Solvers II — Preconditioning and Deflation

Lattice Practices 2014

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Outline

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

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

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

$$\mathbf{L}x = f$$

- Depending on PDE order and order of discretization

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

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

$$\kappa(\mathbf{L}) \longrightarrow \infty \quad (a \to 0)$$

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

$$\begin{aligned} S_\ell A S_r y &= S_\ell b \\ x &= S_r y \end{aligned}$$

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

Open questions

- What are the design goals for preconditioners?
- What are suitable choices of S_ℓ, 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 $S = S_\ell$

Preconditioning — Observations

Consider extreme cases

- $S = I$

  $\Rightarrow \; SA = A$ original setting
- $S = A^{-1}$

  $\Rightarrow \; SA = I$ and $\kappa(SA) = 1$ (ideal)
- $S = A^\dagger$

  $\Rightarrow \; SA = A^\dagger A$ hermitian, but $\kappa(SA) = \kappa(A)^2$

In order to speed up convergence preconditioner S should

- approximate A^{-1}
- be cheap to compute $(S\cdot)$

Preconditioning — CG

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

PCG — Algorithm

Preconditioned Conjugate Gradients

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

for $k = 1, 2, \dots$ **do**

$\alpha_{k-1} = \frac{\langle r^{(k-1)}, z^{(k-1)} \rangle_2}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle_2}$

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

$r^{(k)} = r^{(k-1)} - \alpha_{k-1} Ap^{(k-1)}$

$z^{(k)} = Sr^{(k)}$

$\beta_{k-1} = \frac{\langle r^{(k)}, z^{(k)} \rangle_2}{\langle r^{(k-1)}, z^{(k-1)} \rangle_2}$

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

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 $V_m = [v_1 \mid \ldots \mid v_m], H_{m+1,m} = \{h_{i,j}\}_{1 \le j \le m, 1 \le i \le j+1}$
  Solve $y_m = \operatorname{argmin}_y \|\beta e_1 - H_{m+1,m} y\|_2$
  $x^{(0)} = x^{(0)} + V_m y_m$
end while

Preconditioned BiCGstab

$r^{(0)} = b, \beta_0 = 0$

$\hat{r} = r$ shadow residual $\langle r, \hat{r} \rangle_2 \neq 0$

for $k = 0, 1, \dots$ **do**

$\rho_k = \langle r^{(k)}, \hat{r} \rangle_2$

$\beta_k = \frac{\rho_k}{\rho_{k-1}} \cdot \frac{\alpha_{k-1}}{\omega_{k-1}}$

$p^{(k)} = r^{(k)} + \beta_k (p^{k-1} - \omega_{k-1} v^{(k-1)})$

$\hat{p}^{(k)} = S p^{(k)}$

$\alpha_k = \frac{\rho_k}{\langle A\hat{p}^{(k)}, \hat{r} \rangle_2}$

$x^{(k+\frac{1}{2})} = x^{(k)} + \alpha_k \hat{p}^{(k)}$

$s^{(k)} = r^{(k)} - \alpha_k A \hat{p}^{(k)}$ $s^{(k)} \equiv r^{(k+\frac{1}{2})}$

$\hat{s}^{(k)} = S s^{(k)}$

$\omega_k = \frac{\langle s^{(k)}, A\hat{s}^{(k)} \rangle_2}{\langle A\hat{s}^{(k)}, A\hat{s}^{(k)} \rangle_2}$

$x^{(k+1)} = x^{(k+\frac{1}{2})} + \omega_k \hat{s}^{(k)}$

$r^{(k+1)} = s^{(k)} - \omega_k A \hat{s}^{(k)}$

end for

Preconditioners

Aims for the construction of preconditioners S

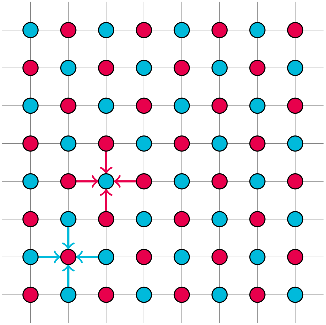
1. $S \approx A^{-1}$ to get speed-up
2. $S\cdot$ should be cheap (1 application per iterate)

