

# Reliable Error Estimation for Cubature Using Sobol' Sequences

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*In honor of Ilya M. Sobol'*

Joint work with Lluís Antoni Jiménez Rugama  
speaking tomorrow, 11:15 am on lattice rules

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# Automatic, Adaptive Quasi-Monte Carlo Cubature

option pricing, statistical physics,  
photon transport, ...

$$\int_{[0,1)^d} f(\boldsymbol{x}) \, d\boldsymbol{x} = ?$$



# Automatic, Adaptive Quasi-Monte Carlo Cubature

option pricing, statistical physics,  
photon transport, ...

$$\int_{[0,1)^d} f(\mathbf{x}) d\mathbf{x} \approx \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{z}_i)$$

$\{\mathbf{z}_i\}$  chosen IID  $\mathcal{U}[0, 1]^d$ ,  
(Richtmyer, 1951), (Korobov, 1959),  
(Halton, 1960), (Sobol', 1967),  
(Faure, 1982), ...

# Automatic, Adaptive Quasi-Monte Carlo Cubature

$\text{err}(f, n, \{\mathbf{z}_i\}) :=$

$$\left| \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{z}_i) \right| \\ \leq \underbrace{D(n, \{\mathbf{z}_i\})}_{\text{quality of } \{\mathbf{z}_i\}} \underbrace{V(f)}_{\text{roughness of } f}$$

option pricing, statistical physics,  
photon transport, ...

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(Richtmyer, 1951), (Korobov, 1959),  
(Halton, 1960), (Sobol', 1967),  
(Faure, 1982), ...

better points, tractability, multi-level  
(Hlawka, 1961), (Niederreiter, 1992),  
(Sloan and Joe, 1994), (Hickernell,  
1998), (Dick and Pillichshammer,  
2010), (Novak and Woźniakowski,  
2010), (Dick et al., 2014) (Giles,  
2014), ...



# Automatic, Adaptive Quasi-Monte Carlo Cubature

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$$\left| \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{z}_i) \right| \\ \leq \underbrace{D(n, \{\mathbf{z}_i\})}_{\text{quality of } \{\mathbf{z}_i\}} \underbrace{V(f)}_{\text{roughness of } f}$$

How to automatically and adaptively choose  $n$  to ensure

$$\text{err}(f, n, \{\mathbf{z}_i\}) \leq \varepsilon?$$

(nonlinear algorithm,  
non-convex set of integrands)

option pricing, statistical physics,  
photon transport, ...

$\{\mathbf{z}_i\}$  chosen IID  $\mathcal{U}[0, 1]^d$ ,  
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2010), (Dick et al., 2014) (Giles,  
2014), ...

guaranteed, automatic, adaptive  
Monte Carlo (Hickernell et al.,  
2014), trapezoidal rule (Clancy et al.,  
2014), GAIL (Choi et al., 2014)



# Sobol' Points

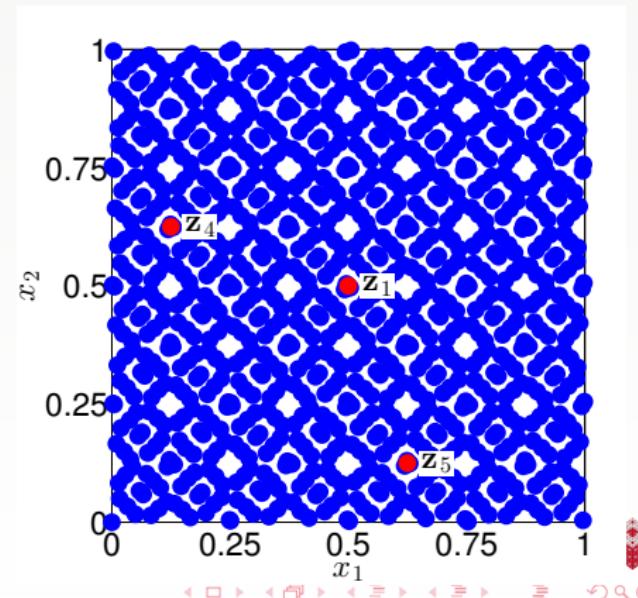
Let  $\oplus$  denote binary **digit by digit** addition modulo 2:

