Parallel Numerics, WT 2012/2013

5 Iterative Methods for Sparse Linear Systems of Equations

Contents

- Disadvantages of direct methods (in parallel):
  - strongly sequential
  - may lead to dense matrices
  - sparsity pattern changes, additional entries necessary
  - indirect addressing
  - storage
  - computational effort
- Iterative solver:
  - choose initial guess = starting vector $x^{(0)}$, e.g., $x^{(0)} = \mathbf{0}$
  - iteration function $x^{(k+1)} := \Phi(x^{(k)})$
- Applied on solving a linear system:
  - Main part of Φ should be a matrix-vector multiplication Ax (matrix-free!?)
  - Easy to parallelize, no change in the pattern of A.

$$x^{(k)} \xrightarrow{k\to\infty} \bar{x} = A^{-1}b$$

  - Main problem: Fast convergence!

5.1. Stationary Methods

5.1.1. Richardson Iteration

- Construct from $Ax = b$ an iteration process:

$$b = Ax = (\underbrace{A - I + I}_{\text{(artificial) splitting of } A})x = x - (I - A)x \quad \Rightarrow \quad x = b + (I - A)x$$

$$= b + Nx$$

- Leads to equation $x = \Phi(x)$ with $\Phi(x) := b + Nx$:

start: $x^{(0)}$;

$$x^{(k+1)} := \Phi(x^{(k)}) = b + Nx^{(k)} = b + (I - A)x^{(k)}$$

Richardson Iteration (cont.)

$$\text{start: } x^{(0)};$$
$$x^{(k+1)} := \Phi(x^{(k)}) = b + Nx^{(k)} = b + (I - A)x^{(k)}$$

If $x^{(k)}$ is convergent, $x^{(k)} \to \tilde{x}$,

then

$$\tilde{x} = \Phi(\tilde{x}) = b + N\tilde{x} = b + (I - A)\tilde{x} \Rightarrow A\tilde{x} = b$$

and therefore it holds

$$x^{(k)} \to \tilde{x} = \bar{x} := A^{-1}b$$

Residual-based formulation:

$$\begin{aligned} x^{(k+1)} &= \Phi(x^{(k)}) = b + (I - A)x^{(k)} = b + x^{(k)} - Ax^{(k)} \\ &= x^{(k)} + \underbrace{(b - Ax^{(k)})}_{r(x) \,=\, \text{residual}} = x^{(k)} + r(x^{(k)}) \end{aligned}$$

Convergence Analysis via Neumann Series

$$\begin{aligned} x^{(k)} &= b + Nx^{(k-1)} = b + N(b + Nx^{(k-2)}) = b + Nb + N^2 x^{(k-2)} = \\ \ldots &= b + Nb + N^2 b + \cdots + N^{k-1} b + N^k x^{(0)} = \\ &= \sum_{j=0}^{k-1} N^j b + N^k x^{(0)} = \left(\sum_{j=0}^{k-1} N^j \right) b + N^k x^{(0)} \end{aligned}$$

Special case $x^{(0)} = 0$:

$$x^{(k)} = \left(\sum_{j=0}^{k-1} N^j \right) b$$

$$\begin{aligned} \Rightarrow x^{(k)} \in \operatorname{span}\{b, Nb, N^2 b, \ldots, N^{k-1} b\} &= \operatorname{span}\{b, Ab, A^2 b, \ldots, A^{k-1} b\} \\ &= K_k(A, b) \end{aligned}$$

which is called the Krylov space to A and b.

For $\|N\| < 1$ holds:

$$\sum_{j=0}^{k-1} N^j \rightarrow \sum_{j=0}^{\infty} N^j = (I - N)^{-1} = (I - (I - A))^{-1} = A^{-1}$$

Convergence Analysis via Neumann Series (cont.)

$$x^{(k)} \rightarrow \left(\sum_{j=0}^{\infty} N^j\right) b = (I-N)^{-1} b = A^{-1} b = \bar{x}$$

Richardson iteration is convergent for $\|N\| < 1$ or $A \approx I$.

Error analysis for $e^{(k)} := x^{(k)} - \bar{x}$:

$$\begin{aligned} e^{(k+1)} &= x^{(k+1)} - \bar{x} = \Phi(x^{(k)}) - \Phi(\bar{x}) = (b + Nx^{(k)}) - (b + N\bar{x}) = \\ &= N(x^{(k)} - \bar{x}) = Ne^{(k)} \end{aligned}$$

$$\|e^{(k)}\| \leq \|N\| \|e^{(k-1)}\| \leq \|N\|^2 \|e^{(k-2)}\| \leq \cdots \leq \|N\|^k \|e^{(0)}\|$$

$$\|N\| < 1 \Rightarrow \|N\|^k \xrightarrow{k \to \infty} 0 \Rightarrow \|e^{(k)}\| \xrightarrow{k \to \infty} 0$$

- Convergence, if $\rho(N) = \rho(I - A) < 1$, where ρ is spectral radius

$$\rho(N) = |\lambda_{\max}| = \max_i(|\lambda_i|) \qquad (\lambda_i \text{ is eigenvalue of } N)$$

- Eigenvalues of A have to be all in circle around 1 with radius 1.

Splittings of A

- Convergence of Richardson only in very special cases!
  Try to improve the iteration for better convergence!
- Write A in form $A := M - N$

$$b = Ax = (M - N)x = Mx - Nx \Leftrightarrow x = M^{-1}b + M^{-1}Nx = \Phi(x)$$

$$\begin{aligned}\Phi(x) &= M^{-1}b + M^{-1}Nx = M^{-1}b + M^{-1}(M - A)x = \\ &= M^{-1}(b - Ax) + x = x + M^{-1}r(x)\end{aligned}$$

- N should be such that Ny can be evaluated efficiently.
- M should be such that $M^{-1}y$ can be evaluated efficiently.

$$x^{(k+1)} = x^{(k)} + M^{-1}r^{(k)}$$

- Iteration with splitting $M - N$ is equivalent to Richardson on

$$M^{-1}Ax = M^{-1}b$$

Convergence

- Iteration with splitting $A = M - N$ is convergent if

$$\rho(M^{-1}N) = \rho(I - M^{-1}A) < 1$$

- For fast convergence it should hold
  - $M^{-1}A \approx I$
  - $M^{-1}A$ should be better conditioned than A itself

- Such a matrix M is called a preconditioner for A.
  Is used in other iterative methods to accelerate convergence.

