Fully symmetric kernel quadrature

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Introduction and summary

Doing kernel quadrature for more than, say, 20,000 nodes is difficult due to the need to solve a large system of linear equations.

- Many approximate fast inversion methods exist, but these are often somewhat complicated.
- If one is doing probabilistic numerics, approximate matrix inversion would have to be also modelled.

We construct the node set using *fully symmetric sets*.

- Solving the kernel quadrature weights is *fast* and involves *no approximations*.
- The algorithm is quite easy to implement.
- The nodes can still be selected in a reasonably flexible manner.

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Fully symmetric sets: the difficult definition

Fully symmetric set

A *generator vector* $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_d) \in \mathbb{R}^d$, composed of *generators* $\lambda_1, \ldots, \lambda_d \geq 0$, generates the *fully symmetric set* $[\boldsymbol{\lambda}] \subset \mathbb{R}^d$:

$$[\boldsymbol{\lambda}] = [\lambda_1, \ldots, \lambda_d] := \bigcup_{\mathbf{q} \in \Pi_d} \bigcup_{\mathbf{s} \in S_d} \left\{ (s_1 \lambda_{q_1}, \ldots, s_d \lambda_{q_d}) \right\} \subset \mathbb{R}^d,$$

where Π_d is the set of all permutations $\mathbf{q} = (q_1, \ldots, q_d)$ of the integers $1, \ldots, d$ and S_d is the set of all vectors of the form $\mathbf{s} = (s_1, \ldots, s_d)$ with each s_i either 1 or -1.

This is, of course, somewhat incomprehensible.

Fully symmetric sets: permutation matrices

Permutation matrix

A permutation (and sign change) matrix $\mathbf{P}$ is a matrix that has exactly one non-zero element on each of its rows and columns and that element is either 1 or -1.

Permutation matrix example:

$$\mathbf{P} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

A fully symmetric set can be expressed as

$$[\boldsymbol{\lambda}] = \bigcup_{\mathbf{P}} \mathbf{P}\boldsymbol{\lambda} \subset \mathbb{R}^d,$$

where the union is over all the set of possible $d \times d$ permutation matrix.

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&\boldsymbol{(\lambda_1, \lambda_2, 0)}, && (-\lambda_1, \lambda_2, 0), && (\lambda_1, -\lambda_2, 0), && (-\lambda_1, -\lambda_2, 0), \\
&(\lambda_2, \lambda_1, 0), && (-\lambda_2, \lambda_1, 0), && (\lambda_2, -\lambda_1, 0), && (-\lambda_2, -\lambda_1, 0), \\
&(0, \lambda_1, \lambda_2), && (0, -\lambda_1, \lambda_2), && (0, \lambda_1, -\lambda_2), && (0, -\lambda_1, -\lambda_2), \\
&(0, \lambda_2, \lambda_1), && (0, -\lambda_2, \lambda_1), && (0, \lambda_2, -\lambda_1), && (0, -\lambda_2, -\lambda_1), \\
&(\lambda_1, 0, \lambda_2), && (-\lambda_1, 0, \lambda_2), && (\lambda_1, 0, -\lambda_2), && (-\lambda_1, 0, -\lambda_2), \\
&(\lambda_2, 0, \lambda_1), && (-\lambda_2, 0, \lambda_1), && (\lambda_2, 0, -\lambda_1), && (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1, \lambda_2, 0), && \boldsymbol{(-\lambda_1, \lambda_2, 0)}, && (\lambda_1, -\lambda_2, 0), && (-\lambda_1, -\lambda_2, 0),\\
&(\lambda_2, \lambda_1, 0), && (-\lambda_2, \lambda_1, 0), && (\lambda_2, -\lambda_1, 0), && (-\lambda_2, -\lambda_1, 0),\\
&(0, \lambda_1, \lambda_2), && (0, -\lambda_1, \lambda_2), && (0, \lambda_1, -\lambda_2), && (0, -\lambda_1, -\lambda_2),\\
&(0, \lambda_2, \lambda_1), && (0, -\lambda_2, \lambda_1), && (0, \lambda_2, -\lambda_1), && (0, -\lambda_2, -\lambda_1),\\
&(\lambda_1, 0, \lambda_2), && (-\lambda_1, 0, \lambda_2), && (\lambda_1, 0, -\lambda_2), && (-\lambda_1, 0, -\lambda_2),\\
&(\lambda_2, 0, \lambda_1), && (-\lambda_2, 0, \lambda_1), && (\lambda_2, 0, -\lambda_1), && (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1, \lambda_2, 0), \quad (-\lambda_1, \lambda_2, 0), \quad \boldsymbol{(\lambda_1, -\lambda_2, 0)}, \quad (-\lambda_1, -\lambda_2, 0), \\
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&(0, \lambda_1, \lambda_2), \quad (0, -\lambda_1, \lambda_2), \quad (0, \lambda_1, -\lambda_2), \quad (0, -\lambda_1, -\lambda_2), \\
&(0, \lambda_2, \lambda_1), \quad (0, -\lambda_2, \lambda_1), \quad (0, \lambda_2, -\lambda_1), \quad (0, -\lambda_2, -\lambda_1), \\
&(\lambda_1, 0, \lambda_2), \quad (-\lambda_1, 0, \lambda_2), \quad (\lambda_1, 0, -\lambda_2), \quad (-\lambda_1, 0, -\lambda_2), \\
&(\lambda_2, 0, \lambda_1), \quad (-\lambda_2, 0, \lambda_1), \quad (\lambda_2, 0, -\lambda_1), \quad (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$\begin{aligned}
\big\{&(\lambda_1,\lambda_2,0), \quad (-\lambda_1,\lambda_2,0), \quad (\lambda_1,-\lambda_2,0), \quad \boldsymbol{(-\lambda_1,-\lambda_2,0)},\\
&(\lambda_2,\lambda_1,0), \quad (-\lambda_2,\lambda_1,0), \quad (\lambda_2,-\lambda_1,0), \quad (-\lambda_2,-\lambda_1,0),\\
&(0,\lambda_1,\lambda_2), \quad (0,-\lambda_1,\lambda_2), \quad (0,\lambda_1,-\lambda_2), \quad (0,-\lambda_1,-\lambda_2),\\
&(0,\lambda_2,\lambda_1), \quad (0,-\lambda_2,\lambda_1), \quad (0,\lambda_2,-\lambda_1), \quad (0,-\lambda_2,-\lambda_1),\\
&(\lambda_1,0,\lambda_2), \quad (-\lambda_1,0,\lambda_2), \quad (\lambda_1,0,-\lambda_2), \quad (-\lambda_1,0,-\lambda_2),\\
&(\lambda_2,0,\lambda_1), \quad (-\lambda_2,0,\lambda_1), \quad (\lambda_2,0,-\lambda_1), \quad (-\lambda_2,0,-\lambda_1)\big\}
\end{aligned}$$

