Iterative Methods in Linear Algebra
(part 2)

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Topics

Projection in Scientific Computing

Sparse matrices, parallel implementations

PDEs, Numerical solution, Tools, etc.

Iterative Methods
Outline

- **Part I**
  Krylov iterative solvers

- **Part II**
  Convergence and preconditioning

- **Part III**
  Iterative eigen-solvers
Part I

Krylov iterative solvers
Building blocks for **Krylov iterative solvers** covered so far

- **Projection/minimization in a subspace**
  - Petrov-Galerkin conditions
  - Least squares minimization, etc.

- **Orthogonalization**
  - CGS and MGS
  - Cholesky or Householder based QR
We also covered abstract formulations for iterative solvers and eigen-solvers

What are the goals of this lecture?

- Give specific examples of Krylov solvers
- Show how examples relate to the abstract formulation
- Show how examples relate to the building blocks covered so far, specifically to
  - Projection, and
  - Orthogonalization
- But we are not going into the details!
Projection and iterative solvers

- The problem: Solve $Ax = b$ in $\mathbb{R}^n$
- Iterative solution: at iteration $i$ extract an approximate $x_i$ from just a subspace $V = \text{span}\{v_1, ..., v_m\}$ of $\mathbb{R}^n$
- How? As on slide 22, impose constraints: $b - Ax \perp$ subspace $W = \text{span}\{w_1, ..., w_m\}$ of $\mathbb{R}^n$, i.e. $$(*) \quad (Ax, w) = (b, w) \quad \text{for all } w \in W = \text{span}\{w_1, ..., w_m\}$$
- Conditions $(*)$ known also as Petrov-Galerkin conditions
- Projection is orthogonal: $V$ and $W$ are the same (Galerkin conditions) or oblique: $V$ and $W$ are different

Remember projection slides 26 & 27, Lecture 7 (left)

- Projection in a subspace is the basis for an iterative method
- Here projection is in $V$
- In Krylov methods $V$ is the Krylov subspace

$$K_m(A, r_0) = \text{span}\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}$$

where $r_0 \equiv b - Ax_0$ and $x_0$ is an initial guess.

- Often $V$ or $W$ are orthonormalized
- The projection is 'easier' to find when we work with an orthonormal basis (e.g. problem 4 from homework 5: projection in general vs orthonormal basis)
- The orthonormalization can be CGS, MGS, Cholesky or Householder based, etc.

Matrix representation

- Let $V = \{v_1, ..., v_m\}$, $W = \{w_1, ..., w_m\}$
- Find $y \in \mathbb{R}^m$ s.t. $x = x_0 + V y$ solves $Ax = b$, i.e.
- $A V y = b - Ax_0 = r_0$
- subject to the orthogonality constraints:
- $W^T A V y = W^T r_0$
- The choice for $V$ and $W$ is crucial and determines various methods (more in Lectures 4 and 5)
To summarize, Krylov iterative methods in general

- expend the Krylov subspace by a matrix-vector product, and
- do a projection in it.

Various methods result by specific choices of the expansion and projection.
A specific example with the

Conjugate Gradient Method (CG)
The method is for SPD matrices

Both $V$ and $W$ are the Krylov subspaces, i.e. at iteration $i$

$$V \equiv W \equiv K_i(A, r_0) \equiv \text{span}\{r_0, Ar_0, \ldots, A^{i-1}r_0\}$$

The projection $x_i \in K_i(A, r_0)$ satisfies the Petrov-Galerkin conditions

$$(Ax_i, \phi) = (b, \phi), \quad \text{for } \forall \phi \in K_i(A, r_0)$$
At every iteration there is a way (to be shown later) to construct a new search direction \( p_i \) such that

\[
\text{span}\{p_0, p_1, \ldots, p_i\} \equiv K_{i+1}(A, r_0) \quad \text{and} \quad (Ap_i, p_j) = 0 \quad \text{for} \quad i \neq j.
\]

**Note:** \( A \) is SPD \( \Rightarrow \) \((Ap_i, p_j) \equiv (p_i, p_j)_A\) can be used as an inner product, i.e. \( p_0, \ldots, p_i \) is an \((\cdot, \cdot)_A\) orthogonal basis for \( K_{i+1}(A, r_0) \)

\[\Rightarrow\] we can easily find \( x_{i+1} \approx x \) as

\[
x_{i+1} = x_0 + \alpha_0 p_0 + \cdots + \alpha_i p_i \quad \text{s.t.} \quad (Ax_{i+1}, p_j) = (b, p_j) \quad \text{for} \quad j = 0, \ldots, i
\]

