

Density estimation by Monte Carlo and randomized quasi-Monte Carlo (RQMC)

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Joint work with **Amal Ben Abdellah, Art B. Owen, and Florian Puchhammer**



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What this talk is about

Monte Carlo (MC) simulation is widely used to estimate the expectation $\mathbb{E}[X]$ of a random variable X and compute a confidence interval on $\mathbb{E}[X]$. $\text{MSE} = \text{Var}[\bar{X}_n] = \mathcal{O}(n^{-1})$.

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But simulation usually provides information to do much more! The output data can be used to estimate the entire distribution of X , e.g., the cumulative distribution function (cdf) F of X , defined by $F(x) = \mathbb{P}[X \leq x]$, or its density f defined by $f(x) = F'(x)$.

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If X_1, \dots, X_n are n indep. realizations of X , the empirical cdf

$$\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{I}[X_i \leq x]$$

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For a continuous r.v. X , the density f provides a better visual idea of the distribution.

Here we focus on estimating f over $[a, b] \subset \mathbb{R}$.

Setting

Classical **density estimation** was developed in the context where independent observations X_1, \dots, X_n of X are **given** and one wishes to estimate the **density** f of X from that.

Best rate: $\text{Var}[\hat{f}_n(x)] = \mathcal{O}(n^{-4/5})$.

Here we assume that X_1, \dots, X_n are **generated by simulation** from a stochastic model. We can choose n and we have some freedom on how the simulation is performed.

The X_i 's are realizations of a random variable $X = g(\mathbf{U}) \in \mathbb{R}$ with density f , where $\mathbf{U} = (U_1, \dots, U_s) \sim U(0, 1)^s$ and $g(\mathbf{u})$ can be computed easily for any $\mathbf{u} \in (0, 1)^s$.

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1. Can we obtain a better estimate of f with **RQMC instead of MC**? How much better?

What about taking a **stratified sample** over $[0, 1)^s$?

2. Is it possible to obtain **unbiased density estimators** that converge as $\mathcal{O}(n^{-1})$ or faster, using clever sampling strategies?

Small example: A stochastic activity network

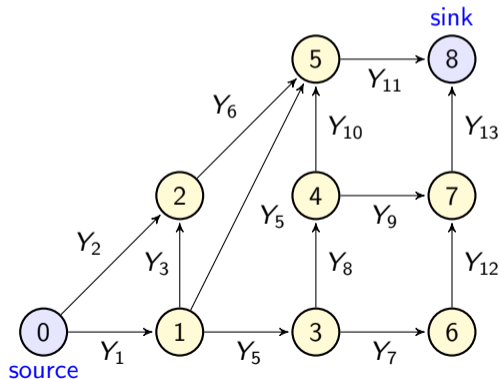
Gives precedence relations between activities. Activity k has random duration Y_k (also length of arc k) with known cdf $F_k(y) := \mathbb{P}[Y_k \leq y]$.

Project duration X = (random) length of longest path from source to sink.

Can look at deterministic equivalent of X , $\mathbb{E}[X]$, cdf, density, ...

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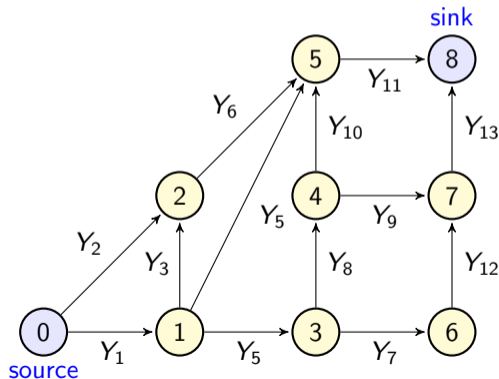
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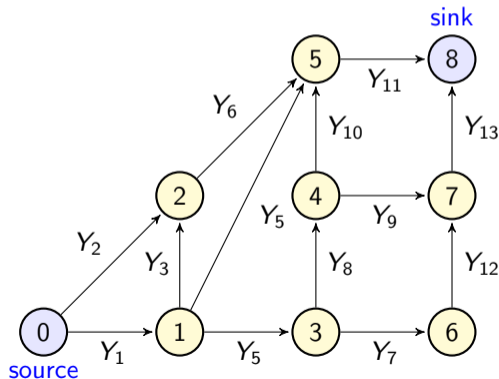
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The sample derivative $\hat{F}'_n(x)$ is **useless** to estimate $f(x)$, because it is 0 almost everywhere.

