Automatic Algorithms for Multidimensional Integration

Fred J. Hickernell
Department of Applied Mathematics
Center for Interdisciplinary Scientific Computation
Illinois Institute of Technology
`hickernell@iit.edu` `mypages.iit.edu/~hickernell`

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When Do We Stop?

Compute an integral

$$\mu(f) = \int_{\mathbb{R}^d} f(\mathbf{x})\, \varrho(\mathbf{x})\, \mathrm{d}\mathbf{x}$$ Bayesian inference, financial risk, statistical physics, ...

Desired solution: An adaptive algorithm, $\hat{\mu}(\cdot,\cdot)$ of the form

$$\hat{\mu}(f,\varepsilon) = w_{0,n} + \sum_{i=1}^{n} w_{i,n} f(\mathbf{x}_i), \qquad \text{e.g., } w_{0,n} = 0,\ w_{1,n} = \cdots = w_{n,n} = \frac{1}{n}$$

where n, $\{\mathbf{x}_i\}_{i=1}^{\infty}$, $w_{0,n}$, and $\boldsymbol{w} = (w_{i,n})_{i=1}^{n}$ are chosen to guarantee

$$\left|\mu(f) - \hat{\mu}(f,\varepsilon)\right| \leqslant \varepsilon \text{ with high probability} \qquad \forall \varepsilon > 0, \text{ reasonable } f$$

When Do We Stop?

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Want $\left|\mu(f) - \hat{\mu}(f,\varepsilon)\right| \leqslant \varepsilon$ with high probability $\forall \varepsilon > 0,$ reasonable f

Possible solutions	Drawbacks
IID sampling: $n = \left(\dfrac{2.58\hat{\sigma}}{\varepsilon}\right)^2$	Does CLT hold yet? How to determine $\hat{\sigma}$?
Low discrepancy sampling: choose n to make $\mathrm{disc}(\{\mathbf{x}_i\}_{i=1}^n)\,\mathrm{Var}(f) \leqslant \varepsilon$	Don't know $\mathrm{Var}(f)$; computing $\mathrm{disc}(\{\mathbf{x}_i\}_{i=1}^n)$ may be expensive
Randomized low discrepancy sampling: look at spread of sample means from random replications of low discrepancy points	How many replications? What measure of spread?

When Do We Stop?

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- Identify a data-driven measure of error
- Identify a cone of nice integrands for which that data-driven error can be proven to hold

Is integrand really in the cone? Well, sometimes there are necessary conditions that can be checked

Automatic IID Sampling[1]

Replace the Central Limit Theorem by Berry-Esseen inequalities:

$$\mu := \int_{\mathcal{X}} f(\mathbf{x})\, \varrho(\mathbf{x}) \mathrm{d}\mathbf{x} =: \mathbb{E}[f(\mathbf{X})], \qquad \mathcal{C} = \{f \in L^4(\mathcal{X}, \varrho) : \mathrm{kurt}(f(\mathbf{X})) \leqslant \kappa_{\mathrm{up}}\}$$

For n_σ determined by κ_{up}, and $\mathbf{x}_1, \mathbf{x}_2, \ldots$ IID let

$$\sigma_{\mathrm{up}}^2 = \frac{(1.2)^2}{n_\sigma - 1} \sum_{i=1}^{n_\sigma} f(\mathbf{x}_i), \qquad \hat{\mu}(f, \varepsilon) = \frac{1}{n_\mu} \sum_{i=n_\sigma+1}^{n_\sigma+n_\mu} f(\mathbf{x}_i), \quad \text{where}$$

$$n_\mu = \min\left\{n \in \mathbb{N} : \Phi\left(-\sqrt{n}\varepsilon/\sigma_{\mathrm{up}}\right) + \frac{1}{\sqrt{n}} \min\left(0.3328(\kappa_{\mathrm{up}}^{3/4} + 0.429), \frac{18.1139\kappa_{\mathrm{up}}^{3/4}}{1 + \left|\sqrt{n}\delta/\sigma_{\mathrm{up}}\right|^3}\right) \leqslant 0.25\%\right\}$$

Then $\mathbb{P}\{|\mu(f) - \hat{\mu}(f, \varepsilon)| \leqslant \varepsilon\} \geqslant 99\%$.