- Condition number:

$$\kappa(A) = \|A^{-1}\| \, \|A\|, \quad \left|\frac{\lambda_{\max}}{\lambda_{\min}}\right|, \quad \text{or} \quad \frac{\sigma_{\max}}{\sigma_{\min}}$$

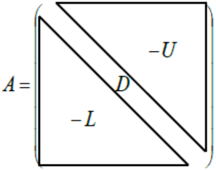
5.1.2. Jacobi (Diagonal) Splitting

Choose $A = M - N = D - (L + U)$ with

$D = \text{diag}(A)$

L the lower triangular part of A, and

U the upper triangular part.



$$\begin{aligned} x^{(k+1)} &= D^{-1}b + D^{-1}(L+U)x^{(k)} = \\ &= D^{-1}b + D^{-1}(D-A)x^{(k)} = x^{(k)} + D^{-1}r^{(k)} \end{aligned}$$

Convergent for $A \approx \text{diag}(A)$ or diagonal dominant matrices:

$$\rho(D^{-1}N) = \rho(I - D^{-1}A) < 1$$

Jacobi (Diagonal) Splitting (cont.)

Iteration process written elementwise:

$$x^{(k+1)} = D^{-1}(b - (A - D)x^{(k)}) \Rightarrow x_j^{(k+1)} = \frac{1}{a_{jj}} \left(b_j - \sum_{m=1, m \neq j}^{n} a_{j,m} x_m^{(k)} \right)$$

$$a_{jj} x_j^{(k+1)} = b_j - \sum\nolimits_{m=1}^{j-1} a_{j,m} x_m^{(k)} - \sum\nolimits_{m=j+1}^{n} a_{j,m} x_m^{(k)}$$

- Damping or relaxation for improving convergence
- Idea: Iterative method as correction of last iterate in search direction.
- Introduce step length for this correction step:

$$x^{(k+1)} = x^{(k)} + D^{-1} r^{(k)} \qquad \to \qquad x^{(k+1)} = x^{(k)} + \omega D^{-1} r^{(k)}$$

  with additional damping parameter ω.
- Damped Jacobi iteration:

$$x_{\text{damped}}^{(k+1)} = (\omega + 1 - \omega) x^{(k)} + \omega D^{-1} r^{(k)} = \omega x^{(k+1)} + (1 - \omega) x^{(k)}$$

Damped Jacobi Iteration

$$
\begin{aligned}
x^{(k+1)} &= x^{(k)} + \omega D^{-1} r^{(k)} = x^{(k)} + \omega D^{-1}(b - Ax^{(k)}) = \\
&= \dots \\
&= \omega D^{-1} b + [(1-\omega) I + \omega D^{-1}(L+U)] x^{(k)}
\end{aligned}
$$

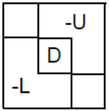
is convergent for

$$
\rho(\underbrace{[(1-\omega) I + \omega D^{-1}(L+U)]}_{\xrightarrow{\omega \to 0} I}) < 1
$$

Look for optimal ω with best convergence (add. degree of freedom).

Parallelism in the Jacobi Iteration

- Jacobi method is easy to parallelize: only Ax and $D^{-1}x$.
- But often too slow convergence!
- Improvement: block Jacobi iteration



5.1.3. Gauss-Seidel Iteration

Always use newest information available!

Jacobi iteration:

$$a_{jj}x_j^{(k+1)} = b_j - \sum_{m=1}^{j-1} a_{j,m} \underbrace{x_m^{(k)}}_{\text{already computed}} - \sum_{m=j+1}^{n} a_{j,m}x_m^{(k)}$$

Gauss-Seidel iteration:

$$a_{jj}x_j^{(k+1)} = b_j - \sum_{m=1}^{j-1} a_{j,m} \underbrace{x_m^{(k+1)}}_{\text{already computed}} - \sum_{m=j+1}^{n} a_{j,m}x_m^{(k)}$$

Gauss-Seidel Iteration (cont.)

- Compare dependancy graphs for general iterative algorithms. Here:

$$x = f(x) = D^{-1}(b + (D - A)x) = D^{-1}(b - (L + U)x)$$

to splitting $A = (D - L) - U = M - N$

$$\begin{aligned} x^{(k+1)} &= (D - L)^{-1}b + (D - L)^{-1}Ux^{(k)} = \\ &= (D - L)^{-1}b + (D - L)^{-1}(D - L - A)x^{(k)} = \\ &= x^{(k)} + (D - L)^{-1}r^{(k)} \end{aligned}$$

- Convergence depends on spectral radius $\rho(I - (D - L)^{-1}A) < 1$

Parallelism in the Gauss-Seidel Iteration

- Linear system in $D - L$ is easy to solve because $D - L$ is lower triangular but
- strongly sequential!
- Use red-black ordering or graph colouring for compromise:

$$\text{parallel} \leftrightarrow \text{convergence}$$

Successive Over Relaxation (SOR)

- Damping or relaxation:

$$x^{(k+1)} = x^{(k)} + \omega(D-L)^{-1}r^{(k)} = \omega(D-L)^{-1}b + [(1-\omega) + \omega(D-L)^{-1}U]x^{(k)}$$

- Convergence depends on spectral radius of iteration matrix

$$(1-\omega) + \omega(D-L)^{-1}U$$

- Parallelization of SOR == parallelization of GS

Stationary Methods (in General)

- Can always be written in the two normal forms

  $$x^{(k+1)} = c + Bx^{(k)}$$

  with convergence depending on $\rho(B)$ and

  $$x^{(k+1)} = x^{(k)} + Fr^{(k)}$$

  with preconditioner F, $B = I - FA$

- For $x^{(0)} = \mathbf{0}$:

  $$x^{(k+1)} \subseteq K_k(B, c),$$

  which is the Krylov space with respect to matrix B and vector c.

- Slow convergence (but good smoothing properties! $\rightarrow$ multigrid)

MATLAB Example

- clear; n=100;k=10;omega=1;stationary
- tridiag($-.5, 1, -.5$):
  - Jacobi norm $|\cos(x)|$
  - GS norm $\frac{\sin(x)}{\sqrt{2(1-\cos(x))}}$
  - both $< 1 \rightarrow$ convergence, but slow
- To improve convergence $\rightarrow$ nonstationary methods (or multigrid)

Chair of Informatics V—SCCS

Efficient Numerical Algorithms—Parallel & HPC

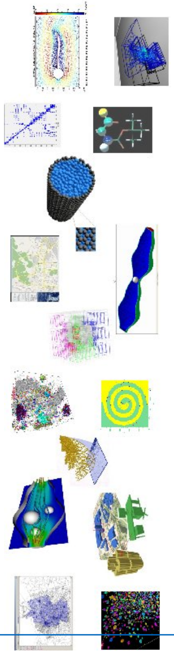
- High-dimensional numerics (sparse grids)
- Fast iterative solvers (multi-level methods, preconditioners)
- Adaptive, octree-based grid generation
- Space-filling curves
- Numerical linear algebra
- Numerical algorithms for image processing
- HW-aware numerical programming

Fields of application in simulation

- CFD (incl. fluid-structure interaction)
- Plasma physics
- Molecular dynamics
- Quantum chemistry

Further info → www5.in.tum.de

Feel free to come around and ask for thesis topics!