$$\frac{1}{8} \oplus \frac{5}{8} = {}_20.001 \oplus {}_20.101 = \oplus_2 0.100 = \frac{1}{2}, \quad 1 \oplus 5 = 001_2 \oplus 101_2 = 100_2 = 4$$

Sobol' points  $\{z_i\}$  satisfy

$$z_0 = \mathbf{0}, \quad z_i \oplus z_\ell = z_{i \oplus \ell} \quad \forall i, \ell \in \mathbb{N}_0$$

$$\begin{aligned} z_1 \oplus z_5 &= ({}_20.100, {}_20.100) \\ &\quad \oplus ({}_20.101, {}_20.001) \\ &= ({}_20.001, {}_20.101) \\ &= z_4 = z_{1 \oplus 5} \end{aligned}$$

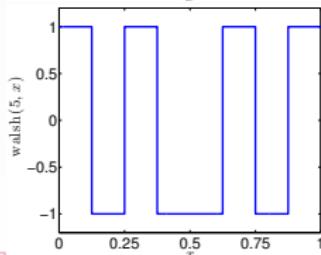
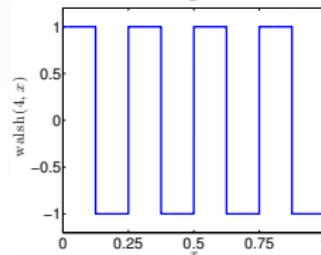
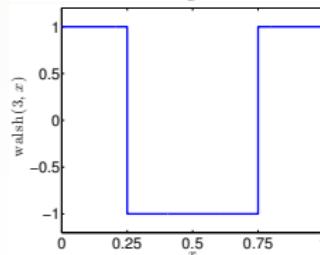
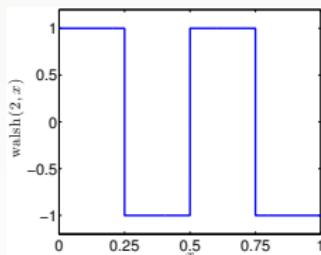
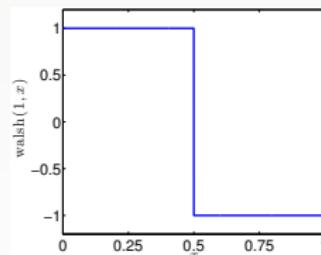
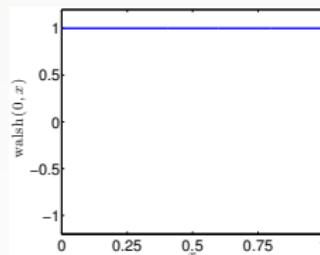


# Walsh Functions

The base-2 Walsh function,  $\text{walsh}(\cdot, \cdot) : (\mathbf{k}, \mathbf{x}) \mapsto (-1)^{\langle \mathbf{k}, \mathbf{x} \rangle}$ , is defined in terms of the a bilinear function  $\langle \cdot, \cdot \rangle : \mathbb{N}_0^d \times [0, 1]^d \rightarrow \{0, 1\}$ :

$$\langle \mathbf{k}, \mathbf{x} \rangle = \langle (k_1, \dots, k_d), (x_1, \dots, x_d) \rangle := \sum_{j=1}^d \langle k_j, x_j \rangle \bmod 2$$

$$\langle k_j, x_j \rangle = \langle (\cdots k_{j1} k_{j0})_2, 20.x_{j1} x_{j2} \cdots \rangle := k_{j0} x_{j1} + k_{j1} x_{j2} + \cdots \bmod 2$$



