Inexact Krylov Subspace Methods
for PDEs and Control Problems

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Problem Statement

Solve a system $Hx = b$, $H$ Hermitian or non-Hermitian using Krylov subspace iterative methods

$$K_m(H, r_0) = \text{span}\{r_0, Hr_0, H^2r_0, \ldots, H^{m-1}r_0\}.$$ 

Given $x_0$, $r_0 = b - Hx_0$, find approximation

$$x_m \in x_0 + K_m(H, r_0),$$

satisfying some property:

Petrov-Galerkin, e.g., GMRES, MINRES:

$$x_m = \arg \min \{\|b - Hx\|_2\}, \quad x \in x_0 + K_m(H, r_0)$$

Galerkin, e.g., FOM, CG:

$$b - Hx_m \perp K_m(H, r_0)$$
Krylov subspace methods (cont.)

- Methods work by suitably choosing a basis of $\mathcal{K}_m(H, r_0)$
- Let $v_1, v_2, \ldots, v_m$ be such a basis, chosen to be orthonormal.
- With $V_m = [v_1, v_2, \ldots, v_m]$, obtain Arnoldi relation:

$$HV_m = V_{m+1}H_{m+1,m} = V_mH_m + h_{m+1,m}v_{m+1}e^T_m$$

$H_{m+1,m}$ is $(m + 1) \times m$ upper Hessenberg

- Each method finds $y_m$ so that $x_m = x_0 + V_m y_m$

- Main costs:
  1. Matrix-vector product: $H v_k$
  2. Orthogonalization
  3. Storage (if there is no recursion)
This Talk

- Consider the case when one does not fully orthogonalize: Truncated methods.
- Reduce the cost of matrix-vector product when $H$ is either
  - Not known exactly
  - Computationally expensive (e.g., Schur complement, reduced Hessian)
  - Preconditioned with variable matrix (i.e., iteration dependent)
Truncated Krylov subspace methods

- Only orthogonalize with respect to some fixed number $k$ of previous vectors [Saad, 1983, 1996].

- $H_{m+1,m}$ banded with upper semiband $k - 2$. Matrix with basis vectors $V_m$ not orthogonal. Can be implemented so that only $O(k)$ vectors are stored.

- Extreme case, $k = 3$, $H_{m+1,m}$ tridiagonal. If $H$ is SPD, FOM reduces to CG (and $V_m$ automatically orthogonal).

- Theory for “non-optimal methods” [Simoncini and Szyld, 2005]
Example: \( L(u) = -u_{xx} - u_{yy} + 100(x + y)u_x + 100(x + y)u_y, \) on \([0, 1]^2\), Dirichlet b.c., centered 5 pts. discretization, \( n = 2500 \).

GMRES, Truncated \( k = 3 \).
Inexact Krylov subspace methods

• At the $k$th iteration of the Krylov space method use

$$(H + D_k) v_{k-1} \text{ instead of } Hv_{k-1},$$

where $\|D_k\|$ can be monitored

• [Bouras, Frayssé, and Giraud, CERFACS reports 2000, SIMAX 2005] show experimentally that as $k$ progresses $\|D_k\|$ can be allowed to be larger; see also [Sleijpen and van der Eshof, 2004]
Inexact Krylov (cont.)

We repeat: \( \|D_k\| \) small at first, \( \|D_k\| \) can be big later. Convergence is maintained!

- Instead of \( HV_m = V_{m+1}H_{m+1,m} \) we have now

\[
[(H + D_1)v_1, (H + D_2)v_2, \ldots, (H + D_m)v_m] = V_{m+1}H_{m+1,m}
\]

- Subspace spanned by \( v_1, v_2, \ldots, v_m \) is not a Krylov subspace, but \( V_m \) orthogonal (in the full case)
Theorem for Inexact FOM
[Simoninci and Szyld, 2003]

True residual: \( r_m = b - Hx_m = r_0 - HV_m y_m \)
Computed residual (e.g.): \( \tilde{r}_m = r_0 - V_{m+1} H_{m+1, m} y_m = r_0 - W_m y_m \)

Let \( \varepsilon > 0 \). If for every \( k \leq m \),
\[
\|D_k\| \leq \frac{\sigma_{\min}(H_{m_*})}{m_*} \frac{1}{\|\tilde{r}_{k-1}\|} \varepsilon \equiv \ell^F_m \frac{1}{\|\tilde{r}_{k-1}\|} \varepsilon ,
\]
then \( \|V_m^T r_m\| \leq \varepsilon \) and \( \|r_m - \tilde{r}_m\| \leq \varepsilon \).

