Sparse Grid Quadrature and Interpolation

Note: We have encountered potentially high dimensional quadrature at several points:

Bayes' Relation: $\pi(q|\upsilon_{obs}) = \dfrac{\pi(\upsilon_{obs}|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon_{obs}|q)\pi_0(q)dq}$

QoI: $y(t,x) = \mathbb{E}[u^K(t,x,Q)] = \int_\Gamma u^K(t,x,q)\rho_Q(q)dq$

Discrete Projection: $u_k(t,x) = \dfrac{1}{\gamma_k}\langle u, \Psi_k\rangle_\rho = \dfrac{1}{\gamma_k}\int_\Gamma u(t,x,q)\Psi_k(q)\rho_Q(q)dq$

Stochastic Quadrature Methods: Monte Carlo

$$\langle u, \Psi_k\rangle_\rho = \frac{1}{R}\sum_{r=1}^{R} u(t,x,q^r)\Psi_k(q^r) + \varepsilon_R$$

Notes:

- Errors satisfy $\mathbb{E}[\varepsilon_R] = 0$ and $\varepsilon_R = \mathcal{O}(\frac{1}{\sqrt{R}})$ for large R
- Optimal for sufficiently large p.

Deterministic Quadrature Methods

1-D Quadrature Relations:

$$I^{(1)}f = \int_{\Gamma_1} f(q)\rho_Q(q)dq \approx \sum_{r=1}^{R} f(q^r)w^r = \mathcal{Q}^{(1)}f$$

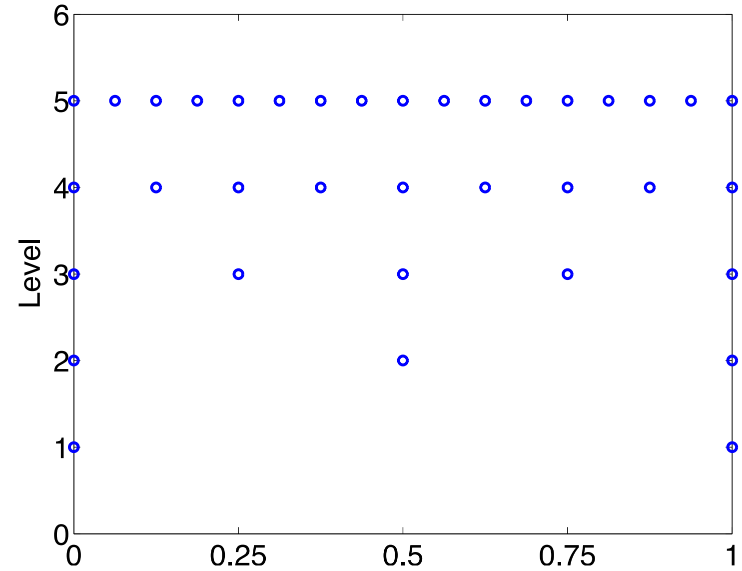
Gaussian Quadrature:

$$I^{(1)}f = \frac{1}{2}\int_{-1}^{1} f(q)dq \approx \frac{1}{2}\sum_{r=1}^{R} f(q^r)w^r,$$

$$I^{(1)}f = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} f(q)e^{-q^2/2}dq \approx \sum_{r=1}^{R} f(q^r)w^r$$

r	Nodes q^r	Weights w^r
1	0	2
2	$\pm\frac{1}{\sqrt{3}}$	1
3	0	$\frac{8}{9}$
	$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
4	$\pm\frac{\sqrt{15+2\sqrt{30}}}{\sqrt{35}}$	$\frac{49}{6(18+\sqrt{30})}$
	$\pm\frac{\sqrt{15-2\sqrt{30}}}{\sqrt{35}}$	$\frac{49}{6(18-\sqrt{30})}$

1-D Quadrature Relations



Nested Quadrature Techniques: Consider on [0,1]