# Sobol' Cubature Error via Fourier-Walsh Expansions

The Fourier-Walsh expansion of an integrand is given by

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} (-1)^{\langle \mathbf{k}, \mathbf{x} \rangle} \hat{f}(\mathbf{k}), \quad \text{where } \hat{f}(\mathbf{k}) := \int_{[0,1)^d} f(\mathbf{x}) (-1)^{\langle \mathbf{k}, \mathbf{x} \rangle} d\mathbf{x}.$$

Sobol' points integrate most Walsh functions perfectly, but some terribly:

$$\frac{1}{2^m} \sum_{i=0}^{2^m-1} (-1)^{\langle \mathbf{k}, \mathbf{z}_i \rangle} = \begin{cases} 1, & \mathbf{k} \in \mathcal{P}_m^\perp := \{\mathbf{k} \in \mathbb{N}_0^d : \langle \mathbf{k}, \mathbf{z}_i \rangle = 0, i = 0, \dots, 2^m - 1\}, \\ 0 & \mathbf{k} \notin \mathcal{P}_m^\perp \end{cases}$$

So Sobol' cubature error depends on the sizes of the Fourier-Walsh coefficients for  $\mathbf{k}$  in the **dual Sobol'** set  $\mathcal{P}_m^\perp$ :

$$\text{err}(f, 2^m, \{\mathbf{z}_i\}) := \left| \int_{[0,1)^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{2^m} \sum_{i=0}^{2^m-1} f(\mathbf{z}_i) \right| = \left| \sum_{\mathbf{k} \in \mathcal{P}_m^\perp \setminus \{\mathbf{0}\}} \hat{f}(\mathbf{k}) \right|$$

How do we reliably bound this error based on the  $f(\mathbf{z}_i)$ ?



# Wavenumber Map

Define a bijective mapping  $\tilde{\mathbf{k}} : \mathbb{N}_0 \rightarrow \mathbb{N}_0^d$  such that for all  $m, \lambda \in \mathbb{N}_0$  and  $\kappa = 0, \dots, 2^m - 1$ ,

$$\tilde{\mathbf{k}}(0) = \mathbf{0}, \quad \tilde{\mathbf{k}}(\kappa + \lambda 2^m) = \tilde{\mathbf{k}}(\kappa) \oplus \mathbf{l} \text{ for some } \mathbf{l} \in \mathcal{P}_m^\perp,$$

e.g.,  $\tilde{\mathbf{k}}(29) = \tilde{\mathbf{k}}(5) \oplus \mathbf{l}$  for some  $\mathbf{l} \in \mathcal{P}_3^\perp$ , but not for some  $\mathbf{l} \in \mathcal{P}_4^\perp$

