Outline

Motivation
The curse of ill-conditioning

Preconditioning
Preconditioning — Basics
Preconditioned Krylov subspace methods
Preconditioners

Deflation

Summary
How to improve an optimal method?

**Solvers I:** Krylov subspace methods are all-duty solvers

- “Optimal” methods for any application
- Fast (i.e., short-recurrence) solvers for many applications
- Convergence dependent on conditioning of $A$, e.g.,
  - Conjugate Gradients

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

How to improve convergence of Krylov subspace methods?

1. Preconditioning
2. Deflation
Scaling issues in Numerical Simulations

Numerical simulations of partial differential equations (PDEs)

\[ \mathcal{L} \psi = \varphi \]

Discretization of \( \mathcal{L} \) on mesh with spacing \( a \) yields

\[ \mathbf{L} \mathbf{x} = \mathbf{f} \]

- Depending on PDE order and order of discretization

\[ \kappa(\mathbf{L}) \sim a^{-\sigma}, \quad \sigma \in \mathbb{N}^+ \]

- Increasing accuracy of discretization \((a \to 0)\)

\[ \kappa(\mathbf{L}) \to \infty \quad (a \to 0) \]

Performance of Krylov methods deteriorates when \( a \to 0 \)!
Preconditioning — Idea

**Idea:** Improve conditioning of $A$ in $Ax = b$!

- Instead of solving $Ax = b$ consider solving
  
  $$S_\ell AS_r y = S_\ell b$$
  
  $$x = S_r y$$

  with preconditioners $S_\ell, S_r$ s.t. $\kappa(S_\ell AS_r) \ll \kappa(A)$

**Open questions**

- What are the design goals for preconditioners?
- What are suitable choices of $S_\ell, S_r$?
- How does the preconditioner fit in the iteration
  
  - Ideally only $A \cdot, S_\ell \cdot$ and $S_r \cdot$ are required

For now consider only left-preconditioning with $S = S_\ell$
Consider extreme cases

- $S = I$
  - $SA = A$ original setting

- $S = A^{-1}$
  - $SA = I$ and $\kappa(SA) = 1$ (ideal)

- $S = A^\dagger$
  - $SA = A^\dagger A$ hermitian, but $\kappa(SA) = \kappa(A)^2$

In order to speed up convergence preconditioner $S$ should

- approximate $A^{-1}$
- be cheap to compute ($S \cdot$)
Recall: Conjugate Gradients requires $A$ hermitian

Problem: $SA$ in general no longer hpd even if $S$ is hpd, but then

$$\langle SAx, y \rangle_{S^{-1}} = \langle Ax, y \rangle_2 = \langle x, Ay \rangle_2 = \langle x, SAy \rangle_{S^{-1}}$$

Solution: Replace all $\langle ., . \rangle_2$ by $\langle ., . \rangle_{S^{-1}}$

- Rewriting the algorithm one even gets rid of $\langle ., . \rangle_{S^{-1}}$
- CG variants exist for any $A$ hermitian in some $\langle ., . \rangle_B$

Changing the inner product also works when preconditioning other methods which require a special relation between $A$ and its adjoint $A^\dagger$, e.g., MINRES, SUMR
Motivation
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Preconditioning — Basics
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PCG — Algorithm

Preconditioned Conjugate Gradients

\[ \begin{align*}
    r^{(0)} &= b - Ax^{(0)}, \quad z^{(0)} = Sr^{(0)}, \quad p^{(0)} = z^{(0)} \\
    \text{for } k = 1, 2, \ldots \text{ do} & \\
    \alpha_{k-1} &= \frac{\langle r^{(k-1)}, z^{(k-1)} \rangle_2}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle_2} \\
    x^{(k)} &= x^{(k-1)} + \alpha_{k-1} p^{(k-1)} \\
    r^{(k)} &= r^{(k-1)} - \alpha_{k-1} Ap^{(k-1)} \\
    z^{(k)} &= Sr^{(k)} \\
    \beta_{k-1} &= \frac{\langle r^{(k)}, z^{(k)} \rangle_2}{\langle r^{(k-1)}, z^{(k-1)} \rangle_2} \\
    p^{(k)} &= z^{(k)} + \beta_{k-1} p^{(k-1)} \\
    \text{end for}
\]
Preconditioned GMRES($m$)

