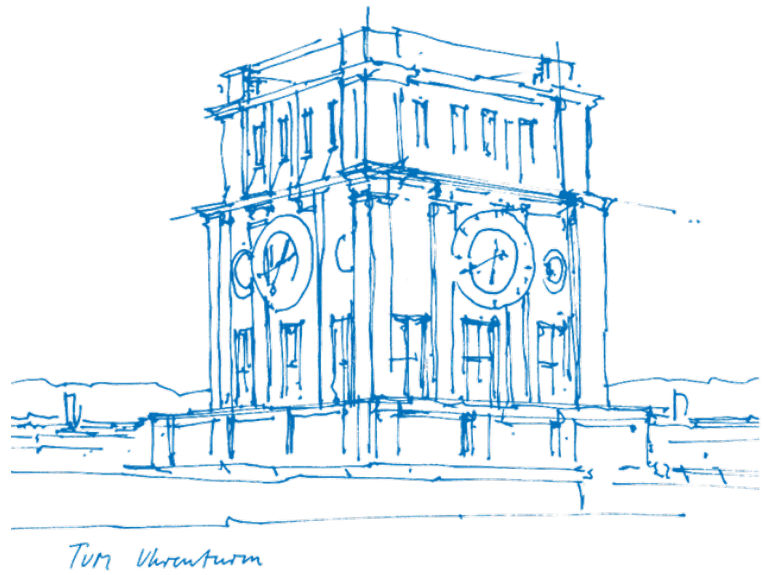
Scientific Computing II

Conjugate Gradient Methods

Michael Bader
Technical University of Munich

Summer 2018



Families of Iterative Solvers

- **relaxation methods**:
  - Jacobi-, Gauss-Seidel-Relaxation, ...
  - Over-Relaxation-Methods
- **Krylov methods**:
  - Steepest Descent, Conjugate Gradient, ...
  - GMRES, ...
- **Multilevel/Multigrid methods**,
  Domain Decomposition, ...

Remember: The Residual Equation

- for $Ax = b$, we defined the **residual** as:

$$r^{(i)} = b - Ax^{(i)}$$

- and the error: $e^{(i)} := x - x^{(i)}$
- leads to the **residual equation:**

$$Ae^{(i)} = r^{(i)}$$

- relaxation methods: solve a modified (easier) SLE:

$$B\,\hat{e}^{(i)} = r^{(i)} \qquad \text{where} \quad B \sim A$$

- multigrid methods: coarse-grid correction on residual equation

$$A_H e_H^{(i)} = r_H^{(i)} \qquad \text{and} \quad x^{(i+1)} := x^{(i)} + I_H^h e_H^{(i)}$$

Part I

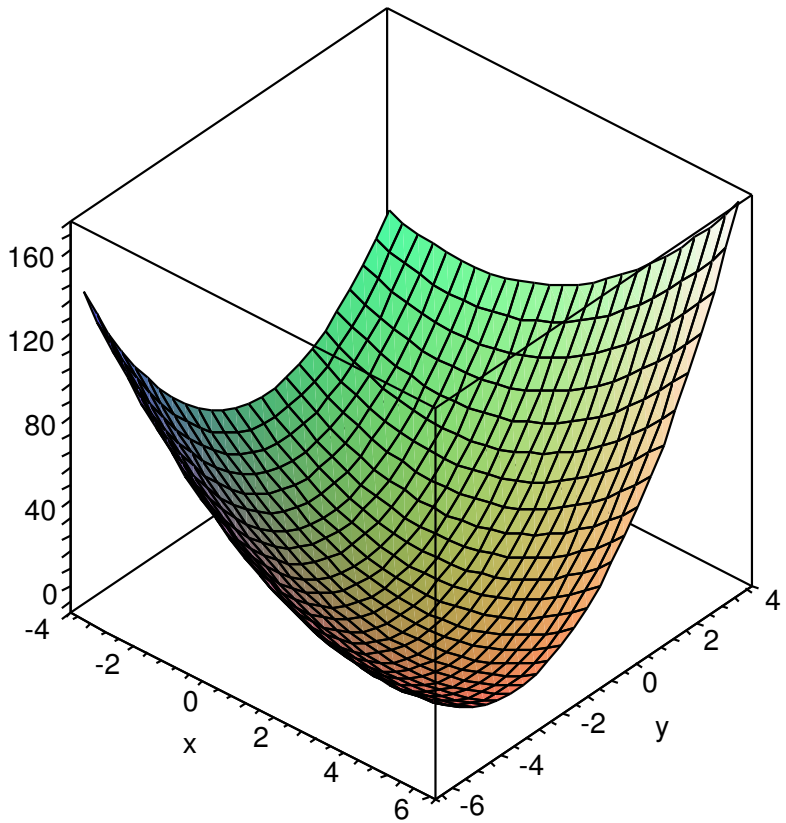
Quadratic Forms and Steepest Descent

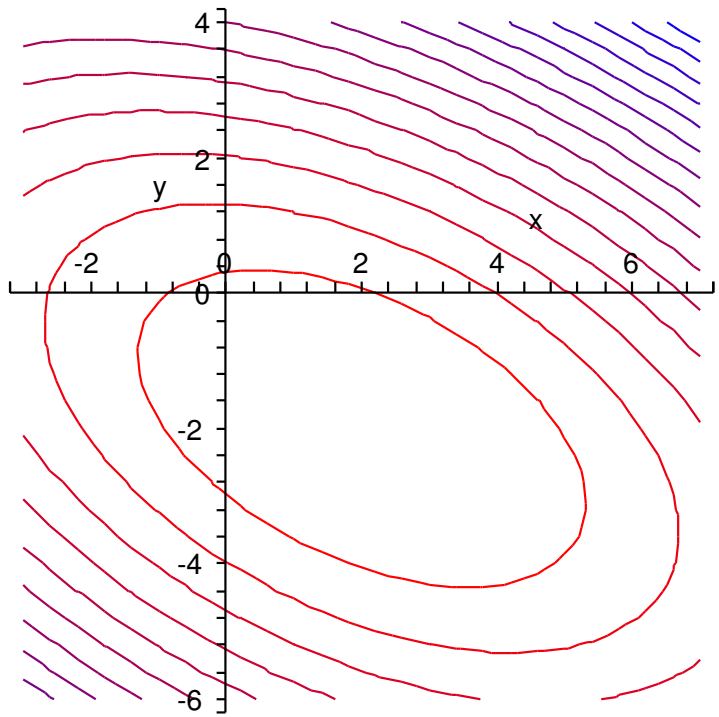
Quadratic Forms
Direction of Steepest Descent
Steepest Descent

Quadratic Forms

A *quadratic form* is a scalar, quadratic function of a vector of the form:

$$f(x) = \frac{1}{2}x^T Ax - b^T x + c, \qquad \text{where } A = A^T$$





Quadratic Forms (2)

The *gradient* of a quadratic form is defined as

$$f'(x) = \begin{pmatrix} \frac{\partial}{\partial x_1} f(x) \\ \vdots \\ \frac{\partial}{\partial x_n} f(x) \end{pmatrix}$$