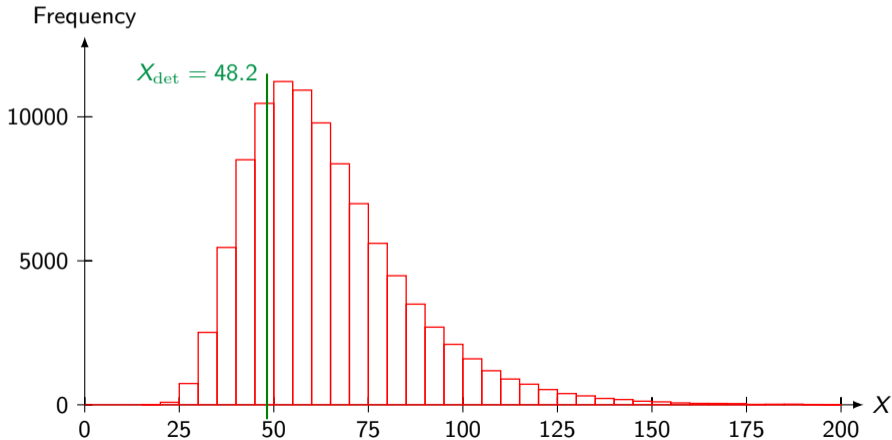


Numerical illustration from Elmaghraby (1977):

$Y_k \sim N(\mu_k, \sigma_k^2)$ for $k = 1, 2, 4, 11, 12$, and $Y_k \sim \text{Expon}(1/\mu_k)$ otherwise.

μ_1, \dots, μ_{13} : 13.0, 5.5, 7.0, 5.2, 16.5, 14.7, 10.3, 6.0, 4.0, 20.0, 3.2, 3.2, 16.5.

Results of an experiment with $n = 100\,000$. Note: X is not normal!

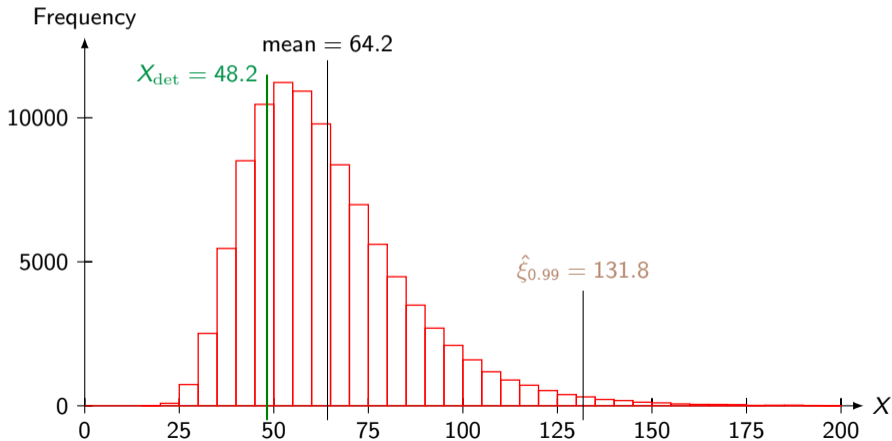


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Density Estimation

Suppose we estimate the density f over a finite interval $[a, b]$.

Let $\hat{f}_n(x)$ denote the density estimator at x , with sample size n .

We use the following measures of error:

$$\text{MISE} = \text{mean integrated squared error} = \int_a^b \mathbb{E}[(\hat{f}_n(x) - f(x))^2] dx$$

$$= \text{IV} + \text{ISB}$$

$$\text{IV} = \text{integrated variance} = \int_a^b \text{Var}[\hat{f}_n(x)] dx$$

$$\text{ISB} = \text{integrated squared bias} = \int_a^b (\mathbb{E}[\hat{f}_n(x)] - f(x))^2 dx$$

To minimize the MISE, we need to balance the IV and ISB.

Density Estimation

Simple **histogram**: Partition $[a, b]$ in m intervals of size $h = (b - a)/m$ and define

$$\hat{f}_n(x) = \frac{n_j}{nh} \text{ for } x \in I_j = [a + (j - 1)h, a + jh), \quad j = 1, \dots, m$$

where n_j is the number of observations X_i that fall in interval j .

Kernel Density Estimator (KDE) : Select kernel k (unimodal symmetric density centered at 0) and **bandwidth** $h > 0$ (horizontal stretching factor for the kernel). The KDE is

$$\hat{f}_n(x) = \frac{1}{nh} \sum_{i=1}^n k\left(\frac{x - X_i}{h}\right) = \frac{1}{nh} \sum_{i=1}^n k\left(\frac{x - g(\mathbf{U}_i)}{h}\right).$$

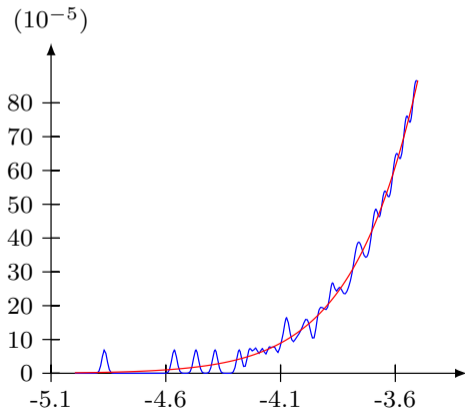
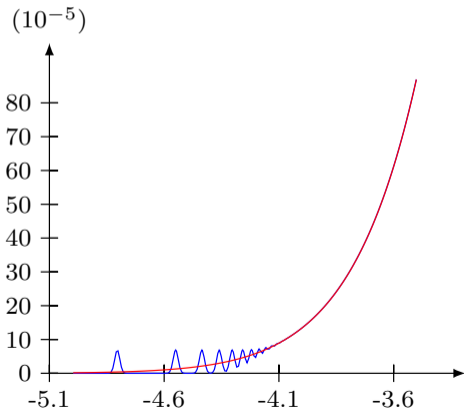
Example of a KDE in $s = 1$ dimension

KDE (blue) vs true density (red) with $n = 2^{19}$:

Here we take U_1, \dots, U_n in $(0, 1)$ and put $X_i = F^{-1}(U_i)$.

midpoint rule (left)

stratified sample of $U = F(X)$ (right).



