SF2520 — Applied numerical methods

Lecture 15

Numerical linear algebra Iterative methods, convergence

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Today's lecture

- Iterative methods for linear systems of equations
 - Search methods (Krylov subspace methods)
 - Steepest descent
 - Conjugate gradient
 - GMRES
- Convergence theory
- Preconditioning

Iterative methods for linear systems of equations

We consider

$$A\mathbf{x} = \mathbf{b}, \qquad A \in \mathbb{R}^{N \times N}, \quad \mathbf{x}, \mathbf{b} \in \mathbb{R}^{N}.$$

Solve this via iteration ⇒

$$x_0, x_1, x_2, \dots$$

- Primarily used for sparse linear systems. Methods are mostly insensitive to the precise sparsity structure. No need to worry about "fill-in" as in direct methods.
- Stationary methods: Split A = M - T, so that Mx = Tx + b and iterate

$$M\mathbf{x}_{k+1} = T\mathbf{x}_k + \mathbf{b}.$$

- Example 1: M = diagonal of A gives "Jacobi method"
- Example 2: M = lower triangular part of A gives "Gauss-Seidel method"

Search methods

In search methods, the iteration is of the form

$$\mathbf{X}_{k+1} = \mathbf{X}_k + \alpha_k \mathbf{p}_k, \qquad \alpha_k \in \mathbb{R}, \quad \mathbf{p}_k \in \mathbb{R}^N,$$

where α_k and \boldsymbol{p}_k (the search direction) are computed based on the residual(s) $\boldsymbol{r}_\ell = \boldsymbol{b} - A\boldsymbol{x}_\ell$, with $\ell \leq k$.

- Examples:
 - Steepest descent method (SD)
 - Conjugate gradient method (CG)
 - GMRES ("generalized minimum residual" method)
- SD and CG require symmetric positive definite matrices. GMRES works for any nonsingular matrix.

Let A be a symmetric positive definite matrix. We note first that then

$$A\mathbf{x} = \mathbf{b}$$
 \Leftrightarrow \mathbf{x} minimizes $\frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T \mathbf{b} =: \phi(\mathbf{x}),$

since

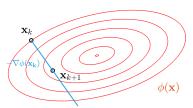
$$abla \phi(\mathbf{x}) = A\mathbf{x} - \mathbf{b}, \qquad D^2 \phi(\mathbf{x}) = A > 0.$$

In steepest descent we iterate

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla \phi(\mathbf{x}_k), \qquad \mathbf{x}_0 = 0,$$

where α_k is chosen to minimize ϕ along the gradient direction,

$$\alpha_k = \operatorname{argmin}_{\alpha} \phi(\mathbf{x}_k - \alpha \nabla \phi(\mathbf{x}_k)).$$



Intuition: Move in direction of largest change $(\nabla \phi)$ to lowest point in that direction.

We have

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k,$$

where

The search direction is the residual,

$$\boldsymbol{p}_k = -\nabla \phi(\boldsymbol{x}_k) = \boldsymbol{b} - A \boldsymbol{x}_k = \boldsymbol{r}_k.$$

• α_k minimizes $\phi(\mathbf{x}_k + \alpha \mathbf{p}_k)$, i.e.

$$0 = \frac{d}{d\alpha}\phi(\mathbf{x}_k + \alpha\mathbf{p}_k) = \mathbf{p}_k^T \nabla \phi(\mathbf{x}_k + \alpha\mathbf{p}_k) = \mathbf{p}_k^T (A(\mathbf{x}_k + \alpha\mathbf{p}_k) - \mathbf{b})$$
$$= -\mathbf{p}_k^T \mathbf{r}_k + \alpha\mathbf{p}_k^T A \mathbf{p}_k.$$

• Therefore,

$$\alpha_k = \frac{\boldsymbol{p}_k^T \boldsymbol{r}_k}{\boldsymbol{p}_k^T A \boldsymbol{p}_k} = \frac{\boldsymbol{r}_k^T \boldsymbol{r}_k}{\boldsymbol{r}_k^T A \boldsymbol{r}_k}.$$