One can express the Fourier-Walsh expansion for the integrand and the error as

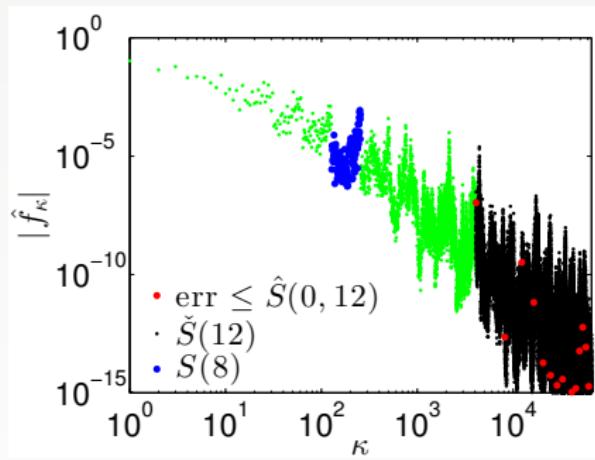
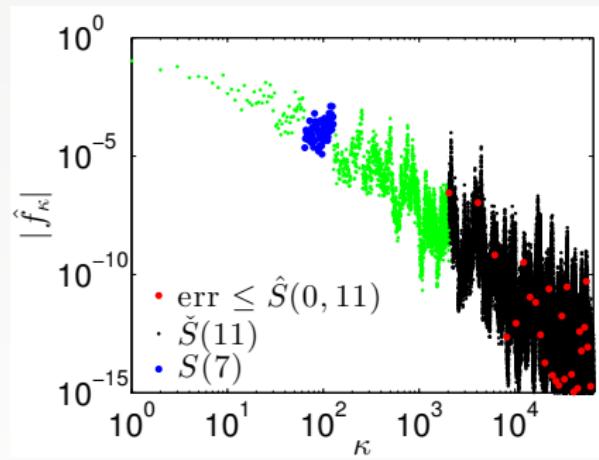
$$f(\mathbf{x}) = \sum_{\kappa=0}^{\infty} (-1)^{\langle \tilde{\mathbf{k}}(\kappa), \mathbf{x} \rangle} \hat{f}_{\kappa}, \quad \hat{f}_{\kappa} := \hat{f}(\tilde{\mathbf{k}}(\kappa)), \quad \text{err}(f, 2^m, \{\mathbf{z}_i\}) = \left| \sum_{\lambda=1}^{\infty} \hat{f}_{\lambda 2^m} \right|$$

Large  $\kappa$  implies typically smaller  $\hat{f}_{\kappa}$  in a way that is made explicit on the next slide. Moreover, the discrete Fourier-Walsh coefficients are aliased as follows:

$$\tilde{f}_{m,\kappa} := \frac{1}{2^m} \sum_{i=0}^{2^m-1} (-1)^{\langle \tilde{\mathbf{k}}(\kappa), \mathbf{z}_i \rangle} f(\mathbf{z}_i) \quad \tilde{f}_{m,\kappa+\lambda 2^m} = \tilde{f}_{m,\kappa},$$

e.g.,  $\tilde{f}_{3,29} = \tilde{f}_{3,5}$ , but generally  $\hat{f}_{29} \neq \hat{f}_5$  and  $\hat{f}_{4,29} \neq \hat{f}_{4,5}$

# Cone Assumptions on Decay of Fourier Walsh Coefficients



Make **cone** assumptions on how the  $\hat{f}_\kappa$  decay. There exist non-increasing  $\hat{\omega}$  and  $\check{\omega}$  such that for all  $0 \leq \ell \leq m$

$$\hat{S}(\ell, m) := \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^m}|, \quad \check{S}(m) := \sum_{\kappa=2^m}^{\infty} |\hat{f}_\kappa| \quad S(\ell) := \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} |\hat{f}_\kappa|$$

$$\hat{S}(\ell, m) \leq \hat{\omega}(m - \ell) \check{S}(m), \quad \check{S}(m) \leq \check{\omega}(\ell) S(m - \ell) \quad \forall m \geq \ell + \ell_*$$

# Error Bound in Terms of Discrete Fourier-Walsh Coeff.

Cone conditions:

$$\widehat{S}(\ell, m) := \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^m}|, \quad \check{S}(m) := \sum_{\kappa=2^m}^{\infty} |\hat{f}_{\kappa}| \quad S(\ell) := \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} |\hat{f}_{\kappa}|$$

$$\widehat{S}(\ell, m) \leq \widehat{\omega}(m - \ell) \check{S}(m) \quad \forall \ell, \quad \check{S}(m) \leq \check{\omega}(\ell) S(m - \ell) \quad \forall m \geq \ell + \ell_*.$$