while not converged do
  $r^{(0)} = S(b - Ax^{(0)})$, $\beta = \|r^{(0)}\|_2$, $v_1 = \beta^{-1}r^{(0)}$
  for $j = 1, \ldots, m$ do
    $w = SAv_j$
    for $i = 1, \ldots, j$ do
      $h_{i,j} = \langle w, v_j \rangle_2$
      $w = w - h_{i,j}v_j$
    end for
    $h_{j+1,j} = \|w\|_2$
    $v_{j+1} = h_{j+1,j}^{-1}w$
  end for
  Define $V_m = [v_1 | \ldots | v_m]$, $H_{m+1,m} = \{h_{i,j}\}_{1 \leq j \leq m, 1 \leq i \leq j+1}$
  Solve $y_m = \text{argmin}_y \|\beta e_1 - H_{m+1,m}y\|_2$
  $x^{(0)} = x^{(0)} + V_m y_m$
end while
Preconditioned BiCGstab

\[ r^{(0)} = b, \beta_0 = 0 \]
\[ \hat{r} = r \]

\textbf{for } k = 0, 1, \ldots \textbf{ do}

\[ \rho_k = \langle r^{(k)}, \hat{r} \rangle_2 \]
\[ \beta_k = \frac{\rho_k}{\rho_{k-1}} \cdot \frac{\alpha_{k-1}}{\omega_{k-1}} \]
\[ p^{(k)} = r^{(k)} + \beta_k \left( p^{k-1} - \omega_{k-1} v^{(k-1)} \right) \]
\[ \hat{p}^{(k)} = S p^{(k)} \]
\[ \alpha_k = \frac{\rho_k}{\langle A \hat{p}^{(k)}, \hat{r} \rangle_2} \]
\[ x^{(k+\frac{1}{2})} = x^{(k)} + \alpha_k \hat{p}^{(k)} \]
\[ s^{(k)} = r^{(k)} - \alpha_k A \hat{p}^{(k)} \]
\[ \hat{s}^{(k)} = S s^{(k)} \]
\[ \omega_k = \frac{\langle s^{(k)}, A \hat{s}^{(k)} \rangle_2}{\langle A \hat{s}^{(k)}, A \hat{s}^{(k)} \rangle_2} \]
\[ x^{(k+1)} = x^{(k+\frac{1}{2})} + \omega_k \hat{s}^{(k)} \]
\[ r^{(k+1)} = s^{(k)} - \omega_k A \hat{s}^{(k)} \]

\textbf{end for}
Preconditioners

Aims for the construction of preconditioners $S$

1. $S \approx A^{-1}$ to get speed-up
2. $S \cdot$ should be cheap (1 application per iterate)

Classes of preconditioners to be discussed

- Structural preconditioners
- Splitting-based preconditioners
- Domain decomposition preconditioners
- Multigrid preconditioners
- Incomplete decomposition preconditioners
Odd-even preconditioning

Discretizations on lattices with next neighbor coupling

Ordering by odd-even

\[ A = \begin{bmatrix} A_{oo} & A_{oe} \\ A_{eo} & A_{ee} \end{bmatrix} \]

with diagonal \( A_{oo} \) and \( A_{ee} \)

- \( A_{oo}^{-1}, A_{ee}^{-1} \) trivial
- odd decoupled
- even decoupled

Solve first even then odd

- Nodes are odd or even
Odd-even preconditioning

With $\hat{A}_{ee} = A_{ee} - A_{eo}A_{oo}^{-1}A_{oe}$ solution of $Ax = b$ given by

Odd-Even Reduction

\begin{align*}
y_o &= A_{oo}^{-1}b_o \\
\text{Solve } \hat{A}_{ee}x_e &= b_e - A_{eo}y_o \\
x_o &= y_o - A_{oo}^{-1}A_{oe}x_e
\end{align*}