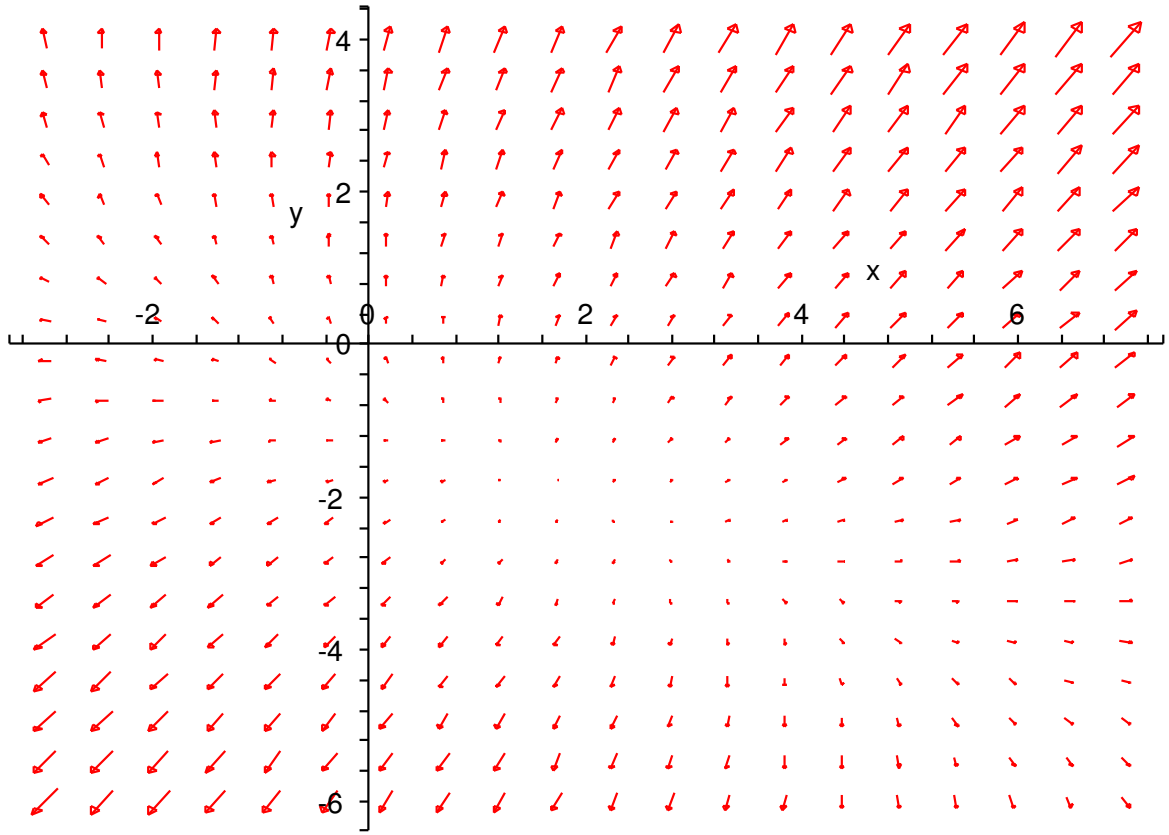
- apply to $f(x) = \frac{1}{2} x^T A x - b^T x + c$, then
- $f'(x) = Ax - b$
- $f'(x) = 0 \quad \Leftrightarrow \quad Ax - b = 0 \quad \Leftrightarrow \quad Ax = b$

$\Rightarrow Ax = b$ equivalent to a **minimisation problem**

$\Rightarrow$ proper minimum **only if A positive definite**

Direction of Steepest Descent

- gradient $f'(x)$: direction of “steepest ascent”
- $f'(x) = Ax - b = -r$ (with residual $r = b - Ax$)
- residual r: direction of “steepest descent”



Solving SLE via Minimum Search

- basic idea to find minimum:
  move into direction of steepest descent
- most simple scheme:
$$x^{(i+1)} = x^{(i)} + \alpha r^{(i)}$$
- α constant $\Rightarrow$ **Richardson** iteration
  (usually considered as a relaxation method)
- better choice of α:
  move to lowest point in that direction
  $\Rightarrow$ **Steepest Descent**

Steepest Descent – find an optimal α

- task: *line search* along the line $x^{(1)} = x^{(0)} + \alpha r^{(0)}$
- choose α such that $f(x^{(1)})$ is minimal:

$$\frac{\partial}{\partial \alpha} f(x^{(1)}) = 0$$

- use chain rule:

$$\frac{\partial}{\partial \alpha} f(x^{(1)}) = f'(x^{(1)})^T \frac{\partial}{\partial \alpha} x^{(1)} = f'(x^{(1)})^T r^{(0)}$$

- remember $f'(x^{(1)}) = -r^{(1)}$, thus:

$$-\left(r^{(1)}\right)^T r^{(0)} \stackrel{!}{=} 0$$

hence, $f'(x^{(1)}) = -r^{(1)}$ should be orthogonal to $r^{(0)}$

Steepest Descent – find α (2)

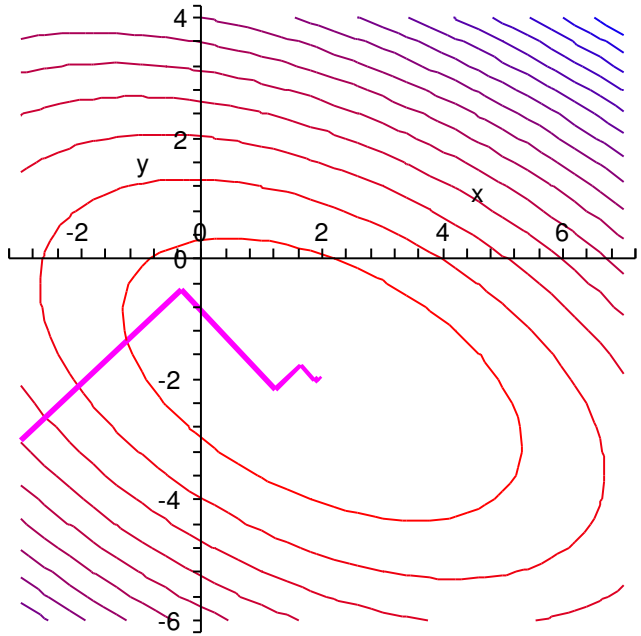
$$
\begin{aligned}
\left(r^{(1)}\right)^T r^{(0)} = \left(b - Ax^{(1)}\right)^T r^{(0)} &= 0 \\
\left(b - A(x^{(0)} + \alpha r^{(0)})\right)^T r^{(0)} &= 0 \\
\left(b - Ax^{(0)}\right)^T r^{(0)} - \alpha \left(Ar^{(0)}\right)^T r^{(0)} &= 0 \\
\left(r^{(0)}\right)^T r^{(0)} - \alpha \left(r^{(0)}\right)^T Ar^{(0)} &= 0
\end{aligned}
$$