Namely, because of the \((\cdot, \cdot)_A\) orthogonality of \( p_0, \ldots, p_i \) at iteration \( i + 1 \) we have to find only \( \alpha_i \)

\[
(Ax_{i+1}, p_j) = (A(x_i + \alpha_i p_i), p_i) = (b, p_i), \quad \Rightarrow \quad \alpha_i = \frac{(r_i, p_i)}{(Ap_i, p_i)}
\]

**Note:** \( x_i \) above actually can be replaced by any \( x_0 + v, v \in K_i(A, r_0) \) \( \text{(Why?)} \)
Conjugate Gradient Method

1: Compute $r_0 = b - Ax_0$ for some initial guess $x_0$
2: for $i = 0$ to ... do
3: $\rho_i = r_i^T r_i$
4: if $i = 0$ then
5: $p_0 = r_0$
6: else
7: $p_i = r_i + \frac{\rho_i}{\rho_{i-1}} p_{i-1}$
8: end if
9: $q_i = Ap_i$
10: $\alpha_i = \frac{\rho_i}{p_i^T q_i}$
11: $x_{i+1} = x_i + \alpha_i p_i$
12: $r_{i+1} = r_i - \alpha_i q_i$
13: check convergence; continue if necessary
14: end for

Note:
- One matrix vector product/iteration (at line 9)
- Two inner-products/iteration (lines 3 and 10)
- In exact arithmetic $r_{i+1} = b - Ax_{i+1}$ (Apply $A$ to both sides of 11 and subtract from $b$ to get line 12)
- Update for $x_{i+1}$ is as pointed out before, i.e. with

$$\alpha_i = \frac{(r_i, r_i)}{(Ap_i, p_i)} = \frac{(r_i, p_i)}{(Ap_i, p_i)}$$

since $(r_i, p_{i-1}) = 0$ (exercise)
- Other relations to be proved (exercise)
  - $p_i$'s span the Krylov space
  - $p_i$'s are $(\cdot, \cdot)_A$ orthogonal, etc.
Conjugate Gradient Method (continued)

To sum it up:

- In exact arithmetic we get the exact solution in at most $n$ steps, i.e.

\[ x = x_0 + \alpha_0 p_0 + \cdots + \alpha_i p_i + \alpha_{i+1} p_{i+1} + \cdots + \alpha_{n-1} p_{n-1} \]

- At every iteration one more term $\alpha_j p_j$ is added to the current approximation

\[
\begin{align*}
x_i & = x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} \\
x_{i+1} & = x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} + \alpha_i p_i \equiv x_i + \alpha_i p_i
\end{align*}
\]

- Note: we do not have to solve linear system at every iteration because of the $A$-orthogonal basis that we manage to maintain and expend at every iteration

- It can be proved that the error $e_i = x - x_i$ satisfies

\[
||e_i||_A \leq 2 \left( \frac{\sqrt{k(A)} - 1}{\sqrt{k(A)} + 1} \right)^i ||e_0||_A
\]
Building orthogonal basis for a Krylov subspace

We have seen the importance in:
- Defining projections
  - not just for linear solvers
- Abstract linear solvers and eigen-solver formulations
- A specific example
  - in CG where the basis for the Krylov subspaces is A-orthogonal (A is SPD)

We have seen how to build it:
- CGS, MGS, Cholesky or Householder based, etc.
- These techniques can be used in a method specifically designed for Krylov subspaces (general non-Hermitian matrix), namely in the Arnoldi’s Method.
Arnoldi’s Method

Arnoldi’s method:

Build an orthogonal basis for $K_m(A, r_0)$

$A$ can be general, non-Hermitian

1: $v_1 = r_0$
2: for $j = 1$ to $m$
3:   $h_{ij} = (Av_j, v_i)$ for $i = 1, \ldots, j$
4:   $w_j = Av_j - h_{1j}v_1 - \ldots - h_{jj}v_j$
5:   $h_{j+1,j} = ||w_j||_2$
6:   if $h_{j+1,j} = 0$ Stop
7:   $v_{j+1} = \frac{w_j}{h_{j+1,j}}$
8: end for

Note:

- This orthogonalization is based on CGS (line 4)
  
  $$w_j = Av_j - (Av_j, v_1)v_1 - \ldots - (Av_j, v_j)v_j$$

- $\Rightarrow$ up to iteration $j$ vectors
  
  $v_1, \ldots, v_j$

  are orthogonal

- The space of this orthogonal basis grows by taking the next vector to be $Av_j$

- If we do not exit at step 6 we will have

  $$K_m(A, r_0) = span\{v_1, v_2, \ldots, v_m\}$$

(exercise)
Arnoldi’s method in matrix notation

- Denote

\[ V_m \equiv [v_1, \ldots, v_m], \quad H_{m+1} = \{h_{ij}\}_{m+1 \times m} \]

and by \( H_m \) the matrix \( H_{m+1} \) without the last row.