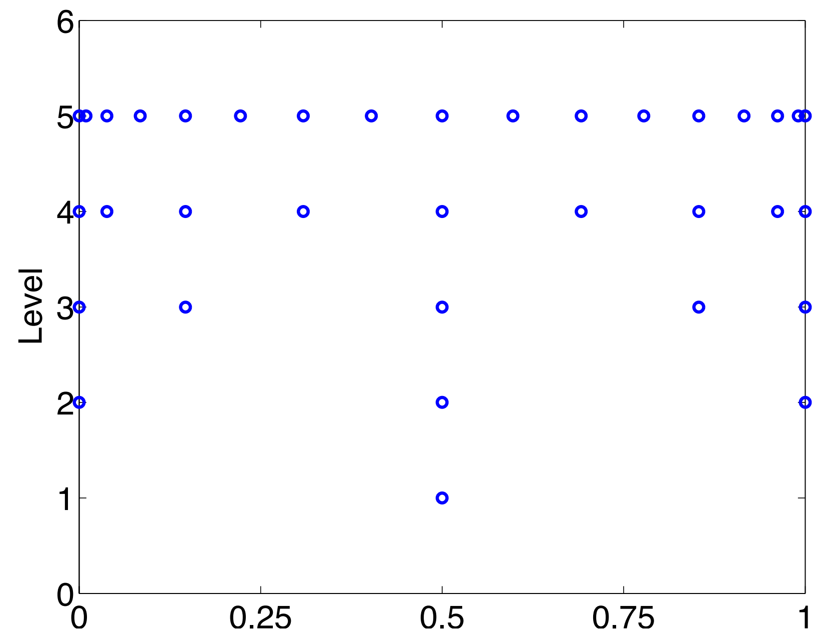
$$\mathcal{Q}_\ell^{(1)} f = \sum_{r=1}^{R_\ell} f(q_\ell^r) w_\ell^r$$

Trapezoid Rule: $r = 1, \ldots, R_\ell$

$$\mathcal{Q}_\ell^{(1)} f = \frac{h_\ell}{2}\left[f(0) + f(1) + 2\sum_{r=1}^{R_\ell - 2} f(q_\ell^r) \right]$$

where

$$h_\ell = \frac{1}{2^{\ell-1}} \;,\; R_\ell = 2^{\ell-1}+1 \;,\; q_\ell^r = r h_\ell = \frac{r-1}{2^{\ell-1}} \;,\; w^r = \left[\frac{h_\ell}{2}, h_\ell, \ldots, h_\ell, \frac{h_\ell}{2} \right]$$



Clenshaw--Curtis:

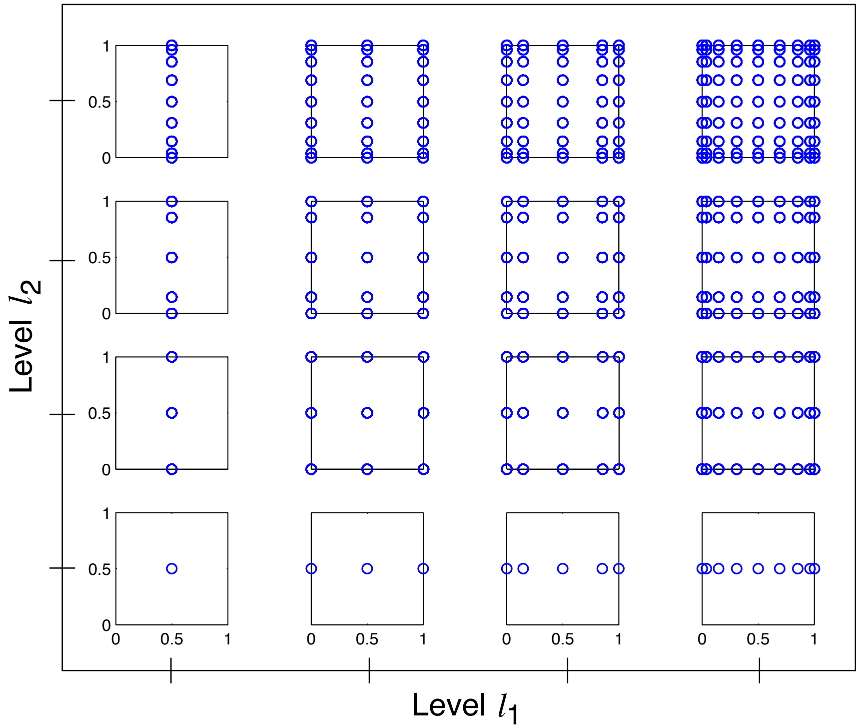
$$q_\ell^r = \frac{1}{2}\left[1 - \cos\frac{\pi(r-1)}{R_\ell - 1} \right] \;,\; r = 1, \ldots, R_\ell$$

