

# Monte Carlo Algorithms Where the Integrand Size is Unknown

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Joint work with Lan Jiang, Yuewei Liu, and Art Owen

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Feb. 16, 2012



# Hypothetical Conversation

Practitioner

You, the Expert

I need to evaluate **integrals**

$$\mu = \int_{\mathbb{R}^d} f(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x},$$

for many different  $f$ , where  $\rho$  is a given probability density function.



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$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{X}_i),$$

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As large as your computational budget allows.



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The **Central Limit Theorem** says

$$n = \left\lceil \left( \frac{1.96\sigma}{\varepsilon} \right)^2 \right\rceil$$

where  $\sigma^2$  is the variance of the integrand.



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where the  $\mathbf{X}_i$  are i.i.d.  $\sim \rho$ .

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$$n = \left\lceil \left( \frac{1.96 \hat{\sigma}}{\varepsilon} \right)^2 \right\rceil$$

Try the **sample variance** times a **variance inflation factor**:

$$\hat{\sigma}^2 = \frac{n_\sigma}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} [f(\mathbf{X}_i) - \hat{\mu}_\sigma]^2.$$





## Hypothetical Conversation

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Does theory **guarantee** that this algorithm works (at least 95% of the time)?

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The **Central Limit Theorem** says

$$n = \left\lceil \left( \frac{1.96\hat{\sigma}}{\varepsilon} \right)^2 \right\rceil$$

Try the **sample variance** times a **variance inflation factor**:

$$\hat{\sigma}^2 = \frac{n}{n-1} \sum_{i=1}^n [f(\mathbf{X}_i) - \hat{\mu}]^2.$$

**Yes!** This algorithm, with minor modifications, carries a **limited warranty**. ☰ ↺ ↻ ↶ ↷



## Three Perspectives

$$\mu = E[f(\mathbf{X})] = \int_{\mathbb{R}^d} f(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} = ?$$

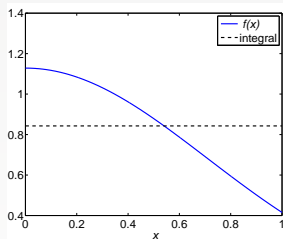
**Algorithm Design** Construct an automatic multivariate integrator analogous to MATLAB's **quad** for univariate integrals.

**Information-Based Complexity** Construct an algorithm,  $A$ , satisfying  $|\mu - A(f)| \leq \epsilon$  (definitely, with high probability, or on average) with  $\text{cost}(\epsilon, A, f)$  depending reasonably on  $\epsilon$  and the **unknown**  $\text{size}(f)$ .

**Statistics** Find a nonparametric confidence interval of **prescribed half-width**  $\epsilon$  for  $\mu$  from a reasonable number of samples  $Y_i = f(\mathbf{X}_i)$ .



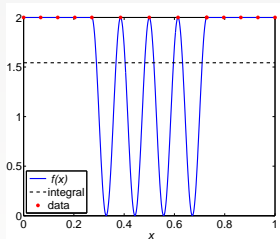
# MATLAB's Quadrature Routine quad Works Well, *but It Can Be Fooled*



$$\frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2} dx = 0.8427007929497149$$

quad →

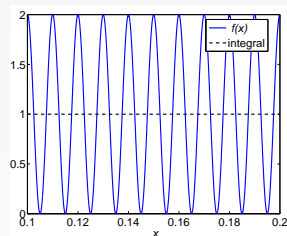
0.8427007929497149 in  
0.160521 seconds.



$$\int_0^1 f(x) dx = 1.5436$$

but quad →

2  
in 0.007092 seconds.



$$\int_0^1 [1 + \cos(200\pi x)] dx = 1$$

but quad →

0.7636784919876782  
in 0.205272 seconds.



## Can We Have a **Guarantee** Like This?

For nice integrands,  $f$ , **quad** will provide  $\int_a^b f(x) dx$  with an error  $\leq \varepsilon$  in a reasonable amount of time, or your money back.

A nice integrand,  $f$ , satisfies the following conditions:

- ▶ ..., i.e., **quad** won't be fooled,
- ▶ ..., i.e., the number of function values required is moderate.

If  $f$  is not nice (nasty), then this guarantee is void, and **quad** may return an incorrect answer.



## An Impractical Guarantee

For integrands,  $f$ , satisfying  $\|f''\|_{\infty} \leq M$ , a trapezoidal rule with  $n = \sqrt{(b-a)^3 M / (12\varepsilon)}$  trapezoids will provide  $\int_a^b f(x) dx$  with an absolute error  $\leq \varepsilon$ .

To apply this guarantee, one must know  $M$  in advance, which is impractical. This is why **quad** (adaptive recursive Simpson's rule) estimates the error and **adaptively** determines the number of function evaluations,  $n$ .

