Numerical Simulation

Sparse Grids

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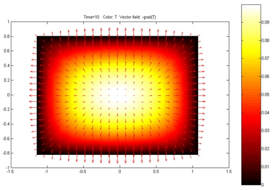
Course 2: Numerical Simulation – From Models to Visualizations

Outline

Some Example Problems

- PDE: $\triangle u = f$ in Ω and $u|_{\partial\Omega} = 0$



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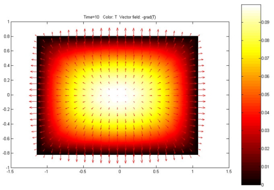

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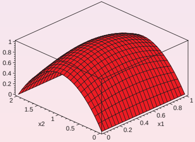
- numerical quadrature



compute $\int_\Omega f(x)\,dx$

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So do what we have to do ?

- evaluate $f(x)$ for many different states $x \in \Omega$
- but: evaluation of f is expensive

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With a naive approach (n sample points in each dimension):

- 1-dim: n evaluations of f
- d-dim: n^d evaluations of f

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Challenge

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- keep quality of u_S still as high as possible

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$$S = \mathrm{span}\{\phi_i : 1 \leq i \leq n\}$$

- $\Rightarrow$ get an approximative u_S as linear combination of basis functions:

$$u_S = \sum_{i=1}^{n} \alpha_i \cdot \phi_i$$

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- the ϕ_i should be inexpensive to evaluate
- $\dim(S)$ should be small for an optimal approximation
- w.l.o.g. we set $\Omega := [0, 1], \quad u(0) = u(1) = 0$

Piecewise Linear Approach

- consider $n = 2^\ell - 1$ equidistant (inner) knots

$$x_{\ell,i} = i \cdot h_\ell \qquad \text{with } h_\ell = 2^{-\ell} \text{ and } 1 \le i \le 2^\ell - 1$$

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- for every point $x_{\ell,i}$ we construct a function $\phi_{\ell,i}(x) : \Omega \to \mathbb{R}$

$$\phi_{\ell,i}(x) = \phi\left(\frac{x - x_{\ell,i}}{h_\ell}\right), \qquad T_{\ell,i} := \operatorname{supp}(\phi_{\ell,i}) = [x_{\ell,i-1}, x_{\ell,i+1}]$$

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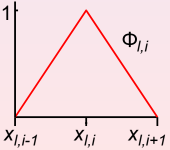
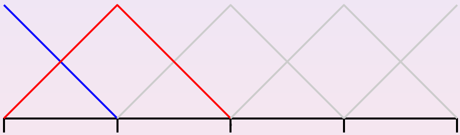


Nodal Point Basis

- the nodal point basis

$$\Phi_\ell := \{\phi_{\ell,i}, i = 1, \dots, 2^\ell - 1\}$$



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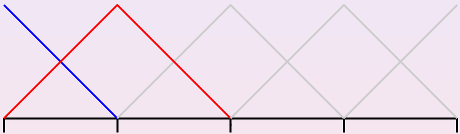

- the resulting subspace of V:

$$S_\ell := \mathrm{span}(\Phi_\ell), \qquad \dim(S_\ell) = 2^\ell - 1$$

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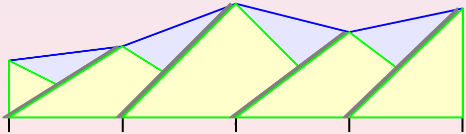
- example for an arbitrary function $u_\ell \in S_\ell$



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For the function $u(x) = 4x(1-x)$ we have the following coefficients:

	$\alpha_i = u_\ell(x_{\ell,i})$						
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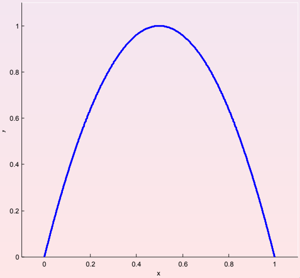
$\ell = 2$		$3/4$		1		$3/4$	
$\ell = 3$	$7/16$	$3/4$	$15/16$	1	$15/16$	$3/4$	$7/16$



