Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids

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Part VI

Finite Elements: An Introduction to the Most Common Prejudices

Solving Differential Equations

- Solution of differential equations (DEs) as another application for sparse grids (apart from integration)
- Algorithmically much more interesting than quadrature
- First, we have to introduce the method of finite elements (FE) to (discretize and) numerically solve DEs
  - There, we can directly plug in our hierarchical basis

Solving Differential Equations

- Solution of differential equations (DEs) as another application for sparse grids (apart from integration)
- Algorithmically much more interesting than quadrature
- First, we have to introduce the method of finite elements (FE) to (discretize and) numerically solve DEs
  - There, we can directly plug in our hierarchical basis
- As an example, we consider a simple linear ordinary differential equation (ODE):

$$u(x) - u''(x) = f(x) \text{ for } x \in (0,1); \quad u(0) = u(1) = 0$$

Finite-Dimensional Function Space

- To represent a function in a computer, only finite number of coefficients possible

$\Rightarrow$ Choose function space V_h with finite dimension N
  - Think of V_n:
  - Continuous, piecewise linear functions u w.r.t. grid with mesh-width $h = 2^{-n}$
  - $u(0) = u(1) = 0 \rightsquigarrow N = 1/h - 1 = 2^n - 1$
- Define basis $\{\phi_j\}_{1 \leq j \leq N}$ (think of hat functions $\phi_j := \phi_{n,j}$)
- Task: determine N coefficients u_j in

$$u_h = \sum_{j=1}^{N} u_j \phi_j$$

such that u_h approximates exact solution u well

Conditions for u_h

- Derive N conditions for u_h from ODE
  $\Rightarrow$determine N coefficients
- Straightforward approach:
  - Demand that ODE is fulfilled at grid points x_i

$$u_h(x_i) - u_h''(x_i) = f(x_i), 1 \leq i \leq N$$

  - Fails – u_h'' does not make sense for functions in V_h with bends at grid points

Conditions for u_h (2)

More reasonable conditions:

- Multiply ODE with ϕ_i (so-called *test functions*)
- Demand that integral over $[0, 1]$ fulfills ODE:

$$\int_0^1 [u_h(x) - u_h''(x)]\, \phi_i(x)\, dx = \int_0^1 f(x)\phi_i(x)\, dx$$

- Replace critical term u'' according to partial integration

$$\int_0^1 -u_h''(x)\phi_i(x)\, dx \rightsquigarrow \int_0^1 u_h'(x)\phi_i'(x)\, dx$$

  - For sufficiently smooth u this is the same ($\phi_i(0) = \phi_i(1) = 0$, as $\phi_i \in V_h$)
  - We just take form on the right, without further considerations

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  - We just take form on the right, without further considerations
- We obtain N equations

$$\int_0^1 u_h(x)\phi_i(x)\, dx + \int_0^1 u_h'(x)\phi_i'(x)\, dx = \int_0^1 f(x)\phi_i(x)\, dx$$

Conditions for u_h (3)

- Note: if u_h fulfills these N conditions, it holds for arbitrary $v_h \in V_h$:

$$\int_0^1 u_h(x)v_h(x)\,dx + \int_0^1 u_h'(x)v_h'(x)\,dx = \int_0^1 f(x)v_h(x)\,dx$$

  - We can expand equation by $v_h = \sum_{j=1}^N v_j\phi_j$ into linear combination of equations with test functions ϕ_i

$\Rightarrow$ No matter which basis of V_h used for test functions: the equations for u_h are equivalent.

- Solutions u_h just depends on ansatz space, not on basis used
- We'll always use same basis for test functions as for u_h

Determining the Coefficients

- Obtain system of linear equations for coefficients u_j by substituting $u_h(x) = \sum_{j=1}^N u_j\phi_j(x)$ in each equation

$$\int_0^1 \underbrace{\left(\sum_{j=1}^N u_j\phi_j(x)\right)}_{u_h(x)} \phi_i(x)\,dx + \int_0^1 \underbrace{\left(\sum_{j=1}^N u_j\phi_j'(x)\right)}_{u_h'(x)} \phi_i'(x)\,dx = \int_0^1 f(x)\phi_i(x)\,dx$$

- Looks bad, but is good – a linear equation in the u_j:

$$\sum_{j=1}^N \left(\underbrace{\int_0^1 \phi_j(x)\phi_i(x)\,dx}_{=:b_{i,j}} + \underbrace{\int_0^1 \phi_j'(x)\phi_i'(x)\,dx}_{=:a_{i,j}}\right) u_j = \underbrace{\int_0^1 f(x)\phi_i(x)\,dx}_{=:f_i}$$

Determining the Coefficients (2)

- Integral-free slide!
- We obtained a $N \times N$ system of linear equations
- Assemble coefficients in two $N \times N$ matrices

$$A := (a_{i,j})_{1 \le i,j \le N}, \qquad B := (b_{i,j})_{1 \le i,j \le N}$$

and vector of length N

$$\vec{f} := (f_i)_{1 \le i \le N)}$$

$\Rightarrow$ System of linear equations

$$(B + A)\vec{u} = \vec{f}$$

- Solution $\vec{u}$ will contain coefficients of u_h in our basis

Determining the Coefficients – Side Note

Only of minor interest for us is mathematical background of this technique (we're just users!)