Asymptotic convergence with Monte Carlo for smooth f

Here we assume independent random samples (Monte Carlo or given data).

For histograms and KDEs, when $n \rightarrow \infty$ and $h \rightarrow 0$:

$$\text{AMISE} = \text{AIV} + \text{AISB} \sim \frac{C}{nh} + Bh^\alpha.$$

For any $g : \mathbb{R} \rightarrow \mathbb{R}$, define

$$R(g) = \int_a^b (g(x))^2 dx, \quad \mu_r(g) = \int_{-\infty}^{\infty} x^r g(x) dx, \quad \text{for } r = 0, 1, 2, \dots$$

	C	B	α
Histogram	1	$R(f') / 12$	2
KDE	$\mu_0(k^2)$	$(\mu_2(k))^2 R(f'') / 4$	4

The asymptotically optimal h is

$$h^* = \left(\frac{C}{B\alpha n} \right)^{1/(\alpha+1)}$$

and it gives $\text{AMISE} = Kn^{-\alpha/(1+\alpha)}$.

	C	B	α	h^*	AMISE
Histogram	1	$\frac{R(f')}{12}$	2	$(nR(f')/6)^{-1/3}$	$\mathcal{O}(n^{-2/3})$
KDE	$\mu_0(k^2)$	$\frac{(\mu_2(k))^2 R(f'')}{4}$	4	$\left(\frac{\mu_0(k^2)}{(\mu_2(k))^2 R(f'') n} \right)^{1/5}$	$\mathcal{O}(n^{-4/5})$

To estimate h^* , one can estimate $R(f')$ and $R(f'')$ via KDE (plugin).

This is true under the simplifying assumption that h must be the same all over $[a, b]$.

Can we take the stochastic derivative of an estimator of F ?

Can we estimate the density $f(x) = F'(x)$ by the derivative of an estimator of $F(x)$.

A simple candidate cdf estimator is the empirical cdf

$$\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{I}[X_i \leq x].$$

However $d\hat{F}_n(x)/dx = 0$ almost everywhere, so this cannot be a useful density estimator!

We need a smoother estimator of F .

Conditional Monte Carlo (CMC) for Derivative Estimation

Idea: Replace indicator $\mathbb{I}[X_i \leq x]$ by its conditional cdf given filtered information:

$$F(x | \mathcal{G}) \stackrel{\text{def}}{=} \mathbb{P}[X \leq x | \mathcal{G}]$$

where the sigma-field \mathcal{G} contains not enough information to reveal X but enough to compute $F(x | \mathcal{G})$, and is chosen so that the following holds:

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Assumption 1. For all realizations of \mathcal{G} , $F(x | \mathcal{G})$ is a continuous function of x over $[a, b]$, differentiable except perhaps over a denumerable set of points $D(\mathcal{G}) \subset [a, b]$, and for which $F'(x | \mathcal{G}) = dF(x | \mathcal{G})/dx$ (when it exists) is bounded uniformly in x by a random variable Γ such that $\mathbb{E}[\Gamma^2] \leq K_\gamma < \infty$.

Theorem 1: Under Ass. 1, for $x \in [a, b]$, $\mathbb{E}[F'(x | \mathcal{G})] = f(x)$ and $\text{Var}[F'(x | \mathcal{G})] < K_\gamma$.

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Conditional density estimator (CDE) with sample size n : $\hat{f}_{\text{cde},n}(x) = \frac{1}{n} \sum_{i=1}^n F'(x | \mathcal{G}^{(i)})$

where $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(n)}$ are n independent “realizations” of \mathcal{G} . $\text{Var}[\hat{f}_{\text{cde},n}(x)] = \mathcal{O}(n^{-1})$.

Example 1. A sum of independent random variables

$X = Y_1 + \cdots + Y_d$, where the Y_j are independent and continuous with cdf F_j and density f_j , and \mathcal{G} is defined by hiding Y_k for an arbitrary k :

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We have

$$F(x | \mathcal{G}_k) = \mathbb{P}[X \leq x | S_{-k}] = \mathbb{P}[Y_k \leq x - S_{-k}] = F_k(x - S_{-k}).$$

Continuous and differentiable if Y_k has a density.

The density estimator for X becomes $F'(x | \mathcal{G}_k) = f_k(x - S_{-k})$. Shifted density of Y_k .