- Iteratively solving $\hat{A}_{ee}x_e = b_e - A_{eo}y_o$
  \Rightarrow \text{ Odd-Even preconditioner}
- If $A$ has constant diagonal $\kappa(\hat{A}_{ee}) < \kappa(A)$
  \Rightarrow \text{ Solving } \hat{A}_{ee} \text{ is easier than solving } A
- Since $A_{oo}^{-1}$ is cheap (diagonal!)
  \Rightarrow \text{ Cost for } \hat{A}_{ee} \cdot \approx \text{ Cost for } A \cdot
Splitting methods

Splitting methods use the additive decomposition of $A$

$$A = L + D + U$$

- Jacobi: $x^{(k+1)} = x^{(k)} + D^{-1}r^{(k)}$
- Gauss-Seidel: $x^{(k+1)} = x^{(k)} + (D + L)^{-1}r^{(k)}$
- SOR: $x^{(k+1)} = x^{(k)} + \left(\frac{1}{\omega}D + L\right)^{-1}r^{(k)}$

**General splitting method:** $A = M + N$

$$x^{(k+1)} = x^{(k)} + M^{-1}r^{(k)} \implies e^{(k+1)} = e^{(k)} - M^{-1}Ae^{(k)}$$

Convergent iff $\|I - M^{-1}A\| < 1$ for some norm $\| \cdot \|$

$\|I - M^{-1}A\|$ small $\Rightarrow M^{-1}A \approx I \Rightarrow M^{-1}$ preconditioner
Domain Decomposition*

- Split the computational domain into subdomains $B_i$
- Solve system iteratively on each subdomain

```
  B_1   B_2  B_3   B_4
  ▶  Canonical injection $I_j$

  $I_j e_i = e (B_j)_i$

  ▶  Restriction of $x$ onto $B_j$

  $x_{B_j} = I_j^\dagger x$

  ▶  Restriction of $A$ onto $B_j$

  $A_{B_j} = I_j^\dagger A I_j$
```

*Domain decomposition dates back to H. Schwarz (1870)
Additive and Multiplicativ Schwarz

**Additive Schwarz**

```latex
\begin{align*}
\text{for } k &= 0, 1, \ldots \text{ do} \\
&\quad r^{(k)} = b - Ax^{(k)} \\
&\quad \text{for } j = 1, 2, \ldots, n_B \text{ do} \\
&\quad\quad x^{(k+1)}_{B_j} = x^{(k)}_{B_j} + A^{-1}_{B_j} r^{(k)}_{B_j} \\
&\quad \text{end for} \\
&\text{end for}
\end{align*}
```

- Block-Jacobi
- Embarrassingly parallel

**Multiplicativ Schwarz**

```latex
\begin{align*}
\text{for } k &= 0, 1, \ldots \text{ do} \\
&\quad r = b - Ax \\
&\quad \text{for } j = 1, 2, \ldots, n_B \text{ do} \\
&\quad\quad r_{B_j} = b - A x_{B_j} \\
&\quad\quad x_{B_j} = x_{B_j} + A^{-1}_{B_j} r_{B_j} \\
&\quad \text{end for} \\
&\text{end for}
\end{align*}
```

- Block-Gauss-Seidel
- Sequential (→ coloring)

Schwarz methods in general
- Data parallel
- Computation parallel
Multigrid

Smooth

Finest Grid

The Multigrid V-cycle

Restriction

Fewer Dofs

First Coarse Grid

Prolongation
(Algebraic) Multigrid

**Given:**
- \(Ax = b\)
- Iterative method \(S\) ("smoother")

**Wanted:**
- Hierarchy of systems
  \[A_\ell x_\ell = b_\ell, \quad \ell = 0, \ldots, L\]
- Intergrid transfer operators
  \[P_{\ell+1}^\ell : \mathbb{C}^{n_{\ell+1}} \rightarrow \mathbb{C}^{n_\ell}\]
  \[R_{\ell+1}^\ell : \mathbb{C}^{n_\ell} \rightarrow \mathbb{C}^{n_{\ell+1}}\]

**Smøother**

\[S_\ell : \mathbb{C}^{n_\ell} \rightarrow \mathbb{C}^{n_\ell}\]

"High modes"