If the algorithm works for  $f$ , it should normally work for  $cf$ .



## Recall Our Hypothetical Conversation

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for many different  $f$ , where  $\rho$  is a given probability density function.

How large should I make  $n$  to obtain  $|\mu - \hat{\mu}| \leq \varepsilon$ ?

How do I find  $\sigma^2$ ?

Does theory **guarantee** that this algorithm works (at least 95% of the time)?

You, the Expert

Try a **sample average**,

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{X}_{i+n_\sigma}),$$

where the  $\mathbf{X}_i$  are i.i.d.  $\sim \rho$ .

The **Central Limit Theorem** says

$$n = \left\lceil \left( \frac{1.96\hat{\sigma}}{\varepsilon} \right)^2 \right\rceil$$

Try the **sample variance** times a **variance inflation factor**:

$$\hat{\sigma}^2 = \frac{n_\sigma}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} [f(\mathbf{X}_i) - \hat{\mu}_\sigma]^2.$$

**Yes!** This algorithm, with minor modifications, carries a **limited warranty**. ☰ ↺ ↻ ↶ ↷



## Guarantee the Variance

The **sample variance**,  $v$  is an unbiased estimate of  $\sigma^2 = \int_{\mathbb{R}^d} [f(\mathbf{x}) - \mu]^2 \rho(\mathbf{x}) \, d\mathbf{x}$ .

$$v = \frac{1}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} [f(\mathbf{X}_i) - \hat{\mu}_{n_\sigma}]^2, \quad \hat{\mu}_{n_\sigma} = \frac{1}{n_\sigma} \sum_{i=1}^{n_\sigma} f(\mathbf{X}_i), \quad \mathbf{X}_1, \mathbf{X}_2, \dots \text{ i.i.d. } \sim \rho$$

$$E[v] = \sigma^2, \quad \text{var}(v) = \frac{\sigma^4}{n_\sigma} \left( \kappa - \frac{n_\sigma - 3}{n_\sigma - 1} \right), \quad \kappa := \frac{\int_{\mathbb{R}^d} [f(\mathbf{x}) - \mu]^4 \rho(\mathbf{x}) \, d\mathbf{x}}{\sigma^4}$$

**Cantelli's Inequality** (Lin and Bai, 2010, 6.1e) guarantees that an inflated sample variance bounds the variance from above with uncertainty  $\tilde{\alpha}$ ,

$$\hat{\sigma}^2 := \mathfrak{C}^2 v, \quad \text{Prob}(\hat{\sigma}^2 \geq \sigma^2) \geq 1 - \tilde{\alpha}, \quad \mathfrak{C} > 1$$

provided that the **kurtosis** of the integrand,  $\kappa$ , is not too large, i.e.,

$$\kappa \leq \frac{n_\sigma - 3}{n_\sigma - 1} + \left( \frac{\tilde{\alpha} n_\sigma}{1 - \tilde{\alpha}} \right) \left( 1 - \frac{1}{\mathfrak{C}^2} \right)^2 =: \kappa_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C}).$$



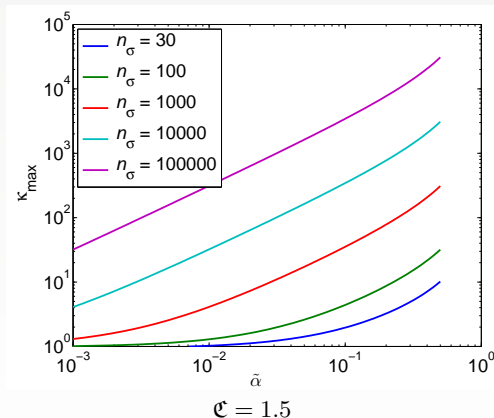


## Guarantee the Variance

$$\hat{\sigma}^2 = \frac{\mathfrak{C}^2}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} [f(\mathbf{X}_i) - \hat{\mu}_{n_\sigma}]^2,$$

$$\text{Prob}(\hat{\sigma}^2 \geq \sigma^2) \geq 1 - \tilde{\alpha}$$

if  $\kappa \leq \kappa_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})$



## Guarantee the Integral (Mean)

The **Central Limit Theorem** gives an asymptotic result for fixed  $z \geq 0$ :

$$\text{Prob} \left[ \left| \underbrace{\int_{\mathbb{R}^d} f(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x}}_{\mu} - \underbrace{\frac{1}{n} \sum_{i=1}^n f(\mathbf{X}_{i+n_\sigma})}_{\hat{\mu}} \right| \leq \frac{z\sigma}{\sqrt{n}} \right] \rightarrow 1 - 2\Phi(-z) \quad \text{as } n \rightarrow \infty$$