Solve for α:

$$
\alpha = \frac{\left(r^{(0)}\right)^T r^{(0)}}{\left(r^{(0)}\right)^T Ar^{(0)}}
$$

Steepest Descent – Algorithm

1. $r^{(i)} = b - Ax^{(i)}$
2. $\alpha_i = \dfrac{\left(r^{(i)}\right)^T r^{(i)}}{\left(r^{(i)}\right)^T Ar^{(i)}}$
3. $x^{(i+1)} = x^{(i)} + \alpha_i r^{(i)}$

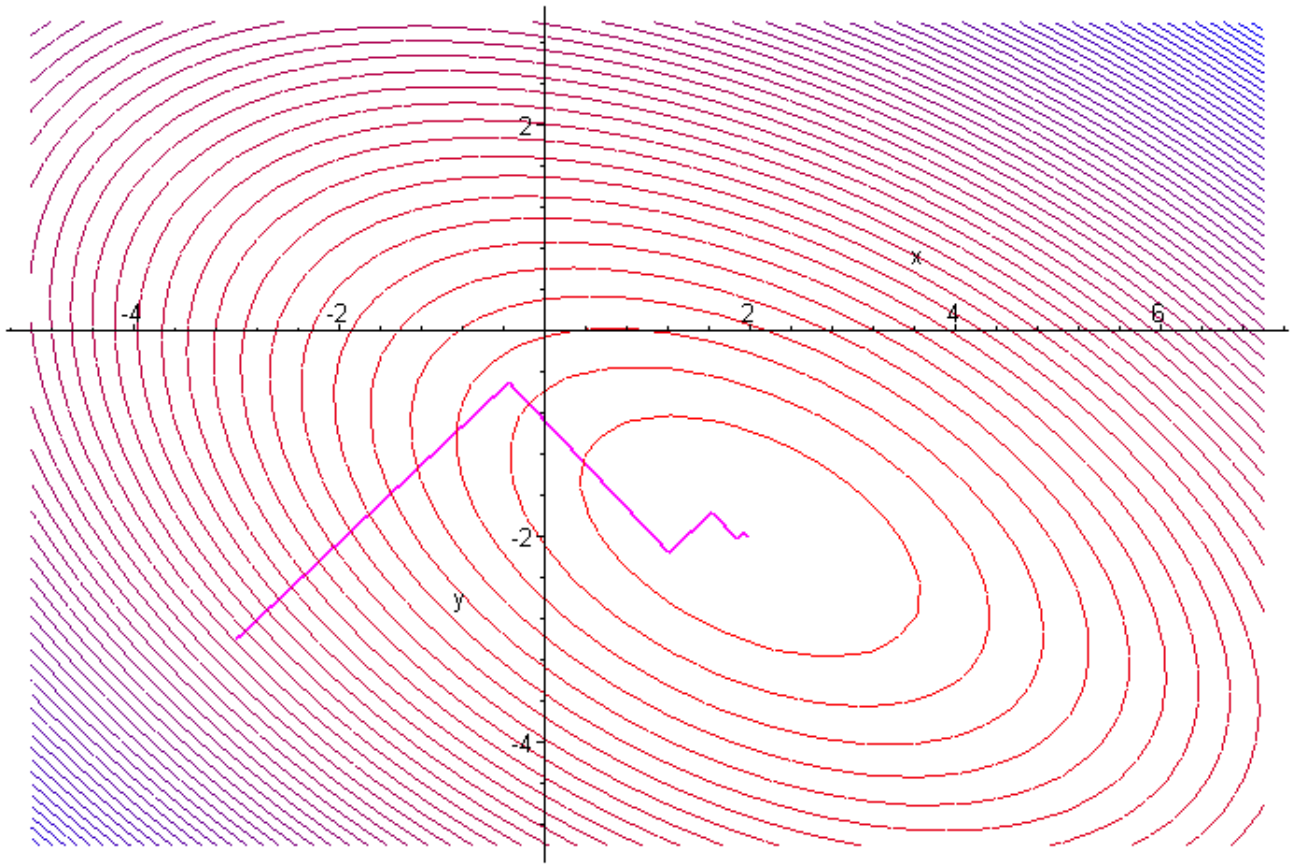


Observations:

- slow convergence (sim. to Jacobi relaxation)
- detailed analysis reveals: $\left\|e^{(i)}\right\|_A \leq \left(\frac{\kappa-1}{\kappa+1}\right)^i \left\|e^{(0)}\right\|_A$
- with $\kappa = \lambda_{\max}/\lambda_{\min}$
  (largest/smallest eigenvalues of A; for positive definite A)
- many steps in the same direction