$$[\boldsymbol{\lambda}]_4 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1, \lambda_2, 0), \quad (-\lambda_1, \lambda_2, 0), \quad (\lambda_1, -\lambda_2, 0), \quad (-\lambda_1, -\lambda_2, 0),\\
&\boldsymbol{(\lambda_2, \lambda_1, 0)}, \quad (-\lambda_2, \lambda_1, 0), \quad (\lambda_2, -\lambda_1, 0), \quad (-\lambda_2, -\lambda_1, 0),\\
&(0, \lambda_1, \lambda_2), \quad (0, -\lambda_1, \lambda_2), \quad (0, \lambda_1, -\lambda_2), \quad (0, -\lambda_1, -\lambda_2),\\
&(0, \lambda_2, \lambda_1), \quad (0, -\lambda_2, \lambda_1), \quad (0, \lambda_2, -\lambda_1), \quad (0, -\lambda_2, -\lambda_1),\\
&(\lambda_1, 0, \lambda_2), \quad (-\lambda_1, 0, \lambda_2), \quad (\lambda_1, 0, -\lambda_2), \quad (-\lambda_1, 0, -\lambda_2),\\
&(\lambda_2, 0, \lambda_1), \quad (-\lambda_2, 0, \lambda_1), \quad (\lambda_2, 0, -\lambda_1), \quad (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_5 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1,\lambda_2,0), && (-\lambda_1,\lambda_2,0), && (\lambda_1,-\lambda_2,0), && (-\lambda_1,-\lambda_2,0),\\
&(\lambda_2,\lambda_1,0), && \boldsymbol{(-\lambda_2,\lambda_1,0)}, && (\lambda_2,-\lambda_1,0), && (-\lambda_2,-\lambda_1,0),\\
&(0,\lambda_1,\lambda_2), && (0,-\lambda_1,\lambda_2), && (0,\lambda_1,-\lambda_2), && (0,-\lambda_1,-\lambda_2),\\
&(0,\lambda_2,\lambda_1), && (0,-\lambda_2,\lambda_1), && (0,\lambda_2,-\lambda_1), && (0,-\lambda_2,-\lambda_1),\\
&(\lambda_1,0,\lambda_2), && (-\lambda_1,0,\lambda_2), && (\lambda_1,0,-\lambda_2), && (-\lambda_1,0,-\lambda_2),\\
&(\lambda_2,0,\lambda_1), && (-\lambda_2,0,\lambda_1), && (\lambda_2,0,-\lambda_1), && (-\lambda_2,0,-\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_6 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$\begin{aligned}
\{&(\lambda_1,\lambda_2,0), && (-\lambda_1,\lambda_2,0), && (\lambda_1,-\lambda_2,0), && (-\lambda_1,-\lambda_2,0),\\
&(\lambda_2,\lambda_1,0), && (-\lambda_2,\lambda_1,0), && (\lambda_2,-\lambda_1,0), && (-\lambda_2,-\lambda_1,0),\\
&(0,\lambda_1,\lambda_2), && (0,-\lambda_1,\lambda_2), && \boldsymbol{(0,\lambda_1,-\lambda_2)}, && (0,-\lambda_1,-\lambda_2),\\
&(0,\lambda_2,\lambda_1), && (0,-\lambda_2,\lambda_1), && (0,\lambda_2,-\lambda_1), && (0,-\lambda_2,-\lambda_1),\\
&(\lambda_1,0,\lambda_2), && (-\lambda_1,0,\lambda_2), && (\lambda_1,0,-\lambda_2), && (-\lambda_1,0,-\lambda_2),\\
&(\lambda_2,0,\lambda_1), && (-\lambda_2,0,\lambda_1), && (\lambda_2,0,-\lambda_1), && (-\lambda_2,0,-\lambda_1)\}
\end{aligned}$$