[1] H., F. J. *et al.* *Guaranteed Conservative Fixed Width Confidence Intervals Via Monte Carlo Sampling.* in *Monte Carlo and Quasi-Monte Carlo Methods 2012* (eds Dick, J. *et al.*) **65** (Springer-Verlag, Berlin, 2013), 105–128.

Automatic Quasi-Monte Carlo Sampling[2]

$$\mu = \int_{[0,1]^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x} = \widehat{f}(\mathbf{0}), \qquad f(\mathbf{x}) = \sum_{\mathbf{k}} \widehat{f}(\mathbf{k})\phi_{\mathbf{k}}(\mathbf{x}), \quad \widehat{f}(\mathbf{k}) = \int_{[0,1]^d} f(\mathbf{x})\overline{\phi}_{\mathbf{k}}(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$\phi_{\mathbf{k}}$ are complex exponentials (for lattices) or Walsh functions (for nets)

$\mathcal{C} =$ integrands whose true Fourier coefficients do not decay erratically

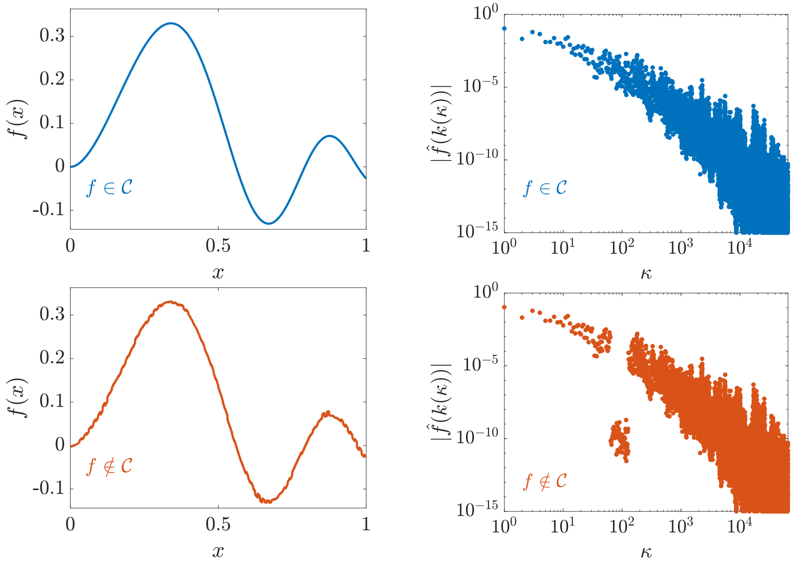
The error bound is derived in terms of

discrete transform, $\widetilde{f}_n(\mathbf{k}) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} f(\mathbf{x}_i)\overline{\phi}_{\mathbf{k}}(\mathbf{x}_i)\ \forall \mathbf{k}$, can be computed in $\mathcal{O}(n\log(n))$ operations

$$\mathfrak{C}(n) \sum_{\text{moderate}\,\mathbf{k}} \left|\widetilde{f}_n(\mathbf{k})\right| \leqslant \varepsilon \implies |\mu(f) - \hat{\mu}(f,\varepsilon)| \leqslant \varepsilon$$

[2] H., F. J. & Ll. A. Jiménez Rugama. *Reliable Adaptive Cubature Using Digital Sequences.* in *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Leuven, Belgium, April 2014* (eds Cools, R. & Nuyens, D.) **163.** arXiv:1410.8615 [math.NA] (Springer-Verlag, Berlin, 2016), 367–383, Ll. A. Jiménez Rugama & H., F. J. *Adaptive Multidimensional Integration Based on Rank-1 Lattices.* in *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Leuven, Belgium, April 2014* (eds Cools, R. & Nuyens, D.) **163.** arXiv:1411.1966 (Springer-Verlag, Berlin, 2016), 407–422, H., F. J. *et al. Adaptive Quasi-Monte Carlo Methods for Cubature.* in *Contemporary Computational Mathematics — a celebration of the 80th birthday of Ian Sloan* (eds Dick, J. *et al.*) (Springer-Verlag, 2018), 597–619. doi:10.1007/978-3-319-72456-0.