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Example 2: generalization

Let $X = h(Y_1, \dots, Y_d)$ and define \mathcal{G}_k again by erasing a continuous Y_k ;
 $\mathcal{G}_k = (Y_1, \dots, Y_{k-1}, Y_{k+1}, \dots, Y_d)$.

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If $k = 3$, since $X \leq x$ if and only if $Y_3 \geq (Y_1 + Y_2^2)/x$,
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If $k = 2$, then $F(x | \mathcal{G}_2) = \mathbb{P}(X \leq x | Y_1, Y_3) = \mathbb{P}(|Y_2| \leq (Y_3x - Y_1)^{1/2}) = F_2(Z) - F_2(-Z)$
 where $Z = (Y_3x - Y_1)^{1/2}$, and the density estimator at x is
 $F'(x | \mathcal{G}_2) = (f_2(Z) + f_2(-Z))dZ/dx = (f_2(Z) - f_2(-Z))Y_3/(2Z)$.

This second estimator can have a huge variance if Z can take values near 0; this shows that a good choice of k can be crucial in general.

Example 3: discontinuity issues

Let $X = \max(Y_1, Y_2)$ where Y_1 and Y_2 are independent and continuous. With $\mathcal{G} = \mathcal{G}_2$ (we hide Y_2):

$$\mathbb{P}[X \leq x \mid Y_1 = y] = \begin{cases} \mathbb{P}[Y_2 \leq x \mid Y_1 = y] = F_2(x) & \text{if } x \geq y; \\ 0 & \text{if } x < y. \end{cases}$$

If $F_2(y) > 0$, this function is discontinuous at $x = y$, so Assumption 1 does not hold. The method does not work in this case.

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Same problem if $X = \min(Y_1, Y_2)$. With $\mathcal{G} = \mathcal{G}_2$, we have

$$\mathbb{P}[X \leq x \mid Y_1 = y) = \begin{cases} F_2(x) & \text{if } x < y; \\ 1 & \text{if } x \geq y. \end{cases}$$

If $F_2(y) < 1$, this function is also discontinuous at $x = y$.

Elementary quasi-Monte Carlo (QMC) Bounds (Recall)

Integration error for $g : [0, 1]^s \rightarrow \mathbb{R}$ with point set $P_n = \{\mathbf{u}_0, \dots, \mathbf{u}_{n-1}\} \subset [0, 1]^s$:

$$E_n = \frac{1}{n} \sum_{i=0}^{n-1} g(\mathbf{u}_i) - \int_{[0,1]^s} g(\mathbf{u}) d\mathbf{u}.$$

Koksma-Hlawka inequality: $|E_n| \leq V_{\text{HK}}(g) D^*(P_n)$ where

$$V_{\text{HK}}(g) = \sum_{\emptyset \neq \mathbf{v} \subseteq \mathcal{S}} \int_{[0,1]^s} \left| \frac{\partial^{|\mathbf{v}|} g}{\partial \mathbf{v}}(\mathbf{u}) \right| d\mathbf{u}, \quad (\text{Hardy-Krause (HK) variation})$$

$$D^*(P_n) = \sup_{\mathbf{u} \in [0,1]^s} \left| \text{vol}[\mathbf{0}, \mathbf{u}] - \frac{|P_n \cap [\mathbf{0}, \mathbf{u}]|}{n} \right| \quad (\text{star-discrepancy}).$$

There are explicit point sets for which $D^*(P_n) = \mathcal{O}(n^{-1}(\log n)^{s-1}) = \mathcal{O}(n^{-1+\epsilon})$, $\forall \epsilon > 0$.

Explicit RQMC constructions for which $\mathbb{E}[E_n] = 0$ and $\text{Var}[E_n] = \mathcal{O}(n^{-2+\epsilon})$, $\forall \epsilon > 0$.

With ordinary Monte Carlo (MC), one has $\text{Var}[E_n] = \mathcal{O}(n^{-1})$.

Bounding the AIV under RQMC for a KDE

KDE density estimator at a single point x :

$$\hat{f}_n(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h} k\left(\frac{x - g(\mathbf{U}_i)}{h}\right) = \frac{1}{n} \sum_{i=1}^n \tilde{g}(\mathbf{U}_i).$$

With RQMC points \mathbf{U}_i , this is an RQMC estimator of $\mathbb{E}[\tilde{g}(\mathbf{U})] = \int_{[0,1]^s} \tilde{g}(\mathbf{u}) d\mathbf{u} = \mathbb{E}[\hat{f}_n(x)]$.

RQMC **does not change the bias**, but **may reduce** $\text{Var}[\hat{f}_n(x)]$, and then the IV.

To get RQMC variance bounds, we need **bounds on the variation of \tilde{g}** .

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We assume they exist and are uniformly bounded. E.g., Gaussian kernel k .

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We assume they exist and are uniformly bounded. E.g., Gaussian kernel k .

By expanding via the chain rule, we obtain terms in h^{-j} for $j = 2, \dots, |\mathbf{v}| + 1$.

The term for $\mathbf{v} = \mathcal{S}$ grows as $h^{-s-1} k^{(s)}((g(\mathbf{u}) - x)/h) \prod_{j=1}^s g_j(\mathbf{u}) = \mathcal{O}(h^{-s-1})$ when $h \rightarrow 0$.