$$[\boldsymbol{\lambda}]_{11} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1,\lambda_2,0), && (-\lambda_1,\lambda_2,0), && (\lambda_1,-\lambda_2,0), && (-\lambda_1,-\lambda_2,0),\\
&(\lambda_2,\lambda_1,0), && (-\lambda_2,\lambda_1,0), && (\lambda_2,-\lambda_1,0), && (-\lambda_2,-\lambda_1,0),\\
&(0,\lambda_1,\lambda_2), && (0,-\lambda_1,\lambda_2), && (0,\lambda_1,-\lambda_2), && (0,-\lambda_1,-\lambda_2),\\
&(0,\lambda_2,\lambda_1), && (0,-\lambda_2,\lambda_1), && (0,\lambda_2,-\lambda_1), && \boldsymbol{(0,-\lambda_2,-\lambda_1)},\\
&(\lambda_1,0,\lambda_2), && (-\lambda_1,0,\lambda_2), && (\lambda_1,0,-\lambda_2), && (-\lambda_1,0,-\lambda_2),\\
&(\lambda_2,0,\lambda_1), && (-\lambda_2,0,\lambda_1), && (\lambda_2,0,-\lambda_1), && (-\lambda_2,0,-\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_{16} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$
\begin{aligned}
\{&(\lambda_1, \lambda_2, 0), && (-\lambda_1, \lambda_2, 0), && (\lambda_1, -\lambda_2, 0), && (-\lambda_1, -\lambda_2, 0),\\
&(\lambda_2, \lambda_1, 0), && (-\lambda_2, \lambda_1, 0), && (\lambda_2, -\lambda_1, 0), && (-\lambda_2, -\lambda_1, 0),\\
&(0, \lambda_1, \lambda_2), && (0, -\lambda_1, \lambda_2), && (0, \lambda_1, -\lambda_2), && (0, -\lambda_1, -\lambda_2),\\
&(0, \lambda_2, \lambda_1), && (0, -\lambda_2, \lambda_1), && (0, \lambda_2, -\lambda_1), && (0, -\lambda_2, -\lambda_1),\\
&\boldsymbol{(\lambda_1, 0, \lambda_2)}, && (-\lambda_1, 0, \lambda_2), && (\lambda_1, 0, -\lambda_2), && (-\lambda_1, 0, -\lambda_2),\\
&(\lambda_2, 0, \lambda_1), && (-\lambda_2, 0, \lambda_1), && (\lambda_2, 0, -\lambda_1), && (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}
$$

$$
[\boldsymbol{\lambda}]_{17} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}
$$

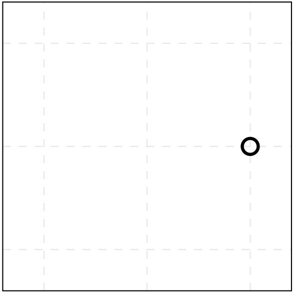
Fully symmetric sets: symbolic example

Consider the generator $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, 0) \in \mathbb{R}^3$ with $\lambda_1 \neq \lambda_2$ non-zero.