- Has the linear system a unique solution?
  (in our example: yes)
- Is u_h a reasonable approximation of the exact solution?
  (yes; one can even show that it's the best possible approximation in V_h, measured in a suitable norm)
- And much more, we're not interested in. . .

Finite Elements in a Nutshell

Steps to solve the DE using FE

- Transform equation to integral representation (“weak form”)
- Choose ansatz space V_h (typically: choose grid, select ansatz functions)
- Now we have determined u_h, we only have to compute the coefficients
- Choose basis $\{\phi_i\}_{1 \leq i \leq N}$
- Assemble matrix (here $B + A$), and right-hand-side $\vec{f}$
- Solve system of linear equations
- Construct the function u_h using $\vec{u}$, and plot a colorful picture

Example: ODE

Previous example

- $u(x) - u''(x) = f(x)$ für $x \in (0, 1)$; $u(0) = u(1) = 0$
- V_h: continuous, piecewise linear functions defined on grid with mesh-width h with $u(0) = u(1) = 0$
- Nodal point basis: $\phi_{n,i}$, $1 \leq i \leq 2^n - 1$ ($h = 2^{-n}$)

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$$b_{i,j} := \int_0^1 \phi_j(x)\phi_i(x)\,dx = \begin{cases} \frac{2}{3}h & \text{if } i = j \\ \frac{1}{6}h & \text{if } |i-j| = 1 \\ 0 & \text{else} \end{cases}$$

$$a_{i,j} := \int_0^1 \phi_j'(x)\phi_i'(x)\,dx = \begin{cases} \frac{2}{h} & \text{if } i = j \\ -\frac{1}{h} & \text{if } |i-j| = 1 \\ 0 & \text{else} \end{cases}$$

Stencil

- More intuitive: Write as stencil
- Notate coefficients for an equation ordered corresponding to the grid points:

$$B \rightsquigarrow \begin{bmatrix} \frac{1}{6}h & \frac{2}{3}h & \frac{1}{6}h \end{bmatrix} \quad \text{or} \quad \frac{h}{6}\begin{bmatrix} 1 & 4 & 1 \end{bmatrix}$$

and

$$A \rightsquigarrow \begin{bmatrix} -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \end{bmatrix} \quad \text{or} \quad \frac{1}{h}\begin{bmatrix} -1 & 2 & -1 \end{bmatrix}$$

- Make sure to know how the matrices look like!
  - Order grid points in their natural order

Partial Differential Equations

- Now: transition to partial differential equations (PDEs, more than one variable)
  - Notation a bit more complicated, but for the (elliptic) PDEs under consideration nothing substantially new
- Domain $\Omega := [0, 1]^d$
- Again, we consider only functions which are 0 on $\partial\Omega$
- Our model problem transfered to *d* dimensions contains *Laplace* operator

$$\Delta u := \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \ldots + \frac{\partial^2 u}{\partial x_d^2},$$

- Can be "partially integrated" as well (Green's first identity, ∇: gradient):

$$-\int_\Omega \Delta u(\vec{x}) \cdot \phi(\vec{x})\, d\vec{x} = \int_\Omega \nabla u(\vec{x}) \nabla \phi(\vec{x})\, d\vec{x}.$$

Model Problem

Back to our previous example, but d-dimensional

- We now dare to solve the PDE

$$u(\vec{x}) - \Delta u(\vec{x}) = f(\vec{x}).$$

- With grid with mesh-width $h = 2^{-n}$, function space V_n with nodal point basis $\Psi_{\vec{n}}$

Model Problem

Back to our previous example, but d-dimensional

- We now dare to solve the PDE

$$u(\vec{x}) - \Delta u(\vec{x}) = f(\vec{x}).$$

- With grid with mesh-width $h = 2^{-n}$, function space V_n with nodal point basis $\Psi_{\vec{n}}$
- To assemble the matrices: compute d-dimensional integrals for all pairs of basis functions (ϕ_i, ϕ_j):

$$b_{i,j} = \int_\Omega \phi_i(\vec{x})\phi_j(\vec{x})\, d\vec{x}, \quad a_{i,j} = \int_\Omega \nabla\phi_i(\vec{x})\nabla\phi_j(\vec{x})\, d\vec{x}$$

- Nice property: in each row of the matrix, at most 3^d coefficients $\neq 0$
  - Corresponds to grid point and all neighbors

Stencil ($d = 2$)

- For $d = 2$, they can be still written as stencil

$$B \rightsquigarrow \frac{h^2}{36} \begin{bmatrix} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{bmatrix} \text{ und } A \rightsquigarrow \frac{1}{3} \begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

- More important than the calculations leading to those entries:
  - How do matrices A and B look like?
  - Best to order grid points lexicographically (e.g. row-wise)