- Note that \( H_m \) is upper Hessenberg (0s below the lower second sub-diagonal) and

\[ AV_m = V_m H_m + w_m e_m^T \]

\[ V_m^T AV_m = H_m \]

(exercise)
Arnoldi’s Method (continued)

Variations:
- Explained using CGS
- Can be implemented with MGS, Householder, etc.

How to use it in linear solvers?
- Example with the **Full Orthogonalization Method (FOM)**
Look for solution in the form

\[ x_m = x_0 + y_m(1)v_1 + \cdots + y_m(m)v_m \]

\[ \equiv x_0 + V_m y_m \]

Petrov-Galerkin conditions will be

\[ V_m^T A x_m = V_m^T b \]
\[ \Rightarrow V_m^T A (x_0 + V_m y_m) = V_m^T b \]
\[ \Rightarrow V_m^T A V_m y_m = V_m^T r_0 \]
\[ \Rightarrow H_m y_m = V_m^T r_0 = \beta e_1 \]

which is given by steps 3 and 4 of the algorithm
What happens when $m$ increases?

- computation grows as at least $O(m^2)n$
- memory is $O(mn)$

A remedy is to restart the algorithm, leading to restarted FOM

FOM$(m)$

1: $\beta = \|r_0\|_2$
2: Compute $v_1, \ldots, v_m$ with Arnoldi
3: $y_m = \beta H_m^{-1} e_1$
4: $x_m = x_0 + V_m y_m$. Stop if residual is small enough.
5: Set $x_0 := x_m$ and go to 1
Generalized Minimum Residual Method (GMRES)

- Similar to FOM
  - Again look for solution
    \[ x_m = x_0 + V_m y_m \]
    where \( V_m \) is from the Arnoldi process (i.e. \( K_m(A, r_0) \))
- The test conditions \( W_m \) from the abstract formulation (slide 27, Lecture 7)
  \[ W_m^T A V_m y_m = W_m^T r_0 \]
  are \( W_m = AV_m \).
- The difference results in step 3 from FOM, namely
  \[ y_m = \beta H_m^{-1} e_1 \]
  being replaced by
  \[ y_m = \text{argmin}_y \| \beta e_1 - H_{m+1} y \|_2 \]
Similarly to FOM, GMRES can be defined with
- Various orthogonalizations in the Arnoldi process
- Restart

Note:
- Solving the least squares (LS) problem

$$\arg\min_y \| \beta e_1 - H_{m+1} y \|_2$$

can be done with QR factorization as discussed in Lecture 7, Slide 25
Can we improve on Arnoldi if $A$ is symmetric?

- Yes! $H_m$ becomes symmetric so it will be just 3 diagonal
- the simplification of Arnoldi in this case leads to the Lanczos Algorithm
- Lanczos can be used in deriving CG

The Lanczos Algorithm

1: $v_1 = \frac{r_0}{\|r_0\|_2}$, $\beta_1 = 0$, $v_0 = 0$
2: for $j = 1$ to $m$ do
3: $w_j = Av_j - \beta_j v_{j-1}$
4: $\alpha_j = (w_j, v_j)$
5: $w_j = w_j - \alpha_j v_j$
6: $\beta_{j+1} = \|w_j\|_2$. If $\beta_{j+1} = 0$ then Stop
7: $v_{j+1} = \frac{w_j}{\beta_{j+1}}$
8: end for

- Matrix $H_m$ here is 3-diagonal with diagonal $h_{ii} = \alpha_i$ and off diagonal $h_{i,i+1} = \beta_{i+1}$
- In exact arithmetic $v_i$’s are orthogonal but in reality orthogonalization gets lost rapidly
We saw how different basis for the Krylov spaces is characteristic for various methods, e.g.

- GMRES uses orthogonal
- CG uses $A$-orthogonal

This is true for other methods as well

- Conjugate Residual (CR; for symmetric problems) uses $A^TA$-orthogonal (i.e. $Ap_i$’s are orthogonal)
- $A^TA$-orthogonal basis can be generalized to the non-symmetric case as well, e.g. in the Generalized Conjugate Residual (GCR)
Other Krylov methods

We considered various methods that construct a basis for the Krylov subspaces

Another big class of methods is based on biorthogonalization (algorithm due to Lanczos)

- For non-symmetric matrices build a pair of bi-orthogonal bases for the two subspaces

  \[ K_m(A, v_1) = \text{span}\{v_1, Av_1, \ldots, A^{m-1}v_1\} \]

  \[ K_m(A^T, w_1) = \text{span}\{w_1, A^T w_1, \ldots, (A^T)^{m-1}w_1\} \]