A non-uniform **Berry-Esseen Inequality** (Petrov, 1995, Theorem 5.16, p. 168) gives a hard upper bound:

$$\text{Prob} \left[ |\mu - \hat{\mu}| \leq \frac{z\sigma}{\sqrt{n}} \right] \geq 1 - 2 \left( \Phi(-z) + \frac{0.56\kappa^{3/4}}{\sqrt{n}} (1 + |z|)^{-3} \right)$$

This guarantees that  $\text{Prob} [|\mu - \hat{\mu}| \leq \varepsilon] \geq 1 - \tilde{\alpha}$  if the sample size is large enough:

$$n \geq N_B(\varepsilon/\sigma, \tilde{\alpha}, \kappa) := \min \left\{ m \in \mathbb{N} : \Phi(-\varepsilon\sqrt{m}/\sigma) + \frac{0.56\kappa^{3/4}}{\sqrt{m}(1 + \varepsilon\sqrt{m}/\sigma)^3} \leq \frac{\tilde{\alpha}}{2} \right\}$$
$$\asymp \frac{\sigma^2}{\varepsilon^2} \quad \text{as } \frac{\varepsilon}{\sigma} \rightarrow 0$$



## cubMC

To evaluate  $\mu = \int_{\mathbb{R}^d} f(\mathbf{x}) \rho(\mathbf{x}) \, d\mathbf{x}$

given input  $f, \rho, \varepsilon, \alpha, n_\sigma, \mathfrak{C}$ , and  $N_{\max}$ :

- ▶ Compute  $\tilde{\alpha} = 1 - \sqrt{1 - \alpha}$ , and the maximum kurtosis allowed,  $\kappa_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})$ .
- ▶ Overestimate the variance:  $\hat{\sigma}^2 = \frac{\mathfrak{C}^2}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} [f(\mathbf{X}_i) - \hat{\mu}_{n_\sigma}]^2$ .
- ▶ Choose the new sample size,  $n = \min(\max(n_\sigma, N_B(\varepsilon/\hat{\sigma}, \tilde{\alpha}, \kappa_{\max})), N_{\max})$ , for the sample mean.
- ▶ Finally, compute the sample mean:  $\hat{\mu} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{X}_{i+n_\sigma})$ .

Then  $\text{Prob}[|\mu - \hat{\mu}| \leq \varepsilon] \geq 1 - \alpha$  provided  $\kappa \leq \kappa_{\max}$  and  $n < N_{\max}$ .



## Guarantee the Time (Sample Size)

Cantelli's inequality also tells us that the estimated variance,  $\hat{\sigma}^2$ , will not overestimate the true variance,  $\sigma^2$ , by much, and so the number of function values needed is not unnecessarily large:

$$\begin{aligned}\text{cost}(\varepsilon, \text{cubMC}, \sigma) &= \sup_{f: \kappa \leq \kappa_{\max}} \min_N \{ \text{Prob}[n_\sigma + n \leq N] \geq 1 - \beta \} \\ &\leq n_\sigma + \max(n_\sigma, N_B(\varepsilon/(\sigma\gamma), \tilde{\alpha}, \kappa_{\max}^{3/4})) \asymp \frac{\sigma^2}{\varepsilon^2}, \\ \gamma &:= \mathfrak{C} \left\{ 1 + \sqrt{\left(\frac{\tilde{\alpha}}{1 - \tilde{\alpha}}\right) \left(\frac{1 - \beta}{\beta}\right) \left(1 - \frac{1}{\mathfrak{C}^2}\right)^2} \right\}^{1/2}.\end{aligned}$$

Cost depends on  $\sigma^2 = \text{var}(f)$ , but the algorithm **does not need to know**  $\sigma^2$ .



## Guarantee for cubMC

For nice integrands **cubMC** will provide the value of  $\mu = \int_{\mathbb{R}^d} f(x) \rho(x) dx$  with an absolute error of  $\leq \varepsilon$ , with probability  $1 - \alpha$ , in time  $\asymp (\sigma/\varepsilon)^2$  with probability  $1 - \beta$ , or your money back.

A nice integrand,  $f$ , satisfies the following conditions:

- ▶ the kurtosis is not too large, i.e.,  $\kappa \leq \kappa_{\max}(\tilde{\alpha}, n_{\sigma}, \mathcal{C})$ , and
- ▶ the variance is not overwhelming, i.e.,  $\sigma^2 \leq c\varepsilon^2 N_{\max}/d$ , where  $N_{\max}$  is the maximum number of scalar samples.

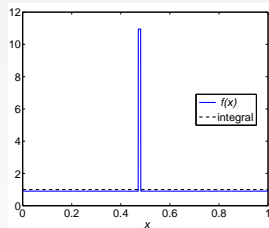
If  $f$  is not nice (nasty), **cubMC** may return the wrong answer.