Then we can bound the error as follows:

$$\begin{aligned} \text{err}(f, 2^m, \{\mathbf{z}_i\}) &= \left| \sum_{\lambda=1}^{\infty} \hat{f}_{\lambda 2^m} \right| \leq \sum_{\lambda=1}^{\infty} |\hat{f}_{\lambda 2^m}| = \widehat{S}(0, m) \\ &\leq \widehat{\omega}(m) \check{S}(m) \leq \widehat{\omega}(m) \check{\omega}(\ell) S(m - \ell) \\ &\leq \frac{\widehat{\omega}(m) \check{\omega}(\ell) \check{S}(m - \ell, m)}{1 - \widehat{\omega}(\ell) \check{\omega}(\ell)} \end{aligned}$$
proof

where

$$\check{S}(\ell, m) := \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} |\tilde{f}_{m, \kappa}|, \quad \tilde{f}_{m, \kappa} := \frac{1}{2^m} \sum_{i=0}^{2^m-1} (-1)^{\langle \bar{k}(\kappa), \mathbf{z}_i \rangle} f(\mathbf{z}_i)$$



# cubSobol\_g—Guaranteed, Adaptive, Sobol' Cubature

Given an error tolerance  $\varepsilon > 0$  and an integrand  $f$ , fix the lag  $\ell \in \mathbb{N}$  and let

$$\mathfrak{C} = \frac{\check{\omega}(\ell)}{1 - \hat{\omega}(\ell)\check{\omega}(\ell)}, \quad m = \ell + \ell_*,$$

**Step 1.** Compute the sum of the (data-based) discrete Fourier-Walsh coefficients  $\tilde{S}(m - \ell, m)$ .

**Step 2.** If the error tolerance is satisfied,

$$\mathfrak{C}\hat{\omega}(m)\tilde{S}(m - \ell, m) \leq \varepsilon,$$

then return the Sobol' cubature answer.

**Step 3.** Otherwise, increase  $m$  by one, and return to Step 1.

**Theorem.** If  $f$  satisfies the cone conditions on its Fourier-Walsh coefficients, then

$$\left| \int_{[0,1)^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{2^m} \sum_{i=1}^m f(\mathbf{z}_i) \right| \leq \varepsilon$$

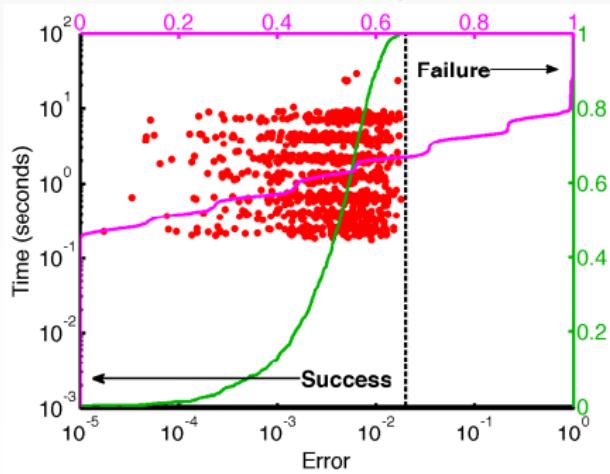
with  $m \leq \min\{m' : \mathfrak{C}\hat{\omega}(m')[1 + \hat{\omega}(\ell)\check{\omega}(\ell)]S(m') \leq \varepsilon\}$

proof

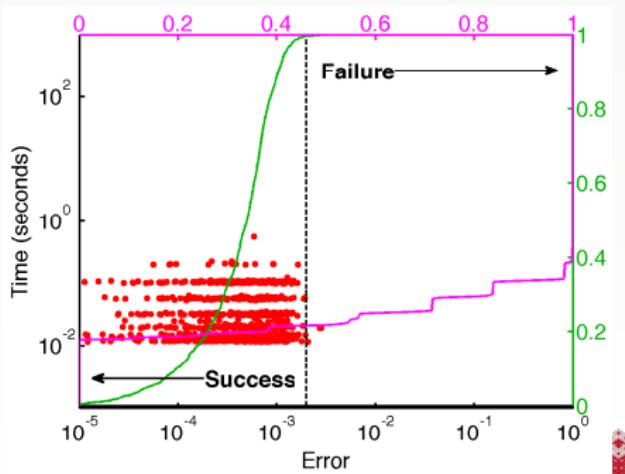
# Asian Geometric Mean Call Option

$S(0) = K = 100, \quad T = 1, \quad r = 0.03, \quad \text{volatility} \sim \mathcal{U}[0.1, 0.7],$   
 $d = \# \text{ time steps} \sim \mathcal{U}\{1, 2, 4, 8, 16, 32, 64\}$