An AIV upper bound that we were able to prove

Assumptions. Let $g : [0, 1]^s \rightarrow \mathbb{R}$ be **piecewise monotone** in each coordinate u_j when the other coordinates are fixed, with at most M_j pieces. Assume that all first-order partial derivatives of g are continuous and that $\|g_{\mathfrak{w}_1} g_{\mathfrak{w}_2} \cdots g_{\mathfrak{w}_\ell}\|_1 < \infty$ for all selections of non-empty, mutually disjoint index sets $\mathfrak{w}_1, \dots, \mathfrak{w}_\ell \subseteq \mathcal{S} = \{1, \dots, s\}$.

For each $j \in \mathcal{S}$, let $G_j = \left\| \prod_{\ell \in \mathcal{S} \setminus \{j\}} g_{\{\ell\}} \right\|_1$ and $c_j = M_j \|k^{(s)}\|_\infty (G_j + \mathbb{I}(s=2) \|g_{\{1,2\}}\|_1)$.

Proposition Then the Hardy-Krause variation of \tilde{g} satisfies

$$V_{\text{HK}}(\tilde{g}) \leq c_j h^{-s} + \mathcal{O}(h^{-s+1}) \quad \text{for each } j.$$

Corollary. With RQMC point sets having $D^*(P_n) = \mathcal{O}(n^{-1+\epsilon})$ for all $\epsilon > 0$ when $n \rightarrow \infty$, using KH and squaring gives the bound

$$\text{AIV} = \mathcal{O}(n^{-2+\epsilon} h^{-2s}) \quad \text{for all } \epsilon > 0.$$

By picking h to minimize the AMISE bound, we obtain $\text{AMISE} = \mathcal{O}(n^{-4/(2+s)+\epsilon})$.

Worst than MC when $s \geq 4$. The factor h^{-2s} hurts! **But this is only an upper bound.**

Stratification of the unit cube, for the KDE

Partition $[0, 1]^s$ into $n = b^s$ congruent cubic cells $S_{\mathbf{i}} := \prod_{j=1}^s [i_j/b, (i_j + 1)/b)$ for $\mathbf{i} = (i_1, i_2, \dots, i_s)$, $0 \leq i_j < b$ for each j , for some $b \geq 2$.

Construct $P_n = \{\mathbf{U}_1, \dots, \mathbf{U}_n\}$ by sampling one point uniformly in each subcube $S_{\mathbf{i}}$, independently, and put $X_i = g(\mathbf{U}_i)$ for $i = 1, \dots, n$.

Proposition. The IV of a KDE under stratification never exceeds the IV of the same estimator under MC.

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Proposition. Suppose g is monotone. Then the KDE obtained from those points has

$$\text{IV} \leq (b - a)s \cdot k^2(0) \cdot h^{-2} n^{-(s+1)/s}.$$

Corollary. By taking $h = \kappa n^{-(s+1)/(6s)}$, one has $\text{AMISE} = \mathcal{O}(n^{-(2/3)(s+1)/s})$.

This bound has a better rate than MC for $s < 5$ and same rate for $s = 5$.

The factor h^{-2} in the IV bound hurts, but much less than h^{-2s} .

Applying RQMC to the CDE

To apply RQMC to the CDE, we must be able to write the density estimator as a function of $\mathbf{u} \in [0, 1)^s$:

$$\begin{aligned}F(x | \mathcal{G}) &= \tilde{g}(x, \mathbf{u}), \\F'(x | \mathcal{G}) &= \tilde{g}'(x, \mathbf{u}) = d\tilde{g}(x, \mathbf{u})/dx\end{aligned}$$

for some $\tilde{g} : [a, b] \times [0, 1)^s$ for which $\tilde{g}'(x, \cdot)$ has bounded HK variation for each x .

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CDE sample: $\tilde{g}'(x, \mathbf{U}_1), \dots, \tilde{g}'(x, \mathbf{U}_n)$ where $\{\mathbf{U}_1, \dots, \mathbf{U}_n\}$ is an RQMC point set over $[0, 1)^s$.

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If $\tilde{g}'(x, \cdot)$ has **unbounded variation**, RQMC may still reduce the IV, but there is no guarantee.

Example: sum of independent random variables

$X = Y_1 + \dots + Y_d$, where the Y_j are independent and continuous with cdf F_j and density f_j , and \mathcal{G} is defined by hiding Y_k for an arbitrary k :

$$\mathcal{G}_k = S_{-k} \stackrel{\text{def}}{=} Y_1 + \dots + Y_k + \dots + Y_d = F_1^{-1}(U_1) + \dots + F_k^{-1}(U_k) + \dots + F_d^{-1}(U_d).$$

We have $\tilde{g}(x, \cdot) = F(x | \mathcal{G}_k) = F_k(x - S_{-k})$
and the density estimator is $\tilde{g}'(x, \mathbf{U}) = F'(x | \mathcal{G}_k) = f_k(x - S_{-k})$ where $\mathbf{U} = (U_1, \dots, U_d)$.

