Iterative Methods in Linear Algebra
(part 2)

Stan Tomov

Innovative Computing Laboratory
Computer Science Department
The University of Tennessee

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Topics

Projection in Scientific Computing

Sparse matrices, parallel implementations

PDEs, Numerical solution, Tools, etc.

Iterative Methods
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!
Krylov iterative solvers

How are these techniques related to Krylov iterative solvers?

Projection and iterative solvers

- The problem: Solve
  \[ Ax = b \quad \text{in } \mathbb{R}^n \]
- Iterative solution: at iteration \( k \) extract an approximate
  \( x_k \) from just a subspace \( V = \text{span}\{v_1, \ldots, v_m\} \) of \( \mathbb{R}^n \)
- How? As on slide 22, impose constraints:
  \[ b - Ax \perp \text{subspace } W = \text{span}\{w_1, \ldots, w_m\} \text{ of } \mathbb{R}^n, \text{i.e.} \]
  \[ (Ax, w) = (b, w) \quad \text{for } \forall w \in W = \text{span}\{w_1, \ldots, w_m\} \]
- 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

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

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 \( V = [v_1, \ldots, v_m] \), \( W = [w_1, \ldots, w_m] \)
  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 $x_0 + v$, $v \in K_i(A, r_0)$ (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.
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
  \[
  x_i = x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} \\
  x_{i+1} = x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} + \alpha_i p_i \equiv x_i + \alpha_i p_i
  \]

- 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 $m$ do
3: \[ h_{ij} = (Av_j, v_i) \text{ for } i = 1, \ldots, j \]
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

\[ K_m(A, r_0) = \text{span}\{v_1, v_2, \ldots, v_m\} \]

(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

\[ V_m^T Ax_m = V_m^T b \]

\[ \Rightarrow V_m^T A(x_0 + V_m y_m) = V_m^T b \]

\[ \Rightarrow V_m^T AV_m y_m = V_m^T r_0 \]

\[ \Rightarrow H_m y_m = V_m^T r_0 = \beta e_1 \]

which is given by steps 3 and 4 of the algorithm
Restarted FOM

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)

\[ W_m^T AV_m y_m = W_m^T r_0 \]

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 biortogonalization (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

$$APx = b, \quad x = Pu$$

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)
Preconditioning

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
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 $V = \text{span}\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$
- How? As on slides 22 and 26, impose constraints:

  $$\lambda x - Ax \perp \text{subspace } W = \text{span}\{w_1, \ldots, w_m\} \text{ of } \mathbb{R}^n$$

  i.e.,

  $$V \setminus W = \{ (Ax, w) = (\lambda x, w) : \forall w \in W = \text{span}\{w_1, \ldots, w_m\} \}$$

- This procedure is known as **Rayleigh-Ritz**
- Again projection can be **orthogonal or oblique**

**Matrix representation**

- Let $V = [v_1, \ldots, v_m]$, $W = [w_1, \ldots, w_m]$;

  Find $y \in \mathbb{R}^n$ 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)

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**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 $r_0 \equiv b - Ax_0$ 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.)