Note also:

$$\mathbf{r}_{k+1} = \mathbf{b} - A\mathbf{x}_{k+1} = \mathbf{b} - A(\mathbf{x}_k + \alpha_k \mathbf{p}_k) = \mathbf{r}_k - \alpha_k A\mathbf{p}_k.$$

In summary, the method can be written

Steepest descent method

$$\mathbf{0} \ \mathbf{x}_0 = 0, \ \mathbf{r}_0 = \mathbf{b}.$$

$$\mathbf{2} \ \alpha_k = \frac{\boldsymbol{p}_k^{\mathsf{T}} \boldsymbol{r}_k}{\boldsymbol{p}_k^{\mathsf{T}} \boldsymbol{A} \boldsymbol{p}_k}$$

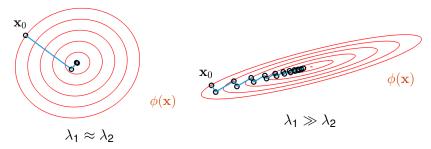
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Note: The main cost of the iteration is the matrix-vector multiply Ap_k . This should only be computed once per iteration!

(Of course in practice we would simplify and only keep r_k , not p_k in the algorithm. I kept p_k here for comparison with the conjugate gradient method later on.)

Remark:

When the eigenvalues of A differ a lot, $\lambda_1 \gg \lambda_2$, the contour lines of ϕ become very elongated ellipses. This can lead to slow convergence. Compare:



Note that $\lambda_1 \gg \lambda_2$ means that the condition number $\kappa(A) \gg 1$. In general a large condition number of A leads to slow convergence.

Conjugate gradient method

The conjugate gradient method (CG) uses more optimally chosen search directions p_k in

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k, \qquad \boldsymbol{x}_0 = 0.$$

In the end, the rest of the algorithm will be the same as SD.

• Observation: Regardless of how p_k are chosen we have

$$\mathbf{x}_{k+1} = \alpha_0 \mathbf{p}_0 + \alpha_1 \mathbf{p}_1 + \dots + \alpha_k \mathbf{p}_k \in \operatorname{span}\{\mathbf{p}_0, \dots, \mathbf{p}_k\}.$$

- Conjugate gradient idea:
 - Let \mathbf{x}_{k+1} be the best value in all of span $\{\mathbf{p}_0, \dots, \mathbf{p}_k\}$,

$$m{x}_{k+1} = \underset{m{x} \in \operatorname{span}\{m{p}_0, ..., m{p}_k\}}{\operatorname{argmin}} \phi(m{x}).$$

- Choose p_k so that:
 - All {p_k} are linearly independent. (This implies full convergence in at most N iterations.)
 - p_{k+1} and x_{k+1} can be computed easily from p_k and x_k .

Conjugate gradient method – sketch of derivation

• Let P be the matrix of search directions upto k-1

$$P = \begin{pmatrix} | & | & & | \\ \boldsymbol{p}_0 & \boldsymbol{p}_1 & \cdots & \boldsymbol{p}_{k-1} \\ | & | & & | \end{pmatrix}$$

and, since \mathbf{x}_{k+1} should be in span{ \mathbf{p}_i }, make the ansatz

$$\mathbf{x}_{k+1} = P\mathbf{y} + \alpha \mathbf{p}_k.$$

We need to determine \mathbf{y} , α and \mathbf{p}_k .

- They should be selected so that

 - We minimize

$$\phi(\boldsymbol{x}_{k+1}) = \ldots = \phi(\boldsymbol{P}\boldsymbol{y}) + \alpha \boldsymbol{y}^T \boldsymbol{P}^T \boldsymbol{A} \boldsymbol{p}_k + \frac{1}{2} \alpha^2 \boldsymbol{p}_k^T \boldsymbol{A} \boldsymbol{p}_k - \alpha \boldsymbol{p}_k^T \boldsymbol{b}.$$

• We therefore pick p_k such that it is "A conjugate" to p_i , j < k,

$$p_i^T A p_k = 0, \quad j = 0, ..., k-1$$

 $\Rightarrow \{ \boldsymbol{p}_k \}$ are linearly independent and $\alpha \boldsymbol{y}^T P^T A \boldsymbol{p}_k = 0$.

