Algorithms for Scientific Computing

Hierarchical Methods and Sparse Grids
– 1D Hierarchical Basis –

Michael Bader
Technical University of Munich

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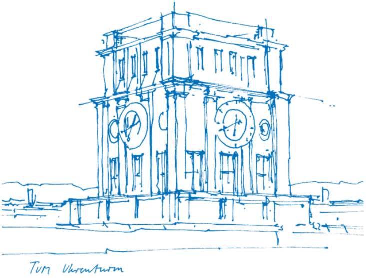
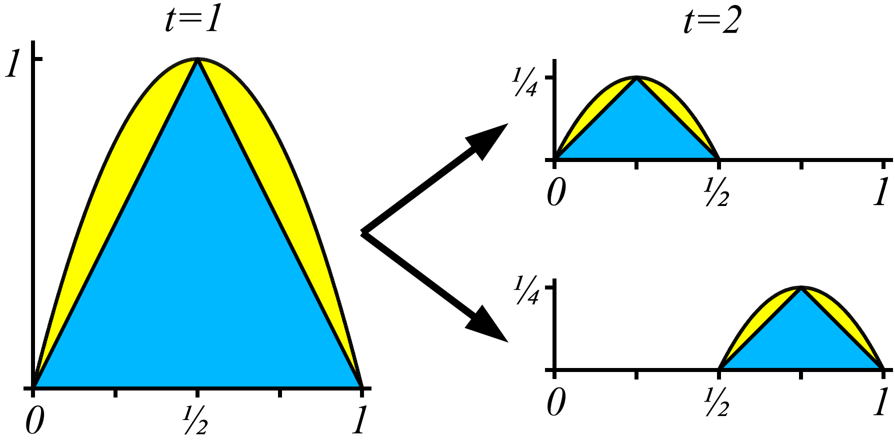


Archimedes' Quadrature

Compute an approximation of $F_1 := \int_0^1 4 \cdot x \cdot (1 - x)\, dx = \dfrac{2}{3}$



Archimedes' Quadrature (2)

- Integrating $4x(1-x)$, we have to consider several quantities
- Ordered by (recursive) level t:

Level-depth	1	2	3	4	...	t
Mesh-width h	1/2	1/4	1/8	1/16	...	2^{-t}
# triangles	1	2	4	8	...	$\frac{1}{2}2^t$
surplus v	1	1/4	1/16	1/64	...	$4 \cdot 2^{-2t}$
Area of triangle D_1	1/2	1/16	1/128	1/1024	...	$4 \cdot 2^{-3t}$
Sum (current t)	1/2	1/8	1/32	1/128	...	$2 \cdot 2^{-2t}$
Sum ($\leq t$)	1/2	5/8	21/32	85/128	...	$\frac{2}{3}\left(1-2^{-2t}\right)$
Error	1/6	1/24	1/96	1/384	...	$\frac{2}{3}2^{-2t}$

Approximation of Functions

- Goal: analyze Archimedes' quadrature rule for more general functions
- We need a representation of the (approximating) function $u(x)$:

  $\rightarrow$ u as linear combination of ansatz functions ϕ_i:

$$u(x) = \sum_{i=1}^{N} \alpha_i \cdot \phi_i(x)$$

- Integrating $u(x)$:

$$\int_a^b u(x)\,dx = \sum_{i=1}^{N} \alpha_i \int_a^b \phi_i(x)\,dx,$$

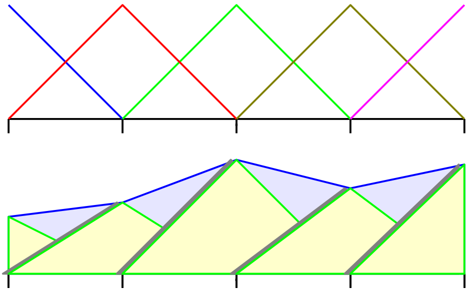
  $\rightarrow$ Weighted sum of α_i

- Compare to Newton-Cotes: integrate the interpolant (polynomial)
  $\Rightarrow$ leads to a weighted sum of function evaluations

Composite Trapezoidal Rule: Function

Interpolant

- Continuous, piecewise linear function
- Represent u in nodal point (hat) basis



- Coefficients α_i are function values at grid points
- Basis functions have area h ($h/2$ at boundaries)