Integrands Inside and Outside the Cone



Automatic QMC Sampling Assuming a Random f

Assume $f \sim \mathcal{GP}(m, s^2 C_\theta)$, a sample from a Gaussian process. Defining

$$c = \int_{[0,1]^d} \int_{[0,1]^d} C_\theta(\mathbf{t}, \mathbf{x}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{x}, \qquad \mathbf{c} = \left(\int_{[0,1]^d} C_\theta(\mathbf{t}, \mathbf{x}_i) \, \mathrm{d}\mathbf{t} \right)_{i=1}^n, \qquad \mathsf{C} = \left(C_\theta(\mathbf{x}_i, \mathbf{x}_j) \right)_{i,j=1}^n$$

and choosing the weights as

$$w_0 = m[1 - \mathbf{c}^T \mathsf{C}^{-1} \mathbf{1}], \quad \boldsymbol{w} = \mathsf{C}^{-1} \mathbf{c}, \qquad \hat{\mu}(f, \varepsilon) = w_0 + \boldsymbol{w}^T \mathbf{f}, \quad \mathbf{f} = \left(f(\mathbf{x}_i) \right)_{i=1}^n.$$

yields an unbiased approximation:

$$\mu(f) - \hat{\mu}(f, \varepsilon) \, \big| \, \mathbf{f} = \boldsymbol{y} \sim \mathcal{N}\Big(0, s^2 (c - \mathbf{c}^T \mathsf{C}^{-1} \mathbf{c})\Big)$$

Choosing n large enough to make

$$2.58 s \sqrt{c - \mathbf{c}^T \mathsf{C}^{-1} \mathbf{c}} \leqslant \varepsilon,$$

assures us that

$$\mathbb{P}_f \left[|\mu(f) - \hat{\mu}(f, \varepsilon)| \leqslant \varepsilon \right] \geqslant 99\%.$$

Issues requiring attention: choosing parameters of the covariance kernel, expensive matrix operations

To Make This Approach Practical[3]

- Use MLE to estimate parameters
- Choose covariance kernels that match the low discrepancy design

$$c = \int_{[0,1]^d} \int_{[0,1]^d} C_\theta(\mathbf{t}, \mathbf{x}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{x} = 1, \qquad \mathbf{c} = \left(\int_{[0,1]^d} C_\theta(\mathbf{t}, \mathbf{x}_i) \, \mathrm{d}\mathbf{t} \right)_{i=1}^n = \mathbf{1}$$

$$\mathsf{C} = \Big(C_\theta(\mathbf{x}_i, \mathbf{x}_j) \Big)_{i,j=1}^n = \frac{1}{n} \mathsf{V} \Lambda \mathsf{V}^H, \quad \Lambda = \mathrm{diag}(\boldsymbol{\lambda}), \quad \boldsymbol{V}_1 = \boldsymbol{v}_1 = \mathbf{1}$$

$$\mathsf{V}^T \boldsymbol{z} \text{ is } \mathcal{O}(n \log n), \qquad \boldsymbol{\lambda} = \mathsf{V}^T \boldsymbol{C}_1, \qquad \mathsf{C}^{-1}\mathbf{1} = \frac{\mathbf{1}}{\lambda_1}$$