$$\begin{aligned}
\{&(\lambda_1, \lambda_2, 0), \quad (-\lambda_1, \lambda_2, 0), \quad (\lambda_1, -\lambda_2, 0), \quad (-\lambda_1, -\lambda_2, 0),\\
&(\lambda_2, \lambda_1, 0), \quad (-\lambda_2, \lambda_1, 0), \quad (\lambda_2, -\lambda_1, 0), \quad (-\lambda_2, -\lambda_1, 0),\\
&(0, \lambda_1, \lambda_2), \quad (0, -\lambda_1, \lambda_2), \quad (0, \lambda_1, -\lambda_2), \quad (0, -\lambda_1, -\lambda_2),\\
&(0, \lambda_2, \lambda_1), \quad (0, -\lambda_2, \lambda_1), \quad (0, \lambda_2, -\lambda_1), \quad (0, -\lambda_2, -\lambda_1),\\
&(\lambda_1, 0, \lambda_2), \quad (-\lambda_1, 0, \lambda_2), \quad (\lambda_1, 0, -\lambda_2), \quad (-\lambda_1, 0, -\lambda_2),\\
&(\lambda_2, 0, \lambda_1), \quad \boldsymbol{(-\lambda_2, 0, \lambda_1)}, \quad (\lambda_2, 0, -\lambda_1), \quad (-\lambda_2, 0, -\lambda_1)\}
\end{aligned}$$

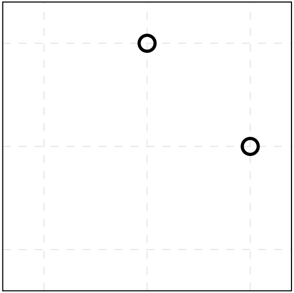
$$[\boldsymbol{\lambda}]_{22} = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ 0 \end{pmatrix}$$