If $\tilde{g}'(x, \cdot)$ has bounded HK variation, then $\text{MISE} = \mathcal{O}(n^{-2+\epsilon})$.

Experimental setting for numerical experiments

We tested the methods on some examples. For each n considered, we compute the KDE or CDE with n samples, evaluate it at a set of n_e evaluation points over $[a, b]$, repeat this n_r times, compute the variance at each evaluation point, and estimate the IV.

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We repeat this for $n = 2^{14}, \dots, 2^{19}$ and fit the model $\text{MISE} = \kappa n^{-\nu}$ by linear regression: $\log_2 \text{MISE} \approx \log_2 \kappa - \nu \log_2 n$. We report $\hat{\nu}$ and also the MISE for $n = 2^{19}$.

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MC and RQMC Point sets:

- ▶ MC: Independent points,
- ▶ Strat: stratification,
- ▶ Lat+s: lattice rule with a random shift modulo 1,
- ▶ Lat+s+b: lattice rule with a random shift modulo 1 + baker's transformation,
- ▶ LMS: Sobol' points with left matrix scrambling (LMS) + digital random shift.

Displacement of a cantilever beam (Bingham 2017)

Displacement X of a cantilever beam with horizontal load Y_2 and vertical load Y_3 :

$$X = h(Y_1, Y_2, Y_3) = \frac{\kappa}{Y_1} \sqrt{\frac{Y_2^2}{w^4} + \frac{Y_3^2}{t^4}}$$

where $\kappa = 5 \times 10^5$, $w = 4$, $t = 2$, Y_1, Y_2, Y_3 independent normal, $Y_j \sim \mathcal{N}(\mu_j, \sigma_j^2)$,

Description	Symbol	μ_j	σ_j
Young's modulus	Y_1	2.9×10^7	1.45×10^6
Horizontal load	Y_2	500	100
Vertical load	Y_3	1000	100

The goal is to estimate the density of X over $[3.1707, 5.6675]$, which covers about 99% of the density (it clips 0.5% on each side).

Using RQMC with CMC

Conditioning on $\mathcal{G}_1 = \{Y_2, Y_3\}$ means **hiding** Y_1 . We have

$$X = \frac{\kappa}{Y_1} \sqrt{\frac{Y_2^2}{w^4} + \frac{Y_3^2}{t^4}} \leq x \quad \text{if and only if} \quad Y_1 \geq \frac{\kappa}{x} \sqrt{\frac{Y_2^2}{w^4} + \frac{Y_3^2}{t^4}} \stackrel{\text{def}}{=} W_1(x).$$

For $x > 0$,

$$F(x | \mathcal{G}_1) = \mathbb{P}[Y_1 \geq W_1(x) | \mathcal{G}_1] = 1 - \Phi((W_1(x) - \mu_1)/\sigma_1)$$

and

$$F'(x | \mathcal{G}_1) = -\frac{\phi((W_1(x) - \mu_1)/\sigma_1) W_1'(x)}{\sigma_1} = \frac{\phi((W_1(x) - \mu_1)/\sigma_1) W_1(x)}{x\sigma_1}.$$

Suppose we condition on $\mathcal{G}_2 = \{Y_1, Y_3\}$ instead, i.e., hide Y_2 . We have

$$X \leq x \quad \text{if and only if} \quad Y_2^2 \leq w^4 \left((xY_1/\kappa)^2 - Y_3^2/t^4 \right) \stackrel{\text{def}}{=} W_2.$$

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If $W_2 \leq 0$, then $F'(x | \mathcal{G}_2) = 0$. If $W_2 > 0$,

$$F(x | \mathcal{G}_2) = \mathbb{P}[-\sqrt{W_2} \leq Y_2 \leq \sqrt{W_2} | W_2] = \Phi((\sqrt{W_2} - \mu_2)/\sigma_2) - \Phi(-(\sqrt{W_2} + \mu_2)/\sigma_2)$$

and

$$F'(x | \mathcal{G}_2) = \frac{\phi((\sqrt{W_2} - \mu_2)/\sigma_2) + \phi(-(\sqrt{W_2} + \mu_2)/\sigma_2)}{w^4 x (Y_1/\kappa)^2 / (\sigma_2 \sqrt{W_2})} > 0.$$

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For conditioning on \mathcal{G}_3 , the analysis is the same as for \mathcal{G}_2 , by symmetry, and we get

$$F'(x | \mathcal{G}_3) = \frac{\phi((\sqrt{W_3} - \mu_3)/\sigma_3) + \phi(-(\sqrt{W_3} + \mu_3)/\sigma_3)}{t^4 x (Y_1/\kappa)^2 / (\sigma_3 \sqrt{W_3})} > 0.$$

for $W_3 > 0$, where W_3 is defined in a similar way as W_2 .