\( m_* \) being the maximum number of iterations allowed
(Similar results for inexact GMRES)
Theorem for Inexact Truncated FOM

\[ \|D_k\| \leq \frac{\sigma_{\min}(H_{m*}) \sigma_{\min}(V_m)}{m*} \frac{1}{\|\tilde{r}_{k-1}\|} \varepsilon \equiv \ell_m^T \frac{1}{\|\tilde{r}_{k-1}\|} \varepsilon, \]

implies \( \|V_m^T r_m\| \leq \varepsilon \) and \( \delta_m = \|r_m - \tilde{r}_m\| \leq \varepsilon. \)

**Notes:**

- This result applies in particular to Inexact CG
  Better criterion than above for ICG [Du, 2007]

- \( \ell_m \) can be estimated from problem, if information is available.
First Experiment

\[ H = \text{diag}([10^{-4}, 2, 3, \cdots, 100]) \]
\[ D_k = \text{symm} \left[ \alpha_k \text{randn}(100, 100) \right] \]
\[ b = \text{randn}(100, 1) \]

We chose \( \varepsilon = 10^{-8} \)

- Our condition (e.g. for FOM)

\[
\| D_k \| \leq \frac{\sigma_{\min}(H)}{m_\star} \frac{1}{\| \tilde{r}_{k-1} \|} \varepsilon
\]

is very conservative. In most cases it is too strict.

However, \( \sigma_{\min}(H) \) does play a role.
CG: condition $\|D_k\| \leq \frac{\sigma_{\min}(H)}{m_*} \frac{1}{\|\tilde{r}_k - 1\|} \varepsilon$

$\|V_m^T r_m\| \ll \varepsilon$
Applications:

I. Schur complement systems

\[
\begin{bmatrix}
A & B \\
B^T & 0
\end{bmatrix}
\begin{bmatrix}
w \\
x
\end{bmatrix}
= 
\begin{bmatrix}
f \\
0
\end{bmatrix},
\]

\[
B^T A^{-1} B x = B^T A^{-1} f; \quad A w = f - B x
\]

\[
H x = b
\]

\(A^{-1}\) not exactly (use Krylov method).
Applications: I. Schur complement systems (cont.)

- $A^{-1}$ not exactly (use Krylov method).

- Replace $Hv$ with $Hv = B^T z_j^{(k)}$, where $z_j^{(k)}$ is the approximation obtained at the $j$th (inner) iteration of the solution to the equation $Az = Bv$

- Question is then: **How many inner iterations?**
  i.e., at what value of $j$ stop?

  "Translate" conditions on $\|D_k\|$ to conditions on norm of inner residual.

Let $r_{k}^{inner} = Az_j^{(k)} - Bv$ be the inner residual

Take
\[
\|r_{k}^{inner}\| < \sigma_{m_\star}(H_{m_\star}) \frac{1}{\|B^T A^{-1}\| m_\star} \frac{1}{\|\tilde{r}_{k-1}^{fom}\|} \varepsilon \equiv \varepsilon_{inner}
\]
- Two-dim. saddle point magnetostatic problem from [Perugia, Simoncini, Arioli, 1999], $A$ is $1272 \times 1272$
- Inexact FOM, $m_\star = 120$, $\varepsilon = 10^{-4}$
Applications:

II. Inexact Preconditioning

\[ Hx = b \quad \rightarrow \quad H \mathcal{P}^{-1} \bar{x} = b, \quad x = \mathcal{P}^{-1} \bar{x} \]

\( \mathcal{P}^{-1} \) not performed exactly (use Krylov method)