Fully symmetric sets: visual example



$$[1,0] = \{(1,0)\}$$

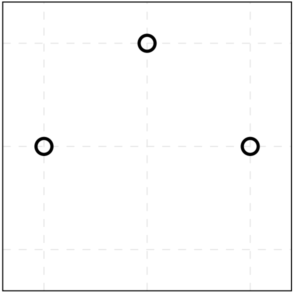
Fully symmetric sets: visual example



$$[1, 0] =$$

$$\{(1, 0), (0, 1)\}$$

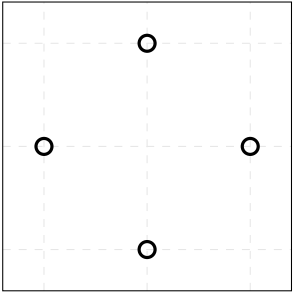
Fully symmetric sets: visual example



$$[1, 0] =$$

$$\{(1, 0), (0, 1), (-1, 0)\}$$

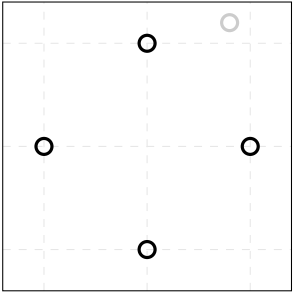
Fully symmetric sets: visual example



$$[1, 0] =$$

$$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$$

Fully symmetric sets: visual example



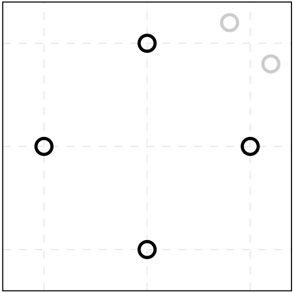
$[1, 0] =$

$$\{(1,0),(0,1),(-1,0),(0,-1)\}$$

$[0.8, 1.2] =$

$$\{(0.8, 1.2)\}$$

Fully symmetric sets: visual example



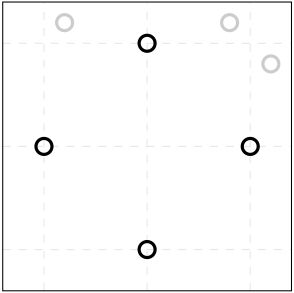
$[1, 0] =$

$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$

$[0.8, 1.2] =$

$\{(0.8, 1.2), (1.2, 0.8)\}$

Fully symmetric sets: visual example



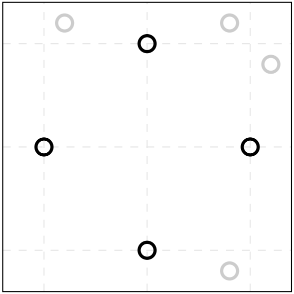
$[1, 0] =$

$\{(1,0),(0,1),(-1,0),(0,-1)\}$

$[0.8, 1.2] =$

$\{(0.8,1.2),(1.2,0.8),(-0.8,1.2)\}$

Fully symmetric sets: visual example



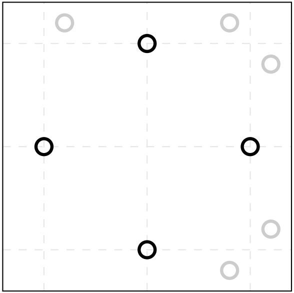
$[1, 0] =$

$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$

$[0.8, 1.2] =$

$\{(0.8, 1.2), (1.2, 0.8), (-0.8, 1.2),$
$(0.8, -1.2)\}$

Fully symmetric sets: visual example



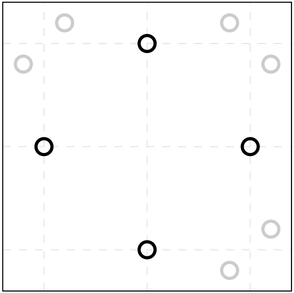
$[1, 0] =$

$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$

$[0.8, 1.2] =$

$\{(0.8, 1.2), (1.2, 0.8), (-0.8, 1.2),$
$(0.8, -1.2), (1.2, -0.8)\}$

Fully symmetric sets: visual example



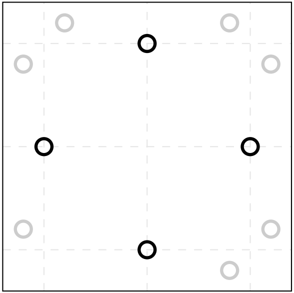
$[1,0] =$

$\{(1,0),(0,1),(-1,0),(0,-1)\}$

$[0.8,1.2] =$

$\{(0.8,1.2),(1.2,0.8),(-0.8,1.2),$
$(0.8,-1.2),(1.2,-0.8),$
$(-1.2,0.8)\}$

Fully symmetric sets: visual example



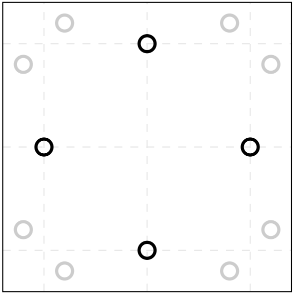
$[1, 0] =$

$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$

$[0.8, 1.2] =$

$\{(0.8, 1.2), (1.2, 0.8), (-0.8, 1.2),$
$(0.8, -1.2), (1.2, -0.8),$
$(-1.2, 0.8), (-1.2, -0.8)\}$

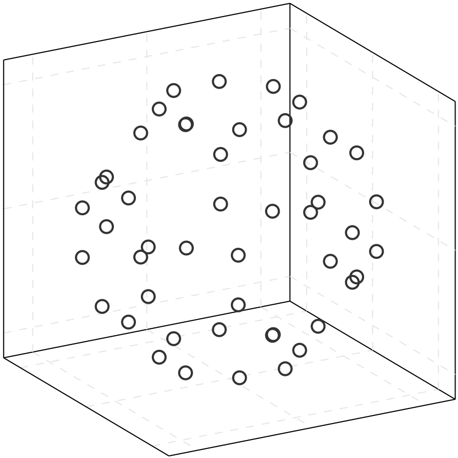
Fully symmetric sets: visual example



$[1, 0] =$
$\{(1, 0), (0, 1), (-1, 0), (0, -1)\}$

$[0.8, 1.2] =$
$\{(0.8, 1.2), (1.2, 0.8), (-0.8, 1.2),$
$(0.8, -1.2), (1.2, -0.8),$
$(-1.2, 0.8), (-1.2, -0.8),$
$(-0.8, -1.2)\}$

A fully symmetric set in $\mathbb{R}^3$



Generator vector: $\mathbf{(1, 0.5, 0.2)}$; number of elements: **48**

How many points?

If m is the number of non-zero generators and $m_1, \ldots, m_l$ are multiplicities of distinct generators, the fully symmetric set contains $\mathbf{2^m d!/(m_1! \cdots m_l!)}$ points.

Figure: Cardinalities of fully symmetric sets generated by $m = 1, \ldots, 9$ distinct non-zero generators for dimensions $d = 2, \ldots, 9$.

	Dimension							
m	2	3	4	5	6	7	8	9
1	4	6	8	10	12	14	16	18
2	8	24	48	80	120	168	224	288
3		48	192	480	960	1,680	2,688	4,032
4			384	1,920	5,760	13,440	26,880	48,384
5				3,840	23,040	80,640	215,040	483,840
6					46,080	322,560	1,290,240	3,870,720
7						645,120	5,160,960	23,224,320
8							10,321,920	92,897,280
9								185,794,560

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Fully symmetric quadrature rules

Fully symmetric quadrature rule

The node set of a fully symmetric quadrature rule is a union of fully symmetric sets and all the nodes of a particular FSS are assigned equal weights:

$$\mu(f) := \int_\Omega f \, \mathrm{d}\mu \approx \sum_{j=1}^{J} w_j f[\boldsymbol{\lambda}_j] := \sum_{j=1}^{J} w_j \sum_{\boldsymbol{\xi} \in [\boldsymbol{\lambda}_j]} f(\boldsymbol{\xi}),$$

where $\Omega \subset \mathbb{R}^d$, μ is a measure on Ω, and the full node set $\mathcal{X}$ is a union of J fully symmetric sets $[\boldsymbol{\lambda}_1], \ldots, [\boldsymbol{\lambda}_J]$.