Note: Recall Runge function

Tensor Product Formulation

Integrals:

$$I^{(p)}f = \int_\Gamma f(q)\rho_Q(q)dq$$



Tensor Product Quadrature:

$$\mathcal{Q}_\ell^{(p)} f = \left(\mathcal{Q}_{\ell_1}^{(1)} \otimes \cdots \otimes \mathcal{Q}_{\ell_p}^{(1)}\right) f$$

$$\equiv \sum_{r_1=1}^{R_{\ell_1}} \cdots \sum_{r_p=1}^{R_{\ell_p}} f\left(q_1^{r_1}, \cdots, q_p^{r_p}\right) w_{\ell_1}^{r_1} \cdots w_{\ell_p}^{r_p}$$

where

$$R = \prod_{i=1}^{p} R_{\ell_i}$$

Errors:

$$\left| I^{(p)}f - \mathcal{Q}_\ell^{(p)} f \right| = \mathcal{O}(R_\ell^{-\alpha/p})$$

Note: Convergence stagnates as parameter dimension p gets large!

for functions f in the space

$$C^\alpha([0,1]^p) = \left\{ f : [0,1]^p \to \mathbb{R} \,\middle|\, \max_{|\mathbf{k}'| \le \alpha} \left\| \frac{\partial^{|\mathbf{k}'|} f}{\partial q_1^{k_1} \cdots \partial q_p^{k_p}} \right\|_\infty < \infty \right\}$$

Sparse Grid Construction

Motivation:

R									
0					1				
1				x		y			
2			x^2		xy		y^2		
3		x^3		x^2y		xy^2		y^3	
4	x^4		x^3y		x^2y^2		xy^3		y^4

Difference Relations: Define

$$\Delta_\ell^{(1)} f = \left(\mathcal{Q}_\ell^{(1)} - \mathcal{Q}_{\ell-1}^{(1)} \right) f$$

where

$$\mathcal{Q}_\ell^{(1)} f = \sum_{r=1}^{R_\ell} f(q_\ell^r) w_\ell^r$$

1-D Nodal Points

$$\Theta_\ell^{(1)} = \left\{ q_\ell^1, \cdots, q_\ell^{R_\ell} \right\}$$

Example: Trapezoid rule

$\ell = 2$: $\Theta_2^{(1)} = \{0, \frac{1}{2}, 1\}$ and $w = [\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$

$\ell = 1 : \Theta_1^{(1)} = \{0, 1\}$ and $w = [\frac{1}{2}, \frac{1}{2}]$

Thus

$$\Delta_2^{(1)} f = -\frac{1}{4} f(0) + \frac{1}{2} f(1/2) - \frac{1}{4} f(1)$$

Note: Weights can be negative

Sparse Grid Construction

Sparse Grid Quadrature Rule:

$$\mathcal{Q}_\ell^{(p)} f = \sum_{|\ell'| \le \ell + p - 1} \left(\Delta_{\ell_1}^{(1)} \otimes \cdots \otimes \Delta_{\ell_p}^{(1)} \right) f$$

where $\ell' = (\ell_1, \cdots, \ell_p) \in \mathbb{N}^p$ is a multi-index with $|\ell'| = \sum_{i=1}^p \ell_i$.