5.2. Nonstationary Methods

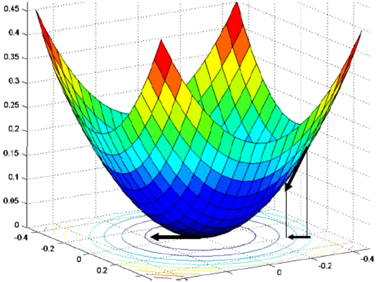
5.2.1. Gradient Method

- Consider $A = A^T > 0$ (A SPD)

$$\text{Function} \quad \Phi(x) = \frac{1}{2} x^T A x - b^T x$$

- n-dim. paraboloid $\mathbb{R}^n \to \mathbb{R}$
- Gradient $\nabla\Phi(x) = Ax - b$
- Position with $\nabla\Phi(x) = 0$ is exactly minimum of paraboloid
- Instead of solving $Ax = b$ consider $\min_x \Phi(x)$
- Local descent direction in y: $\nabla\Phi(x) \cdot y$ is minimum for

$$y = -\nabla\Phi(x)$$



Gradient Method (cont.)

- Optimization: start with $x^{(0)}$

$$x^{(k+1)} := x^{(k)} + \alpha_k d^{(k)}$$

with search direction $d^{(k)}$ and step size α_k.

- In view of previous results the optimal (local) search direction is

$$-\nabla\Phi(x^{(k)}) =: d^{(k)}$$

- To define α_k:

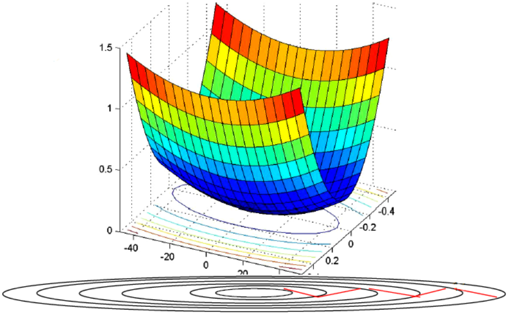
$$\begin{aligned}
\min_\alpha g(\alpha) &:= \min_\alpha(\Phi(x^{(k)} + \alpha(b - Ax^{(k)}))) \\
&= \min_\alpha \left(\frac{1}{2}(x^{(k)} + \alpha d^{(k)})^T A(x^{(k)} + \alpha d^{(k)}) - b^T(x^{(k)} + \alpha d^{(k)})\right) \\
&= \min_\alpha \left(\frac{1}{2}\alpha^2 {d^{(k)}}^T A d^{(k)} - \alpha {d^{(k)}}^T d^{(k)} + \frac{1}{2}{x^{(k)}}^T A x^{(k)} - {x^{(k)}}^T b\right)
\end{aligned}$$

$$\alpha_k = \frac{{d^{(k)}}^T d^{(k)}}{{d^{(k)}}^T A d^{(k)}} \qquad d^{(k)} = -\nabla\Phi(x^{(k)}) = b - Ax^{(k)}$$

Gradient Method (cont. 2)

$$x^{(k+1)} = x^{(k)} + \frac{\|b - Ax^{(k)}\|_2^2}{(b - Ax^{(k)})^T A (b - Ax^{(k)})}(b - Ax^{(k)})$$

- Method of steepest descent.
- Disadvantage: Distorted contour lines.
- Slow convergence (zig zag path)
- Local descent direction is not globally optimal



Analysis of the Gradient Method

- Definition A-norm:

$$\|x\|_A := \sqrt{x^T A x}$$

- Consider error:

$$\begin{aligned} \|x - \bar{x}\|_A^2 &= \|x - A^{-1}b\|_A^2 = (x^T - b^T A^{-1})A(x - A^{-1}b) \\ &= x^T A x - 2b^T x + b^T A^{-1} b \\ &= 2\Phi(x) + b^T A^{-1} b \end{aligned}$$

- Therefore, minimizing Φ is equivalent to minimizing the error in the A-norm! More detailed analysis reveals:

$$\|x^{(k+1)} - \bar{x}\|_A^2 \leq \left(1 - \frac{1}{\kappa(A)}\right) \cdot \|x^{(k)} - \bar{x}\|_A^2$$

- Therefore, for $\kappa(A) \gg 1$ very slow convergence!

5.2.2. The Conjugate Gradient Method

- Improving descent direction being globally optimal.
- $x^{(k+1)} := x^{(k)} + \alpha_k p^{(k)}$ with search direction not being negative gradient, but projection of gradient that is A-conjugate to all previous search directions:

$$
\begin{aligned}
& p^{(k)} \perp Ap^{(j)} \text{ for all } j < k \text{ or} \\
& p^{(k)} \perp_A p^{(j)} \text{ or} \\
& p^{(k)^T} Ap^{(j)} = 0 \text{ for } j < k
\end{aligned}
$$

- We choose new search direction as component of last residual that is A-conjugate to all previous search directions.
- α_k again by 1-dim. minimization as before (for chosen $p^{(k)}$)

The Conjugate Gradient Algorithm

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

for $k = 1, 2, \ldots$ do

$$\alpha^{(k)} = -\frac{\langle r^{(k)}, r^{(k)}\rangle}{\langle p^{(k)}, Ap^{(k)}\rangle}$$

$$x^{(k+1)} = x^{(k)} - \alpha^{(k)} p^{(k)}$$

$$r^{(k+1)} = r^{(k)} + \alpha^{(k)} Ap^{(k)}$$

if $\|r^{(k+1)}\|_2^2 \leq \epsilon$ **then break**

$$\beta^{(k)} = \frac{\langle r^{(k+1)}, r^{(k+1)}\rangle}{\langle r^{(k)}, r^{(k)}\rangle}$$

$$p^{(k+1)} = r^{(k+1)} + \beta^{(k)} p^{(k)}$$

Properties of Conjugate Gradients

- It holds
$$p^{(j)^T} A p^{(k)} = 0 = r^{(j)^T} r^{(k)} \quad \text{for} \quad j \neq k$$
- and
$$\begin{aligned} \operatorname{span}(p^{(1)}, \ldots, p^{(j)}) &= \operatorname{span}(r^{(0)}, \ldots, r^{(j-1)}) = \\ &= \operatorname{span}(r^{(0)}, Ar^{(0)}, \ldots, A^{j-1} r^{(0)}) = K_j(A, r^{(0)}) \end{aligned}$$
- Especially for $x^{(0)} = \mathbf{0}$ it holds
$$K_j(A, r^{(0)}) = \operatorname{span}(b, Ab, \ldots, A^{j-1} b)$$
- $x^{(k)}$ is best approximate solution to $Ax = b$ in subspace $K_k(A, r^{(0)})$. For $x^{(0)} = \mathbf{0}$: $\quad x^{(k)} \in K_k(A, b)$
- Error:
$$\|x^{(k)} - \bar{x}\|_A = \min_{x \in K_k(A,b)} \|x - \bar{x}\|_A$$
- Cheap 1-dim. minimization gives optimal k-dim. solution for free!

