

Outlines

Part I: Quadratic
Forms and Steepest
Descent

Part II: Conjugate
Gradients

Part III:
Preconditioning

Scientific Computing II

Conjugate Gradient Methods

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

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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:

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

- multigrid methods: coarse-grid correction on residual equation

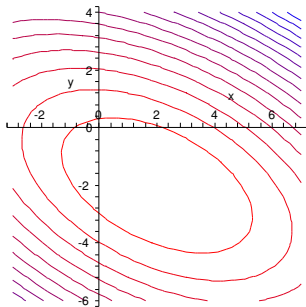
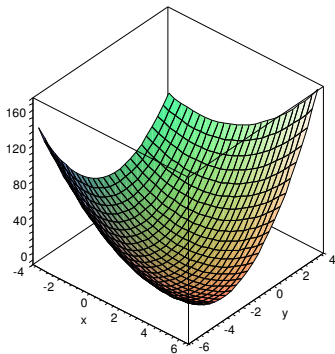
Part I

Quadratic Forms and Steepest Descent

Quadratic Forms

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

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



Quadratic Forms (2)

The *gradient* of a quadratic form is defined as

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

- $f'(x) = Ax - b$

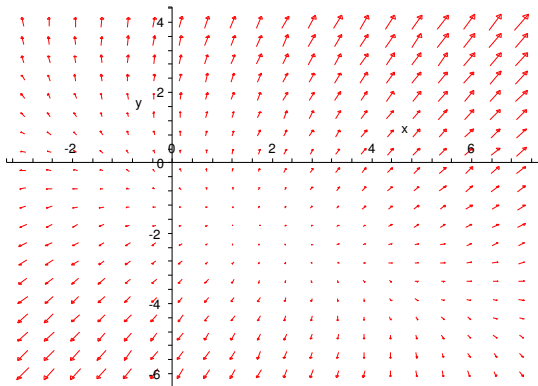
- $f'(x) = 0 \Leftrightarrow Ax - b = 0 \Leftrightarrow Ax = b$

$\Rightarrow Ax = b$ 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
(often 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:

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

Steepest Descent – find α (2)

$$(r^{(1)})^T r^{(0)} = (b - Ax^{(1)})^T r^{(0)} = 0$$

$$(b - A(x^{(0)} + \alpha r^{(0)}))^T r^{(0)} = 0$$

$$(b - Ax^{(0)})^T r^{(0)} - \alpha (Ar^{(0)})^T r^{(0)} = 0$$

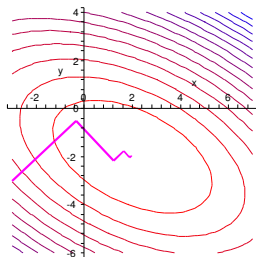
$$(r^{(0)})^T r^{(0)} - \alpha (r^{(0)})^T Ar^{(0)} = 0$$

Solve for α :

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

Steepest Descent – Algorithm

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



Observations:

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

Part II

Conjugate Gradients

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
 $d^{(0)} \perp d^{(1)} \perp d^{(2)} \perp \dots$
- notice: errors orthogonal to previous directions:
 $e^{(1)} \perp d^{(0)}, e^{(2)} \perp d^{(1)} \perp d^{(0)}, \dots$

Conjugate Directions (2)

- compute α from

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

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 :

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

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

A-Orthogonality

- make the search directions *A-orthogonal*:

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

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

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

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

$$\frac{\partial}{\partial \alpha} f(x^{(i+1)}) = \left(f'(x^{(i+1)}) \right)^T \frac{\partial}{\partial \alpha} x^{(i+1)} = 0$$

$$\Leftrightarrow - (r^{(i+1)})^T d^{(i)} = 0$$

$$\Leftrightarrow - (d^{(i)})^T A e^{(i+1)} = 0$$

A-Conjugate Directions

- remember the formula for conjugate directions:

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

- same computation, but with A -orthogonality:

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

(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 $u^{(0)}, u^{(1)}, \dots, u^{(i-1)}$
- construct orthogonal directions $d^{(0)}, d^{(1)}, \dots, d^{(i-1)}$

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

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

Conjugate Gradients

- use residuals (i.e., $u^{(i)} := r^{(0)}$) 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 $d^{(j)}$:

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

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

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

Conjugate Gradients – Status

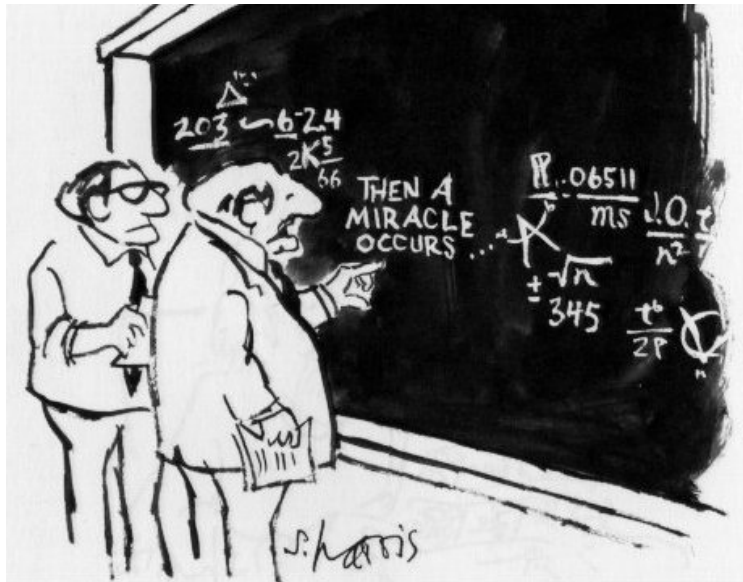
- 1 conjugate directions:

$$\alpha_i = \frac{(d^{(i)})^T r^{(i)}}{(d^{(i)})^T A d^{(i)}}$$
$$x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$$

- 2 use residuals to compute search directions:

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

→ **still infeasible**, as we need to store all vectors $d^{(k)}$



“I think you should be more explicit here in step two.”

from *What's so Funny about Science?* by Sidney Harris (1977)

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

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

A Miracle Occurs – Part 2

Orthogonality of the residuals:

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

$$(r^{(i)})^T r^{(j)} = 0, \quad i < j$$

A Miracle Occurs – Part 3

- combine orthogonality and recurrence for residuals:

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

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

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

A Miracle Occurs – Part 4

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

$$\begin{aligned}\beta_{ik} &= -\frac{(r^{(i)})^T Ad^{(k)}}{(d^{(k)})^T Ad^{(k)}} \\ &= \begin{cases} \frac{(r^{(i)})^T r^{(i)}}{\alpha_{i-1} (d^{(i-1)})^T Ad^{(i-1)}}, & i = k + 1 \\ 0 & i > k + 1 \end{cases}\end{aligned}$$

- thus: search directions

$$d^{(i)} = r^{(i)} + \sum_{k=0}^{i-1} \beta_{ik} d^{(k)} = r^{(i)} + \beta_{i,i-1} d^{(i-1)}$$
$$\beta_i := \beta_{i,i-1} = \frac{(r^{(i)})^T r^{(i)}}{\alpha_{i-1} (d^{(i-1)})^T Ad^{(i-1)}}$$

A Miracle Occurs – Part 5

- build search directions

$$d^{(i+1)} = r^{(i+1)} + \beta_i d^{(i)}$$
$$\beta_{i+1} = \frac{(r^{(i+1)})^T r^{(i+1)}}{\alpha_i (d^{(i)})^T A d^{(i)}}$$

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

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

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

Conjugate Gradients – Algorithm

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

$$\textcircled{1} \quad \alpha_i = \frac{(r^{(i)})^T r^{(i)}}{(d^{(i)})^T A d^{(i)}}$$

$$\textcircled{2} \quad x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$$

$$\textcircled{3} \quad r^{(i+1)} = r^{(i)} - \alpha_i A d^{(i)}$$

$$\textcircled{4} \quad \beta_{i+1} = \frac{(r^{(i+1)})^T r^{(i+1)}}{(r^{(i)})^T r^{(i)}}$$

$$\textcircled{5} \quad d^{(i+1)} = r^{(i+1)} + \beta_{i+1} d^{(i)}$$

Part III

Preconditioning

Conjugate Gradients – Convergence

Convergence Analysis:

- uses *Krylow subspace*:

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

- “Krylow subspace method”

Convergence Results:

- in principle: direct method (n steps)
- in practice: iterative scheme

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

Preconditioning

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

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

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}

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

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

- Note: for Finite Element discretization, this corresponds to a change of basis functions!
- requires some re-computations in the CG algorithm (see following slides)

"Change-of-Basis" Preconditioning

- preconditioned system of equations:

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

- computation of residual:

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

- computation of α for new system:

$$\alpha_i := \frac{(\hat{r}^{(i)})^T \hat{r}^{(i)}}{(\hat{d}^{(i)})^T \hat{A} \hat{d}^{(i)}} = \frac{(\hat{r}^{(i)})^T \hat{r}^{(i)}}{(\hat{d}^{(i)})^T L^T AL \hat{d}^{(i)}} = \frac{(\hat{r}^{(i)})^T \hat{r}^{(i)}}{(\tilde{d}^{(i)})^T A \tilde{d}^{(i)}}$$

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} :

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

- computation of β_i :

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

- 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 Convergence

Preconditioning

CG with
“Change-of-Basis”
PreconditioningCG with Matrix
PreconditionerPreconditioners –
Examples

CG with "Change-of-Basis" Preconditioning

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

$$\textcircled{1} \quad \alpha_j = \frac{(\hat{r}^{(j)})^T \hat{r}^{(j)}}{(\tilde{d}^{(j)})^T A \tilde{d}^{(j)}}$$

$$\textcircled{2} \quad x^{(j+1)} = x^{(j)} + \alpha_j \tilde{d}^{(j)}$$

$$\textcircled{3} \quad \hat{r}^{(j+1)} = \hat{r}^{(j)} - \alpha_j L^T A \tilde{d}^{(j)}$$

$$\textcircled{4} \quad \beta_{j+1} = \frac{(\hat{r}^{(j+1)})^T \hat{r}^{(j+1)}}{(\hat{r}^{(j)})^T \hat{r}^{(j)}}$$

$$\textcircled{5} \quad \tilde{d}^{(j+1)} = L\hat{r}^{(j+1)} + \beta_j \tilde{d}^{(j)}$$

Hierarchical Basis Preconditioning

Some specifics for the CG implementation:

- L transforms vector from nodal basis to hierarchical basis, for example $\hat{r} = Lr$
- L^T transforms the vector of basis functions from nodal basis to hierarchical basis (cmp. FEM)
- 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 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
(requires some re-computations)

CG with Preconditioner

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

$$\textcircled{1} \quad \alpha_i = \frac{(r^{(i)})^T M^{-1}r^{(i)}}{(d^{(i)})^T Ad^{(i)}}$$

$$\textcircled{2} \quad x^{(i+1)} = x^{(i)} + \alpha_i d^{(i)}$$

$$\textcircled{3} \quad r^{(i+1)} = r^{(i)} - \alpha_i Ad^{(i)}$$

$$\textcircled{4} \quad \beta_{i+1} = \frac{(r^{(i+1)})^T M^{-1}r^{(i+1)}}{(r^{(i)})^T M^{-1}r^{(i)}}$$

$$\textcircled{5} \quad d^{(i+1)} = M^{-1}r^{(i+1)} + \beta_{i+1}d^{(i)}$$

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!
→ any approximate solver for $Ae = r^{(i)}$
 - algorithm to compute M^{-1} is sufficient!
→ compute (sparse) approximate inverse (SPAI)
- Examples: Multigrid, Jacobi, ILU, SPAI, ...

Preconditioners for CG – Examples

- find $M \approx A$ and compute effect of M^{-1} :
 - Jacobi preconditioning: $M := D_A$
 - Gauss-Seidel preconditioning: $M := L_A$, etc.
- just compute effect of M^{-1} :
 - any approximate solver might do
 - incl. multigrid methods
 - incomplete LU -decomposition (ILU)
 - use a multigrid method as preconditioner(?)
 - 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

General:

- Gander, Hrebicek: *Solving Problems in Scientific Computing Using Maple and MATLAB.*
- Golub, Ortega: *Scientific Computing and Differential Equations.*
- Dongarra, et. al.: *Numerical linear algebra for high-performance computers.*

Literature (2)

Multigrid:

- Briggs, Henson, McCormick: *A Multigrid Tutorial* (2nd ed.).

Conjugate Gradients:

- Shewchuk: *An Introduction to the Conjugate Gradient Method Without the Agonizing Pain.*