Note: Tensor product formula can be expressed as

$$\mathcal{Q}_\ell^{(p)} f = \sum_{\max \ell' \le \ell} \left(\Delta_{\ell_1}^{(1)} \otimes \cdots \otimes \Delta_{\ell_p}^{(1)} \right) f$$

where $\max \ell' \equiv \max\{\ell_1, \cdots, \ell_p\}$.

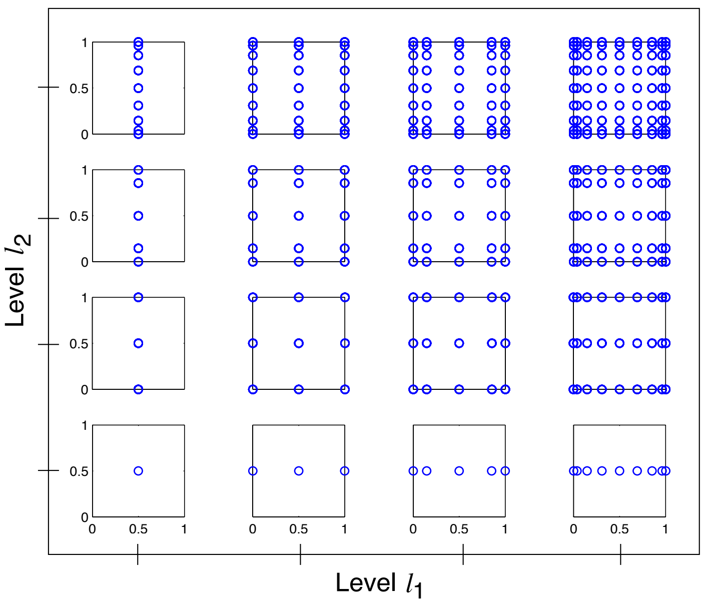
Sparse Grid Nodal Set:

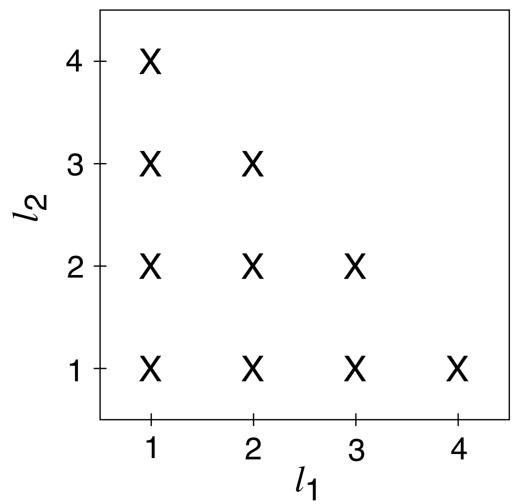
$$\Theta_\ell^{(p)} = \bigcup_{|\ell'| \le \ell + p - 1} \Theta_{\ell_1}^{(1)} \times \cdots \times \Theta_{\ell_p}^{(1)}.$$