Dealing with the fast transformed data, $\hat{\mathbf{y}} = \mathsf{V}^T \mathbf{y}$, where $\mathbf{y} = \big(f(\mathbf{x}_i)\big)_{i=1}^n$, it follows that

$$\hat{\mu}(f, \varepsilon) = \frac{\hat{y}_1}{n} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i), \qquad \mathbb{P}_f \left[|\mu(f) - \hat{\mu}(f, \varepsilon)| \leqslant \varepsilon \right] \geqslant 99\%.,$$

$$\text{provided} \qquad 2.58 \sqrt{\left(1 - \frac{n}{\lambda_1}\right) \frac{1}{n^2} \sum_{i=2}^n \frac{|\hat{y}_i|^2}{\lambda_i}} \leqslant \varepsilon$$

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[3] Jagadeeswaran, R. & H., F. J. *Automatic Bayesian Cubature.* in preparation. 2018+.

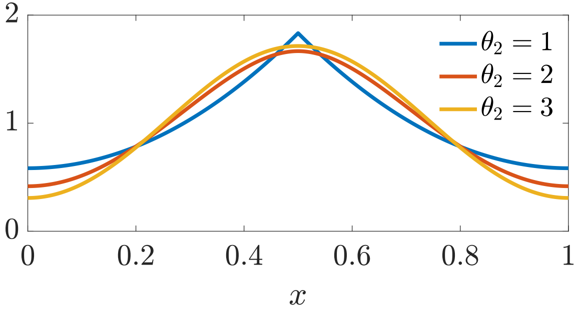
Form of Matching Covariance Kernels

Typically the domain of f is $[0,1)^d$, and

$$C(\mathbf{t},\mathbf{x}) = \begin{cases} \widetilde{C}(\mathbf{x}-\mathbf{t} \bmod 1) & \text{integration lattices} \\ \widetilde{C}(\mathbf{x} \oplus \mathbf{t}) & \text{Sobol' sequences, } \oplus \text{ means digitwise addition modulo 2} \end{cases}$$

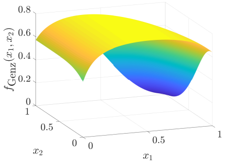
E.g., for integration lattices

$$C(\mathbf{x},\mathbf{t}) = \prod_{k=1}^{d} [1 - \theta_1 (-1)^{\theta_2} B_{2\theta_2}(x_k - t_k \bmod 1)], \qquad \theta_1 > 0, \theta_2 \in \mathbb{N}$$



Gaussian Probability

$$\mu = \int_{[\mathbf{a},\mathbf{b}]} \frac{\exp\left(-\frac{1}{2}\mathbf{t}^T\Sigma^{-1}\mathbf{t}\right)}{\sqrt{(2\pi)^d \det(\Sigma)}}\, \mathrm{d}\mathbf{t} \; = \int_{[0,1]^{d-1}} f(\mathbf{x})\, \mathrm{d}\mathbf{x}$$



For some typical choice of $\mathbf{a}$, $\mathbf{b}$, Σ, $d = 3$; $\mu \approx 0.6763$

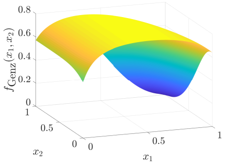
Rel. Error Tolerance	Method	Median Error	Accuracy	Worst 10% n	Worst 10% Time (s)
1E−2	IID	5E−4	100%	8.1E4	0.020
1E−2	Sh. Latt.	1E−5	100%	1.0E3	0.004
1E−2	Scr. Sobol'	4E−5	100%	1.0E3	0.005
1E−2	Bayes. Latt.	1E−5	100%	1.0E3	0.002

These algorithms are implemented in GAIL[4]

[4] Choi, S.-C. T. *et al.* *GAIL: Guaranteed Automatic Integration Library (Versions 1.0–2.2).* MATLAB software. 2013–2017. http://gailgithub.github.io/GAIL_Dev/.