IID, cubMC\_g

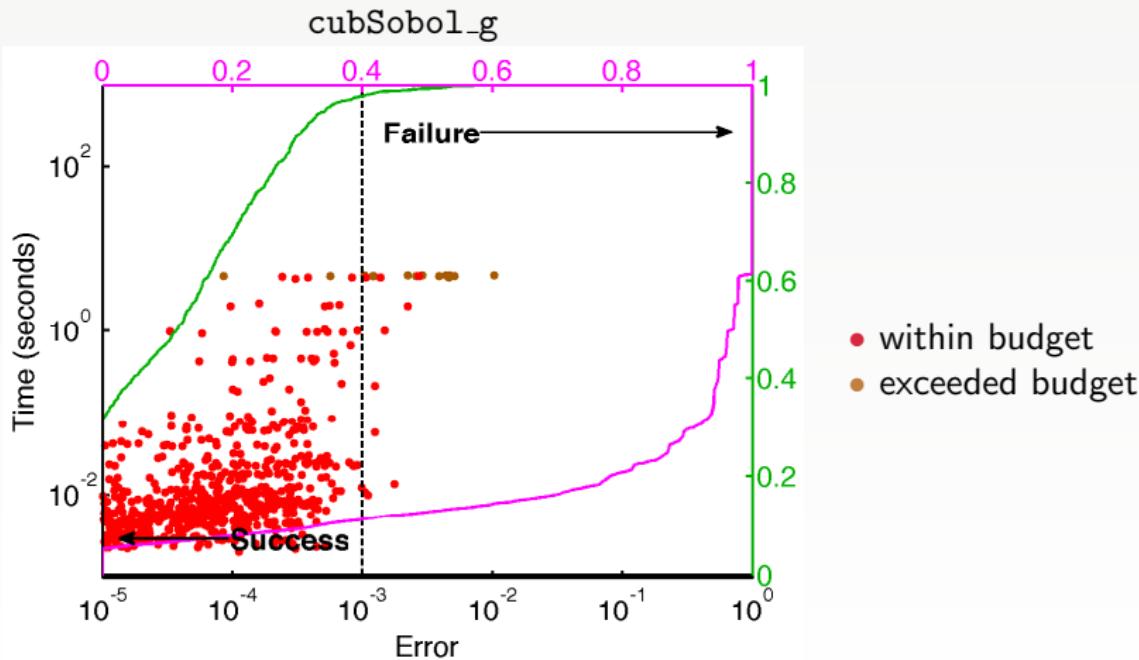


Sobol', cubSobol\_g



# Genz and Keister Examples

These examples come from Genz (1987) and Keister (1996)



# What's Missing for cubSobol\_g?

- ▶ Connections between our cone conditions and **familiar spaces** of integrands, such as Korobov spaces
- ▶ Lower bound on the **computational complexity**
- ▶ **Relative** error criterion
- ▶ Justification for our heuristic determination of the map  $\kappa$



# Why Not Replications to Estimate Error?

$$\left| \int_{[0,1)^d} f(\boldsymbol{x}) d\boldsymbol{x} - \hat{\mu}_n \right| \leq \mathfrak{C} \sqrt{\frac{1}{R-1} \sum_{r=1}^R (Y_r - \hat{\mu}_n)^2}, \quad \hat{\mu}_n := \frac{1}{R} \sum_{i=0}^{R-1} Y_r$$

**IID Replications**  $Y_r = \frac{R}{n} \sum_{i=0}^{n/R-1} f(\boldsymbol{z}_i^{(r)})$ , where  $\{\boldsymbol{z}_i^{(r)}\}$  are independent randomizations.

