ for each dimension...
 - Disadvantage: the term $\mathcal{O}\left(\frac{(\log N)^s}{N}\right)$ becomes worse.
 - Advantage: the samples will be ordered, so for Algorithm 2, the term $\frac{N}{n}$ can be replaced by $\frac{1}{2n}$.

Thank you for your attention!

Questions? Suggestions?

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