\( H \mathcal{P}^{-1} v_k \) replaced with \( H \tilde{z}_k, \quad \tilde{z}_k \approx \mathcal{P}^{-1} v_k \)

Arnoldi relation

\[ H \mathcal{P}^{-1} V_m = V_{m+1} H_{m+1,m} \quad \text{is transformed into} \]

\[ H[\tilde{z}_1, \cdots, \tilde{z}_m] = V_{m+1} H_{m+1,m}. \]

Use Flexible Krylov subspace method

\( r^{inner}_k = v_k - \mathcal{P} \tilde{z}_k \) inner residual

\[ \| r^{inner}_k \| \leq \frac{\sigma_{m_k}(H_{m_k})}{\| H \mathcal{P}^{-1} v_k \| m_k} \frac{1}{\| \tilde{r}^g_{m, k-1} \| \tilde{r}^g_{m, k-1} \|} \varepsilon \equiv \varepsilon^{inner} \]
For some 2D saddle point, use $P = \begin{bmatrix} I & 0 \\ 0 & B^T B \end{bmatrix}$. Solve

$B^T B p_k = rhs$ iteratively, $m_* = 80$, $\varepsilon = 10^{-9}$, tolerance $\varepsilon_{inner}$.
Some CPU Times: Same Magnetostatic 2D Problem

Outer tolerance: $10^{-8}$

**Elapsed Time**

CPU in seconds of a Sun Enterprise 4500 (Fortran code)
(4 CPU 400MHertz, 2GBytes RAM) CG iterations.

<table>
<thead>
<tr>
<th>Problem Size</th>
<th>Fixed Inner Tol $\varepsilon_{inner} = 10^{-10}$</th>
<th>Var. Inner Tol. $10^{-10}/|r|$</th>
<th>Var. Inner Tol. $10^{-12}/|r|$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3810</td>
<td>17.0 (54)</td>
<td>11.4 (54)</td>
<td>14.7 (54)</td>
</tr>
<tr>
<td>9102</td>
<td>82.9 (58)</td>
<td>62.8 (58)</td>
<td>70.7 (58)</td>
</tr>
<tr>
<td>14880</td>
<td>198.4 (54)</td>
<td>156.5 (54)</td>
<td>170.1 (54)</td>
</tr>
</tbody>
</table>
Applications:

III. Parabolic Control Problems (W i P)

First Example

Inverse problem: Recover control $u(x)$ based on field (state) $z(x)$ related by the forward problem (3D):

\[ \Delta z = z_t, \quad x \in \Omega \]
\[ z = u, \quad x \in \partial \Omega \]
\[ z = z_0, \quad x \in \Omega \setminus \partial \Omega, \quad \text{for } t = 0 \]
Discretized forward problem (FD)

\[ Ez - \delta t Nu = c. \]

\[
\begin{bmatrix}
B \\
-I & B \\
-I & B \\
\vdots & \ddots & \ddots \\
-I & B
\end{bmatrix}
\begin{bmatrix}
z_1 \\
z_2 \\
\vdots \\
z_s
\end{bmatrix}
\begin{bmatrix}
M \\
M \\
\vdots \\
M
\end{bmatrix}
\begin{bmatrix}
z_0 \\
0
\end{bmatrix}
\]

where \( z_i \approx z(t_i) \), \( B = (I + \delta t A_h) \), with \( A_h \) discretization of \( \triangle \).
Optimization problem

\[
\min \phi = \frac{1}{2} \|Qz - d^{obs}\|^2 \\
\text{subject to} \quad E z - \delta t N u = c.
\]

Lagrangian \[ L(z, u, \lambda) = \frac{1}{2} \|Qz - d^{obs}\|^2 + \lambda^T (E z - \delta t N u - c) \]

Linearize to obtain

\[
\begin{bmatrix}
Q^T Q & 0 & E^T \\
0 & 0 & N^T \\
E & N & 0
\end{bmatrix}
\begin{bmatrix}
z \\
u \\
\lambda
\end{bmatrix}
= -
\begin{bmatrix}
L_u \\
L_m \\
L_\lambda
\end{bmatrix}
\]
Reduced Hessian

After elimination one has $Hu = -p$

$$H \ u = N^T E^{-T} Q^T Q E^{-1} N \ u = -p.$$ 

Use, e.g., with inexact CG, approximating each of the the systems with $E$ and $E^T$ with CG with varying (increasing) tolerance.