**Internal Replications**  $Y_r = \frac{R}{n} \sum_{i=(r-1)n/R}^{rn/R-1} f(\boldsymbol{z}_i)$ .

Want  $R$  small to take advantage of Sobol' point evenness, but need  $R$  large to ensure that sample variance of  $Y_r$  represents error (Deng, 2013; Hickernell et al., 2014).

# Guaranteed Automatic Integration Library (GAIL)

<http://code.google.com/p/gail/>

- ▶ Version 1.3 (February 14, 2014) (Choi et al., 2014) includes `integral_g.m`, `meanMC_g.m`, `cubMC_g.m`, and `funappx_g.m`
- ▶ Version 2.0 (exp. September 2014) will hopefully include some of the following:
  - ▶ quasi-Monte Carlo—`cubSobol_g.m`, `cubLattice_g.m`
  - ▶ Monte Carlo for Bernoulli—`meanBernoulli_g.m`
  - ▶ multi-level Monte Carlo—`meanMLMC_g.m`
  - ▶ multivariate function approximation
  - ▶ relative error criterion
  - ▶ higher order methods (for one dimensional problems)
  - ▶ local adaption (for one dimensional problems)
- ▶ Theory developed in Hickernell et al. (2014) and Clancy et al. (2014). Should apply to other problems where

$$\text{solution}(cf) = |c| \text{ solution}(f).$$



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# Bounding $S(\ell)$ in Terms of $\tilde{S}(\ell, m)$

$$\begin{aligned}
 S(\ell) &= \sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} |\hat{f}_\kappa| = \sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} \left| \tilde{f}_{m,\kappa} - \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda 2^m} \right| \\
 &\leq \underbrace{\sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} |\tilde{f}_{m,\kappa}|}_{\tilde{S}(\ell, m)} + \underbrace{\sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^m}|}_{\hat{S}(\ell, m)} \\
 &\leq \tilde{S}(\ell, m) + \hat{\omega}(m-\ell) \check{\omega}(m-\ell) S(\ell) \\
 S(\ell) &\leq \frac{\tilde{S}(\ell, m)}{1 - \hat{\omega}(m-\ell) \check{\omega}(m-\ell)} \quad \text{provided that } \hat{\omega}(m-\ell) \check{\omega}(m-\ell) < 1
 \end{aligned}$$

◀ back



## Bounding $\tilde{S}(\ell, m)$ in Terms of $S(\ell)$

$$\begin{aligned} \widetilde{S}(\ell, m) &= \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} |\tilde{f}_{m,\kappa}| = \sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} \left| \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda 2^m} \right| \\ &\leq \underbrace{\sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} |\hat{f}_\kappa|}_{\hat{S}(\ell)} + \underbrace{\sum_{\kappa=[2^{\ell-1}]}^{2^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^m}|}_{\hat{S}(\ell, m)} \\ &\leq [1 + \hat{\omega}(m-\ell)\check{\omega}(m-\ell)] \color{blue}{S(\ell)} \end{aligned}$$

◀ back



# Computing the Discrete Fourier Walsh Coefficients

$$\begin{aligned}\widetilde{S}(\ell, m) &= \sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} |\tilde{f}_{m,\kappa}| = \sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} \left| \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda 2^m} \right| \\ &\leq \underbrace{\sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} |\hat{f}_\kappa|}_{\hat{S}(\ell)} + \underbrace{\sum_{\kappa=\lfloor 2^{\ell-1} \rfloor}^{2^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^m}|}_{\hat{S}(\ell, m)} \\ &\leq [1 + \hat{\omega}(m-\ell)\check{\omega}(m-\ell)] S(\ell)\end{aligned}$$