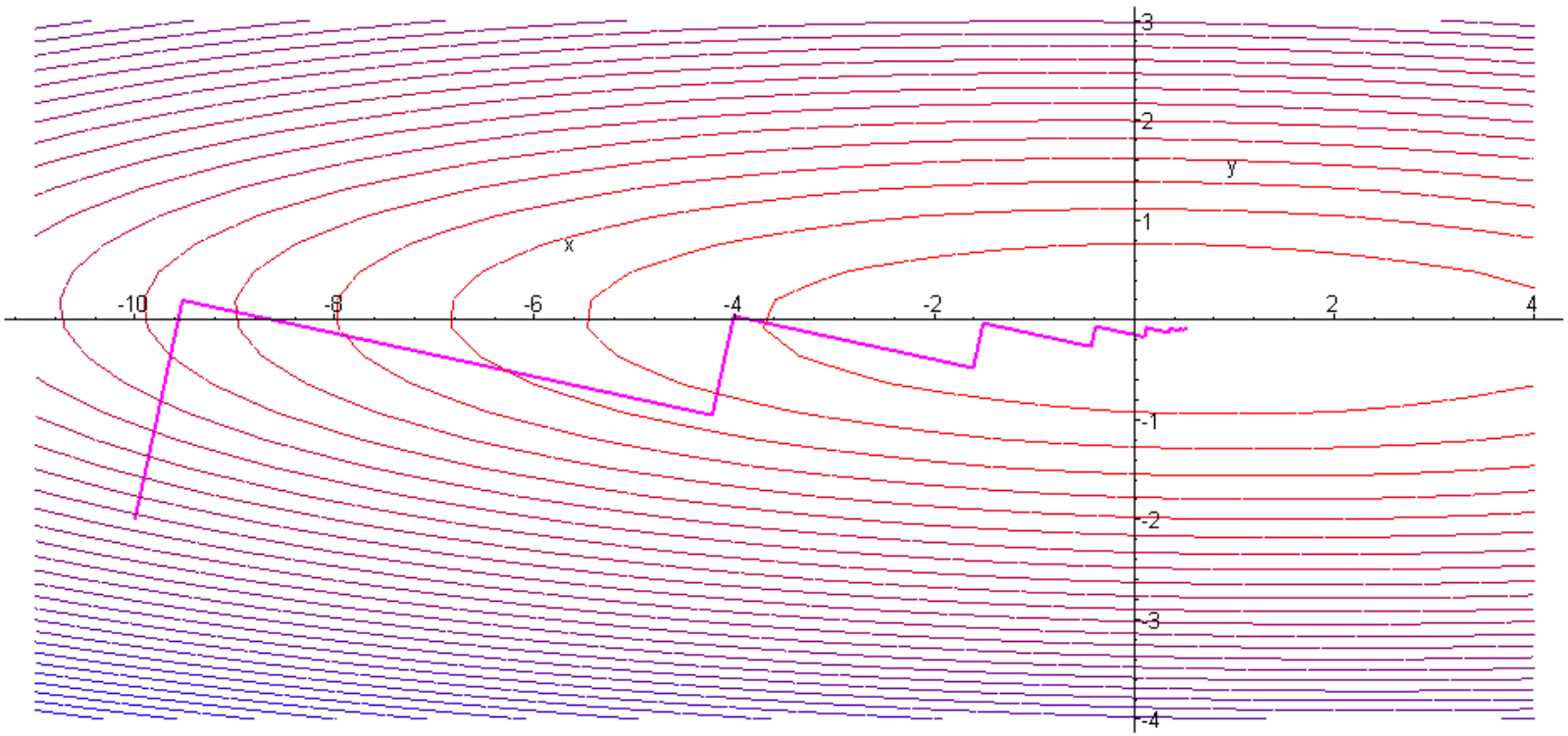
Steepest Descent – Example 1

Consider example $\begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} x = \begin{pmatrix} 2 \\ -8 \end{pmatrix}$, starting solution $\begin{pmatrix} -3 \\ -3 \end{pmatrix}$



Steepest Descent – Example 2

Consider example $\begin{pmatrix} 3 & 2 \\ 2 & 100 \end{pmatrix} x = \begin{pmatrix} 2 \\ -8 \end{pmatrix}$, starting solution $\begin{pmatrix} -10 \\ -2 \end{pmatrix}$



Multiple steps in the same search direction!

Part II

Conjugate Gradients

Conjugate Directions
***A*-Orthogonality**
Conjugate Gradients
A Miracle Occurs . . .
CG Algorithm

Conjugate Directions

- observation:
  Steepest Descent takes repeated steps in the same direction
- obvious idea:
  try to do only one step in each direction
- possible approach:
  choose orthogonal search directions $d^{(0)} \perp d^{(1)} \perp d^{(2)} \perp \ldots$
- notice:
  errors then orthogonal to previous directions:

$$e^{(1)} \perp d^{(0)}, e^{(2)} \perp d^{(1)} \perp d^{(0)}, \ldots$$

Conjugate Directions (2)

- wanted: best-possible α for correction $x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$
- use orthogonality criterion $\rightsquigarrow$ determine α from

$$\left(d^{(0)}\right)^T e^{(1)} = \left(d^{(0)}\right)^T \left(e^{(0)} - \alpha d^{(0)}\right) = 0$$

requires propagation of the error $e^{(1)} = x - x^{(1)}$

$$\begin{aligned} x^{(1)} &= x^{(0)} + \alpha_i d^{(0)} \\ x - x^{(1)} &= x - x^{(0)} - \alpha_i d^{(0)} \\ e^{(1)} &= e^{(0)} - \alpha_i d^{(0)} \end{aligned}$$

- formula for α:

$$\alpha = \frac{\left(d^{(0)}\right)^T e^{(0)}}{\left(d^{(0)}\right)^T d^{(0)}}$$

- **but:** we don't know $e^{(0)}$

A-Orthogonality

- make the search directions *A-orthogonal*:

$$\left(d^{(i)}\right)^T A d^{(j)} = 0$$

- again: errors *A*-orthogonal to previous directions:

$$\left(e^{(i+1)}\right)^T A d^{(i)} \stackrel{!}{=} 0$$

- equiv. to minimisation in search direction $d^{(i)}$:

$$\begin{aligned}
\frac{\partial}{\partial \alpha} f\left(x^{(i+1)}\right) = \left(f'\left(x^{(i+1)}\right)\right)^T \frac{\partial}{\partial \alpha} x^{(i+1)} &= 0 \\
\Leftrightarrow \quad -\left(r^{(i+1)}\right)^T d^{(i)} &= 0 \\
\Leftrightarrow \quad -\left(d^{(i)}\right)^T A e^{(i+1)} &= 0
\end{aligned}$$

A-Conjugate Directions

- remember the formula for conjugate directions:

$$\alpha = \frac{\left(d^{(0)}\right)^T e^{(0)}}{\left(d^{(0)}\right)^T d^{(0)}}$$

- same computation, but with A-orthogonality:

$$\alpha_i = \frac{\left(d^{(i)}\right)^T A e^{(i)}}{\left(d^{(i)}\right)^T A d^{(i)}} = \frac{\left(d^{(i)}\right)^T r^{(i)}}{\left(d^{(i)}\right)^T A d^{(i)}}$$

  (for the i-th iteration)
- **these α_i can be computed!**
- still to do: find A-orthogonal search directions

A-Conjugate Directions (2)

classical approach to find orthogonal directions $\rightarrow$
conjugate Gram-Schmidt process:

- from linearly independent vectors $u^{(0)}, u^{(1)}, \ldots, u^{(i-1)}$
- construct orthogonal directions $d^{(0)}, d^{(1)}, \ldots, d^{(i-1)}$

$$
\begin{aligned}
d^{(i)} &= u^{(i)} + \sum_{k=0}^{i-1} \beta_{ik} d^{(k)} \\
\beta_{ik} &= -\frac{(u^{(i)})^T A d^{(k)}}{(d^{(k)})^T A d^{(k)}}
\end{aligned}
$$

- needs to keep all old search vectors in memory
- $\mathcal{O}(n^3)$ computational complexity $\Rightarrow$ infeasible

Conjugate Gradients

- use residuals (i.e., $u^{(i)} := r^{(i)}$) to construct conjugate directions:

$$d^{(i)} = r^{(i)} + \sum_{k=0}^{i-1} \beta_{ik} d^{(k)}$$

- new direction $d^{(i)}$ should be A-orthogonal to all $d^{(j)}$:

$$0 \overset{!}{=} \left(d^{(i)}\right)^T A d^{(j)} = \left(r^{(i)}\right)^T A d^{(j)} + \sum_{k=0}^{i-1} \beta_{ik} \left(d^{(k)}\right)^T A d^{(j)}$$

- all directions $d^{(k)}$ (for $k = 0, \ldots, i-1$) are already A-orthogonal (and $j < i$), hence:

$$0 = \left(r^{(i)}\right)^T A d^{(j)} + \beta_{ij} \left(d^{(j)}\right)^T A d^{(j)} \Rightarrow \beta_{ij} = -\frac{\left(r^{(i)}\right)^T A d^{(j)}}{\left(d^{(j)}\right)^T A d^{(j)}}$$

Conjugate Gradients – Status

1. conjugate directions and computation of α_i:

$$\begin{aligned} \alpha_i &= \frac{\left(d^{(i)}\right)^T r^{(i)}}{\left(d^{(i)}\right)^T A d^{(i)}} \\ x^{(i+1)} &= x^{(i)} + \alpha_i d^{(i)} \end{aligned}$$