**Interpolation**

\[P_{\ell+1}^\ell : \mathbb{C}^{n_{\ell+1}} \rightarrow \mathbb{C}^{n_\ell}\]

"Low modes"

**Complementarity of Smøother and Interpolation**
Generic Multigrid Algorithm — \( \text{MG}_\ell(A_\ell, b_\ell) \)

```
if \( \ell = L \) then
  \( x_L = A_L^{-1} b_L \)
else
  \( x_\ell = 0 \)
  for \( i = 1, \ldots, \nu_1 \) do
    \( x_\ell = S_\ell(x_\ell, b_\ell) \)  
      \( (x_\ell \leftarrow x_\ell + M_\ell^{-1} r_\ell, r_\ell = b_\ell - A_\ell x_\ell) \)  
      "Pre-smoothing"
  end for
  \( x_{\ell+1} = \text{MG}(A_{\ell+1}, R_{\ell+1}^\ell(b_\ell - A x_\ell)) \)
  \( x_\ell = x_\ell + P_{\ell+1}^\ell x_{\ell+1} \)
  for \( i = 1, \ldots, \nu_2 \) do
    \( x_\ell = S_\ell(x_\ell, b_\ell) \)
  end for
end if
```
Optimality of Multigrid

For certain classes of discretizations of certain types of PDEs and appropriate variants of **multigrid** we have

- Multigrid can be used as a **stand alone** solver (no wrapping as a preconditioner into a Krylov subspace method)

- no. of iterations for given accuracy **independent** of no. of variables.

  **“optimal method”**

Even when not optimal as a stand alone solver, multigrid is often a very efficient preconditioner.
To be efficient, **domain decomposition** needs an additional small system $A_C$ which couples the boundaries of the domains.

For certain classes of discretizations of certain types of PDEs and appropriate variants of **domain decomposition** we have

- Domain decomp. can be used as a **stand alone** solver
- no. of iterations for given accuracy $\propto \log(H/h)$
Incomplete LU (ILU)

**Recall:** Direct methods are based on factorization of $A$

\[
A = L \cdot U
\]

**Drawback:** Fill-In in $L$ and $U$ for sparse $A$

**Idea:** Incomplete factorizations with sparse $L$ and $U$

1. Prescribe the non-zero pattern (e.g., non-zeroes of $A$)
   - Minimize the error-matrix $E$ in $A = \tilde{L} \tilde{U} + E$
2. Use drop-tolerance $\theta$ to drop small entries in $L$ and $U$
   - Often: $(A^{-1})_{i,j} \sim \alpha^{\text{dist}_G(i,j)}, \quad \alpha < 1$
     \[\Rightarrow\] If $i$ is “far” from $j$, $L_{ij}$ and $U_{ij}$ will be dropped

**ILU is a black-box preconditioner**
Flexible Krylov subspace methods

The preconditioner may be an iterative process by itself

- choice 1: fixed no. of iterations or stopping criterion?
- choice 2: stationary or non-stationary iteration
- For red choices: $S \cdot$ changes in each iteration $\rightarrow S = S_k$
- There is no longer a Krylov subspace defined by

$$K_k(SA, b) = \{b, SAb, (SA)^2b, \ldots, (SA)^{k-1}b\}$$

$\Rightarrow$ Convergence theory does not hold anymore

- Algorithmic realizations have to be modified!
  $\Rightarrow$ Flexible Krylov subspace methods
Flexible CG — Algorithm

Flexible Conjugate Gradients

\[ r^{(0)} = b - Ax^{(0)}, \quad z^{(0)} = S_0 r^{(0)}, \quad p^{(0)} = z^{(0)} \]

\[ \text{for } k = 1, 2, \ldots \text{ do} \]

\[ \alpha_{k-1} = \frac{\langle r^{(k-1)}, z^{(k-1)} \rangle}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle} \]

\[ x^{(k)} = x^{(k-1)} + \alpha_{k-1} p^{(k-1)} \]

\[ r^{(k)} = r^{(k-1)} - \alpha_{k-1} A p^{(k-1)} \]

\[ z^{(k)} = S_k r^{(k)} \]

\[ \beta_{k-1} = \frac{\langle r^{(k)} - r^{(k-1)}, z^{(k)} \rangle}{\langle r^{(k-1)}, z^{(k-1)} \rangle} \]

\[ p^{(k)} = z^{(k)} + \beta_{k-1} p^{(k-1)} \]

\[ \text{end for} \]