The fully symmetric sets and their weights are usually selected so that the rule is exact whenever f is a low-degree polynomial.

Kernel quadrature

Given a positive-definite kernel $k\colon \Omega \times \Omega \to \mathbb{R}$, the kernel quadrature rule Q_k is

$$Q_k(f) := \sum_{i=1}^{n} w_i f(\mathbf{x}_i) \approx \mu(f) = \int_\Omega f \, \mathrm{d}\mu.$$

The weights $w_1, \ldots, w_n$ are solved from

$$\begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \mu\big[k(\mathbf{x}_1, \cdot)\big] \\ \vdots \\ \mu\big[k(\mathbf{x}_n, \cdot)\big] \end{pmatrix} = \begin{pmatrix} \mu_k(\mathbf{x}_1) \\ \vdots \\ \mu_k(\mathbf{x}_n) \end{pmatrix}$$

$$\mathbf{K}\mathbf{w} = \mu_k(\mathcal{X}).$$

The associated worst-case error (posterior standard deviation) is

$$e(Q_k) = \sup_{\|f\|_{\mathcal{H}(k)} \leq 1} |\mu(f) - Q_k(f)| = \sqrt{\mu(\mu_k) - Q_k(\mu_k)}.$$

Fully symmetric kernel quadrature

Theorem

Suppose that for any permutation matrix $\mathbf{P}$

1. $\Omega = \mathbf{P}\Omega = \{\mathbf{P}\omega : \omega \in \Omega\}$;
2. *The density* w *of* μ *satisfies* $w(\mathbf{x}) = w(\mathbf{P}\mathbf{x})$;
3. *The kernel* k *satisfies* $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{P}\mathbf{x}, \mathbf{P}\mathbf{x}')$.

If the nodeset $\mathcal{X}$ *is a union of fully symmetric sets, then the kernel quadrature rule is a fully symmetric quadrature rule.*

Examples:

Kernel: isotropic or a product/sum of 1D isotropics.

Domain: Whole of $\mathbb{R}^d$ or $[-1, 1]^d$.

Measure: Uniform, standard Gaussian/Student's t.

Fully symmetric kernel quadrature: computation I

$$\begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \mu_k(\mathbf{x}_1) \\ \vdots \\ \mu_k(\mathbf{x}_n) \end{pmatrix}$$

Fully symmetric kernel quadrature: computation I

$$\begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \mu_k(\mathbf{x}_1) \\ \vdots \\ \mu_k(\mathbf{x}_n) \end{pmatrix}$$

Let the node set be a union of fully symmetric sets, $\mathcal{X} = \cup_{j=1}^{J} [\boldsymbol{\lambda}_j]$.

Fully symmetric kernel quadrature: computation I

$$\begin{pmatrix} k(\mathsf{x}_1, \mathsf{x}_1) & \cdots & k(\mathsf{x}_1, \mathsf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathsf{x}_n, \mathsf{x}_1) & \cdots & k(\mathsf{x}_n, \mathsf{x}_n) \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \mu_k(\mathsf{x}_1) \\ \vdots \\ \mu_k(\mathsf{x}_n) \end{pmatrix}$$

Let the node set be a union of fully symmetric sets, $\mathcal{X} = \cup_{j=1}^{J} [\boldsymbol{\lambda}_j]$.

$\Longrightarrow$ The kernel mean vector is $\mu_k(\mathcal{X}) = (\boldsymbol{\mu}^1, \ldots, \boldsymbol{\mu}^J)$, all the elements of each $\boldsymbol{\mu}^j$ are equal to μ^j, and $\#\boldsymbol{\mu}^j = \#[\boldsymbol{\lambda}_j]$.

$\Longrightarrow$ The weight vector $\mathbf{w} = (w_1, \ldots, w_n)$ is of the same structure as $(\boldsymbol{\mu}^1, \ldots, \boldsymbol{\mu}^J)$. That is, $\mathbf{w} = (\mathbf{w}^1, \ldots, \mathbf{w}^J)$, $\#\mathbf{w}^j = \#[\boldsymbol{\lambda}_j]$.

Fully symmetric kernel quadrature: computation I

$$\begin{pmatrix} \mathsf{K}_{11} & \cdots & \mathsf{K}_{1J} \\ \vdots & \ddots & \vdots \\ \mathsf{K}_{J1} & \cdots & \mathsf{K}_{JJ} \end{pmatrix} \begin{pmatrix} \mathbf{w}^1 \\ \vdots \\ \mathbf{w}^J \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu}^1 \\ \vdots \\ \boldsymbol{\mu}^J \end{pmatrix}$$

Let the node set be a union of fully symmetric sets, $\mathcal{X} = \cup_{j=1}^{J} [\boldsymbol{\lambda}_j]$.