## Peak Function — cubMC

$$f(x) = \begin{cases} 1 + \sigma \sqrt{\frac{1-p}{p}}, & 0 \leq x - z \pmod{1} \leq p, \\ 1 - \sigma \sqrt{\frac{p}{1-p}}, & p < x - z \pmod{1} \leq 1, \end{cases}$$

$$\mu = 1, \quad \kappa = \frac{1}{p(1-p)} - 3$$



$$z \sim U(0,1)$$

$$p \in [10^{-5}, 1/2], \quad \sigma \in [0.1, 10]$$

$$\log(p), \log(\sigma) \sim \text{Uniform}$$

$$\alpha = 5\%, \quad \mathfrak{C} = 1.5,$$

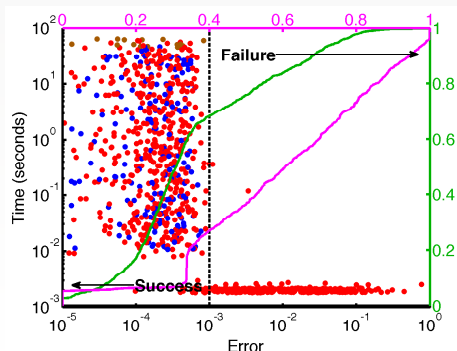
$$n_\sigma = 1024, \quad \varepsilon = 0.001$$

$$\kappa_{\max} = 9.2, \quad N_{\max} = 10^9$$

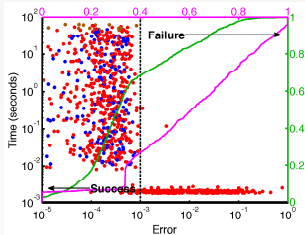
covered by guarantee

kurtosis too large

truncated sample



## Peak Function — cubMC vs. quad & quadgk



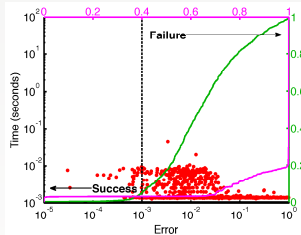
my cubMC

$\varepsilon = 0.001$

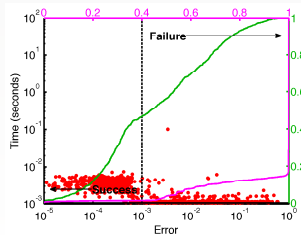
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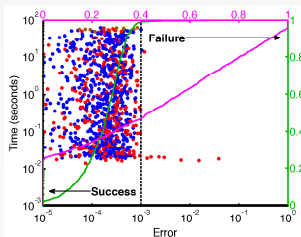
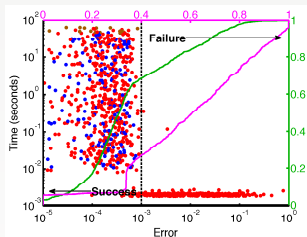
{ MATLAB's quad  
 $\varepsilon = 0.001$   
fast  
tolerance rarely met  
no guarantee



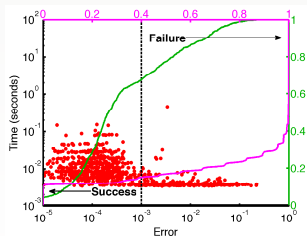
{ MATLAB's quadgk  
 $\varepsilon = 0.001$   
fast  
tolerance rarely met  
no guarantee



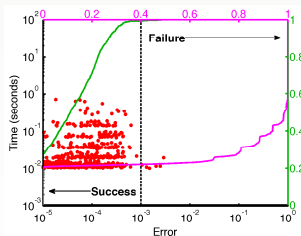
# Peak Function — cubMC i.i.d. vs. Sobol', Plus More Robustness



i.i.d. sampling  
covered by guarantee  
kurtosis too large  
truncated sample



$$n_{\sigma} = 1024, \kappa_{\max} = 9.2$$



Sobol' sampling  
no guarantee yet  
faster

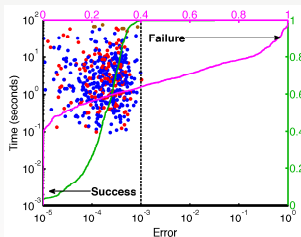
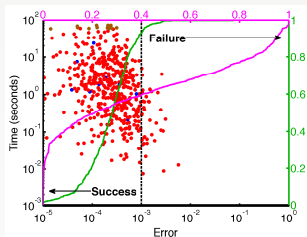
$$n_{\sigma} = 131072, \kappa_{\max} = 1050$$

$$\varepsilon = 0.001$$

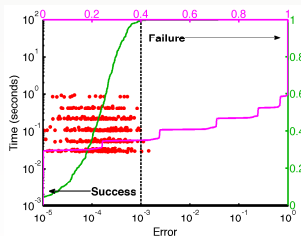
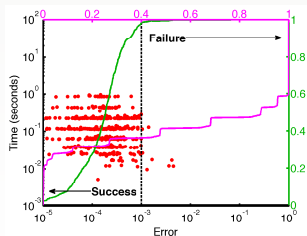