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



- Nodes are odd or even

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

Odd-even preconditioning

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

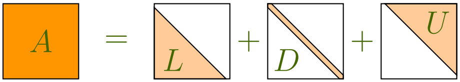
Odd-Even Reduction

$y_o = A_{oo}^{-1}b_o$
Solve $\hat{A}_{ee}x_e = b_e - A_{eo}y_o$
$x_o = y_o - A_{oo}^{-1}A_{oe}x_e$

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

Splitting methods

Splitting methods use the additive decomposition of A



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

General splitting method: $A = M + N$

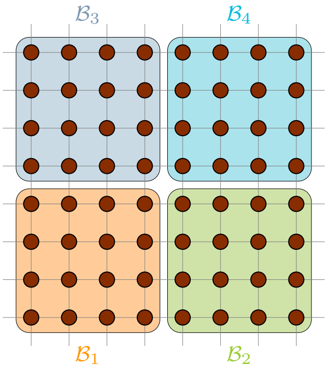
$$x^{(k+1)} = x^{(k)} + M^{-1}r^{(k)} \Longrightarrow e^{(k+1} = e^{(k)} - M^{-1}Ae^{(k)}$$

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 $\mathcal{B}_i$
- Solve system iteratively on each subdomain



- Canonical injection $\mathcal{I}_j$

$$\mathcal{I}_j e_i = e_{(B_j)_i}$$

- Restriction of x onto $\mathcal{B}_j$

$$x_{\mathcal{B}_j} = \mathcal{I}_j^\dagger x$$

- Restriction of A onto $\mathcal{B}_j$

$$A_{\mathcal{B}_j} = \mathcal{I}_j^\dagger A \mathcal{I}_j$$

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

Additive and Multiplicative Schwarz

Additive Schwarz

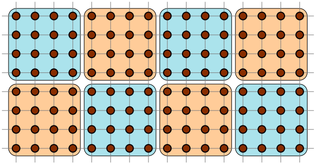
for $k = 0, 1, \dots$ **do**
  $r^{(k)} = b - Ax^{(k)}$
  for $j = 1, 2, \dots, n_B$ **do**
    $x^{(k+1)}_{\mathcal{B}_j} = x^{(k)}_{\mathcal{B}_j} + A^{-1}_{\mathcal{B}_j} r^{(k)}_{\mathcal{B}_j}$
  end for
end for

- Block-Jacobi
- Embarrassingly parallel

Multiplicative Schwarz

for $k = 0, 1, \dots$ **do**
  for $j = 1, 2, \dots, n_B$ **do**
    $r = b - Ax$
    $x_{\mathcal{B}_j} = x_{\mathcal{B}_j} + A^{-1}_{\mathcal{B}_j} r_{\mathcal{B}_j}$
  end for
end for

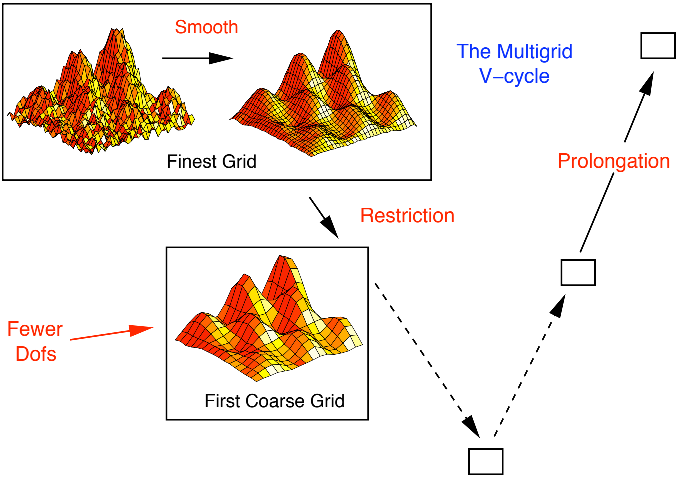
- Block-Gauss-Seidel
- Sequential ($\rightarrow$ coloring)



Schwarz methods in general

- $\oplus$ Data parallel
- $\oplus$ Computation parallel

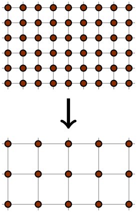
Multigrid


Smooth
Finest Grid
The Multigrid
V–cycle
Prolongation
Restriction
Fewer
Dofs
First Coarse Grid