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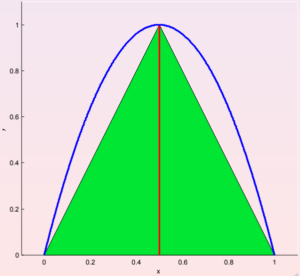

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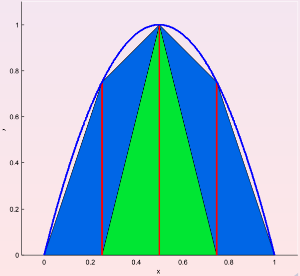

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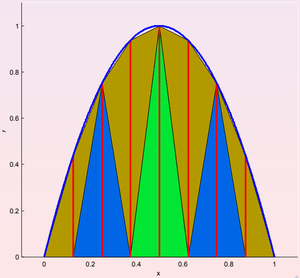

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What do we have so far ?

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Search for an alternative basis for S_ℓ !

Hierarchical Increments

- we define the hierarchical increments

$$W_\ell := \mathrm{span}\{\phi_{\ell,i} : i \in I_\ell\} \qquad I_\ell := \{i : 1 \leq i \leq 2^\ell - 1, i \text{ odd}\}$$

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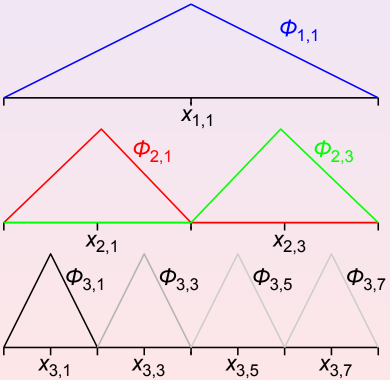
- the basis functions for the hierarchical increments W_1, W_2, W_3:



Hierarchical Basis and Hierarchical Surpluses

- we get a new view of S_ℓ and V

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- with the hierarchical surpluses w_ℓ

$$u(x) = \sum_{\ell=1}^{\infty} w_\ell(x), \qquad w_\ell = \sum_{i \in I_\ell} v_{\ell,i} \cdot \phi_{\ell,i} \in W_\ell$$

$$v_{\ell,i} = u(x_{\ell,i}) - \frac{u(x_{\ell,i-1}) + u(x_{\ell,i+1})}{2}$$

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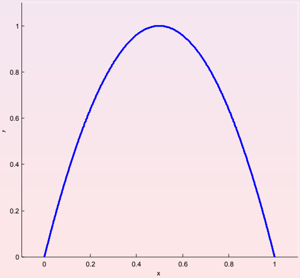

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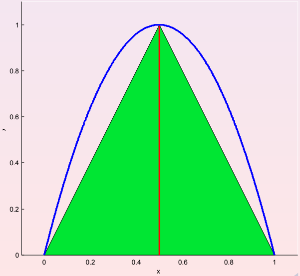

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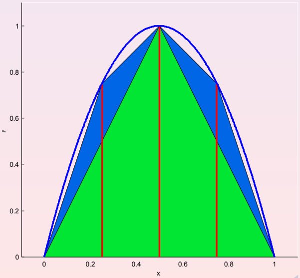

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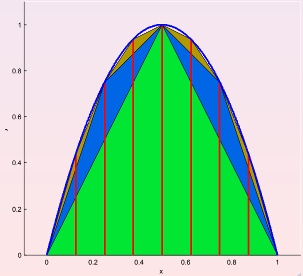

Convergence

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- it seems that the $v_{\ell,i}$ decrease very fast with increasing ℓ
- are the w_ℓ really less important for large ℓ ?
- to decide about the importance of each w_ℓ: define some norms

Norms

There are different possibilities to define norms in V

Important norms in our applications:

maximum norm:

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energy norm:

$$\|\phi_{\ell,i}\|_E := \sqrt{\int_\Omega (\phi'_{\ell,i}(x))^2\,dx} = \sqrt{\frac{2}{h_\ell}}$$

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- we need another representation of $v_{\ell,i}$:

$$v_{\ell,i} = \int_0^1 -\frac{h_\ell}{2} \cdot \phi_{\ell,i} \cdot u''(x)\, dx$$