$\Longrightarrow$ The kernel mean vector is $\mu_k(\mathcal{X}) = (\boldsymbol{\mu}^1, \ldots, \boldsymbol{\mu}^J)$, all the elements of each $\boldsymbol{\mu}^j$ are equal to μ^j, and $\#\boldsymbol{\mu}^j = \#[\boldsymbol{\lambda}_j]$.

$\Longrightarrow$ The weight vector $\mathbf{w} = (w_1, \ldots, w_n)$ is of the same structure as $(\boldsymbol{\mu}^1, \ldots, \boldsymbol{\mu}^J)$. That is, $\mathbf{w} = (\mathbf{w}^1, \ldots, \mathbf{w}^J)$, $\#\mathbf{w}^j = \#[\boldsymbol{\lambda}_j]$.

The submatrices K_{ij} contain kernel evaluations for $[\boldsymbol{\lambda}_i]$ and $[\boldsymbol{\lambda}_j]$:

$$\begin{aligned} [\mathsf{K}_{ij}]_{pq} &= k(\mathsf{x}_p, \mathsf{x}'_q), \\ \mathsf{x}_p &= p\text{th element of } [\boldsymbol{\lambda}_i], \\ \mathsf{x}'_q &= q\text{th element of } [\boldsymbol{\lambda}_j]. \end{aligned}$$

Fully symmetric kernel quadrature: computation II

$$\begin{pmatrix} \mathsf{K}_{11} & \cdots & \mathsf{K}_{1J} \\ \vdots & \ddots & \vdots \\ \mathsf{K}_{J1} & \cdots & \mathsf{K}_{JJ} \end{pmatrix} \begin{pmatrix} \mathbf{w}^1 \\ \vdots \\ \mathbf{w}^J \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu}^1 \\ \vdots \\ \boldsymbol{\mu}^J \end{pmatrix}$$

Each of the submatrices K_{ij} has **identical row sums**. That is, $\sum_{q=1}^{\#[\boldsymbol{\lambda}_j]} [\mathsf{K}_{ij}]_{pq} = S_{ij}$ does not depend on the row p.

$\implies$ The J "block rows" are $\mathsf{K}_{i1}\mathbf{w}^1 + \cdots + \mathsf{K}_{iJ}\mathbf{w}^J = \boldsymbol{\mu}^i$ for $i = 1, \ldots, J$.

$\implies$ But each of these is just $\#[\boldsymbol{\lambda}_j]$ equations $S_{i1}w^1 + \cdots S_{iJ}w^J = \mu^J$!

Fully symmetric kernel quadrature: computation III

The system of n equations

$$\begin{pmatrix} \mathsf{K}_{11} & \cdots & \mathsf{K}_{1J} \\ \vdots & \ddots & \vdots \\ \mathsf{K}_{J1} & \cdots & \mathsf{K}_{JJ} \end{pmatrix} \begin{pmatrix} \mathbf{w}^1 \\ \vdots \\ \mathbf{w}^J \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu}^1 \\ \vdots \\ \boldsymbol{\mu}^J \end{pmatrix}$$

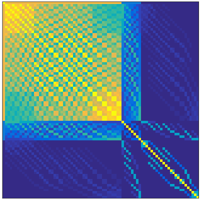
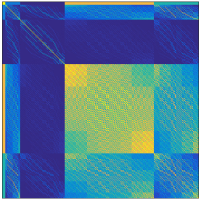
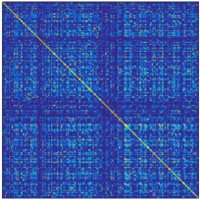
is converted into the system

$$\begin{pmatrix} S_{11} & \cdots & S_{1J} \\ \vdots & \ddots & \vdots \\ S_{J1} & \cdots & S_{JJ} \end{pmatrix} \begin{pmatrix} w^1 \\ \vdots \\ w^J \end{pmatrix} = \begin{pmatrix} \mu^1 \\ \vdots \\ \mu^J \end{pmatrix}$$

of J equations, where $S_{ij} = \sum_q [\mathsf{K}_{ij}]_{pq}$ for any p.

The J distinct weights $w^1, \ldots, w^J$ can be solved very efficiently because typically $J \ll n$.

What do the kernel matrices look like?

Gaussian kernel matrices for the node sets

$\mathcal{X} = [0] \cup [0.5, 0.4, 0.1] \cup [1, 1, 1] \cup [2, 1, 2] \subset \mathbb{R}^3$, $\#\mathcal{X} = 81$;

$\mathcal{X} = [0.05] \cup [1, 1, 1] \cup [2, 1, 2] \cup [0.5, 0.4, 0.1] \cup [0.5, 0.5, 1] \subset \mathbb{R}^4$, $\#\mathcal{X} = 424$;

$\mathcal{X} =$ 200 standard normal points in $\mathbb{R}^4$.