## Peak Function for $d = 3$



i.i.d. sampling  
covered by guarantee  
kurtosis too large  
truncated sample



Sobol' sampling  
quasi-standard error  
no guarantee yet  
faster

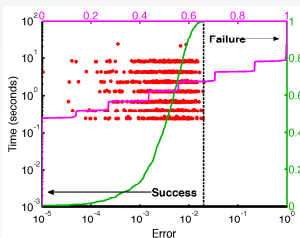
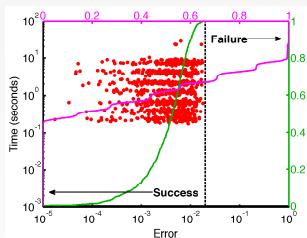
$$n_{\sigma} = 1024, \kappa_{\max} = 9.2$$

$$n_{\sigma} = 131072, \kappa_{\max} = 1050$$

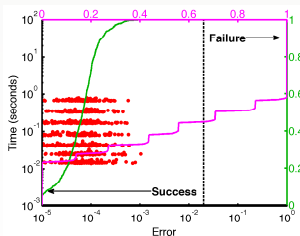
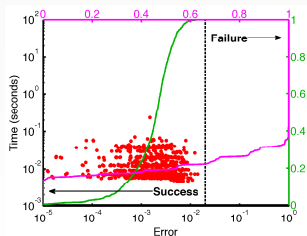
$$\varepsilon = 0.001$$



# Asian Geometric Mean Call, $d = 1, 2, 4, \dots, 64$



{ i.i.d. sampling



{ Sobol' sampling

$$n_{\sigma} = 1024, \kappa_{\max} = 9.2$$

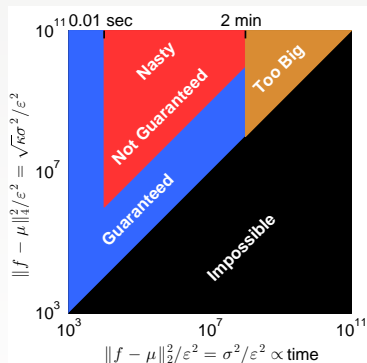
$$n_{\sigma} = 131072, \kappa_{\max} = 1050$$

$$\varepsilon = 0.02$$

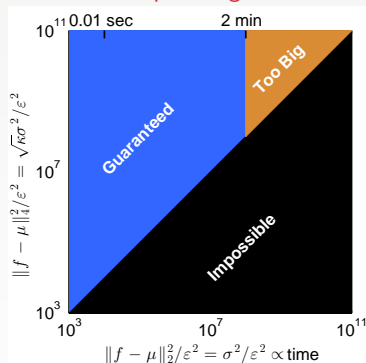


# Why an Adaptive Algorithm?

cubMC



non-adaptive algorithm



- ▶ Cost depends on size of integrand
- ▶ Algorithm parameters determine robustness to nasty integrands
- ▶ Tiny integrands handled regardless
- ▶ Huge integrands cannot be handled

- ▶ Cost is fixed and high if you want it reach tolerance for lots of integrands
- ▶ Huge integrands cannot be handled



## Why Make cubMC Dependent on Kurtosis?

$$\sigma = \text{difficulty} \quad \kappa = \text{nastiness}$$

The kurtosis of a random variable or function,

$$\kappa = \frac{E[(Y - \mu)^4]}{\underbrace{\{E[(Y - \mu)^2]\}^2}_{\sigma^4}} \quad \text{or} \quad \kappa := \frac{\int_{\mathbb{R}^d} [f(\mathbf{x}) - \mu]^4 \rho(\mathbf{x}) \, d\mathbf{x}}{\underbrace{\left\{ \int_{\mathbb{R}^d} [f(\mathbf{x}) - \mu]^2 \rho(\mathbf{x}) \, d\mathbf{x} \right\}^2}_{\sigma^4}}$$

is difficult to estimate. Why should cubMC's guarantee depend on bounded  $\kappa$ ?