- now we can find some upper bounds for the $v_{\ell,i}$

$$|v_{\ell,i}| \leq \frac{h_\ell^2}{2} \cdot \|u''|_{T_{\ell,i}}\|_\infty$$

$$|v_{\ell,i}| \leq \frac{h_\ell^3}{6} \cdot \|u''|_{T_{\ell,i}}\|_2$$

Norms

And what we originally wanted to quantify:

$$
\begin{aligned}
\|w_\ell\|_\infty &\leq \frac{h_\ell^2}{2} \cdot \quad \|u''\|_\infty \\
\|w_\ell\|_2 &\leq \frac{h_\ell^2}{3} \cdot \quad \|u''\|_2 \\
\|w_\ell\|_W &\leq \frac{h_\ell}{2} \cdot \quad \|u''\|_\infty
\end{aligned}
$$

Approximation Error

With these results it is possible to quantify the approximation error:

approximation error

$$\|u - u_n\|_\infty \leq \frac{\|u''\|_\infty}{6} \cdot h_n^2 = \mathcal{O}(h_n^2)$$

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\|u - u_n\|_E &\leq \frac{\|u''\|_\infty}{2} \cdot h_n = \mathcal{O}(h_n)
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(with $d = 1$: $n = \ell$)

Approximation Error

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$$\begin{array}{lclcl} \|u-u_n\|_\infty & \leq & \frac{\|u''\|_\infty}{6} \cdot & h_n^2 & = & \mathcal{O}(h_n^2) \\ \|u-u_n\|_2 & \leq & \frac{\|u''\|_2}{9} \cdot & h_n^2 & = & \mathcal{O}(h_n^2) \\ \|u-u_n\|_E & \leq & \frac{\|u''\|_\infty}{2} \cdot & h_n & = & \mathcal{O}(h_n) \end{array}$$

(with $d = 1$: $n = \ell$)

Often an estimation of the error is possible:

- e.g. finite elements $u'' = f$

$$\Rightarrow \quad \|u''\|_* = \|f\|_*$$

Outline

Some Definitions

- w.l.o.g. $\Omega = [0,1]^d$, $u|_{\partial\Omega} = 0$ and $u(x) = u(x_1, \ldots, x_d)$
- now ℓ is a grid vector:

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- the grid points:

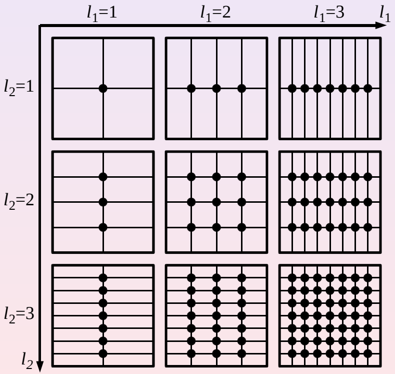
$$x_{\ell,i} := (i_1 \cdot h_{\ell_1}, \dots, i_d \cdot h_{\ell_d}) \text{ with } 1 \leq i < 2^\ell$$

(the $\leq$ is componentwise, i.e. $\forall j : 1 \leq i_j \leq 2^{\ell_j} - 1$)

Some Definitions

Here are the first grid points for $d = 2$ $(\ell$ up to $(3,3))$:

$$x_{\ell,i} := (i_1 \cdot h_{\ell_1}, \ldots, i_d \cdot h_{\ell_d}) \text{ with } 1 \leq i < 2^{\ell}$$



d-linear Functions

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$$\phi_{\ell,i}(x) = \prod_{j=1}^{d} \phi_{\ell_j,i_j}(x_j)$$

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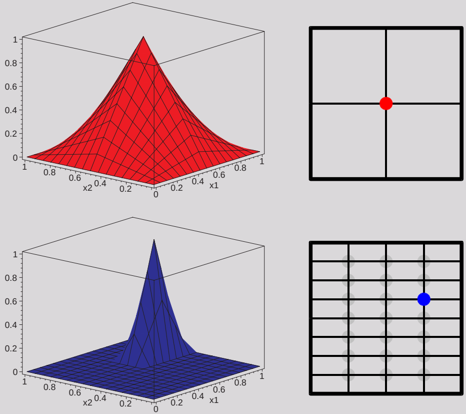
- get d-linear basis functions
  (i.e. for fixed $(d-1)$ *coordinates, function is linear in the remaining variable)*