Instead of choosing a single conditioning k , we can take a convex combination:

$$\hat{f}(x) = \alpha_1 F'(x | \mathcal{G}_1) + \alpha_2 F'(x | \mathcal{G}_2) + \alpha_3 F'(x | \mathcal{G}_3),$$

where $\alpha_1 + \alpha_2 + \alpha_3 = 1$. This is equivalent to taking $F'(x | \mathcal{G}_1)$ as the main estimator and the other two as **control variates (CV)**. We can use CV theory to optimize the α_j 's.

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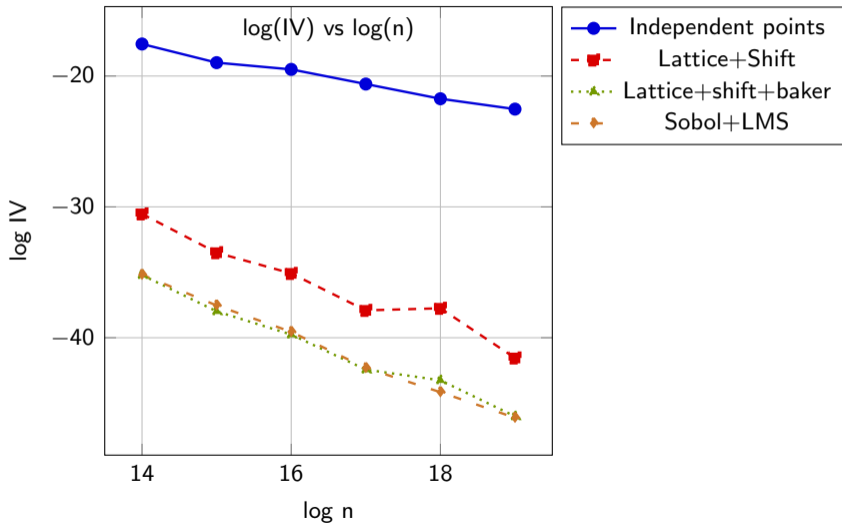
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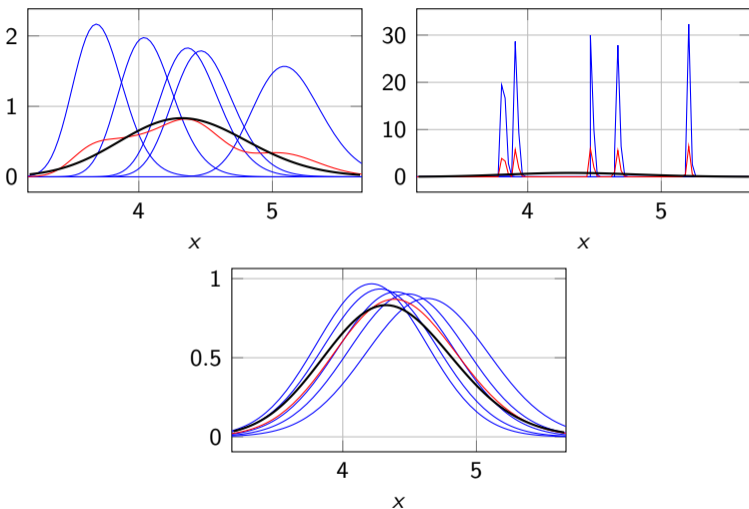
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	\hat{v}					$-\log_2 \text{MISE} (n = 2^{19})$				
	KDE	\mathcal{G}_1	\mathcal{G}_2	\mathcal{G}_3	comb.	KDE	\mathcal{G}_1	\mathcal{G}_2	\mathcal{G}_3	comb.
MC	0.80	0.97	0.98	0.99	0.98	14.7	19.3	14.5	22.8	22.5
stratif.	0.90					17.4				
Lat+s	—	2.06	2.82	2.04	2.02	—	38.9	25.4	41.5	41.5
Lat+s+b	—	2.26	2.55	1.98	2.07	—	44.3	23.3	45.5	46.0
Sob+LMS	0.96	2.21	2.03	2.21	2.21	20.5	44.0	23.6	45.7	46.1

For $n = 2^{19}$, the MISE is about $2^{-14.7}$ for the usual KDE+MC and 2^{-46} for the new CDE+RQMC; i.e., **MISE is divided by more than $2^{31} \approx 2$ millions.**

MISE Comparison for CDE with linear combination of 3 estimators, for cantilever.





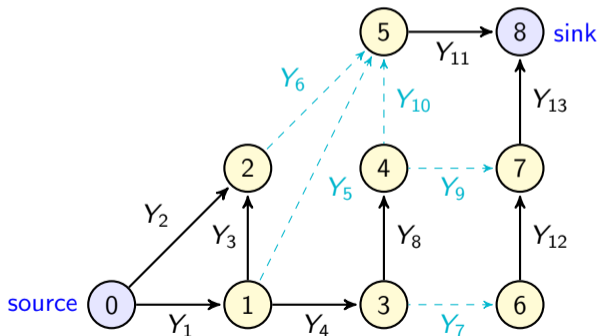
Five realizations of the density conditional on \mathcal{G}_k (blue), their average (red), and the true density (thick black) for $k = 1$ (left), $k = 2$ (middle), and $k = 3$ (right).