2. use residuals to compute search directions:

$$\begin{aligned} d^{(i)} &= r^{(i)} + \sum_{k=0}^{i-1} \beta_{ik} d^{(k)} \\ \beta_{ik} &= -\frac{\left(r^{(i)}\right)^T A d^{(k)}}{\left(d^{(k)}\right)^T A d^{(k)}} \end{aligned}$$

$\rightarrow$ **still too expensive**, as we need to store all vectors $d^{(k)}$

A Miracle Occurs – Part 1

Two small contributions:

1. propagation of the error $e^{(i)} = x - x^{(i)}$

$$\begin{aligned} x^{(i+1)} &= x^{(i)} + \alpha_i d^{(i)} \\ x - x^{(i+1)} &= x - x^{(i)} - \alpha_i d^{(i)} \\ e^{(i+1)} &= e^{(i)} - \alpha_i d^{(i)} \end{aligned}$$

   (we have used this once, already)

2. propagation of residuals

$$\begin{aligned} r^{(i+1)} &= Ae^{(i+1)} = A\left(e^{(i)} - \alpha_i d^{(i)}\right) \\ \Rightarrow r^{(i+1)} &= r^{(i)} - \alpha_i A d^{(i)} \end{aligned}$$

A Miracle Occurs – Part 2

Orthogonality of the residuals:

- search directions are A-orthogonal
- only one step in each direction
- hence: error is A-orthogonal to all previous search directions:
  $\left(d^{(i)}\right)^T A e^{(j)} = 0$, for $i < j$
- residuals are orthogonal to all previous search directions:
  $\left(d^{(i)}\right)^T r^{(j)} = 0$, for $i < j$
- search directions are built from residuals:
  $\text{span}\left\{d^{(0)}, \ldots, d^{(i-1)}\right\} = \text{span}\left\{r^{(0)}, \ldots, r^{(i-1)}\right\}$
- hence: **residuals are orthogonal**

$$\left(r^{(i)}\right)^T r^{(j)} = 0, \qquad i < j$$

A Miracle Occurs – Part 3

- combine orthogonality and recurrence for residuals:

$$\begin{aligned} \left(r^{(i)}\right)^T r^{(j+1)} &= \left(r^{(i)}\right)^T r^{(j)} - \alpha_j \left(r^{(i)}\right)^T A d^{(j)} \\ \Rightarrow \alpha_j \left(r^{(i)}\right)^T A d^{(j)} &= \left(r^{(i)}\right)^T r^{(j)} - \left(r^{(i)}\right)^T r^{(j+1)} \end{aligned}$$

- $\left(r^{(i)}\right)^T r^{(j)} = 0$, if $i \neq j$:

$$\left(r^{(i)}\right)^T A d^{(j)} = \begin{cases} \frac{1}{\alpha_i}\left(r^{(i)}\right)^T r^{(i)}, & i = j \\ -\frac{1}{\alpha_{i-1}}\left(r^{(i)}\right)^T r^{(i)}, & i = j+1 \\ 0 & \text{otherwise.} \end{cases}$$

A Miracle Occurs – Part 4

- computation of β_{ik} (for $k = 0, \ldots, i-1$):

$$\beta_{ik} = -\frac{\left(r^{(i)}\right)^T A d^{(k)}}{\left(d^{(k)}\right)^T A d^{(k)}} = \begin{cases} \dfrac{\left(r^{(i)}\right)^T r^{(i)}}{\alpha_{i-1}\left(d^{(i-1)}\right)^T A d^{(i-1)}}, & \text{if } i = k+1 \\ 0, & \text{if } i > k+1 \end{cases}$$

- thus: search directions

$$d^{(i)} = r^{(i)} + \sum_{k=0}^{i-1} \beta_{ik} d^{(k)} = r^{(i)} + \beta_{i,i-1} d^{(i-1)}$$

$$\beta_i := \beta_{i,i-1} = \frac{\left(r^{(i)}\right)^T r^{(i)}}{\alpha_{i-1}\left(d^{(i-1)}\right)^T A d^{(i-1)}}$$

$\Rightarrow$ reduces to a **simple iterative scheme for** β_i

A Miracle Occurs – Part 5

- build search directions

$$\begin{aligned} d^{(i+1)} &= r^{(i+1)} + \beta_i d^{(i)} \\ \beta_{i+1} &= \frac{\left(r^{(i+1)}\right)^T r^{(i+1)}}{\alpha_i \left(d^{(i)}\right)^T A d^{(i)}} \end{aligned}$$

- remember: $\alpha_i = \dfrac{(d^{(i)})^T r^{(i)}}{(d^{(i)})^T A d^{(i)}}$
- thus: $\alpha_i (d^{(i)})^T A d^{(i)} = (d^{(i)})^T r^{(i)}$

$$\Rightarrow \beta_{i+1} = \frac{\left(r^{(i+1)}\right)^T r^{(i+1)}}{\left(d^{(i)}\right)^T r^{(i)}} = \frac{\left(r^{(i+1)}\right)^T r^{(i+1)}}{\left(r^{(i)}\right)^T r^{(i)}}$$

- last step: $\left(d^{(i)}\right)^T r^{(i)} = \left(r^{(i)} + \beta_{i-1} d^{(i-1)}\right)^T r^{(i)} = \left(r^{(i)}\right)^T r^{(i)} + \beta_{i-1} \left(d^{(i-1)}\right)^T r^{(i)} = \left(r^{(i)}\right)^T r^{(i)}$
  (residual $r^{(i)}$ orthogonal to previous search direction $d^{(i-1)}$)