(Algebraic) Multigrid

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

Wanted:
- Hierarchy of systems
  $A_\ell x_\ell = b_\ell, \quad \ell = 0, \dots, L$
- Intergrid transfer operators
  $P_{\ell+1}^{\ell} : \mathbb{C}^{n_{\ell+1}} \longrightarrow \mathbb{C}^{n_\ell}$
  $R_\ell^{\ell+1} : \mathbb{C}^{n_\ell} \longrightarrow \mathbb{C}^{n_{\ell+1}}$



Smoother

$$S_\ell : \mathbb{C}^{n_\ell} \longrightarrow \mathbb{C}^{n_\ell}$$

"High modes"

Interpolation

$$P_{\ell+1}^{\ell} : \mathbb{C}^{n_{\ell+1}} \longrightarrow \mathbb{C}^{n_\ell}$$

"Low modes"

Complementarity of Smoother and Interpolation

Generic Multigrid Algorithm — $\mathsf{MG}_\ell(A_\ell, b_\ell)$

if $\ell = L$ **then**
  $x_L = A_L^{-1} b_L$
else
  $x_\ell = 0$
  for $i = 1, \ldots, \nu_1$ **do**
    $x_\ell = S_\ell(x_\ell, b_\ell)$ $\quad (x_\ell \leftarrow x_\ell + M_\ell^{-1} r_\ell, r_\ell = b_\ell - A_\ell x_\ell)$
    "Pre-smooothing"
  end for
  $x_{\ell+1} = \mathsf{MG}(A_{\ell+1}, R_{\ell+1}^{\ell}(b_\ell - A x_\ell))$
  $x_\ell = x_\ell + P_{\ell+1}^{\ell} x_{\ell+1}$ "Coarse-grid correction"
  for $i = 1, \ldots, \nu_2$ **do**
    $x_\ell = S_\ell(x_\ell, b_\ell)$ "Post-smoothing"
  end for
end if

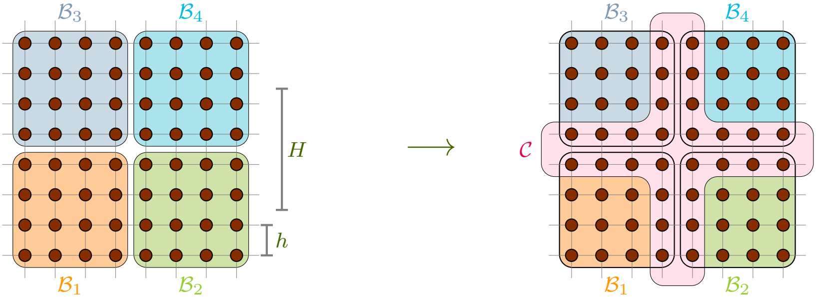
Optimality of Multigrid

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 $A_{\mathcal{C}}$ which couples the boundaries of the domains.

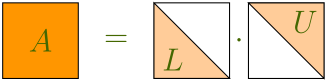


For certain classes of discretizations of certain types of PDEs and appropriate variants of **domain decomposition** we have

- 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



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 θ to drop small entries in L and U
   - Often: $\left(A^{-1}\right)_{i,j} \sim \alpha^{\mathrm{dist}_G(i,j)}, \quad \alpha < 1$

     $\Rightarrow$ 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

$$\mathcal{K}_k(SA, b) = \{b, SAb, (SA)^2 b, \dots, (SA)^{k-1} b\}$$

$\Rightarrow$ Convergence theory does not hold anymore

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

Flexible CG — Algorithm

Flexible Conjugate Gradients

$r^{(0)} = b - Ax^{(0)}, z^{(0)} = S_0 r^{(0)}, p^{(0)} = z^{(0)}$

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

$$\alpha_{k-1} = \frac{\langle r^{(k-1)}, z^{(k-1)} \rangle_2}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle_2}$$

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

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

$$z^{(k)} = S_k r^{(k)}$$

$$\beta_{k-1} = \frac{\langle r^{(k)} - r^{(k-1)}, z^{(k)} \rangle_2}{\langle r^{(k-1)}, z^{(k-1)} \rangle_2}$$

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

end for

- If $S_k = S$ for all k $\implies$ $z^{(k)} \perp r^{(k-1)}$
- Flexible CG preserves local optimality