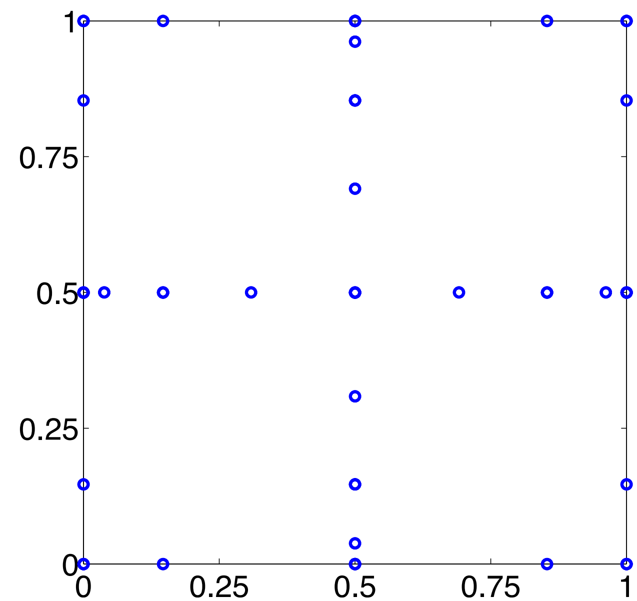
Sparse Grid Construction

Example: Consider Clenshaw-Curtis with $\Theta_1^{(1)} = \{\frac{1}{2}\}$ and $\Theta_2^{(1)} = \{0, \frac{1}{2}, 1\}$. For $p = 2$, $\ell' = (\ell_1, \ell_2)$ so $|\ell'| = \ell_1 + \ell_2$. For $\ell = 4$, the sparse grid nodal set is

$$
\begin{aligned}
\Theta_4^{(2)} = &\left(\Theta_1^{(1)} \times \Theta_1^{(1)}\right) \quad , \quad (\ell_1 = 1, \ell_2 = 1) \\
&\cup \left(\Theta_1^{(1)} \times \Theta_2^{(1)}\right) \cup \left(\Theta_2^{(1)} \times \Theta_1^{(1)}\right) \\
&\cup \left(\Theta_1^{(1)} \times \Theta_3^{(1)}\right) \cup \left(\Theta_2^{(1)} \times \Theta_2^{(1)}\right) \cup \left(\Theta_1^{(1)} \times \Theta_3^{(1)}\right) \\
&\cup \left(\Theta_1^{(1)} \times \Theta_4^{(1)}\right) \cup \left(\Theta_2^{(1)} \times \Theta_3^{(1)}\right) \cup \left(\Theta_3^{(1)} \times \Theta_2^{(1)}\right) \cup \left(\Theta_4^{(1)} \times \Theta_1^{(1)}\right)
\end{aligned}
$$







Sparse Grid: 29 points

Tensored Grid: 81 points

Sparse Grid Construction

Error Analysis:

$$\|\mathcal{I}f - \mathcal{A}(q,p)f\| = \mathcal{O}\left(\mathcal{R}^{-\alpha}\log(\mathcal{R})^{(p-1)(\alpha+1)}\right)$$

Grid Sizes:

p	R_ℓ	Sparse Grid $\mathcal{R}$	Tensored Grid $R = (R_\ell)^p$
2	5	13	25
	9	29	81
5	5	61	3125
	9	241	59,049
10	5	221	9,765,625
	9	1581	$> 3 \times 10^9$
50	5	5101	$> 8 \times 10^{34}$
	9	171,901	$> 5 \times 10^{47}$
100	5	20,201	$> 7 \times 10^{69}$
	9	1,353,801	$> 2 \times 10^{95}$

Numerical Quadrature

Problem:

- Accuracy of methods diminishes as parameter dimension p increases
- Suppose $f \in C^{\alpha}([0,1]^p)$
- Tensor products: Take R_ℓ points in each dimension so $R = (R_\ell)^p$ total points
- Quadrature errors:

$$\text{Newton-Cotes: } E \sim \mathcal{O}(R_\ell^{-\alpha}) = \mathcal{O}(R^{-\alpha/p})$$

$$\text{Gaussian: } E \sim \mathcal{O}(e^{-\beta R_\ell}) = \mathcal{O}\left(e^{-\beta \sqrt[p]{R}}\right)$$

$$\text{Sparse Grid: } E \sim \mathcal{O}\left(\mathcal{R}^{-\alpha} \log{(\mathcal{R})}^{(p-1)(\alpha+1)}\right)$$

- Alternative: Monte Carlo quadrature

$$\int_{\mathbb{R}^p} f(q)\rho(q)dq \approx \frac{1}{R}\sum_{r=1}^{R} f(q^r) \quad , \quad E \sim \left(\frac{1}{\sqrt{R}}\right)$$

- Advantage: Errors independent of dimension p
- Disadvantage: Convergence is very slow!