Properties of Conjugate Gradients (cont.)

- Consequence: After n steps $K_n(A, b) = \mathbb{R}^n$ and therefore $x^{(n)} = A^{-1}b$ is solution in exact arithmetic.
- Unfortunately, this is not true in floating point arithmetic.
- Furthermore, $\mathcal{O}(n)$ iteration steps would be too costly:
  costs: #iterations $*$ matrix-vector-product
- Matrix-vector-product easy in parallel.
- But, how to get fast convergence and reduce #iterations?

Error Estimation ($x^{(0)} = 0$)

$$
\begin{aligned}
\|e^{(k)}\|_A &= \|x^{(k)} - \bar{x}\|_A = \min_{x \in K_k(A,b)} \|x - \bar{x}\|_A = \\
&= \min_{\alpha_0,\ldots,\alpha_{k-1}} \left\| \sum_{j=0}^{k-1} \alpha_j (A^j b) - \bar{x} \right\|_A = \\
&= \min_{\mathcal{P}^{(k-1)}(x)} \left\| \mathcal{P}^{(k-1)}(A) b - \bar{x} \right\|_A = \\
&= \min_{\mathcal{P}^{(k-1)}(x)} \left\| \mathcal{P}^{(k-1)}(A) A \bar{x} - \bar{x} \right\|_A = \\
&= \min_{\mathcal{P}^{(k-1)}(x)} \left\| (\mathcal{P}^{(k-1)}(A) A - I)(\bar{x} - x^{(0)}) \right\|_A = \\
&= \min_{\mathcal{Q}^{(k)}(x), \mathcal{Q}^{(k)}(0)=1} \left\| \mathcal{Q}^{(k)}(A) e^{(0)} \right\|_A
\end{aligned}
$$

for polynomial $\mathcal{Q}^{(k)}(x)$ of degree k with $\mathcal{Q}^{(k)}(0) = 1$.

Error Estimation

- Matrix A has orthonormal basis of eigenvectors $u_j,\ j = 1, \ldots, n$, eigenvalues λ_j
- It holds

$$Au_j = \lambda_j u_j, \quad j = 1, \ldots, n, \quad \text{and} \quad u_j^T u_k = 0 \ \text{ for } \ j \neq k \ \text{ and } \ 1 \ \text{ for } \ j = k$$

- Start error in ONB: $e^{(0)} = \sum_{j=1}^{n} \rho_j u_j$

$$\begin{aligned}
\|e^{(k)}\|_A &= \min_{\mathcal{Q}^{(k)}(0)=1} \left\| \mathcal{Q}^{(k)}(A) \sum_{j=1}^{n} \rho_j u_j \right\|_A = \min_{\mathcal{Q}^{(k)}(0)=1} \left\| \sum_{j=1}^{n} \rho_j \mathcal{Q}^{(k)}(A) u_j \right\|_A = \\
&= \min_{\mathcal{Q}^{(k)}(0)=1} \left\| \sum_{j=1}^{n} \rho_j \mathcal{Q}^{(k)}(\lambda_j) u_j \right\|_A \leq \min_{\mathcal{Q}^{(k)}(0)=1} \left\{ \max_{j=1,\ldots,n} \left| \mathcal{Q}^{(k)}(\lambda_j) \right| \right\} \left\| \sum_{j=1}^{n} \rho_j u_j \right\|_A = \\
&= \min_{\mathcal{Q}^{(k)}(0)=1} \left\{ \max_{j=1,\ldots,n} |\mathcal{Q}^{(k)}(\lambda_j)| \right\} \left\| e^{(0)} \right\|_A
\end{aligned}$$

Error Estimates

By choosing polynomials with $\mathcal{Q}^{(k)}(0) = 1$, we can derive error estimates for the error after the kth step:

$$\text{Choose, e.g. } \mathcal{Q}^{(k)}(x) := \left|1 - \frac{2}{\lambda_{\max} + \lambda_{\min}} x\right|^k$$

$$\begin{aligned} \|e^{(k)}\|_A &\leq \max_{j=1,\ldots,n} |\mathcal{Q}^{(k)}(\lambda_j)| \left\|e^{(0)}\right\|_A = \left|1 - \frac{2\lambda_{\max}}{\lambda_{\max} + \lambda_{\min}}\right|^k \|e^{(0)}\|_A \\ &= \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}\right)^k \|e^{(0)}\|_A = \left(\frac{\kappa(A) - 1}{\kappa(A) + 1}\right)^k \|e^{(0)}\|_A \end{aligned}$$

Better Estimates

- Choose normalized Chebyshev polynomials
  $T_n(x) = \cos(n \arccos(x))$

$$\|e^{(k)}\|_A \leq \frac{1}{T_k\left(\frac{\kappa(A)+1}{\kappa(A)-1}\right)}\|e^{(0)}\|_A \leq 2\left(\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}\right)^k \|e^{(0)}\|_A$$

- For clustered eigenvalues choose special polynomial, e.g. assume that A has only two eigenvalues λ_1 and λ_2:

$$\mathcal{Q}^{(2)}(x) := \frac{(\lambda_1 - x)(\lambda_2 - x)}{\lambda_1 \lambda_2}$$

$$\|e^{(2)}\|_A \leq \max_{j=1,2} \left|\mathcal{Q}^{(2)}(\lambda_j)\right| \|e^{(0)}\|_A = 0$$

Convergence of CG after two steps!

Outliers/Cluster

Assume the matrix has an eigenvalue $\lambda_1 > 1$ and all other eigenvalues are contained in an ϵ-neighborhood of 1:

$$\forall \lambda \neq \lambda_1 : \quad |\lambda - 1| < \epsilon$$

$$\mathcal{Q}^{(2)}(x) := \frac{(\lambda_1 - x)(1 - x)}{\lambda_1}$$

$$\|e^{(2)}\|_A \leq \max_{|\lambda - 1| < \epsilon} \left| \frac{(\lambda_1 - \lambda)(1 - \lambda)}{\lambda_1} \right| \|e^{(0)}\|_A \leq \frac{(\lambda_1 - 1 + \epsilon)\epsilon}{\lambda_1} = \mathcal{O}(\epsilon)$$

Very good approximation of CG after only two steps!

Important: small number of outliers combined with cluster.

Conjugate Gradients Summary

- To get fast convergence and reduce the number of iterations: $\rightarrow$ find preconditioner M, such that $M^{-1}Ax = M^{-1}b$ with clustered eigenvalues.
- Conjugate gradients (CG) is always the method of choice for symmetric positive definite A (in general).
- To improve convergence, include preconditioning (PCG).
- CG has two important properties: optimal and cheap.