Basis Functions in 2 Dimensions

Example

the functions $\phi_{(1,1),(1,1)}$ and $\phi_{(2,3),(3,5)}$



Basis and Subspaces

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for a fixed $\ell \in \mathbb{N}^d$ we define:

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Now we have to make some definitions, analog to the 1 dimensional case

for a fixed $\ell \in \mathbb{N}^d$ we define:

- we get the subspace

$$S_\ell := \mathrm{span}\{\Phi_\ell\} = \mathrm{span}\{\psi_\ell\} = \bigoplus_{k \le \ell} W_k$$

- the dimension of S_ℓ

$$\dim(S_\ell) = (2^{\ell_1} - 1) \cdot \dots \cdot (2^{\ell_d} - 1) = \mathcal{O}(2^{|\ell|_1})$$

- the whole space can be represented by the W_k

$$V = S_\infty = \bigoplus_{k \in \mathbb{N}^d} W_k$$

Basis and Subspaces

Now we have to make some definitions, analog to the 1 dimensional case

for a fixed $\ell \in \mathbb{N}^d$ we define:

- the hierarchical surpluses of $u \in V$

$$u(x) = \sum_{\ell \in \mathbb{N}^d} w_\ell(x), \qquad w_\ell = \sum_{i \in I_\ell} v_{\ell,i} \cdot \phi_{\ell,i} \in W_\ell$$

- and the $v_{\ell,i}$, same as in 1 dimension *(maybe a litte more complicated ;-))*

$$v_{\ell,i} = \left(\prod_{j=1}^{d} \begin{bmatrix} -\frac{1}{2} & 1 & -\frac{1}{2} \end{bmatrix}_{x_{\ell_j,i_j},\ell_j} \right) u$$

Hierarchical Surpluses

Example

for 2 dimensions, $v_{\ell,(i_1,i_2)}$ is as follows:

$$v_{\ell,(i_1,i_2)} = \frac{u(x_{\ell,(i_1-1,i_2-1)}) - 2u(x_{\ell,(i_1,i_2-1)}) + u(x_{\ell,(i_1+1,i_2-1)})}{4} + \frac{-2u(x_{\ell,(i_1-1,i_2)}) + 4u(x_{\ell,(i_1,i_2)}) - 2u(x_{\ell,(i_1+1,i_2)})}{4} + \frac{u(x_{\ell,(i_1-1,i_2+1)}) - 2u(x_{\ell,(i_1,i_2+1)}) + u(x_{\ell,(i_1+1,i_2+1)})}{4}$$

$v_{\ell,i}$ - Another Representation

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$v_{\ell,i}$ - Another Representation

There is an integral representation for $v_{\ell,i}$, analogious to 1-dim

- first of all, a different definition for u'':

$$u'' := \frac{\partial^{2d} u}{\partial x_1^2 \cdots \partial x_d^2}$$

- the new representation:

$$v_{\ell,i} = \int_\Omega \left(\prod_{j=1}^{d} -\frac{h_{\ell_j}}{2} \cdot \phi_{\ell_j,i_j}(x_j) \right) u''(x)\, dx$$

Norms – d Dimensions

for the basis functions we have:

$$
\begin{aligned}
\|\phi_{\ell,i}\|_\infty &= 1 \\
\|\phi_{\ell,i}\|_2 &= \left(\tfrac{2}{3}\right)^{\frac{d}{2}} \cdot \quad 2^{-|\ell|_1/2} \\
\|\phi_{\ell,i}\|_E &= \sqrt{2} \cdot \left(\tfrac{2}{3}\right)^{\frac{d-1}{2}} \cdot \quad 2^{-|\ell|_1/2} \quad \left(\textstyle\sum_{j=1}^{d} 2^{2\ell_j}\right)^{\frac{1}{2}}
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\end{aligned}
$$

and for the coefficients:

$$
\begin{aligned}
|v_{\ell,i}| &\leq 2^{-d} \cdot 2^{-2|\ell|_1} \cdot \|u''\|_\infty \\
|v_{\ell,i}| &\leq 2^{-d} \cdot \left(\tfrac{2}{3}\right)^{\frac{d}{2}} 2^{-3/2|\ell|_1} \cdot \|u''|_{T_{\ell,i}}\|_2
\end{aligned}
$$