Conjugate Gradients – Algorithm

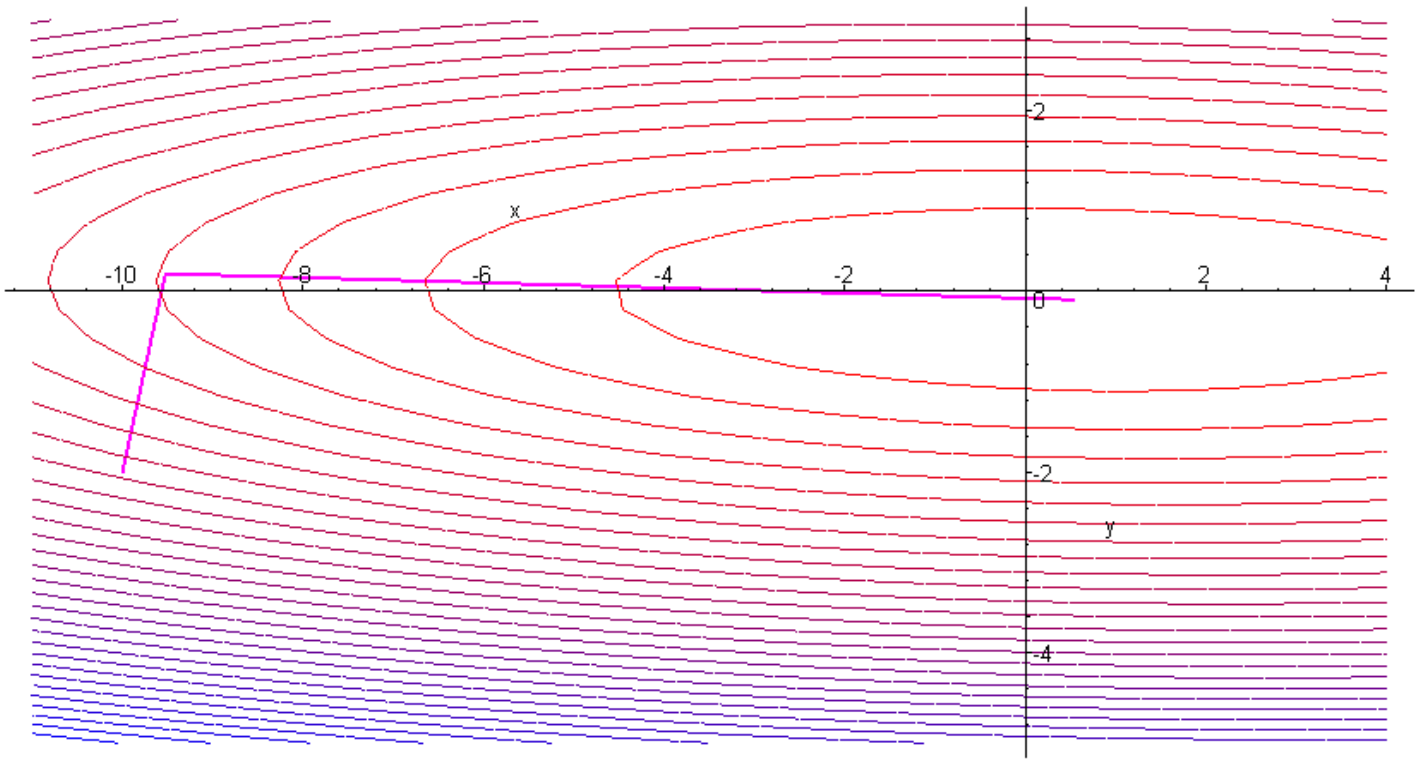
Start with $d^{(0)} = r^{(0)} = b - Ax^{(0)}$

While $r^{(i)} > \epsilon$ iterate over:

1. $\alpha_i = \dfrac{(r^{(i)})^T r^{(i)}}{(d^{(i)})^T A d^{(i)}}$
2. $x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$
3. $r^{(i+1)} = r^{(i)} - \alpha_i A d^{(i)}$
4. $\beta_{i+1} = \dfrac{\left(r^{(i+1)}\right)^T r^{(i+1)}}{\left(r^{(i)}\right)^T r^{(i)}}$
5. $d^{(i+1)} = r^{(i+1)} + \beta_{i+1} d^{(i)}$

Conjugate Gradients – Example

Consider example $\begin{pmatrix} 3 & 2 \\ 2 & 100 \end{pmatrix} x = \begin{pmatrix} 2 \\ -8 \end{pmatrix}$, starting solution $\begin{pmatrix} -10 \\ -2 \end{pmatrix}$



Convergence to solution after $n = 2$ steps!

Part III

Preconditioning

CG Convergence
Preconditioning
CG with “Change-of-Basis” Preconditioning
Hierarchical Transforms
CG with Matrix Preconditioner
Preconditioners – Examples
ILU and Incomplete Cholesky

Conjugate Gradients – Convergence

Convergence Analysis:

- uses *Krylov subspace*:

$$\text{span}\left\{r^{(0)}, Ar^{(0)}, A^2 r^{(0)}, \ldots, A^{i-1} r^{(0)}\right\}$$

- "Krylov subspace method"

Convergence Results:

- in principle: direct method (n steps)
  (however: orthogonality lost due to round-off errors $\rightarrow$ exact solution not found)
- in practice: iterative scheme

$$\left\|e^{(i)}\right\|_A \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^i \left\|e^{(0)}\right\|_A, \quad \kappa = \lambda_{\text{max}}/\lambda_{\text{min}}$$

Preconditioning

- convergence depends on matrix A
- idea: modify linear system

$$Ax = b \quad \rightsquigarrow \quad M^{-1}Ax = M^{-1}b,$$

  then: convergence depends on matrix $M^{-1}A$
- optimal preconditioner: $M^{-1} = A^{-1}$:

$$A^{-1}Ax = A^{-1}b \Leftrightarrow x = A^{-1}b.$$

- in practice:
  - avoid explicit computation of $M^{-1}A$
  - find an M similar to A, compute effect of M^{-1} (i.e., approximate solution of SLE)
  - or: find an M^{-1} similar to A^{-1}
- also possible: solve $AMy = b$ for y, and then $x = My$

CG and Preconditioning

- just replace A by $M^{-1}A$ in the algorithm??
- problem: $M^{-1}A$ not necessarily symmetric
  (even if M and A both are)
- we will try an alternative first:
  symmetric preconditioning

$$Ax = b \quad \rightsquigarrow \quad L^T AL\hat{x} = L^T b, \quad x = L\hat{x}$$

- Remember: for Finite Element discretization, this corresponds to a change of basis functions!
- can we implement CG without having to set up $L^T AL$?
- requires some re-computations in the CG algorithm
  (see following slides)

“Change-of-Basis” Preconditioning

- preconditioned system of equations:

$$Ax = b \quad \rightsquigarrow \quad \underbrace{(L^T A L)}_{=:\widehat{A}} \hat{x} = \underbrace{L^T b}_{=:\hat{b}}, \quad x = L\hat{x}$$

- computation of residual:

$$\hat{r} = \hat{b} - \widehat{A}\,\hat{x} = L^T b - L^T A L \hat{x} = L^T (b - Ax) = L^T r$$

- computation of α (for preconditioned system):

$$\alpha_i := \frac{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}{\left(\hat{d}^{(i)}\right)^T \widehat{A}\,\hat{d}^{(i)}} = \frac{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}{\left(\hat{d}^{(i)}\right)^T L^T A L\,\hat{d}^{(i)}} = \frac{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}{\left(\tilde{d}^{(i)}\right)^T A\,\tilde{d}^{(i)}}$$

  where we defined $L\hat{d}^{(i)} =: \tilde{d}^{(i)}$

- update of solution:

$$\begin{aligned} \hat{x}^{(i+1)} &= \hat{x}^{(i)} + \alpha_i \hat{d}^{(i)} \\ \Rightarrow x^{(i+1)} = L\hat{x}^{(i+1)} &= L\hat{x}^{(i)} + L\alpha_i \hat{d}^{(i)} = x^{(i)} + \alpha_i \tilde{d}^{(i)} \end{aligned}$$

“Change-of-Basis” Preconditioning (2)

- update residuals $\hat{r}$:

$$\begin{aligned}\hat{r}^{(i+1)} &= \hat{r}^{(i)} - \alpha_i \widehat{A}\hat{d}^{(i)} = \hat{r}^{(i)} - \alpha_i L^T A L\, \hat{d}^{(i)} \\ &= \hat{r}^{(i)} - \alpha_i L^T A\, \tilde{d}^{(i)}\end{aligned}$$