Gaussian Probability

$$\mu = \int_{[\mathbf{a},\mathbf{b}]} \frac{\exp\left(-\frac{1}{2}\mathbf{t}^T\Sigma^{-1}\mathbf{t}\right)}{\sqrt{(2\pi)^d \det(\Sigma)}}\,\mathrm{d}\mathbf{t} = \int_{[0,1]^{d-1}} f(\mathbf{x})\,\mathrm{d}\mathbf{x}$$



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Rel. Error Tolerance	Method	Median Error	Accuracy	Worst 10% n	Worst 10% Time (s)
1E−3	IID	9E−5	100%	2.0E6	0.400
1E−3	Sh. Latt.	8E−6	100%	2.0E3	0.007
1E−3	Scr. Sobol’	2E−5	100%	2.0E3	0.006
1E−3	Bayes. Latt.	1E−5	100%	1.0E3	0.002

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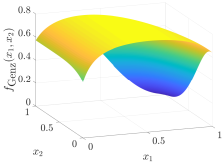

For some typical choice of $\mathbf{a}$, $\mathbf{b}$, Σ, $d = 3$; $\mu \approx 0.6763$

Rel. Error Tolerance	Method	Median Error	Accuracy	Worst 10% n	Worst 10% Time (s)
1E−4	Sh. Latt.	4E−7	100%	8.2E3	0.014
1E−4	Scr. Sobol'	4E−7	100%	1.6E4	0.018
1E−4	Bayes. Latt.	5E−7	100%	8.2E3	0.010

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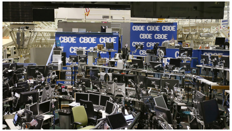
Option Pricing



$$\mu = \text{fair price} = \int_{\mathbb{R}^d} e^{-rT} \max\left(\frac{1}{d}\sum_{j=1}^{d} S_j - K, 0\right) \frac{e^{-z^T z/2}}{(2\pi)^{d/2}}\, dz \approx \$13.12$$

$$S_j = S_0 e^{(r-\sigma^2/2)jT/d+\sigma x_j} = \text{stock price at time } jT/d,$$

$$x = Az, \quad AA^T = \Sigma = \left(\min(i,j)T/d\right)_{i,j=1}^{d}, \quad T = 1/4,\ d = 13 \text{ here}$$

Abs. Error Tolerance	Method		Median Error	Accuracy	Worst 10% n	Worst 10% Time (s)
1E−2	IID	diff	2E−3	100%	6.1E7	33.000
1E−2	Scr. Sobol'	PCA	1E−3	100%	1.6E4	0.040
1E−2	Scr. Sob. cont. var.	PCA	2E−3	100%	4.1E3	0.019
1E−2	Bayes. Latt.	PCA	2E−3	99%	1.6E4	0.051

Future Work

- Bayesian cubature with higher order nets and smoother kernels, control variates
- Stopping criteria for multilevel and multivariate decomposition methods
- Community QMC software that combines the efforts of several research groups
  - Skeleton with clearly defined properties for different kinds of objects
  - Plug-and-play functionality

```
%% Example
stopObj = CLTStopping %stopping criterion
distribObj = IIDDistribution; %IID sampling with uniform distribution
[sol, out] = integrate(KeisterFun, distribObj, stopObj)
stopObj.absTol = 1e-3; %decrease tolerance
[sol, out] = integrate(KeisterFun, distribObj, stopObj)
```

```
>> IntegrationExample
sol =
0.428567222603452
sol =
0.425203913946775
```

Thank you

Slides available on SpeakerDeck at
speakerdeck.com/fjhickernell/matrix-week-two-2018-june

- H., F. J., Jiang, L., Liu, Y. & Owen, A. B. *Guaranteed Conservative Fixed Width Confidence Intervals Via Monte Carlo Sampling.* in *Monte Carlo and Quasi-Monte Carlo Methods 2012* (eds Dick, J., Kuo, F. Y., Peters, G. W. & Sloan, I. H.) **65** (Springer-Verlag, Berlin, 2013), 105–128.
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(eds Cools, R. & Nuyens, D.) *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Leuven, Belgium, April 2014.* **163** (Springer-Verlag, Berlin, 2016).