Piecewise Linear Functions

Ansatz space and basis functions

- Only consider $u : [0,1] \to \mathbb{R}$
- Consider discretization level $n \in \mathbb{N}$
- *Mesh-width* $h_n = 2^{-n}$
- *Grid points* $x_{n,i} = i \cdot h_n$
- Define “mother of all hat functions”

$$\phi(x) := \max\{1 - |x|, 0\}$$

$\Rightarrow$ **Basis functions**

$$\phi_{n,i}(x) := \phi\left(\frac{x - x_{n,i}}{h_n}\right)$$

- Nodal point basis $\Phi_n := \{\phi_{n,i}, 0 \leq i \leq 2^n\}$

Piecewise Linear Functions (2)

Towards Function Spaces:

- Space of continuous piecewise linear functions:

$$V_n = \operatorname{span}(\Phi_n)$$

- Interpolants $u_n \in V_n$:

$$u_n(x) = \sum_{i=0}^{2^n} \alpha_{n,i}\phi_{n,i}(x)$$

- V_n the space of all such interpolants u_n

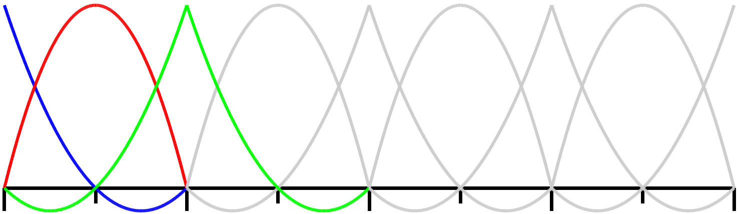
Interpolation with Nodal Basis:

- Interpolation conditions: $u_n(x_j) = \sum \alpha_{n,i}\phi_{n,i}(x_j) \stackrel{!}{=} f(x_{n,j})$
- Due to nodal basis: $\phi_{n,i}(x_j) = 0$ if $i \neq j$, and $\phi_{n,j}(x_j) = 1$
- Thus: all $\alpha_{n,j} = f(x_{n,j})$

Composite Simpson's Rule: Function

Interpolant

- Continuous, piecewise quadratic function
- More complicated basis:



- Basis functions: Lagrangian polynomials, glued together
- α_i: function values at grid points
- Basis functions have area $h/6$ (blue), $4h/6$ (red), $2h/6$ (green)
- We'll not formally define basis functions here ...

From Composite Trapezoidal to Archimedes

Piecewise linear functions

- We restrict our functions u to $u(0) = u(1) = 0$
- Nodal point basis for discretization level n:

$$\Phi_n := \{\phi_{n,i}, 1 \leq i \leq 2^n - 1\}$$

- Wanted: *function space*

$$V := \bigcup_{l=1}^{\infty} V_l$$

  contains all functions which are in V_l for sufficiently large l
- However: generating system of V as

$$\Phi := \bigcup_{l=1}^{\infty} \Phi_l$$

  does not lead to a basis (not linear independent)

Hierarchical Basis

- We are interested in a hierarchical decomposition of V_l
  $\Rightarrow$ Define **hierarchical increment** W_l, such that V_l is a *direct sum*:

$$V_l = V_{l-1} \oplus W_l$$

  Side-note: direct sum

  $\rightarrow$ Every $u_l \in V_l$ can be uniquely decomposed as $u_l = u_{l-1} + w_l$, with $u_{l-1} \in V_{l-1}$ and $w_l \in W_l$

- W_l has to contain 2^{l-1} ansatz functions:

$$\dim V_l = 2^l - 1 = \dim V_{l-1} + \dim W_l$$

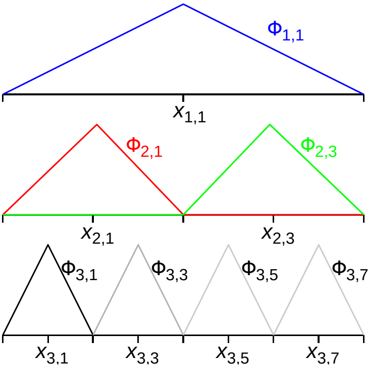
- This holds (introducing index sets $\mathcal{I}_l$) for

$$\mathcal{I}_l := \{i : 1 \leq i < 2^l,\ i \text{ odd}\}$$

$$W_l := \operatorname{span}\{\phi_{l,i} :\ i \in \mathcal{I}_l\}$$

Hierarchical Increments

- Set of hierarchical increments W_l
- For $l = 1$: $W_1 = V_1$
- Example for $l = 1, 2, 3$:



Hierarchical Basis (cont.)