- ▶ Practically, we need  $\kappa$  bounded to justify the estimates of  $\sigma^2$ .
- ▶ Bounded  $\kappa$  yields sets of probability distributions or functions that are **non-convex**.
  - ▶ Nonparametric confidence intervals are **impossible** for **convex** sets of distributions (Bahadur and Savage, 1956, Corollary 2). ▶ How we break convexity
  - ▶ **Adaptive information does not help** for **convex** sets of integrands in the worst case and probabilistic settings (Traub et al, 1988, Chapter 4, Theorem 5.2.1; Chapter 8, Corollary 5.3.1). ▶ How we break convexity

## Quasi-Standard Error (Internal Replications) for Quasi-Random Sequences

Let  $\mathbf{X}_1, \mathbf{X}_2, \dots$  be a (random or deterministic) sequence, let  $r$  be fixed, and let

$$\hat{\mu}_m = \frac{1}{2^m} \sum_{i=1}^{2^m} f(\mathbf{X}_i) = \frac{1}{2^r} \sum_{j=1}^{2^r} \hat{\mu}_{m,j}, \quad \hat{\mu}_{m,j} = \frac{1}{2^{m-r}} \sum_{i=1}^{2^{m-r}} f(\mathbf{X}_{(j-1)2^{m-r}+i})$$

The **quasi-standard error** (Owen, 1997) measures the variation of among the means of parts of the whole sample

$$\text{qse}_m = \sqrt{\frac{1}{2^r(2^r - 1)} \sum_{j=1}^{2^r} (\hat{\mu}_{m,j} - \hat{\mu}_m)^2}$$

Given error tolerance,  $\varepsilon$ , and parameters  $r \in \mathbb{N}$ ,  $m_1 \geq r$ , and  $\mathfrak{C} > 1$ , for  $m = m_1, m_1 + 1, \dots$ ,

- ▶ Compute  $f(\mathbf{X}_{2^{m-1}+1}), \dots, f(\mathbf{X}_{2^m})$ , and  $\hat{\mu}_{m,1}, \dots, \hat{\mu}_{m,2^r}, \hat{\mu}_m$ .
- ▶ If  $\mathfrak{C} \text{qse}_m \leq \varepsilon$ , then stop. Else continue.



## Further Work

**Quasi-Monte Carlo Sampling** — What is a good measure of an integrand being nasty or nice?

**Variance Reduction Techniques** — Can we preserve the guarantee?

**Different Error Criteria** — Worst case? Randomized?

**Lower Bounds on Cost** — The typical fooling functions are nasty (high kurtosis). Does assuming moderate kurtosis make the problem easier?

**Relative Error Tolerances** — Both the variance and the mean are needed to determine the eventual sample size.

**Unbounded or Infinite  $d$**  — Can automatic integrators for finite  $d$  be used in multilevel methods to improve efficiency?

[▶ Look here](#)

**Other Problems** — Are there any guarantees for MATLAB's **quad**, or any other univariate adaptive quadrature routine that estimates error? What about guarantees for function approximation?



## References I

- Bahadur RR, Savage LJ (1956) The nonexistence of certain statistical procedures in nonparametric problems. *Ann Math Stat* 27:1115–1122
- Halton JH (2005) Quasi-probability: Why quasi-Monte-Carlo methods are statistically valid and how their errors can be estimated statistically. *Monte Carlo Methods and Appl* 11:203–350
- Lin Z, Bai Z (2010) *Probability Inequalities*. Science Press and Springer-Verlag, Beijing and Berlin
- Owen AB (1997) Scrambled net variance for integrals of smooth functions. *Ann Stat* 25:1541–1562
- Owen AB (2006) On the Warnock-Halton quasi-standard error. *Monte Carlo Methods and Appl* 12:47–54
- Petrov VV (1995) *Limit Theorems of Probability Theory: Sequences of Independent Random Variables*. Clarendon Press, Oxford
- Snyder WC (2000) Accuracy estimation for quasi-Monte Carlo simulations. *Math Comput Simulation* 54:131–143
- Traub JF, Wasilkowski GW, Woźniakowski H (1988) *Information-Based Complexity*. Academic Press, Boston



# A Set of Distributions with Bounded Kurtosis is Non-Convex

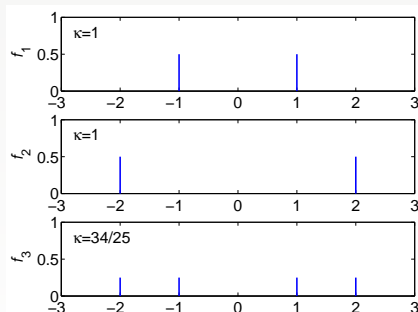
$$\text{Prob}(Y_1 = y) = 0.5, \quad y = \pm 1$$

$$\text{Prob}(Y_2 = y) = 0.5, \quad y = \pm 2$$

$$f_3 = \frac{1}{2}f_1 + \frac{1}{2}f_2$$

$$\text{Prob}(Y_3 = y) = 0.25, \quad y = \pm 1, \pm 2$$

$$\kappa_3 = \frac{34}{25} > 1 = \kappa_1 = \kappa_2$$

[Return](#)