MVP $Hu$

1. Multiply $Nv$
2. Solve $Ez = Nv$ by solving $Ez = Nv$ with an inner tolerance $\epsilon_{in1}$
3. Multiply $Qz$
4. Multiply $Q^T Qz$
5. Solve $E^T w = Q^T Qz$ by solving with an inner tolerance $\epsilon_{in2}$
6. Compute $N^T w$
Experiments

$16 \times 16 \times 16$ grid. control $u$ of order 3375, 10 time steps.

<table>
<thead>
<tr>
<th>fixed</th>
<th>fixed</th>
<th>decreasing</th>
<th>increasing</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-14}$</td>
<td>$10^{-7}$</td>
<td>$10^{-3} \cdot |\tilde{r}_{k-1}|$</td>
<td>$10^{-8}/|\tilde{r}_{k-1}|$</td>
</tr>
<tr>
<td>35/23812</td>
<td>41/15250</td>
<td>48/18982</td>
<td>47/8689</td>
</tr>
</tbody>
</table>

Outer iterations / total inners = total matvecs with Laplacian.

Outer $\varepsilon = 10^{-7}$

There is a “delay”
12 more outer iter. than ”exact”, 6 more than fixed

but savings of 64%, and 43%
Illustration of “delay”, cheaper by a factor of about THREE

- - - exact CG,      ——— inexact CG,      - - - $\varepsilon_{inner}$

$n = 16, \text{tol} = 10^{-7}$
One surface of true and recovered model, and their difference decreasing $\epsilon_{inner} = 10^{-3} \cdot \|\tilde{r}_{k-1}\|$

-error $O(10^{-3})$
One surface of true and recovered model,
and their difference
increasing $\epsilon_{inner} = 10^{-8}/\|\tilde{r}_{k-1}\|$

error $O(10^{-6})$
Parabolic Control Problems, Second Example

General Lagrangian (using FEM)

\[ \mathcal{L}_h(z, u, p) = \frac{1}{2}(e^T Ke^T + u^T Gu) + p^T (Ez + Nu - f) \]

Reduced system: \[ Hu := (G + N^T E^{-T} KE^{-1} N)u = b_u \]

\[ E = \begin{bmatrix} F_h & & \\ -M_h & F_h & \\ & \ddots & \ddots \\ & & -M_h & F_h \end{bmatrix} \]

\[ F_h = M_h + \delta t A_h \]
Here we approximate $E$ with $E_n$, $n$ sweeps of the Parareal Algorithm.

We use our theory to find $\varepsilon_{inner}$ which determine how many sweeps we use.

**Example.** Find $u$ so that $z$ is closest to $z_*$, subject to $z_t - z_{xx} = u$,
$0 < x < 1$, $t > 0$. with initial and boundary data.
Discretize $\delta x = 1/16$ and $\delta t = 1/64$. System size 1024.
Inexact FOM: blue
Inexact FOM − true residual: dotted blue
Exact FOM: dotted black
Inner tol = $10^{-6}$ / res. norm
Computed residual: Inexact truncated FOM, semiband $m = 20$, $m = 8$ and $m = 1$ (ICG) (blue).

For the stopping criteria we use $\ell_n^{(1)} = \ell_n^{(2)} = 1 \left(10^{-6} \| r_0 \| / \| r_{m-1} \| \right)$
Conclusions

- Inexact matrix-vector product (or inexact preconditioning) might be worth trying for your problem
- Truncated methods might be worth trying for your problem
With Valeria Simoncini:

Theory of Inexact Krylov Subspace Methods and Applications to Scientific Computing

On the Occurrence of Superlinear Convergence of Exact and Inexact Krylov Subspace Methods

The Effect of Non-Optimal Bases on the Convergence of Krylov Subspace Methods

Recent computational developments in Krylov Subspace Methods for linear systems

All available at: http://www.math.temple.edu/~szyld

Watch for forthcoming reports on the control problems.