- Then

$$V_n = \bigoplus_{l=1}^{n} W_l$$

  is a direct sum, too:

- $u \in V_n$ can be decomposed uniquely into $w_l \in W_l$:

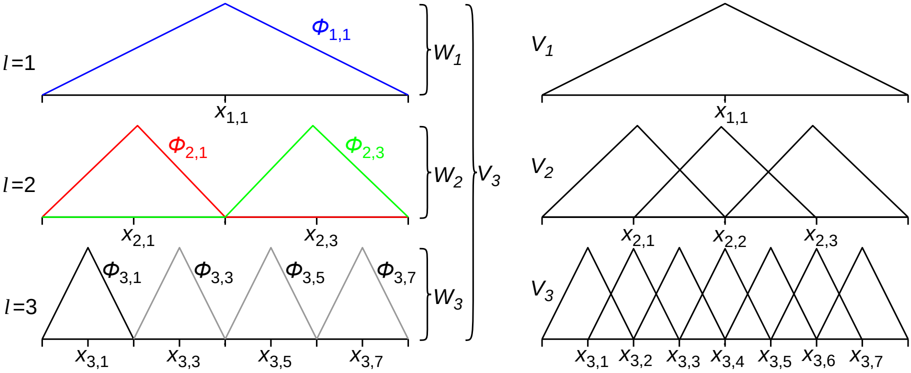
$$u = \sum_{l=1}^{n} w_l = \sum_{l=1}^{n} \sum_{i \in \mathcal{I}_l} v_{l,i} \phi_{l,i}$$

  $\rightarrow$ Coefficients $v_{l,i}$ are **hierarchical surplusses**

- Corresponding basis of V_n (or, with ∞ instead of n, of V)

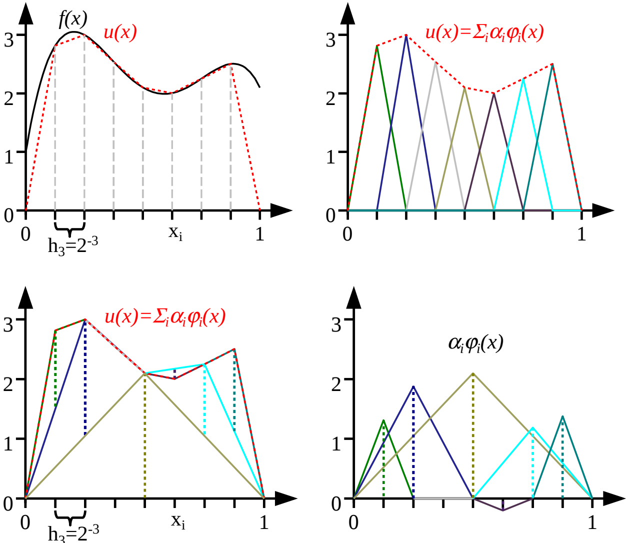
$$\Psi_n := \bigcup_{l=1}^{n} \{\phi_{l,i} : i \in \mathcal{I}_l\}.$$

Comparison



$l=1$
$\Phi_{1,1}$
$x_{1,1}$
W_1
$l=2$
$\Phi_{2,1}$
$\Phi_{2,3}$
$x_{2,1}$
$x_{2,3}$
W_2
V_3
$l=3$
$\Phi_{3,1}$
$\Phi_{3,3}$
$\Phi_{3,5}$
$\Phi_{3,7}$
$x_{3,1}$
$x_{3,3}$
$x_{3,5}$
$x_{3,7}$
W_3
V_1
$x_{1,1}$
V_2
$x_{2,1}$
$x_{2,2}$
$x_{2,3}$
V_3
$x_{3,1}$
$x_{3,2}$
$x_{3,3}$
$x_{3,4}$
$x_{3,5}$
$x_{3,6}$
$x_{3,7}$

Comparison (2)



Part I

Hierarchical Basis in 1D: Integration and Transformations

Numerical Integration with Hierarchical Basis

Key Ingredients:

- Integration of $u(x)$:

$$\int_a^b u(x)\,dx = \int_a^b \sum_i^N \alpha_i \phi_i(x)\,dx = \sum_i^N \alpha_i \int_a^b \phi_i(x)\,dx,$$

- Using a hierarchical basis:

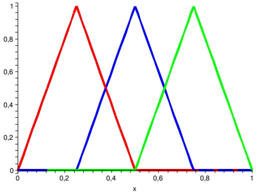
$$\int_a^b u\,dx = \int_a^b \sum_{l=1}^n \sum_{i\in\mathcal{I}_l} v_{l,i}\phi_{l,i}\,dx = \sum_{l=1}^n \sum_{i\in\mathcal{I}_l} v_{l,i} \int_a^b \phi_{l,i}\,dx = \sum_{l=1}^n \sum_{i\in\mathcal{I}_l} v_{l,i} h_l$$

- Computation of hierarchical surpluses:

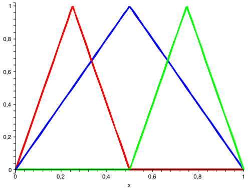
$$v_{l.i} = u(x_{l,i}) - \tfrac{1}{2}\big(u(x_{l,i-1}) + u(x_{l,i+1})\big)$$

i.e., difference between function and linear interpolant (on coarser level) at $x_{l,i} \rightarrow$ **hierarchical surplus**

Hierarchical Basis Transformation



$\longrightarrow$



- represent "wider" hat function $\phi_{1,1}(x)$ via basis functions $\phi_{2,j}(x)$

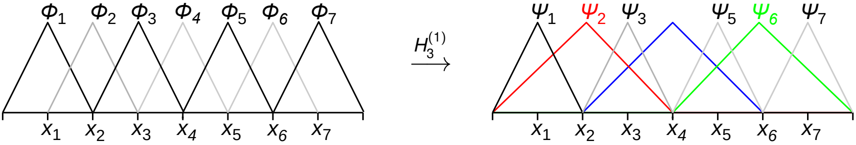
$$\phi_{1,1}(x) = \tfrac{1}{2}\phi_{2,1}(x) + \phi_{2,2}(x) + \tfrac{1}{2}\phi_{2,3}(x)$$

- consider vector of hierarchical/nodal basis functions and write transformation as matrix-vector product:

$$\begin{pmatrix} \psi_{2,1}(x) \\ \psi_{2,2}(x) \\ \psi_{2,3}(x) \end{pmatrix} := \begin{pmatrix} \phi_{2,1}(x) \\ \phi_{1,1}(x) \\ \phi_{2,3}(x) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_{2,1}(x) \\ \phi_{2,2}(x) \\ \phi_{2,3}(x) \end{pmatrix}$$

Hierarchical Basis Transformation (2)

Consider "semi-hierarchical" transform: (step 1)

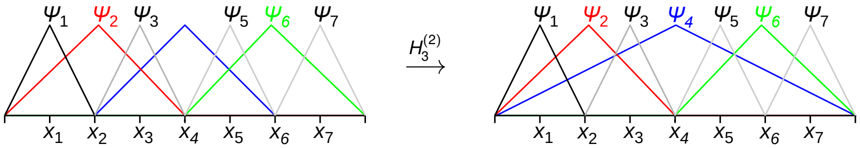


Matrices for change of basis are then: ($H_3^{(2)}$ to transform to hierarchical basis)

$$H_3^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad H_3^{(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 1 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Hierarchical Basis Transformation (2)

Consider "semi-hierarchical" transform: (step 2)



Matrices for change of basis are then: ($H_3^{(2)}$ to transform to hierarchical basis)

$$H_3^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad H_3^{(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 1 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Hierarchical Basis Transformation (3)

Level-wise hierarchical transform:

- hierarchical basis transformation: $\psi_{n,i}(x) = \sum_j H_{i,j}\phi_{n,j}(x)$
- written as matrix-vector product: $\vec{\psi}_n = H_n\vec{\phi}_n$
- $H_n\vec{\phi}_n$ can be performed as a sequence of level-wise transforms:

  For k from 1 to n-1

  $\quad\vec{\phi}_n := H_n^{(k)}\vec{\phi}_n$

- matrix H_n for hierarchical basis transformation is thus:

$$H_n = H_n^{(n-1)}\, H_n^{(n-2)}\, \ldots\, H_n^{(2)}\, H_n^{(1)}$$

- where each level-wise transform $H_n^{(k)}\vec{\phi}_n$ has a simple loop implementation:

  For j from 2^k *to* 2^n *step* 2^k

  $\quad\phi_{n,j} := \frac{1}{2}\phi_{n,j-2^{k-1}} + \phi_{n,j} + \frac{1}{2}\phi_{n,j+2^{k-1}}$

Hierarchical Coordinate Transformation

- consider function $f(x) \approx \sum_i a_i \psi_{n,i}(x)$ represented via hier. basis
- wanted: corresponding representation in nodal basis

$$\sum_j b_j \phi_{n,j}(x) = \sum_i a_i \psi_{n,i}(x) \approx f(x)$$

- with $\psi_{n,i}(x) = \sum_j H_{i,j} \phi_{n,j}(x)$ we obtain

$$\sum_j b_j \phi_{n,j}(x) = \sum_i a_i \sum_j H_{i,j} \phi_{n,j}(x) = \sum_j \sum_i a_i H_{i,j} \phi_{n,j}(x)$$

- compare coordinates and get

$$b_j = \sum_i H_{i,j} a_i = \sum_i \left(H^T\right)_{j,i} a_i$$

- written in vector notation: $b = H^T a$

Hierarchical Coordinate Transformation (2)

- transform $b = H^T a$ turns "hierachical" coefficients a into "nodal" coefficients b:

$$\sum_j b_j \phi_{n,j}(x) = \sum_i a_i \psi_{n,i}(x) \approx f(x)$$

- Recall that $H_n = H_n^{(n-1)} H_n^{(n-2)} \ldots H_n^{(2)} H_n^{(1)}$ has a level-wise representation, therefore:

$$H_n^T = \left(H_n^{(1)}\right)^T \left(H_n^{(2)}\right)^T \ldots \left(H_n^{(n-2)}\right)^T \left(H_n^{(n-1)}\right)^T$$

- use loop-based implementation for $\left(H_n^{(k)}\right)^T a$ to get **fast algorithm**:

For k from n-1 downto 1

For i from 2^{k-1} to 2^n step 2^k

$a_i := \frac{1}{2} a_{i-2^{k-1}} + a_i + \frac{1}{2} a_{i+2^{k-1}}$ *(with $a_0 = a_{2^n} = 0$)*

Hierarchical Coordinate Transformation (3)

Now: transform “nodal” coefficients b into “hierachical” coefficients a

- thus: solve $H^T a = b$ for a (for given b), or $a = \left(H^T\right)^{-1} b = H^{-T} b$
- again via level-wise representation:

$$H_n^{-T} = \left(H_n^{(n-1)}\right)^{-T} \left(H_n^{(n-2)}\right)^{-T} \cdots \left(H_n^{(2)}\right)^{-T} \left(H_n^{(1)}\right)^{-T}$$

- iterate over $a^{\text{new}} = \left(H_n^{(j)}\right)^{-T} a^{\text{old}}$, i.e. repeatedly solve $\left(H_n^{(j)}\right)^T a^{\text{new}} = a^{\text{old}}$ (in-place computation on a, starting with $a^{\text{old}} = b$ for $j = 1$)
- consider example $\left(H_3^{(1)}\right)^T a^{\text{new}} = a^{\text{old}}$:

$$\begin{pmatrix} 1 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} a_1^{\text{new}} \\ \\ \\ \vdots \\ \\ \\ a_7^{\text{new}} \end{pmatrix} = \begin{pmatrix} a_1^{\text{old}} \\ \\ \\ \vdots \\ \\ \\ a_7^{\text{old}} \end{pmatrix}$$

- for row 3 (and similar for rows 1, 5 and 7):

  $\frac{1}{2} a_2^{\text{new}} + a_3^{\text{new}} + \frac{1}{2} a_4^{\text{new}} = a_3^{\text{old}} \quad \Leftrightarrow \quad a_3^{\text{new}} = a_3^{\text{old}} - \frac{1}{2} a_2^{\text{new}} - \frac{1}{2} a_4^{\text{new}} = a_3^{\text{old}} - \frac{1}{2}\left(a_2^{\text{old}} + a_4^{\text{old}}\right)$

  $\rightsquigarrow$ **computation of hierarchical surplus!**