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Sparse grids: definition

Sparse grid

Let $X^1 = \{0\}$ and $X^i \subset X^{i+1} \subset [-1, 1]$ for $i > 1$ be finite, nested and symmetric (i.e. if $x \in X^i$, then $-x \in X^i$) point sets. Then the *sparse grid* of *level* $q \geq 1$ is the set

$$H(q, d) := \bigcup_{|\alpha|=d+q} \left(X^{\alpha_1} \times \cdots \times X^{\alpha_d}\right) \subset [-1, 1]^d, \qquad (*)$$

where $\alpha \in \mathbb{N}^d$ is a d-dimensional multi-index.

The largest X^i appearing is X^{q+1} as a part of $X^1 \times \cdots X^1 \times X^{q+1}$.

The full Cartesian grid would be $X^{q+1} \times \cdots \times X^{q+1}$, which is a significantly larger set than any member of the union in Eq. $(*)$.

Sparse grids: some examples

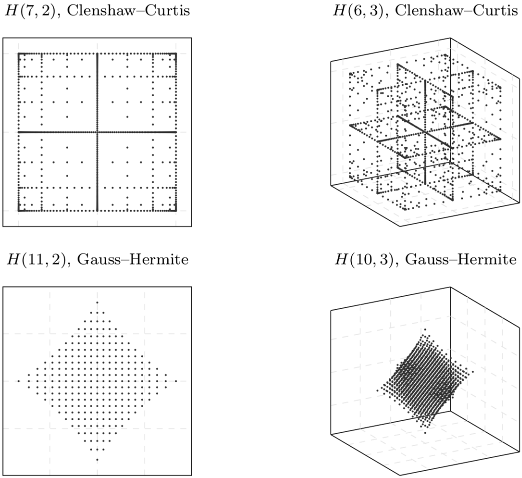


Fig. 4.1: Examples of sparse grids with Clenshaw–Curtis and Gauss–Hermite nodes. The numbers of nodes in the sparse grids are 705 (upper left), 1,073 (upper right), 265 (lower left), and 1,561 (lower right). Compare these to the cardinalities of the corresponding full grids that are $129^2 = 16{,}641$; $65^3 = 274{,}625$; $23^2 = 529$; and $21^3 = 9{,}261$.

Sparse grids: some properties

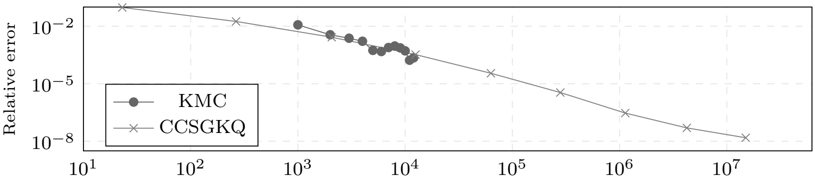
— Sparse grids are "sparsified" versions of full Cartesian product grids and require significantly less points.

— Sparse grids, as defined above, are unions of fully symmetric sets.

— This is not the most general definition: the sets X^i need not be symmetric nor nested and sparse grids can be constructed also for the whole of $\mathbb{R}^d$.

— To obtain high polynomial exactness, the sets X^i come coupled with weights of univariate quadrature rules that are used to construct the sparse grids weights. This construction yields a fully symmetric quadrature rule.

Closed-form numerical example



Integrand: $f(\mathbf{x}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}_f\|^2}{2\ell^2}\right)$, $\ell = 0.8$

Domain and measure: $\Omega = \mathbb{R}^{11}$, $\mu =$ standard Gaussian

Kernel: Gaussian, $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2\ell^2}\right)$

Nodes: Clenshaw–Curtis sparse grids of levels 1 to 9 (23 to 15,005,761 nodes).

Closed-form numerical example continued

level	# of nodes	# of FSSs	computation time
1	23	2	$< 1\,s$
2	265	4	$< 1\,s$
3	2,069	8	$< 1\,s$
4	12,497	17	$< 1\,s$
5	63,097	36	$< 1\,s$
6	280,017	79	$\approx 1.5\,s$
7	1,129,569	172	$\approx 9\,s$
8	4,236,673	379	$\approx 64\,s$
9	15,005,761	832	$\approx 8\,min$

Discussion

Selecting the fully symmetric sets:

— One could select a number of generators vectors of fixed structure and minimize the WCE over the generators.

— The sparse grid 1D point sequences could be selected based on e.g. sequential minimization of the WCE.

Setting the kernel parameters:

— The algorithm does not result in an efficient way of optimizing the kernel parameters.

— In high dimensions setting these parameters via e.g. marginal likelihood maximization seems to be impossible anyway.

— The length-scale needs to be large in high dimension because a) distances are longer and b) the nodes do not cover the space adequately. Use heuristics?

Thank you for your attention!