- computation of β_i:

$$\beta_{i+1} = \frac{\left(\hat{r}^{(i+1)}\right)^T \hat{r}^{(i+1)}}{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}$$

- update of search directions:

$$\begin{aligned}\hat{d}^{(i+1)} &= \hat{r}^{(i+1)} + \beta_i \hat{d}^{(i)} \\ \Rightarrow \tilde{d}^{(i+1)} = L\hat{d}^{(i+1)} &= L\hat{r}^{(i+1)} + L\beta_i \hat{d}^{(i)} \\ &= L\hat{r}^{(i+1)} + \beta_i \tilde{d}^{(i)}\end{aligned}$$

CG with "Change-of-Basis" Preconditioning

Start with $\hat{r}^{(0)} = L^T(b - Ax^{(0)})$ and $\tilde{d}^{(0)} = L\hat{r}^{(0)}$;

While $\hat{r}^{(i)} > \epsilon$ iterate over:

1. $\alpha_i = \dfrac{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}{\left(\tilde{d}^{(i)}\right)^T A \tilde{d}^{(i)}}$
2. $x^{(i+1)} = x^{(i)} + \alpha_i \tilde{d}^{(i)}$
3. $\hat{r}^{(i+1)} = \hat{r}^{(i)} - \alpha_i L^T A \tilde{d}^{(i)}$
4. $\beta_{i+1} = \dfrac{\left(\hat{r}^{(i+1)}\right)^T \hat{r}^{(i+1)}}{\left(\hat{r}^{(i)}\right)^T \hat{r}^{(i)}}$
5. $\tilde{d}^{(i+1)} = L\hat{r}^{(i+1)} + \beta_i \tilde{d}^{(i)}$

Hierarchical Basis Preconditioning

Some specifics for the CG implementation:

- L transforms coefficient vector from hierarchical basis to nodal basis, for example $\hat{x} = L\,x$ or $\tilde{d} = L\,\hat{d}$
- L^T transforms the vector of basis functions from nodal basis to hierarchical basis (cmp. FEM), thus $\hat{r} = L^T\,r$
- effect of L and L^T can be computed in $\mathcal{O}(N)$ operations

HB-CG for the Poisson problem:

- in 1D: convergence after a $\log N$ iterations!
  (in this case: $L^T A L$ diagonal matrix with $\log N$ different eigenvalues)
- in 2D and 3D very fast convergence!
- further improved by additional diagonal preconditioning
- so-called *hierarchical generating systems* (change to a multigrid basis) achieve multigrid-like performance

CG with Hierarchical Generating Systems

Recall: system of linear equations $A^{\mathrm{GS}} v^{\mathrm{GS}} = b^{\mathrm{GS}}$ given as

$$\begin{pmatrix} A_h & A_h P_{2h}^h & A_h P_{4h}^h \\ R_h^{2h} A_h & A_{2h} & A_{2h} P_{4h}^{2h} \\ R_h^{4h} A_h & R_{2h}^{4h} A_{2h} & A_{4h} \end{pmatrix} \begin{pmatrix} v_h \\ v_{2h} \\ v_{4h} \end{pmatrix} = \begin{pmatrix} b_h \\ R_h^{2h} b_h \\ R_h^{4h} b_h \end{pmatrix}$$

Preconditioning for CG?

- system $A^{\mathrm{GS}} v^{\mathrm{GS}} = b^{\mathrm{GS}}$ is singular
  $\rightarrow$ subspace of solutions v^{GS} (minima of the quadratic form!)
- however: any of the solutions will do!
- convergence result:

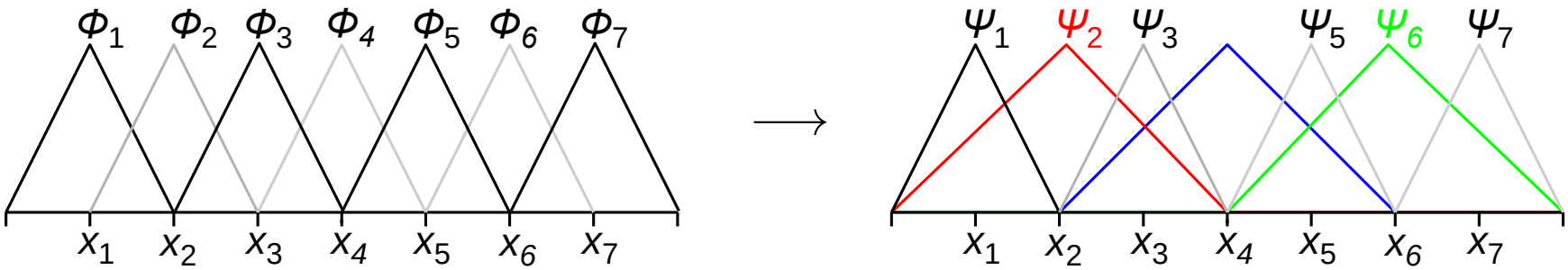
$$\left\| e^{(i)} \right\|_A \leq 2 \left(\frac{\sqrt{\hat{\kappa}_{\mathrm{GS}}} - 1}{\sqrt{\hat{\kappa}_{\mathrm{GS}}} + 1} \right)^i \left\| e^{(0)} \right\|_A, \quad \hat{\kappa}_{\mathrm{GS}} = \hat{\lambda}_{\max} / \hat{\lambda}_{\min}$$

  where $\hat{\kappa}_{\mathrm{GS}}$ is the ratio of largest vs. smallest **non-zero** eigenvalue
- for Poisson eq.: $\hat{\kappa}_{\mathrm{GS}}$ independent of $h \rightsquigarrow$ multigrid convergence

Hierarchical Basis Transformation

Towards level-wise approach

Consider "semi-hierarchical" transform:



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

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:

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

- consider Hierarchical-Basis-Preconditioning for FEM-discretization: $L^T := H_n$ and we need to compute $\hat{r}^{(0)} = L^T r^{(0)}$ and $L^T A\, \tilde{d}^{(i)}$
- each level-wise transform $H_n^{(k)}$ has a simple loop implementation:

For k from 1 to n-1 do
For j from 2^k to 2^n step 2^k
$r_j := \frac{1}{2} r_{j-2^{k-1}} + r_k + \frac{1}{2} r_{j+2^{k-1}}$

Hierarchical Coordinate Transformation

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

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

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

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

- consider Hierarchical-Basis-Preconditioning for FEM-discretization: $L := H_n^T$ for computation of $\tilde{d}^{(0)} = L\,\hat{r}^{(0)}$ and $\tilde{d}^{(i+1)} = L\,\hat{r}^{(i+1)} + \beta_i \tilde{d}^{(i)}$
- again: use loop-based implementations for $\left(H_n^{(k)}\right)^T a$