Flexible GMRES(m)

while not converged **do**
  $r^{(0)} = S_0(b - Ax^{(0)}), \beta = \|r^{(0)}\|_2, v_1 = \beta^{-1} r^{(0)}$
  for $j = 1, \ldots, m$ **do**
    $z_j = S_j v_j$
    $w = Az_j$
    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 $Z_m = [z_1 \mid \ldots \mid z_m], H_{m+1,m} = \{h_{i,j}\}_{1 \leq j \leq m, 1 \leq i \leq j+1}$
  Solve $y_m = \operatorname{argmin}_y \|\beta e_1 - H_{m+1,m} y\|_2$
  $x^{(0)} = x^{(0)} + Z_m y_m$
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 $S\cdot$ cheap

Preconditioning makes Krylov subspace methods **more robust**

- Reducing $\kappa(A)$ helps controlling the error $e^{(k)}$, since

$$\|e\|_2 \leq c\kappa(A)^{-1}\|r\|_2$$

$\Rightarrow$ 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 $v_1, \dots, v_\ell$
  $\Rightarrow$ deflate the subspace $\mathcal{V} = \operatorname{colspan}(\underbrace{[v_1 \mid \dots \mid v_\ell]}_{=V})$

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

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

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

- In case v_i are eigenmodes, $V^\dagger AV = \operatorname{diag}(\lambda_1, \dots, \lambda_\ell)$
  $\Rightarrow$ $(V^\dagger AV)^{-1}$ nothing to worry about

Deflation — Conjugate Gradients Theory

The effective condition number κ_{eff} replaces κ in theory

$$
\begin{aligned}
\kappa_{\text{eff}} &= \frac{\mu_1}{\mu_\ell} \\
\mu_1 &= \max_{x \neq 0} \frac{\langle A(I - \pi_A(V))x, x\rangle_2}{\langle x, x\rangle_2} \\
\mu_\ell &= \min_{x \in \mathcal{V}^\perp \setminus \{0\}} \frac{\langle A(I - \pi_A(V))x, x\rangle_2}{\langle x, x\rangle_2}
\end{aligned}
$$

- If v_i are smallest ℓ eigenmodes

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

where $\lambda_{\ell+1}$ is the $(\ell+1)^{st}$ smallest eigenvalue

Deflated CG — Algorithm

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

$x^{(0)} = x^{(0)} + \pi_A(V)b$
$r^{(0)} = b - Ax^{(0)}$
$p^{(0)} = (I - \pi_A(V))r^{(0)}$
for $k = 1, 2, \dots$ **do**
  $\alpha_{k-1} = \frac{\langle r^{(k-1)}, r^{(k-1)} \rangle_2}{\langle Ap^{(k-1)}, p^{(k-1)} \rangle_2}$
  $x^{(k)} = x^{(k-1)} + \alpha_{k-1} p^{(k-1)}$
  $r^{(k)} = r^{(k-1)} - \alpha_{k-1} Ap^{(k-1)}$
  $\beta_{k-1} = \frac{\langle r^{(k)}, r^{(k)} \rangle_2}{\langle r^{(k-1)}, r^{(k-1)} \rangle_2}$
  $p^{(k)} = (I - \pi_A(V))r^{(k)} + \beta_{k-1} p^{(k-1)}$
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 $V_m^\dagger A V_m = H_{m,m}$ 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

$$H_{mm} w_i = \lambda_i w_i \;\Rightarrow\; V_m^\dagger (A V_m w_i - \lambda_i V_m w_i) = 0$$

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

Idea: Use smallest eigenmodes of $H_{m,m}$ in deflation

Deflated GMRES(m) — Sketch

$\tilde{V} = \emptyset$
for $\ell = 0, 1, \dots$ **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 $V_m w_1, \dots, V_m w_\ell$
  $y_m = \operatorname{argmin}_y \|\beta e_1 - H_{m+1,m} y\|_2$
  $x^{(0)} = x^{(0)} + V_m y_m$
  $\tilde{V} = [V_m w_1 \mid \dots \mid V_m w_\ell]$
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 ($\rightarrow$ ARPACK)
- Analysis of general deflation subspaces $\mathcal{V}$ (cf. [3])

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

- In order to have constant number of iterations for $a \rightarrow 0$

$$\kappa_{\text{eff}} = \text{const} \quad \Longleftrightarrow \quad \lambda_{min}^{\text{eff}} > \sigma$$

- Often number N_σ of eigvalues below threshold σ fulfills

$$N_\sigma \sim \text{system size } n \longrightarrow \infty \quad (a \rightarrow 0)$$

$\Rightarrow$ More eigenmodes need to be computed as $a \rightarrow 0$

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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