- If \( S_k = S \) for all \( k \) \( \implies \) \( z^{(k)} \perp r^{(k-1)} \)

- Flexible CG preserves local optimality
Flexible GMRES($m$)

\[
\textbf{while not converged do}
\]
\[r^{(0)} = b - Ax^{(0)}, \quad \beta = \|r^{(0)}\|_2, \quad v_1 = \beta^{-1} r^{(0)}\]
\[\textbf{for } j = 1, \ldots, m \textbf{ do}
\]
\[z_j = S_j v_j\]
\[w = Az_j\]
\[\textbf{for } i = 1, \ldots, j \textbf{ do}
\]
\[h_{i,j} = \langle w, v_j \rangle_2\]
\[w = w - h_{i,j} v_j\]
\[\textbf{end for}\]
\[h_{j+1,j} = \|w\|_2\]
\[v_{j+1} = h_{j+1,j}^{-1} w\]
\[\textbf{end for}\]
\[\text{Define } Z_m = [z_1 \mid \ldots \mid z_m], \quad H_{m+1,m} = \{h_{i,j}\}_{1 \leq j \leq m, 1 \leq i \leq j+1}\]
\[\text{Solve } y_m = \arg\min_y \|\beta e_1 - H_{m+1,m} y\|_2\]
\[x^{(0)} = x^{(0)} + Z_m y_m\]
\[\textbf{end while}\]
Preconditioners — Summary

Preconditioning **improves convergence** if $\kappa(SA) \ll \kappa(A)$

- There is a wide variety of preconditioners available
  - Most of them require knowledge about $A$ or its origins
- Goals when constructing preconditioners $S$ are
  - $S \approx A^{-1}$ and $S$· cheap

Preconditioning makes Krylov subspace methods **more robust**

- Reducing $\kappa(A)$ helps controlling the error $e^{(k)}$, since
  $$\|e\|_2 \leq c\kappa(A)\|r\|_2$$

  $\Rightarrow$ If $\kappa(A) \gg 1$ results based on $\|r\|_2$ should not be trusted!
  $\Rightarrow$ If $\kappa(A) \gg 1$ a preconditioner is **mandatory**!
Deflation — Idea ($A$ hermitian and positive definite)

Assume $A$ hermitian and positive definite
Then convergence is slowed down by small eigenmodes

- Given the “troublesome” modes $v_1, \ldots, v_\ell$

  $\Rightarrow$ deflate the subspace $V = \text{colspan}([v_1 | \ldots | v_\ell])$

Similar to preconditioning, instead of $Ax = b$ solve

$$A (I - \pi_A(V)) \hat{x} = (I - \pi_A(V)) b$$
$$x = \hat{x} + V (V^\dagger AV)^{-1} V^\dagger b$$

with $\pi_A(V) = V (V^\dagger AV)^{-1} V^\dagger A$

- In case $v_i$ are eigenmodes, $V^\dagger AV = \text{diag}(\lambda_1, \ldots, \lambda_\ell)$

  $\Rightarrow (V^\dagger AV)^{-1}$ nothing to worry about
Deflation — Conjugate Gradients Theory

The effective condition number $\kappa_{\text{eff}}$ replaces $\kappa$ in theory

$$\kappa_{\text{eff}} = \frac{\mu_1}{\mu_\ell}$$

$$\mu_1 = \max_{x \neq 0} \frac{\langle A(I - \pi_A(V))x, x \rangle_2}{\langle x, x \rangle_2}$$

$$\mu_\ell = \min_{x \in V^\perp \setminus \{0\}} \frac{\langle A(I - \pi_A(V))x, x \rangle_2}{\langle x, x \rangle_2}$$

- If $v_i$ are smallest $\ell$ eigenmodes

$$\kappa_{\text{eff}} = \frac{\lambda_{\text{max}}}{\lambda_{\ell+1}}$$

where $\lambda_{\ell+1}$ is the $(\ell + 1)^{st}$ smallest eigenvalue
**Deflated CG — Algorithm**