For k from n-1 downto 1
For i from 2^{k-1} to 2^n step 2^k
$d_i := \frac{1}{2} d_{i-2^{k-1}} + d_i + \frac{1}{2} d_{i+2^{k-1}}$ *(with $d_0 = a_{d^n} = 0$)*

CG and Preconditioning (revisited)

- preconditioning: replace A by $M^{-1}A$
- problem: $M^{-1}A$ not necessarily symmetric
- compare symmetric preconditioning

$$Ax = b \quad \rightsquigarrow \quad L^T AL\hat{x} = Lb, \quad x = L\hat{x}$$

- workaround: find $E^T E = M$ (Cholesky fact.), then

$$Ax = b \quad \rightsquigarrow \quad E^{-T} AE^{-1}\hat{x} = E^{-T} b, \quad \hat{x} = Ex$$

- what if E cannot be computed (efficiently)?
  (neither M nor M^{-1} might be known explicitly!)
- E, E^{-T}, E^{-1} can be eliminated from algorithm
  (again requires some re-computations):

$$\text{set } \hat{d} = Ed \quad \text{and use } \hat{r} = E^{-T} r, \quad \hat{x} = Ex, \quad E^{-1}E^{-T} = M^{-1}$$

CG with Preconditioner

Start: $r^{(0)} = b - Ax^{(0)}$; $d^{(0)} = M^{-1} r^{(0)}$

1. $\alpha_i = \dfrac{(r^{(i)})^T M^{-1} r^{(i)}}{(d^{(i)})^T A d^{(i)}}$
2. $x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$
3. $r^{(i+1)} = r^{(i)} - \alpha_i A d^{(i)}$
4. $\beta_{i+1} = \dfrac{\left(r^{(i+1)}\right)^T M^{-1} r^{(i+1)}}{\left(r^{(i)}\right)^T M^{-1} r^{(i)}}$
5. $d^{(i+1)} = M^{-1} r^{(i+1)} + \beta_{i+1} d^{(i)}$

(for detailed derivation, see Shewchuck)

Implementation

Preconditioning steps: $M^{-1}r^{(i)}, M^{-1}r^{(i+1)}$

- M^{-1} known then multiply $M^{-1}r^{(i)}$
- M known? Then solve $My = r^{(i)}$ to obtain $y = M^{-1}r^{(i)}$
- neither M, nor M^{-1} are known explicitly:
  - algorithm to solve $My = r^{(i)}$ is sufficient!
  - algorithm to compute action of M^{-1} on a vector is sufficient!

  $\Rightarrow$ any approximate solver for $Ae = r^{(i)}$ is sufficient
  (if it is equivalent to applying a symmetric and pos. definite matrix)

Preconditioners for CG – Examples

- find $M \approx A$ and compute effect of M^{-1}:
  - Jacobi preconditioning: $M := D_A$
  - (Symmetric) Gauss-Seidel preconditioning: $M := L_A$ or $M = (D_A + L'_A)D_A^{-1}(D_A + (L'_A)^T)$, etc.
- just compute effect of M^{-1}:
  - any approximate solver might do
    $\rightarrow$ incl. multigrid methods
  - incomplete Cholesky factorization
    $\rightarrow$ i.e., incomplete LU-decomposition (ILU) for symmetric positive definite matrix
  - use a multigrid method as preconditioner(?)
    $\rightarrow$ worthwhile (only) in situations where multigrid does not work (well) as stand-alone solver
- find an M^{-1} similar to A^{-1}
  - "sparse approximate inverse" (SPAI)
  - tries to minimise $\|I - MA\|_F$, where M is a matrix with (given) sparse non-zero pattern

Preconditioners – ILU and Incomplete Cholesky

Recall LU decomposition and Cholesky factorization:

- LU decomposition: given A, find lower/upper triangular matrices L and U such that $A = LU$
- Cholesky factorization: given $A = A^T$, find lower triangular matrix L such that $A = LL^T \rightarrow$ symmetric preconditioning!
- variants with explicit diagonal matrix D:

$$A = LD^{-1}U \qquad \text{or} \qquad A = LD^{-1}L^T,$$

  where $L = D + L'$ and $R = D + R'$ with *strict* lower/upper triangular L', R'
- **but:** for sparse A, **L and U may be non-sparse**

Idea: disregard all fill-in during factorization

Cholesky Factorization

$$\begin{pmatrix} L_{11} & & \\ L_{21} & L_{22} & \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} D_{11}^{-1} & & \\ & D_{22}^{-1} & \\ & & D_{33}^{-1} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{21}^T & L_{31}^T \\ & L_{22}^T & L_{32}^T \\ & & L_{33}^T \end{pmatrix} = \begin{pmatrix} A_{11} & A_{21}^T & A_{31}^T \\ A_{21} & A_{22} & A_{32}^T \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$$

Derive the factorization algorithm:

- assume that $A_{11} \stackrel{!}{=} L_{11} D_{11}^{-1} L_{11}^T$ is already factorized
- let L_{21} be a $1 \times k$ submatrix, i.e., to compute next row of L:

$$L_{21} D_{11}^{-1} L_{11}^T \stackrel{!}{=} A_{21}$$

  $D_{11}^{-1} L_{11}^T$ upper triangular matrix $\rightarrow$ solve triangular system for L_{21}
- by convention $L_{22} = D_{22}$ (1×1 "matrix"), which is computed from:

$$L_{21} D_{11}^{-1} L_{21}^T + L_{22} D_{22}^{-1} L_{22}^{-T} \stackrel{!}{=} A_{22} \quad \Rightarrow \quad L_{22} = D_{22} := A_{22} - L_{21} D_{11}^{-1} L_{21}^T$$

Incomplete Cholesky Factorization

Algorithm: ($A \to LD^{-1}L^T$)

- initialize $D := 0$, $L := 0$
- for $i = 1, \ldots, n$:
  1. for $k = 1, \ldots, i-1$:
     if $(i,k) \in S$ then set $L_{ik} := A_{ik} - \sum_{j<k}{}' L_{ij} D_{jj}^{-1} L_{kj}$
  2. set $L_{ii} = D_{ii} := A_{ii} - \sum_{j<i}{}' L_{ij} D_{jj}^{-1} L_{ij}$
- note: sums $\sum_{j<k}{}'$ and $\sum_{j<i}{}'$ only consider non-zero elements $\in S$
- uses given **pattern** S of non-zero elements in the factorization (frequent choice: use non-zeros of A for S)
- Cholesky factorization computed in $\mathcal{O}(n)$ operations for sparse matrices (with $c \cdot n$ non-zeros)
- frequently used for preconditioning

Literature/References

Conjugate Gradients:

- Shewchuk: *An Introduction to the Conjugate Gradient Method Without the Agonizing Pain*.
- Hackbusch: *Iterative Solution of Large Sparse Systems of Equations*, Springer 1993.
- M. Griebel: *Multilevelmethoden als Iterationsverfahren über Erzeugendensystemen*, Teubner Skripten zur Numerik, 1994

  M. Griebel: *Multilevel algorithms considered as iterative methods on semidefinite systems*, SIAM Int. J. Sci. Stat. Comput. 15(3), 1994.