- Examples here are BCG and QMR (not to be discussed)

- These methods are more difficult to analyze
Part II

Convergence and preconditioning
Convergence can be analyzed by

- Exploit the optimality properties (of projection) when such properties exist
- A useful tool is Chebyshev polynomials
- Depend on the condition number of the matrix, e.g.
  - in CG it is

\[
\|e_i\|_A \leq 2 \left( \frac{\sqrt{k(A)} - 1}{\sqrt{k(A)} + 1} \right)^i \|e_0\|_A
\]
Preconditioning

Convergence can be slow or even stagnate

- for ill-conditioned matrices (with large condition number)

But can be improved with *preconditioning*

\[ x_{i+1} = x_i + P(b - Ax_i) \]

- Think of \( P \) as a preconditioner, an operator/matrix \( P \approx A^{-1} \)
- for \( P = A^{-1} \) it takes 1 iteration
Properties desired in a preconditioner:

- Should approximate $A^{-1}$
- Should be easy to compute, apply to a vector, and store

Iterative solvers can be extended to support preconditioning (How?)
Extending Iterative solvers to support preconditioning

- The same solver can be used but on a modified problem, e.g.
- Problem $Ax = b$ is transformed into $PAX = Pb$

  known as left preconditioning

- Problem $Ax = b$ is transformed into $APX = b, \ x = Pu$

  known as right preconditioning

- Convergence of the modified problem would depend on $k(PA)$
  (e.g. with left preconditioning)
Preconditioning

Examples:
- Incomplete LU factorization (e.g. ILU(0))
- Jacobi (inverse of the diagonal)
- Other stationary iterative solvers (GS, SOR, SSOR)
- Block preconditioners and domain decomposition
  - Additive Schwarz (thing of Block-Jacobi)
  - Multiplicative Schwarz (think of Block-GS)
Examples so far:

- algebraic preconditioners, i.e. exclusively based on the matrix

Often, for problems coming from PDEs, PDE and discretization information can be used in designing a preconditioner, e.g.

- FFTs’ can be involved to approximate differential operators on regular grids (as in Fourier space the operators are diagonal matrices)

- Grid and problem information to define multigrid preconditioners

- Indefinite problems are often composed of sub-blocks that are definite: used in defining specific preconditioners and even modify solvers for these needs, etc.
Part III

Iterative eigen-solvers
How are iterative eigensolvers related to Krylov subspaces?

Projection and Eigen-Solvers

- The problem: Solve \( Ax = \lambda x \) in \( \mathbb{R}^n \)
- As in linear solvers: at iteration \( i \) extract an approximate \( x_i \) from a subspace \( V = \text{span}\{v_1, ..., v_m\} \) of \( \mathbb{R}^n \)
- How? As on slides 22 and 26, impose constraints: \( \lambda x - Ax \perp \text{subspace } W = \text{span}\{w_1, ..., w_m\} \) of \( \mathbb{R}^n \), i.e.
  \[
  (Ax, w_j) = (\lambda x, w_j) \quad \text{for } \forall w_j \in W = \text{span}\{w_1, ..., w_m\}
  \]
- This procedure is known as Rayleigh-Ritz
- Again projection can be orthogonal or oblique

Matrix representation

- Let \( V = \{v_1, ..., v_m\} \), \( W = \{w_1, ..., w_m\} \)
- Find \( y \in \mathbb{R}^m \) s.t. \( x = V y \) solves \( Ax = \lambda x \), i.e.
  \[
  A V y = \lambda V y
  \]
  subject to the orthogonality constraints:
  \[
  W^T A V y = \lambda W^T V y
  \]
- The choice for \( V \) and \( W \) is crucial and determines various methods (more in Lectures 4 and 5)

Remember projection slides 29 & 30, Lecture 7 (left)

- Again, as in linear solvers, Projection in a subspace is the basis for an iterative eigen-solver
  
  - \( V \) and \( W \) are often based on Krylov subspaces
    \[
    K_m(A, r_0) = \text{span}\{r_0, A r_0, A^2 r_0, \ldots, A^{m-1} r_0\}
    \]
    where \( r_0 \equiv b - A x_0 \) and \( x_0 \) is an initial guess.

- Often parts of \( V \) or \( W \) are orthogonalized
  
  - For stability
  
  - The orthogonalization can be CGS, MGS, Cholesky or Householder based, etc.
  
  - The smaller Rayleigh-Ritz are usually solved with LAPACK routines
A brief introduction to Krylov iterative solvers and eigen-solvers

- Links to building blocks that we have already covered
  - Abstract formulation
  - Projection, and
  - Orthogonalization

- Specific examples and issues
  (preconditioning, parallelization, etc.)