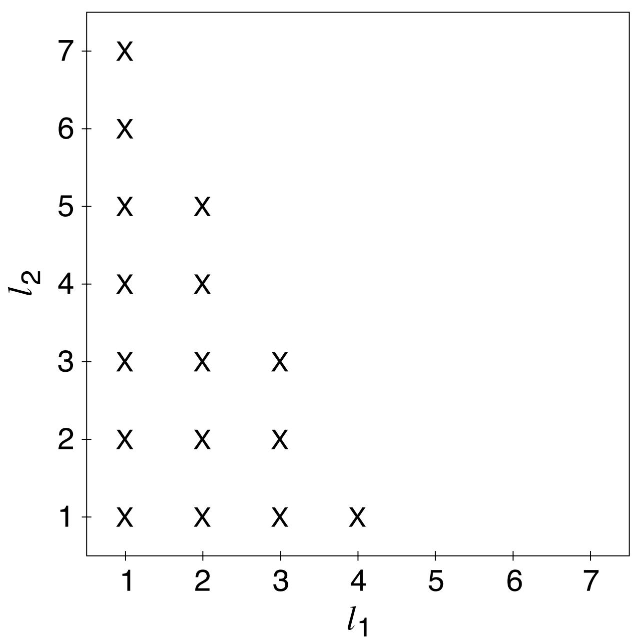
Conclusion: For high enough dimension p, monkeys throwing darts will beat Gaussian and sparse grid techniques!

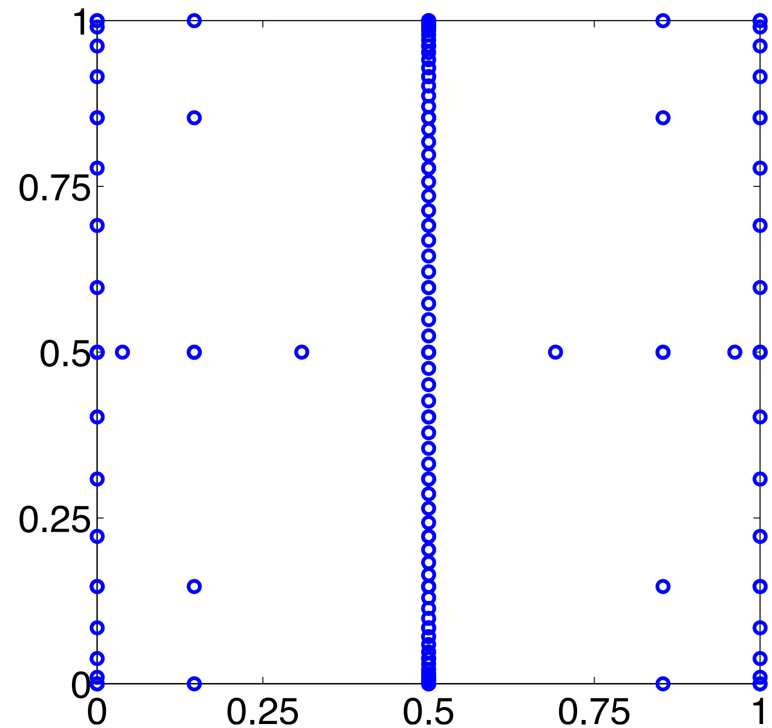
Anisotropic Sparse Grids

Multi-Index Set:

$$\mathbb{I}(\ell) = \left\{ \ell' \in \mathbb{N}^p \,\middle|\, \ell' \cdot \mathbf{a} = \sum_{i=1}^{p} a_i \ell_i \leq \ell + p - 1 \right\}$$

where $\mathbf{a} \in \mathbb{R}_+^p$ is a vector of weights.





Multi-Dimensional Interpolation

Tensor Products and Sparse Grid: Interpolation formulae analogous to quadrature rules.

Uses:

- Spectral collocation methods to propagate input uncertainties.
- Construction of surrogate models.

Sparse Grid Software:

- MATLAB: Sparse Grid Interpolation Toolbox – Be careful of Clenshaw-Curtis, which are actually Newton-Cotes points – versus Chebychev
- Dakota