Parallel Conjugate Gradients Algorithm

```
while ( sqrt(gamma) > epsilon * error_0 ) {
    if (iteration > 1)
      q = r + gamma / gamma_old * q;
    v = A * q;
    delta = dot(v,q);
    alpha = delta / gamma;
    x = x + alpha * q;
    r = r - alpha * v;
    gamma_old = gamma;
    gamma = dot(r,r);
    iteration = iteration + 1;
}
```

MVP

scalar

local vector

synchronisation points

dot product: requires communication (MPI_ALLREDUCE)

Non-Blocking Collective Operations

- Use to hide communication!
- Allows overlap of numerical computations and communcations.
- In MPI-1/MPI-2 only possible for point-to-point communication: `MPI_Isend` and `MPI_Irecv`.

  Additional libraries necessary for collective operations!
  Example: LibNBC (non-blocking collectives)
- Are included in new MPI-3 standard.

Example: Pseudocode for Nonblock. Reduct.

```
MPI_Request req;
int sbuf1[SIZE], rbuf1[SIZE], buf2[SIZE];
// compute sbuf1
compute(sbuf1, SIZE);

// start non-blocking allreduce of subf1
// computation and communication overlap
MPI_Iallreduce(sbuf1,rbuf1,SIZE,MPI_INT,MPI_SUM,MPI_COMM, &req);

// compute buf2 (independent of buf1)
compute(buf2, SIZE);

// synchronization
MPI_WAIT(&req, &stat);

// use data in rbuf1; final computation
evaluate(rbuf1, buf2, SIZE);
```

Iter. Methods for general (nonsymmetric) A: BiCGSTAB

- Applicable if little memory at hand and A^T not available.
- Computational costs per iteration similar to BiCG and CGS.
- Alternative for CGS that avoids irregular convergence patterns of CGS maintaining similar convergence speed.
- Less loss of accuracy in the updated residual.

Iter. Methods for general (nonsymmetric) A: GMRES

- Leads to smallest residual for fixed number of iteration steps, but these steps become increasingly expensive.
- To limit increasing storage requirments and work per iteration step, restarting is necessary. When to do so depends on A and b; it requires skill and experience.
- Requires only matrix-vector products with the coeff. matrix.
- Number of inner products grows linearly with iteration number (up to restart point).
- Implementation based on Gram-Schmidt $\rightarrow$ inner products independent $\rightarrow$ only one synchronization point.
  Using modified Gram-Schmidt $\rightarrow$ one synchronization point per inner product.

We consider GMRES in the following.

5.2.3. GMRES

- Iterative solution method for general A
- Consider small subspace U_m and determine optimal approximate solution for $Ax = b$ in U_m. Hence x is of the form $x := U_m y$

$$\min_{x \in U_m} \|Ax - b\|_2 = \min_y \|A(U_m y) - b\|_2$$

- Can be solved by normal equations: $(U_m^T A^T A U_m) y = U_m^T A^T b$
- Try to find sequence of "good" subspaces $U_1 \to U_2 \to U_3 \to \dots$ such that iteratively we can update the optimal solutions

$$x_1 \to x_2 \to x_3 \to \dots \to A^{-1} b$$

using mainly matrix-vector products.

GMRES: Subspace

What subspace for fast convergence and easy computations?

$$U_m := K_m(A, b) = \text{span}(b, Ab, \ldots, A^{m-1}b) \qquad \text{(Krylov space)}$$

Problem: b, Ab, $A^2 b$, $\ldots$ is bad basis for this subspace!

So we need a first step to compute a good basis for U_m:

Start with $u_1 := \frac{b}{\|b\|_2}$ and do for $j = 2 : m$:

$$\begin{aligned}
\widetilde{u}_j &:= Au_{j-1} - \sum_{k=1}^{j-1}(u_k^T A u_{j-1})u_k = Au_{j-1} - \sum_{k=1}^{j-1} h_{k,j-1} u_k \\
u_j &:= \frac{\widetilde{u}_j}{\|\widetilde{u}_j\|_2} = \frac{\widetilde{u}_j}{h_{j,j-1}}
\end{aligned}$$

which is the standard orthogonalization method (Arnoldi method)

Matrix Form of Arnoldi ONB

$$U_m = \mathrm{span}(b, Ab, \ldots, A^{m-1}b) = \mathrm{span}(u_1, u_2, \ldots, u_m) \quad \text{(ONB)}$$

Write this orthogonalization method in matrix form

$$Au_{j-1} = \sum_{k=1}^{j-1} h_{k,j-1} u_k + \tilde{u}_j = \sum_{k=1}^{j} h_{k,j-1} u_k$$

$$AU_m = A(u_1 \quad \ldots \quad u_m) = (u_1 \quad \ldots \quad u_{m+1})\widetilde{H}_{m+1,m} = U_{m+1}\widetilde{H}_{m+1,m}$$

$$\widetilde{H}_{m+1,m} = \begin{pmatrix} h_{11} & \cdots & \cdots & h_{1m} \\ h_{21} & \ddots & & \vdots \\ 0 & \ddots & \ddots & \vdots \\ & & \ddots & h_{mm} \\ 0 & & 0 & h_{m+1,m} \end{pmatrix}$$

GMRES: Minimization

This leads to minimization problem

$$\begin{aligned}
\min_{x \in U_m} \|Ax - b\| &= \min_y \|AU_m y - b\| \\
&= \min_y \left\| U_{m+1} \widetilde{H}_{m+1,m} y - \|b\| u_1 \right\| \\
&= \min_y \left\| U_{m+1} (\widetilde{H}_{m+1,m} y - \|b\| e_1) \right\| \\
&= \min_y \left\| \widetilde{H}_{m+1,m} y - \|b\| e_1 \right\|
\end{aligned}$$

Because U_{m+1} is part of an orthogonal matrix.

GMRES: QR

Use Givens matrices to compute a QR-factorization of the upper Hessenberg matrix $\widetilde{H}_{m+1,m}$.

$$G_1 \cdot \begin{pmatrix} * & \cdots & * \\ * & \ddots & \vdots \\ & \ddots & * \\ & & * \end{pmatrix} = \begin{pmatrix} * & \cdots & * \\ 0 & \ddots & \vdots \\ & \ddots & * \\ & & * \end{pmatrix} =$$

$$G_m \cdots G_2 G_1 \cdot \widetilde{H}_{m+1,m} = Q \cdot \widetilde{H}_{m+1,m} = \begin{pmatrix} R_m \\ 0 \end{pmatrix}$$

QR via Givens matrices is a simplified version of QR via Householder matrices.

