Iterative Methods in Linear Algebra (part 2)

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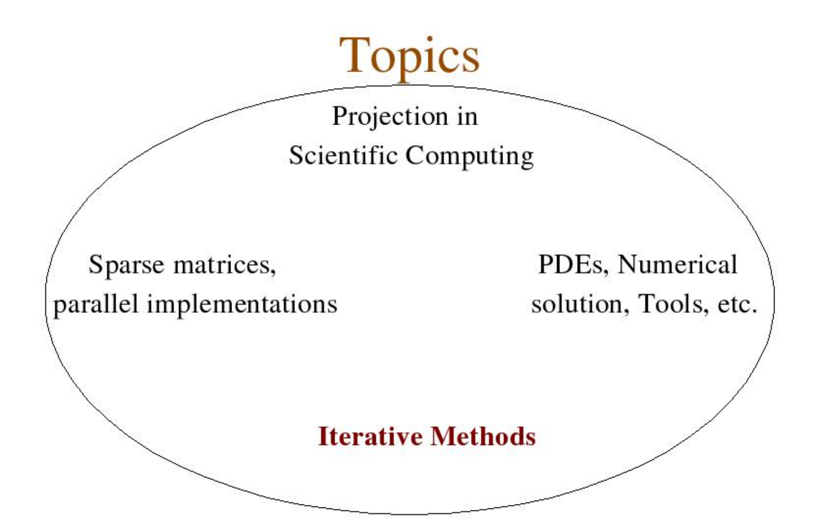
Topics
Projection in
Scientific Computing
Sparse matrices,
parallel implementations
PDEs, Numerical
solution, Tools, etc.
Iterative Methods

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, specidicly to
  - Projection, and
  - Orthogonalization
- But we are not going into the details!

How are these techniques related to Krylov iterative solvers?

Projection and iterative solvers

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

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Matrix representation

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

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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

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

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.

Krylov Iterative Methods

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)

Conjugate Gradient Method

- The method is for SPD matrices
- Both V and W are the Krylov subspaces, i.e. at iteration i

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

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

$$(Ax_i, \phi) = (b, \phi), \quad \text{for } \forall \phi \in K_i(A, r_0)$$

Conjugate Gradient Method (continued)

At every iteration there is a way (to be shown later) to construct a new search direction p_i such that

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

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

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

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

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

Note: x_i above actually can be replaced by any $x_0 + v$, $v \in K_i(A, r_0)$ (Why?)

Conjugate Gradient Method (continued)

Conjugate Gradient Method

1: Compute $r_0 = b - Ax_0$ for some initial guess x_0
2: **for** $i = 0$ to ... **do**
3: $\quad \rho_i = r_i^T r_i$
4: $\quad$ **if** $i = 0$ **then**
5: $\quad\quad p_0 = r_0$
6: $\quad$ **else**
7: $\quad\quad p_i = r_i + \frac{\rho_i}{\rho_{i-1}} p_{i-1}$
8: $\quad$ **end if**
9: $\quad q_i = Ap_i$
10: $\quad \alpha_i = \frac{\rho_i}{p_i^T q_i}$
11: $\quad x_{i+1} = x_i + \alpha_i p_i$
12: $\quad r_{i+1} = r_i - \alpha_i q_i$
13: $\quad$ *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_is' span the Krylov space
  - p_is' 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

$$\begin{aligned} x_i &= x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} \\ x_{i+1} &= x_0 + \alpha_0 p_0 + \cdots + \alpha_{i-1} p_{i-1} \quad + \alpha_i p_i \equiv x_i + \alpha_i p_i \end{aligned}$$

- 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

$$||e_i||_A \le 2 \left(\frac{\sqrt{k(A)} - 1}{\sqrt{k(A)} + 1} \right)^i ||e_0||_A$$

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: $\quad h_{ij} = (Av_j, v_i)$ for $i = 1, .., j$
4: $\quad w_j = Av_j - h_{1j}\mathbf{v_1} - \ldots - h_{jj}\mathbf{v_j}$
5: $\quad h_{j+1,j} = ||w_j||_2$
6: $\quad$ **if** $h_{j+1,j} = 0$ **Stop**
7: $\quad v_{j+1} = \frac{w_j}{h_{j+1,j}}$
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

$$\begin{aligned} AV_m &= V_m Hm + w_m e_m^T \\ V_m^T AV_m &= H_m \end{aligned}$$

(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)

FOM

1: $\beta = ||r_0||_2$
2: Compute $v_1, \ldots, v_m$ with Arnoldi
3: $y_m = \beta H_m^{-1} e_1$
4: $x_m = x_0 + V_m y_m$

- Look for solution in the form

$$\begin{aligned} x_m &= x_0 + y_m(1)v_1 + \cdots + y_m(m)v_m \\ &\equiv x_0 + V_m y_m \end{aligned}$$

- Petrov-Galerkin conditions will be

$$\begin{aligned} V_m^T A x_m &= V_m^T b \\ \Rightarrow \quad V_m^T A(x_0 + V_m y_m) &= V_m^T b \\ \Rightarrow \quad V_m^T A V_m y_m &= V_m^T r_0 \\ \Rightarrow \quad H_m y_m &= V_m^T r_0 = \beta e_1 \end{aligned}$$

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)

$$W_m^T A V_m y_m = W_m^T r_0$$

    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

$$y_m = argmin_y ||\beta e_1 - H_{m+1} y||_2$$

GMRES

Similarly to FOM, GMRES can be defined with

- Various orthogonalizations in the Arnoldi process
- Restart

Note:

- Solving the least squares (LS) problem

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

can be done with QR factorization as discussed in Lecture 7, Slide 25

Lanczos Algorithm

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

```
v_1 = r_0 / ||r_0||_2,  β_1 = 0,  v_0 = 0
for j = 1 to m do
    w_j = A v_j − β_j v_{j−1}
    α_j = (w_j, v_j)
    w_j = w_j − α_j v_j
    β_{j+1} = ||w_j||_2.  If β_{j+1} = 0 then Stop
    v_{j+1} = w_j / β_{j+1}
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_is' are orthogonal but in reality orthogonalization gets lost rapidly

Choice of basis for the Krylov subspace

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 $A^T A$-orthogonal (i.e. Ap_i's are orthogonal)
- $A^T A$-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

$$\begin{aligned} K_m(A, v_1) &= span\{v_1, Av_1, \ldots, A^{m-1}v_1\} \\ K_m(A^T, w_1) &= span\{w_1, A^T w_1, \ldots, (A^T)^{m-1}w_1\} \end{aligned}$$

- Examples here are BCG and QMR (not to be discussed)
- These methods are more difficult to analyze

Part II

Convergence and preconditioning

Convergence

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

Preconditioning

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?)

Preconditioning

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

Slide 29 / 39

Matrix representation

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

Slide 30 / 39

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

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

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

Learning Goals

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.)