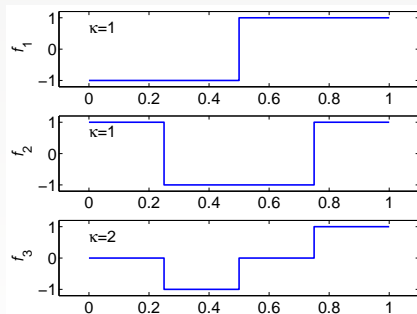
## A Set of Integrands with Bounded Kurtosis is Non-Convex

$$f_1(x) = \begin{cases} -1, & 0 \leq x < 1/2 \\ 1, & 1/2 \leq x \leq 1 \end{cases}$$

$$f_2(x) = \begin{cases} 1, & 0 \leq x < 1/4 \\ -1, & 1/4 \leq x \leq 3/4 \\ 1, & 3/4 \leq x \leq 1 \end{cases}$$

$$\begin{aligned} f_3(x) &= \frac{1}{2}f_1(x) + \frac{1}{2}f_2(x) \\ &= \begin{cases} 0, & 0 \leq x < 1/4, \\ -1, & 1/4 \leq x \leq 1/2, \\ 0, & 1/2 \leq x \leq 3/4, \\ 1, & 3/4 \leq x \leq 1, \end{cases} \end{aligned}$$

$$\kappa_3 = 2 > 1 = \kappa_1 = \kappa_2$$

[Return](#)

## When Does Quasi-Standard Error Work?

Quasi-standard error has been proposed by Warnock and studied by Owen (1997); Snyder (2000); Halton (2005); Owen (2006). Suppose that  $\mathbf{X}_1, \mathbf{X}_2, \dots$  is a scrambled digital  $(t, d)$ -sequence in base 2,  $P_m = \{\mathbf{X}_1, \dots, \mathbf{X}_{2^m}\}$ , and the integrand can be expanded in a Walsh series:

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}, \quad (S_B f)(\mathbf{x}) := \sum_{\mathbf{k} \in B} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}} \quad (\text{filtered } f)$$

$$\mu = \int_{[0,1]^d} f(\mathbf{x}) \, d\mathbf{x} = S_{\{\mathbf{0}\}} f, \quad \hat{\mu}_m = \frac{1}{2^m} \sum_{i=1}^{2^m} f(\mathbf{X}_i) = (S_{P_m^\perp} f)(\mathbf{X}_1),$$

where  $\otimes$  is a bitwise dot product modulo 2, and  $P_m^\perp = \{\mathbf{k} \in \mathbb{N}_0^d : \mathbf{k} \otimes \mathbf{x} = 0 \, \forall \mathbf{x} \in P_m\}$  is the **dual net** (wavenumbers aliased with  $\mathbf{0}$ ). The **quasi-standard error** may be expressed as

$$\text{qse}_m = \sqrt{\frac{1}{2^r - 1} \sum_{\mathbf{l} \in (P_m^\perp - \mathbf{r} / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)}$$

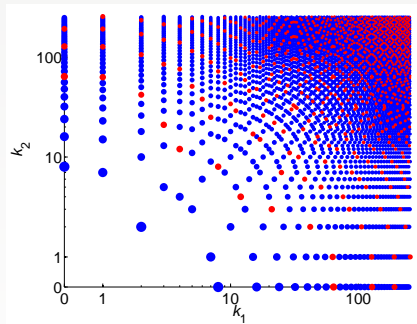
which is a surrogate for  $|\mu - \hat{\mu}_m| = |(S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1)|$ .



# When Does Quasi-Standard Error Work?

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}$$

$$|\mu - \hat{\mu}_m| = \left| (S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1) \right| \quad \bullet P_6^\perp \setminus \{\mathbf{0}\}$$



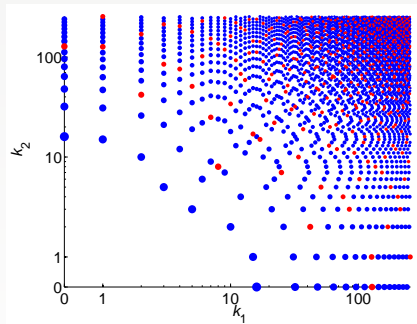
$$\text{qse}_m = \sqrt{\frac{1}{7} \sum_{\mathbf{l} \in (P_{m-3}^\perp / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)} \quad \bullet P_3^\perp \setminus P_6^\perp$$