GMRES

$$
\begin{aligned}
\min_{x\in K_m} \|Ax-b\| &= \min_y \left\| \widetilde{H}_{m+1,m} y - \|b\| e_1 \right\| \\
&= \min_y \left\| Q^T R y - \|b\| e_1 \right\| = \min_y \| Ry - \|b\| Qe_1 \| \\
&= \min_y \left\| \begin{pmatrix} R_m \\ 0 \end{pmatrix} y - \widetilde{b} \right\| = \min_y \left\| \begin{pmatrix} R_m y - \widetilde{b}_m \\ -\widetilde{\beta}_m \end{pmatrix} \right\|
\end{aligned}
$$

Solution:

$$
R_m y = \widetilde{b}_m, \quad x_m = U_m y
$$

GMRES Algorithm

- GMRES is a clever implementation of this sequence of least squares problems.
- Computing step by step for increasing m
  - next Au_m
  - enlarged $H_{m+1,m}$ by Arnoldi orthogonalization (gives new u_{m+1})
  - next Givens matrix G_m
  - update triangular solves to get next y_m and x_m.
- Disadvantage: large Hessenberg matrices!
- Therefore, use restarted GMRES, e.g. GMRES(20).

GMRES Algorithm: First Step

Start: $b,\ u_1 := \frac{b}{\|b\|}$

$$h_{2,1}u_2 = Au_1 - h_{1,1}u_1, \quad H_{2,1} = \begin{pmatrix} h_{1,1} \\ h_{2,1} \end{pmatrix}, \quad G_1 H_{2,1} = \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix},$$

$$\begin{aligned} \|Ax - b\| &= \|AU_1 y_1 - b\| = \|H_{2,1}y_1 - \|b\|e_1\| \\ &= \left\| G_1^T \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix} y_1 - \|b\|e_1 \right\| = \left\| \begin{pmatrix} \nu_{1,1} \\ 0 \end{pmatrix} y_1 - \|b\| G_1 e_1 \right\| \end{aligned}$$

$$y_1 = \frac{(G_1 e_1 \|b\|)_1}{\nu_{1,1}}, \qquad x_1 = u_1 y_1 = U_1 y_1$$

GMRES Algorithm: Second Step

$$h_{3,2}u_3 = Au_2 - h_{2,2}u_2 - h_{1,2}u_1, \qquad H_{3,2} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \\ 0 & h_{32} \end{pmatrix},$$

$$G_1 H_{3,2} = \begin{pmatrix} \nu_1 & * \\ 0 & * \\ 0 & * \end{pmatrix}, \qquad G_2 G_1 H_{3,2} = \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix}$$

$$\|Ax - b\| = \|AU_2 y_2 - b\| = \|H_{3,2} y_2 - \|b\| e_1\|$$

$$= \left\| G_1^T G_2^T \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix} y_2 - \|b\| e_1 \right\| = \left\| \begin{pmatrix} \nu_{1,1} & \nu_{1,2} \\ 0 & \nu_{2,2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_{2,1} \\ y_{2,2} \end{pmatrix} - \|b\| G_2 G_1 e_1 \right\|$$

$$y_{2,2} = \frac{(G_2 G_1 e_1 \|b\|)_2}{\nu_{2,2}}, \qquad y_{2,1} = \frac{(G_2 G_1 e_1 \|b\|)_1 - \nu_{1,2} y_{2,2}}{\nu_{1,1}}$$

$x_2 = U_2 y_2 = u_1 y_{2,1} + u_2 y_{2,2}$ and so forth...

GMRES Error (A diagonalisable)

$$
\begin{aligned}
\|r_m\| &= \|Ax_m - b\| = \min_{x \in U_m} \|Ax - b\| \\
&= \min_{\alpha_1,\dots,\alpha_m} \left\| A \left(\sum_{j=0}^{m-1} \alpha_j A^j b \right) - b \right\| = \min_{\mathcal{P}^{(m-1)}} \left\| A\mathcal{P}^{(m-1)}(A)b - b \right\| \\
&= \min_{\mathcal{Q}^{(m)}(0)=1} \left\| \mathcal{Q}^{(m)}(A)b \right\| = \min_{\mathcal{Q}^{(m)}(0)=1} \left\| V\mathcal{Q}^{(m)}(\Lambda)V^{-1}b \right\| \\
&= \min_{\mathcal{Q}^{(m)}(0)=1} \left\| V \operatorname{diag}(\mathcal{Q}^{(m)}(\lambda_j))V^{-1}b \right\| \leq \\
&\leq \kappa_2(V) \cdot \min_{\mathcal{Q}^{(m)}(0)=1} \left[\max_{j=1,\dots,n} \left| \mathcal{Q}^{(m)}(\lambda_j) \right| \right] \|r_0\|
\end{aligned}
$$

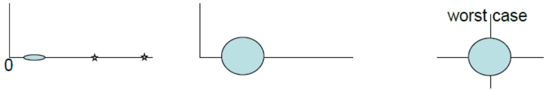
Iterative Methods: Survey

- Basic iterative methods (not considering multigrid!)
- SPD A: PCG (preconditioned conjugate gradient method)
- symmetric indefinite A: MINRES, SYMMLQ, (PCG on normal equations)
- general A:

  GMRES (optimal like CG, but expensive)

  BiCG, BiCGSTAB, CGS (not optimal, but cheap, instable?)

  QMR (quasi optimal, cheap)
- Essential for convergence is position of eigenvalues (singular values)
- Fast convergence for well conditioned problems or matrices with clustered spectrum



5.3. Preconditioning

- Direct solvers: sequential, loosing sparsity
- Iterative solvers: easy parallel and sparse, but possibly slowly convergent
- Combination of both methods (2 variants):
  1. Include preconditioner $M \approx A$ in the form $M^{-1}Ax = M^{-1}b$, such that
     - M is easy to deal with in parallel (reduced approximate direct solver)
     - spectrum of $M^{-1}A$ is much better clustered
  2. Or include preconditioner $M \approx A^{-1}$ in the form $MAx = Mb$, such that
     - M is easy to deal with in parallel (reduced approximate inverse)
     - Spectrum of MA is much better clustered
- General both-sided preconditioning:

$$Ax = b \Leftrightarrow MA(Ky) = Mb \quad \text{and} \quad Ky = x$$

Overview of Following Preconditioners

- Stationary preconditioners
- ILU preconditioner
- Polynomial preconditioners
- Sparse approximate inverse preconditioners:
  - SPAI for the general nonsymmetric case
  - FSPAI for the SPD case
  - MSPAI using SPAI with probing

5.3.1. Stationary Preconditioners

Consider preconditioner $M \approx A$ in the form $M^{-1}Ax = M^{-1}b$.

- Stationary iteration to splitting $A = M - N$. Convergence depends on
$$\|I - M^{-1}A\| < 1$$
- That is exactly a condition for a good preconditioner: spectrum clustered around 1, $M^{-1}A \approx I$
- If splitting leads to fast convergence, than M is also a good preconditioner.
- In this sense, PCG with stationary preconditioner M can be seen as an accelaration of the stationary method with splitting $M - N$.