CMC for the SAN Example

Want to estimate the density of the longest path length X .

CMC estimator of $\mathbb{P}[X \leq x]$: $F(x | \mathcal{G}) = \mathbb{P}[X \leq x | \{Y_j, j \notin \mathcal{L}\}]$ for a minimal cut \mathcal{L} .

Ex.: $\mathcal{L} = \{5, 6, 7, 9, 10\}$ and $Y_j = F_j^{-1}(U_j)$. This estimator continuous in the U_j 's and in x .
(Erasing a single Y_j does not work.)



For each $j \in \mathcal{L}$, let P_j be the length of the longest path that goes through arc j when we exclude Y_j from that length. Then

$$F(x | \mathcal{G}) = \mathbb{P}[X < x | \{Y_j : j \notin \mathcal{L}\}] = \prod_{j \in \mathcal{L}} F_j[x - P_j]$$

and

$$F'(x | \mathcal{G}) = \sum_{j \in \mathcal{L}} f_j[x - P_j] \prod_{l \in \mathcal{L}, l \neq j} F_l[x - P_l],$$

if f_j exists for all $j \in \mathcal{L}$.

Under this conditioning, the cdf of every path length is continuous in x , and so is $F(\cdot | \mathcal{G})$, and Assumption 1 holds, so $F'(x | \mathcal{G})$ is an unbiased density estimator.

Estimated $\text{MISE} = Kn^{-\nu}$, for KDE with CMC.

		$\hat{\nu}$	$-\log_2 \text{MISE} (n = 2^{19})$
KDE	MC	0.77	20.9
	Lat+s	0.75	22.0
	Sobol+LMS	0.76	22.0
CDE	MC	0.99	25.5
	Lat+s	1.26	29.9
	Sobol+LMS	1.25	29.9

With RQMC, we observe a convergence rate near $\mathcal{O}(n^{-1.25})$ for the IV and the MISE.

For $n = 2^{19}$, by using the new CDE+RQMC rather than the usual KDE+MC, the MISE is divided by about $2^9 \approx 500$.

Waiting-time distribution in a single-server queue

FIFO queue, arbitrary arrival process, independent service times with cdf G and density g .

Let W be the waiting time of a “random” customer.

Want to estimate $p_0 = \mathbb{P}[W = 0]$ and density f of W over $(0, \infty)$.

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The system starts empty and evolves over a day of length τ .

T_j = arrival time of customer j , $T_0 = 0$,

$A_j = T_j - T_{j-1}$ = j th interarrival time,

S_j = service time of customer j ,

W_j = waiting time of customer j .

Random number of customers in the day: $N = \max\{j \geq 1 : T_j < \tau\}$.

Lindley recurrence: $W_1 = 0$ and $W_j = \max(0, W_{j-1} + S_{j-1} - A_j)$ for $j \geq 2$.

W has cdf $F(x) = \mathbb{P}[W \leq x] = \mathbb{E}[\mathbb{I}(W \leq x)]$ for $x > 0$.

For a random customer over an infinite number of days, we have (renewal reward theorem): ³¹

$$F(x) = \mathbb{E}[\mathbb{I}(W \leq x)] = \frac{\mathbb{E} [\mathbb{I}[W_1 \leq x] + \cdots + \mathbb{I}[W_N \leq x]]}{\mathbb{E}[N]}.$$

The density $f(x)$ is the derivative of the numerator with respect to x , divided by $\mathbb{E}[N]$.

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Cannot take the derivative inside the expectation. CMC: Replace $\mathbb{I}[W_j \leq x]$ by

$$P_j(x) = \mathbb{P}[W_j \leq x \mid W_{j-1} - A_j] = \mathbb{P}[S_{j-1} \leq x + A_j - W_{j-1}] = G(x + A_j - W_{j-1}) \quad \text{for } x \geq 0.$$

That is, we hide the service time S_{j-1} of the previous customer.

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That is, we hide the service time S_{j-1} of the previous customer.

For $x > 0$, we have $P'_j(x) = dP_j(x)/dx = g(x + A_j - W_{j-1})$ and

$$f(x) = \frac{1}{\mathbb{E}[N]} \sum_{j=1}^N P'_j(x).$$

This is **extended CMC**: we condition on different information for different customers.

We replicate this for n days and take the average.

Other possibilities: Can also hide A_j for customer j , etc.

Conclusion

- ▶ Combining a KDE with RQMC can improve reduce the MISE and sometimes improve its convergence rate, even though our MISE bounds converge faster only when the dimension is small.
- ▶ The CDE is an unbiased density estimator with better convergence rate for the IV and the MISE. Combining it with RQMC can provide an even better rate, and sometimes huge MISE reductions.
- ▶ What if we we cannot find \mathcal{G} for which Assumption 1 holds and $F'(x | \mathcal{G})$ is easy to compute?
Current work: density estimator based on likelihood ratio derivative estimation.
- ▶ Future: Density estimation for a function of the state of a Markov chain, using Array-RQMC.
- ▶ Lots of potential applications.

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