# When Does Quasi-Standard Error Work?

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}$$

$$|\mu - \hat{\mu}_m| = \left| (S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1) \right| \quad \bullet P_7^\perp \setminus \{\mathbf{0}\}$$



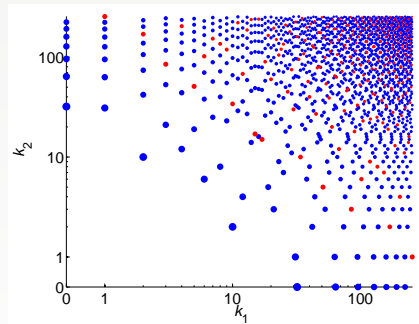
$$\text{qse}_m = \sqrt{\frac{1}{7} \sum_{\mathbf{l} \in (P_{m-3}^\perp / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)} \quad \bullet P_4^\perp \setminus P_7^\perp$$



# When Does Quasi-Standard Error Work?

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}$$

$$|\mu - \hat{\mu}_m| = \left| (S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1) \right| \quad \bullet P_8^\perp \setminus \{\mathbf{0}\}$$



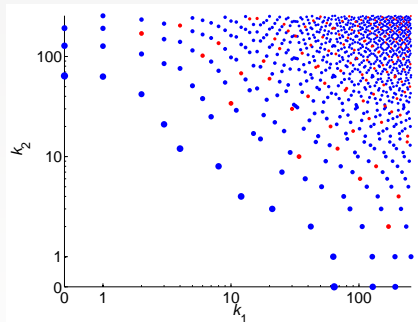
$$\text{qse}_m = \sqrt{\frac{1}{7} \sum_{\mathbf{l} \in (P_{m-3}^\perp / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)} \quad \bullet P_5^\perp \setminus P_8^\perp$$



# When Does Quasi-Standard Error Work?

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}$$

$$|\mu - \hat{\mu}_m| = \left| (S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1) \right| \quad \bullet P_9^\perp \setminus \{\mathbf{0}\}$$



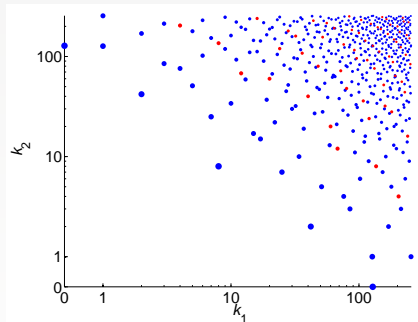
$$\text{qse}_m = \sqrt{\frac{1}{7} \sum_{\mathbf{l} \in (P_{m-3}^\perp / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)} \quad \bullet P_6^\perp \setminus P_9^\perp$$

[Return](#)


# When Does Quasi-Standard Error Work?

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) e^{\pi \sqrt{-1} \mathbf{k} \otimes \mathbf{x}}$$

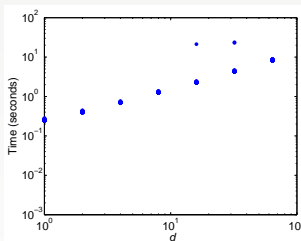
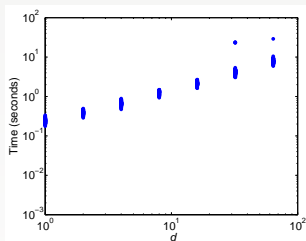
$$|\mu - \hat{\mu}_m| = \left| (S_{P_m^\perp \setminus \{\mathbf{0}\}} f)(\mathbf{X}_1) \right| \quad \bullet P_{10}^\perp \setminus \{\mathbf{0}\}$$



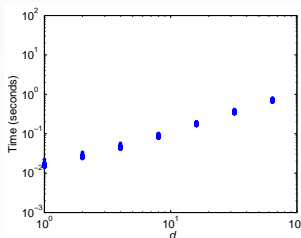
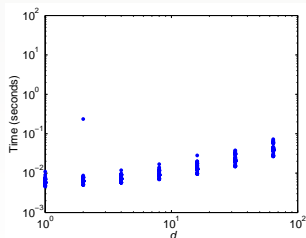
$$\text{qse}_m = \sqrt{\frac{1}{7} \sum_{\mathbf{l} \in (P_{m-3}^\perp / P_m^\perp) \setminus \{\mathbf{0}\}} (S_{P_m^\perp \oplus \mathbf{l}} f)^2(\mathbf{X}_1)} \quad \bullet P_7^\perp \setminus P_{10}^\perp$$

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## Asian Geometric Mean Call Execution Times



{ i.i.d. sampling



{ Sobol' sampling

 $n_{\sigma} = 1024, \kappa_{\max} = 9.2$  $n_{\sigma} = 131072, \kappa_{\max} = 1050$ 

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