Stationary Preconditioners (cont.)

- Jacobi splitting with $D = \text{diag}(A)$ gives Jacobi preconditioner $M := D$.
- Gauss-Seidel splitting $M = D - L$ leads to GS preconditioner.
- Relaxation:
$$x^{(k,\text{new})} := (1-\omega)x^{(k-1)} + \omega x^{(k)}$$
  As convex combination of old and new iterate (Jacobi or GS)
- Symmetrization: first iteration with preconditioner M, second iteration with M^T.
$$M_{\text{new}} := M + M^T - M^T A M$$
- Special case: damped GS $\rightarrow$ SSOR:
$$M_{\text{new}} = \frac{1}{2-\omega}\left(\frac{1}{\omega}D - L\right)\left(\frac{1}{\omega}D\right)^{-1}\left(\frac{1}{\omega}D - L\right)^T$$

5.3.2. ILU Preconditioner

- Apply Gaussian elimination algorithm, but only on allowed pattern $\Rightarrow$ incomplete LU factorization called ILU.
- Reduce in the `for`-loops the indices to the indices with
  - allowed pattern, e.g. ILU(0) for pattern of A
  - values that are not too small, ILUT for ILU with treshold
- Leads to approximate LU factorization

$$A = LU + R, \quad \text{preconditioner} \quad M = LU$$

  with all ignored fill-in entries collected in R.
- MILU (modified ILU): collect all ignored fill-in entries on the related main diagonal elements $\rightarrow$ maintains the row sum or the action on $(1, 1, \ldots, 1)^T$.

Overview Explicit Preconditioners

- ILU and stationary methods use approximations on A itself.
- The resulting preconditioners are given by triangular matrices L, that have to be solved in each iteration step: $L^{-1}x^{(k)}$! Strongly sequential!
- Jacobi easy to parallelize, but slow convergence.
- Question: How to derive preconditioners that lead to fast convergence and are easy to parallelize?
- Until now considered variant 1.; In the following variant 2.:

  Find approximations on $M \approx A^{-1}$. Then the solution of the linear system given by the preconditioner, is only $Mx^{(k)}$, a matrix vector product!

Parallel Preconditioning

- Find preconditioner M, that satisfies three conditions:
  - **(i)** The computation of M is fast in parallel
  - **(ii)** The application Mx in each iteration step is easy in parallel
  - **(iii)** The spectrum AM or MA is clustered $\rightarrow$ fast convergence
- Examples:

  For GS is (i) ok, but not (ii)

  For Jacobi (i) and (ii) ok, but not (iii)

  For ILU (iii) ok, but not (i) and (ii)
- Note that preconditioners also have to be well defined! Zero on diagonals?

5.3.3. Polynomial Preconditioners

- Characteristic polynomial for A:

$$0 = q(A) = \gamma_n A^n + \gamma_{n-1} A^{n-1} + \ldots + \gamma_1 A + \gamma_0 I$$

Gives polynomial representation for A^{-1} ($\gamma_0 \neq 0$):

$$A^{-1} = \frac{1}{\gamma_0}\left(-\gamma_n A^{n-1} - \gamma_{n-1} A^{n-2} - \ldots - \gamma_1 I\right) = p(A)$$

- Therefore, it makes sense to approximate A^{-1} by a polynomial.
- Better approximation by finding region $S \in \mathbb{R}$ or $\mathbb{C}$ that contains nearly all eigenvalues, and then find polynomial p that is near the inverse in S:

$$\min_{p_n} \|P(A)A - I\|, \quad \min_{p_n(x)} \left(\max_{\lambda \text{ eigenvalue}} |p(\lambda)\lambda - 1| \right)$$

- Solution: Normalized Chebyshev polynomials.
- \+ Advant. of pol. prec.: better in parallel (mtx-vec product, BLAS 2)
- \- Disadvantage: non-optimal approximation in Krylov subspace

5.3.4. Sparse Approximate Inverses

- Other approach for approximating A^{-1} by norm minimization

$$\min_{M \in \mathcal{P}} \|AM - I\| \qquad \text{over some sparsity pattern } \mathcal{P}.$$

- Choice of the norm?
  - analytic (to allow the explicit solution of this problem)
  - easy to compute (in parallel)

- Optimal norm is Frobenius norm:

$$\|A\|_F^2 := \sum_{i,j=1}^{n} a_{i,j}^2 = \sum_{j=1}^{n} \|A_{\bullet,j}\|^2 = \text{trace}(A^T A)$$

SPAI in Parallel

- First, we choose pattern $\mathcal{P}$ in a static way a priori, e.g. as the pattern of A

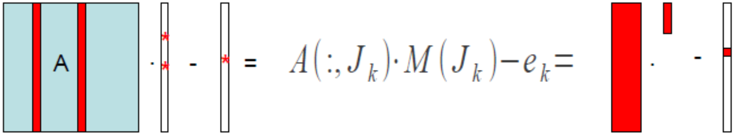
$$\min_{M \in \mathcal{P}} \|AM - I\|_F^2 = \min_{M \in \mathcal{P}} \sum_{k=1}^{n} \|(AM - I)e_k\|_2^2 = \sum_{k=1}^{n} \min_{M_k \in \mathcal{P}_k} \|AM_k - e_k\|_2^2$$

- Hence, to minimize the Frobenius norm, we have to solve n least squares problems in the sparse columns of M!
- This can be done fully in parallel!
- But costs for least squares problems?

SPAI and Least Squares

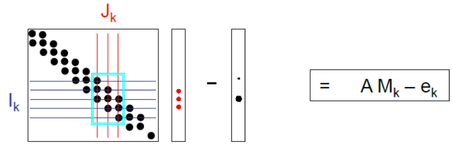
$$\min_{M_k \in \mathcal{P}_k} \|AM_k - e_k\|_2^2 = \min_{M_k \in \mathcal{P}_k} \left\| A \begin{pmatrix} 0 \\ * \\ 0 \\ * \\ 0 \\ 0 \end{pmatrix} - e_k \right\|_2^2 = \min_{M_k \in \mathcal{P}_k} \|A(:, \mathcal{J}_k) M_k(\mathcal{J}_k) - e_k\|_2^2$$

Denote by $\mathcal{J}_k$ the set of allowed indices in the kth column of M.