Norms – d Dimensions

we are interested in the surpluses:

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\begin{aligned}
\|w_\ell\|_\infty &\leq 2^{-d} \cdot 2^{-2|\ell|_1} \cdot \|u''\|_\infty &= \mathcal{O}(h_1^2 \cdots h_d^2) \\
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$$\begin{aligned} \|w_\ell\|_\infty &\leq \frac{1}{2 \cdot 12^{(d-1)/2}} \cdot 2^{-2|\ell|_1} \cdot \left(\sum_{j=1}^{d} 2^{2\ell_j} \right)^{\frac{1}{2}} \cdot \|u''\|_\infty \\ &= \mathcal{O}\left(h_1^2 \cdots h_d^2 \cdot \sqrt{\sum_{j=1}^{d} \frac{1}{h_j^2}} \right) \end{aligned}$$

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- take a set $L \subset \mathbb{N}^d$
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$$\|u - u_L\| \leq \sum_{\ell \notin L} \|w_\ell\|$$

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- approximation error with this L:

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which L is the best to take?

Outline

First Idea

We have to search for an optimal $L \subset \mathbb{N}^d$

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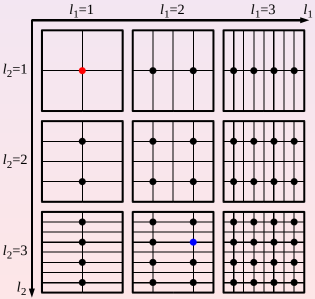

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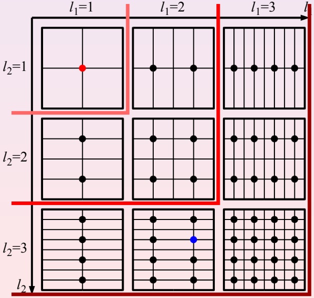

Evaluation – Costs

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the more points $\widehat{=}$ *functions in* W_ℓ*, the higher the costs*

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- Costs of the full grid S_n^∞: In each coordinate $2^n - 1$ possibilities

$$\Rightarrow \quad C(S_n^\infty) = \mathcal{O}(2^{nd})$$

Evaluation – Benefits

- and look at the benefits of each ℓ:

$$\operatorname{maxfail}(L \cup \{\ell\}) - \operatorname{maxfail}(L) = \sum_{k \notin L \cup \{\ell\}} \|w_k\|_* - \sum_{k \notin L} \|w_k\|_* = \|w_\ell\|_*$$

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$$\begin{aligned} b_\infty(\ell) = b_2(\ell) &:= 2^{-2|\ell|_1} \\ b_E(\ell) &:= 2^{-2|\ell|_1} \cdot \left(\sum_{j=1}^{d} 2^{2\ell_j} \right)^{\frac{1}{2}} \end{aligned}$$

benefit $b(\ell)$ is the on ℓ dependend part of the bound of w_ℓ

Cost-Benefit Ratio

Now we can evaluate the quality of each ℓ: the ratio of benefit and cost

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$$cbr_2(\ell) = cbr_\infty(\ell) = \frac{b_*(\ell)}{c(\ell)} = \frac{2^{-2|\ell|_1}}{2^{|\ell|_1 - d}} = 2^{-3|\ell|_1 + d}$$

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- the ratio is best for small $|\ell|_1$
- so we define

$$L_n^1 := \{\ell \in \mathbb{N}^d : |\ell|_1 \leq n + d - 1\}$$

$$S_n^1 := \bigoplus_{\ell \in L_n^1} W_\ell$$

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So, what is a SPARSE GRID ?