**Deflated CG**  
(Deflation space $\mathcal{V} = \text{colspan}(V)$)

\[
\begin{align*}
x^{(0)} &= x^{(0)} + \pi_A(V)b \\
r^{(0)} &= b - Ax^{(0)} \\
p^{(0)} &= (I - \pi_A(V))r^{(0)} \\
\text{for } k = 1, 2, \ldots & \text{ do} \\
\alpha_{k-1} &= \frac{\langle r^{(k-1)}, r^{(k-1)} \rangle}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle} \\
x^{(k)} &= x^{(k-1)} + \alpha_{k-1}p^{(k-1)} \\
r^{(k)} &= r^{(k-1)} - \alpha_{k-1}Ap^{(k-1)} \\
\beta_{k-1} &= \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k-1)}, r^{(k-1)} \rangle} \\
p^{(k)} &= (I - \pi_A(V))r^{(k)} + \beta_{k-1}p^{(k-1)} \\
\text{end for}
\]
GMRES($m$)

On restart all information about $\mathcal{K}_m(A, r^{(0)})$ is lost!

- Use deflation technique to transfer information

Note: Due to the Arnoldi relation $V_m^* A V_m = H_{m,m}$ we have

- Eigenmodes $w_1, \ldots, w_m$ of $H_{m,m}$ give approximations $V_m w_1, \ldots, V_m w_m$ for eigenmodes of $A$

\[ H_{mm} w_i = \lambda_i w_i \implies V_m^* (A V_m w_i - \lambda_i V_m w_i) = 0 \]

- Vectors $V_m w_i$ are called Ritz vectors (→ ARPACK)

Idea: Use smallest eigenmodes of $H_{m,m}$ in deflation
Deflated GMRES($m$) — Sketch

\(\tilde{V} = \emptyset\)

\textbf{for} \(\ell = 0, 1, \ldots\) \textbf{do}

\(r^{(0)} = b - Ax^{(0)}\), \(\beta = \|r^{(0)}\|_2\), \(v_1 = \beta^{-1}r^{(0)}\)

Compute \(V_m, H_{m+1,m}\) based on initial \(\tilde{V}\) (Arnoldi)

Compute smallest Ritz vectors \(V_m w_1, \ldots, V_m w_\ell\)

\(y_m = \arg\min_y \|\beta e_1 - H_{m+1,m} y\|_2\)

\(x^{(0)} = x^{(0)} + V_m y_m\)

\(\tilde{V} = [V_m w_1 \mid \ldots \mid V_m w_\ell]\)

\textbf{end for}

- For a more detailed description see [4]
- Reusing information upon restart is also known as…
  - …recycling
  - …augmenting
Deflation — Summary

Deflation “hides” most difficult part of the problem

- Computation of eigenmodes necessary
  - possibly on-the-fly (Deflated GMRES($m$))
  - possibly a priori knowledge available
  - approximations viable (→ ARPACK)
- Analysis of general deflation subspaces $\mathcal{V}$ (cf. [3])

Eigenmode deflation suffers from scaling (i.e., $a \to 0$)

- In order to have constant number of iterations for $a \to 0$
  \[ \kappa_{\text{eff}} = \text{const} \iff \lambda_{\text{min}}^{\text{eff}} > \sigma \]
- Often number $N_\sigma$ of eigenvalues below threshold $\sigma$ fulfills
  \[ N_\sigma \sim \text{system size } n \to \infty \quad (a \to 0) \]
  \[ \Rightarrow \quad \text{More eigenmodes need to be computed as } a \to 0 \]
Summary

To find an efficient solver is hard, but there are guidelines

- Use as much information about your system as possible
  - In the choice of the Krylov subspace method
    - Short recurrence method available?
    - Optimal method available?
  - In the choice of the preconditioner
- Adjust parameters of your method w.r.t. hardware, e.g.,
  - Restart length in GMRES($m$)
  - Dimension of the deflation subspace
  - Dimension of the subdomains in domain decomposition

Most often there is no obvious optimal choice for the solver!

Construction of optimal solvers is ongoing research!
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