SPAI and Sparse Least Squares

- $A(:, \mathcal{J}_k)$ is a sparse rectangular matrix. $\mathcal{I}_k$ is index set called *shadow* of $\mathcal{J}_k$.
- Delete superfluous zeros in least squares problem:
  - For index set $\mathcal{J}_k$ in M_k keep only $A(:, \mathcal{J}_k)$
  - In $A(:, \mathcal{J}_k)$ keep only nonzero rows $A(\mathcal{I}_k, \mathcal{J}_k)$



- Hence, reduction of sparse LS to $A(\mathcal{I}_k, \mathcal{J}_k)$:

$$\min_{M_k \in \mathcal{P}_k} \|A(\mathcal{I}_k, \mathcal{J}_k)M(\mathcal{J}_k) - e(\mathcal{I}_k)\|_2^2 = \min_{M_k \in \mathcal{P}_k} \left\|\widetilde{A}\widetilde{M}_k - \widetilde{e}_k\right\|_2^2$$

- Solve small LS problem by Householder *QR* for

$$A(\mathcal{I}_k, \mathcal{J}_k) \to \widetilde{M}_k \to M_k$$

Sparsity Pattern: Static A Priori Choice

- A^{-1} will be no more sparse!
- As a priori choice of a good approximate sparsity pattern for M we can choose the pattern of
  - A^k or $(A^T)^k$
  - $(A^T A)^k A^T$ for some $k = 1, 2$
  - A_ϵ with sparsified A
  - a combination of above
- A_ϵ by sparsification of A: delete all entries with $|A_{ij}| < \epsilon$

Sparsity Pattern: Dynamic Pattern Finding

- Start with thin approximate pattern $\mathcal{J}_k$ for M_k
- Compute optimal column $M_{k,\text{opt}}(\mathcal{J}_k)$ by least squares
- Find new entry j for M_k such that $M_{k,\text{opt}}(\mathcal{J}_k) + \lambda e_j$ has smaller residual in the Frobenius norm.

$$\begin{aligned}\min_{M_k \in \mathcal{P}_k} \left\|A(M_k + \lambda e_j) - e_k\right\|_2^2 &= \min_{M_k \in \mathcal{P}_k} \left\|(AM_k - e_k) + \lambda A e_j\right\|_2^2 = \\ &= \min\left(\|r_k\|_2^2 + 2\lambda(r_k^T A_j) + \lambda^2 \|A_j\|_2^2\right)\end{aligned}$$

For each possible index candidate j compute

$$\lambda_j = -\frac{r_k^T A_j}{\|A_j\|_2^2}$$

Choose index j with $r_k^T A_j \neq 0$ and $j = \arg\min(\lambda_j)$ since

$$\min = \|r_k\|_2^2 - \frac{(r_k^T A_j)^2}{\|A_j\|_2^2}.$$

Error Estimates

- Assume that for all columns holds

$$\|r_k\| = \|AM_k - e_k\| < \epsilon$$

- Then

$$\begin{aligned} \|AM - I\|_F &\leq \sqrt{n}\epsilon \\ \|AM - I\|_2 &\leq \sqrt{n}\epsilon \\ \|AM - I\|_1 &\leq \sqrt{p}\epsilon \end{aligned}$$

with p being the maximum number of nonzero entries in r_k, $k = 1, \dots, n$.

Overview Following SPAI Variants

1. Block SPAI
2. Iterative SPAI
3. Factorized SPAI (FSPAI)
4. Modified SPAI (MSPAI)

Further Variants of SPAI

1. Block SPAI
   - Partition the matrix M in small blocks (e.g., 2×2 or 3×3) and apply the Frobenius norm minimization with blockwise pattern.
   - Advantages:
     - Underlying block structure will also appear in the pattern of $A^{-1} \rightarrow$ improved pattern
     - Block operations are more efficient
     - Less least squares problems to solve
2. Iterative SPAI
   - Start with pattern of $A \rightarrow M_1$
   - Construct M_2 relative to new matrix AM_1
   - Construct M_3 relative to new matrix AM_1M_2
   - ...
   - Advantage: cheaper (but inferior approximation)

3. Factorized SPAI, FSPAI

- Parallel Preconditioner for SPD matrices
- Approximate the inverse Cholesky factor of $A = L_A^T L_A$

$$A^{-1} = (L_A^T L_A)^{-1} = L_A^{-1} L_A^{-T} \approx L L^T$$

$$L_A^{-1} \approx L \qquad \rightarrow \qquad \min \| L_A L - I \|_F$$

- Normal equations give $A(\mathcal{J}_k, \mathcal{J}_k) L(\mathcal{J}_k) = \alpha e_k$

4. Modified SPAI, MSPAI: Combining Targeting and Probing in classical SPAI formulation.

Targeting (for MSPAI)

$$\min_{M \in \mathcal{P}} \|AM - T\|_F$$

- Assume, T is a good sparse preconditioner for A. Improve T by computing M and solving the above Frobenius norm minimization.
- Application: Assume that A is given by two parts, e.g. an advection part and a diffusion part.

  We can choose T as Laplacian relative to the diffusion part (easy to solve) and then we add M for improving T relative to the advection part.

Probing (for MSPAI)

- Find preconditioner of special form (tridiag, band) for preconditioning a matrix that is not given explicitly, but only by its action on certain (probing-)vectors, e.g.

$$e^T S = f^T.$$

  Example: S is Schur complement or general matrix.

- Choose, e.g. $e = (1, 1, \ldots, 1)^T$, $e = (1, -1, 1, -1, \ldots)^T$, ...

- Disadvantage: Can use only very special pattern for M and special probing vectors e.
  Example: tridiagonal probing

4. Modified SPAI: SPAI with Targeting and Probing

Generalize Frobenius norm minimization to

$$\min_{M \in \mathcal{P}} \|CM - B\|_F = \min_{M \in \mathcal{P}} \left\| \begin{pmatrix} C_0 \\ \rho u^T \end{pmatrix} M - \begin{pmatrix} B_0 \\ \rho v^T \end{pmatrix} \right\|_F$$

For example: original SPAI extended by an additional norm minimization to deliver especially good results on vector e:

$$\min_{M \in \mathcal{P}} \|CM - B\|_F = \min_{M \in \mathcal{P}} \left\| \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} M - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F$$

Outlook: Further Research

1. Apply MSPAI with the probing feature to multigrid or regularization problems (smoother, preconditioner).
   In connection with domain decomposition:
   - In the small domains use MSPAI as smoother
   - Use MSPAI as preconditioner for Schur complement
2. Find good block pattern
   - that reflects the physical connections
   - combines columns with very similar pattern to one LS problem
3. Factorized SPAI for indefinite matrices
   - Use a priori permutations (perfect matching)
   - and blocking

   to avoid breakdowns.

Available Code

- SPAI, MSPAI, FSPAI available in parallel version (MPI, C/C++)
  - SPAI (University of Basel):
    `http://www.computational.unibas.ch/software/spai/`
  - SPAI, MSPAI (TUM):
    `http://www5.in.tum.de/wiki/index.php/MSPAI`
  - FSPAI (TUM):
    `http://www5.in.tum.de/wiki/index.php/FSPAI`

  Publications on SPAI, MSPAI, FSPAI available on these websites!

- Block SPAI also available for GPU and shared memory (OpenMP, C/C++).
- High priority to port FSPAI to (parallel) block case.