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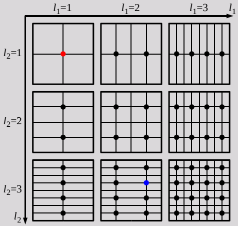
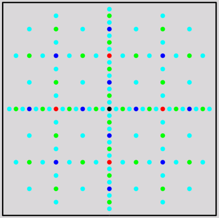
example with $d = 2, n = 5$





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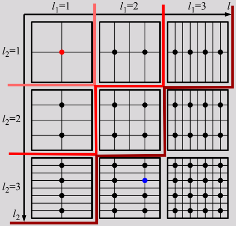

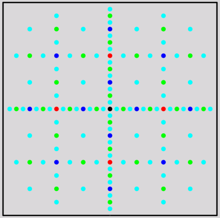

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Comparison: Full – Sparse Grid

How good is a sparse grid ?

Analysis of the approximation error – ∞-norm:

$$\begin{aligned} \|u - u_n^\infty\|_\infty &\leq \frac{d}{6^d} \cdot 2^{-2n} \cdot \|u''\|_\infty \\ \|u - u_n^1\|_\infty &\leq \frac{2}{8^d} \cdot 2^{-2n} \cdot \|u''\|_\infty \cdot \left(\frac{n^{d-1}}{(d-1)!} + \mathcal{O}(n^{d-2}) \right) \end{aligned}$$

$$\|u - u_n^\infty\|_\infty = \mathcal{O}(h_n^2), \qquad \|u - u_n^1\|_\infty = \mathcal{O}(h_n^2 \cdot n^{d-1})$$

Comparison: Full – Sparse Grid

How good is a sparse grid ?

Analysis of the approximation error – L_2-norm:

$$\|u - u_n^\infty\|_2 \leq \frac{d}{9^d} \cdot 2^{-2n} \cdot \|u''\|_2$$

$$\|u - u_n^1\|_2 \leq \frac{2}{12^d} \cdot 2^{-2n} \cdot \|u''\|_2 \cdot \left(\frac{n^{d-1}}{(d-1)!} + \mathcal{O}(n^{d-2}) \right)$$

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Comparison: Full – Sparse Grid

How good is a sparse grid ?

Analysis of the approximation error – E-norm:

$$\|u - u_n^\infty\|_E \leq \frac{d^{3/2}}{2 \cdot 3^{(d-1)/2} \cdot 6^{d-1}} \cdot 2^{-n} \cdot \|u''\|_\infty$$

$$\|u - u_n^1\|_E \leq \frac{d}{2 \cdot 3^{(d-1)/2} \cdot 4^{d-1}} \cdot 2^{-n} \cdot \|u''\|_\infty$$

$$\boxed{\|u - u_n^\infty\|_E = \mathcal{O}(h_n), \qquad \|u - u_n^1\|_E = \mathcal{O}(h_n)}$$

Comparison: Full – Sparse Grid

How good is a sparse grid ?

Indeed – it is very good, especially for high dimensional problems

approximation errors

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\begin{aligned}
\|u - u_n^\infty\|_\infty &= \mathcal{O}(h_n^2), & \|u - u_n^1\|_\infty &= \mathcal{O}(h_n^2 \cdot n^{d-1}) \\
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\end{aligned}
$$

- dimensions:

$$
\dim(S_n^\infty) = \mathcal{O}(2^{nd}), \qquad \dim(S_n^1) = \mathcal{O}(2^n \cdot n^{d-1})
$$

Sizes of Dimensions

Already with small d, the effect is quite drastic

Dimension Comparison

- $d = 2$

n	1	2	3	4	5	...	10
$\dim(S_n^\infty)$	1	9	49	225	961	...	1 046 529
$\dim(S_n^1)$	1	5	17	49	129	...	9 217

- $d = 3$

n	1	2	3	4	...	10
$\dim(S_n^\infty)$	1	27	343	225	...	1 070 590 167
$\dim(S_n^1)$	1	7	17	31	...	47 103

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- we have

$$b_E(\ell) = 2^{-2|\ell|_1} \cdot \left(\sum_{j=1}^{d} 2^{2\ell_j} \right)^{\frac{1}{2}}$$

- one can show

$$\dim(S_n^E) \leq 2^n \cdot \frac{d}{2} \cdot e^d = \mathcal{O}(2^n) \quad , \quad S_n^E \subset S_n^1$$

$$\|u - u_n^E\|_E = \mathcal{O}(h_n) = \|u - u_n^{\infty/1}\|_E$$

Outline

1. Introduction
2. Hierarchical Basis
   - In 1 dimension
   - In 2 or more dimensions
   - Sparse grids
3. Conclusion

Different Ω

We always assumed $\Omega = [0,1]^d$. What's about $\Omega \neq [0,1]^d$?

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- for Ω cuboid: linear transformation of coordinates of $x_{i,\ell}$:

$$x_{i,\ell} = \left(a_j + i_j \cdot \frac{b_j - a_j}{2^\ell} \right)_{j=1,\dots,d}$$

Different Ω

We always assumed $\Omega = [0,1]^d$. What's about $\Omega \neq [0,1]^d$?

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$$x_{i,\ell} = \left(a_j + i_j \cdot \frac{b_j - a_j}{2^\ell} \right)_{j=1,\dots,d}$$

- for abitrary Ω:
  - approximate Ω with cuboids C
    (additional approximation error, take care of special properties of u !)
  - transform cuboid into a fitting shape e.g. circle or sphere

Adaptive Refinement

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- for adaptivity:
  - partition Ω (e.g. halfs, quarters)
  - evaluate error for each part T

$$\|(u-u_n)|_T\|_* = \|u-u_n\|_* \cdot \frac{\|u''|_T\|_*}{\|u''\|_*} \cdot \frac{\text{area}(T)}{\text{area}(\Omega)}, \quad (* = 2/E)$$

  - new sparse grid on T where the error is maximal

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  - new sparse grid on T where the error is maximal
- Caution: we usually don't know $u'' = \frac{\partial^{2d} u}{\partial x_1^2 \cdots \partial x_d^2}$ for $d > 2$

  if at all, we only know $\triangle u := \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}$ *(e.g. PDE: $\triangle u = -f$)*

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- many applications of sparse grids:
  - numerical quadrature
  - solving PDEs
  - data-mining
  - etc.

Thanks for listening!

For further reading:

H.-J. Bungartz, M. Griebel
Sparse grids
Acta Numerica, pp. 147-269, 2004

M. Bader, S. Zimmer
lecture's slides "Algorithmen des Wissenschaftlichen Rechnens"
(http://www5.in.tum.de/lehre/vorlesungen/algowiss/ss05/material.html)
TU München, summer term 2005

Outline

The PDE and it's weak form

- Given a PDE: $\triangle u = f$ in Ω and $u|_{\partial\Omega} = 0$

The PDE and it's weak form

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- Find $u \in V$ with $u|_{\partial\Omega} = 0$ and

$$\int_\Omega u' \cdot v' dx = \int_\Omega f \cdot v \, dx, \forall v \in V$$

$$\Longleftrightarrow \int_\Omega \nabla u^T \cdot \nabla v \, dx = \int_\Omega f \cdot v \, dx, \forall v \in V$$

Galerkin Projection

- Take *finite* n-dimensional subspace $S \subset V$ with

$$S = \mathrm{span}\{\phi_i : 1 \leq i \leq n\}$$

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- Receive an approximative u_S as linear combination of basis functions:

$$u_S = \sum_{i=1}^{n} \alpha_i \cdot \phi_i$$

Linear Equation System

We get a *linear* equation system for $z = (\alpha_1, \dots, \alpha_n)$

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$$A = \left(\int_\Omega \phi_i' \cdot \phi_j' \, dx \right)_{i,j=1,\ldots,n}$$

$$b = \left(\int_\Omega f \cdot \phi_i \, dx \right)_{i=1,\ldots,n}$$

Matrix Conditions

- matrix is sparse, if ϕ has small support - e.g. using the nodal point basis, but then:

$$\mathrm{cond}(A) = \mathcal{O}(h_n^{-2}) \quad \text{and} \quad \dim(A) = \mathcal{O}(2^{dn}) \times \mathcal{O}(2^{dn})$$

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- using iterative linear equation solvers (e.g. CG method):
  $\Rightarrow$ don't need A explicitly but only Av
- there are algorithms for evaluation of Av in $\mathcal{O}(N)$ time

back to talk