Conjugate gradient method – sketch of derivation

• We are left to minimize, over ${\bf y}$ and α

$$\phi(\mathbf{X}_{k+1}) = \underbrace{\phi(P\mathbf{y})}_{\text{only depends on } \mathbf{y}} + \underbrace{\frac{1}{2}\alpha^2\mathbf{p}_k^TA\mathbf{p}_k - \alpha\mathbf{p}_k^T\mathbf{b}}_{\text{only depends on } \alpha}.$$

- We can minimize the two terms independently:
 - Minimum of $\phi(Py) = \phi(x_k)$, the solution in the previous iteration, by the definition of how x_k are chosen. Hence $Py = x_k$.
 - Optimal α in second term obtained by putting α -derivative to zero,

$$\alpha_k = \frac{\boldsymbol{p}_k^T \boldsymbol{b}}{\boldsymbol{p}_k^T A \boldsymbol{p}_k} = \ldots = \frac{\boldsymbol{p}_k^T \boldsymbol{r}_k}{\boldsymbol{p}_k^T A \boldsymbol{p}_k}.$$

We get

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k$$

Finally, one can show that

$$\boldsymbol{p}_k = \boldsymbol{r}_k + \beta_k \boldsymbol{p}_{k-1}, \qquad \beta_k = \frac{\boldsymbol{r}_k^T \boldsymbol{r}_k}{\boldsymbol{r}_{k-1}^T \boldsymbol{r}_{k-1}}$$

is A-conjugate to p_i for i < k (and easy to compute).

Conjugate gradient method

In summary, the method can be written

Conjugate gradient method

1
$$\mathbf{x}_0 = \mathbf{p}_{-1} = 0, \, \mathbf{r}_0 = \mathbf{b}, \, \beta_0 = 0.$$

$$\mathbf{2} \ \alpha_k = \frac{\boldsymbol{p}_k^T \boldsymbol{r}_k}{\boldsymbol{p}_k^T \boldsymbol{A} \boldsymbol{p}_k}$$

$$\mathbf{3} \ \mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k$$

6 Goto 1

Note: As in the steepest descent method, the main cost of the iteration is the matrix-vector multiply Ap_k . It should only be computed once per iteration!

Conjugate gradient method

Remarks:

• The span of p_k satisfies

$$\operatorname{span}\{\boldsymbol{p}_0,\boldsymbol{p}_1,\boldsymbol{p}_2,\ldots,\boldsymbol{p}_k\}=\operatorname{span}\{\boldsymbol{b},A\boldsymbol{b},A^2\boldsymbol{b},\ldots,A^k\boldsymbol{b}\},$$

which is called a Krylov space, denoted by $\mathcal{K}(b, A, k)$.

• x_k in each iteration minimizes the "A-norm" of the error,

$$||\boldsymbol{x}-\boldsymbol{x}^*||_A^2 =: (\boldsymbol{x}-\boldsymbol{x}^*)^T A (\boldsymbol{x}-\boldsymbol{x}^*), \qquad (A\boldsymbol{x}^* = \boldsymbol{b} \text{ here}),$$

over all vectors in $\mathcal{K}(b, A, k)$. (Note $||\cdot||_A$ is a norm since A is symmetric positive definite.)

- CG converges in at most N iterations. (Although this is seldom of practical use.)
- Convergence for CG is much faster than for SD.
- Like SD, convergence is slower for matrices with large condition numbers $\kappa(A)$.
- $\phi(\mathbf{x}_{k+1}) < \phi(\mathbf{x}_k)$, for both SD and CG.
- Keep in mind: SD and CG only work for symmetric positive definite matrices.

- GMRES is a Krylov method for non-symmetric A.
- \mathbf{x}_k minimizes $||A\mathbf{x}_k \mathbf{b}||$ over all vectors in $\mathcal{K}(b, A, k)$.
- Implementation and algorithm much more complicated than CG. E.g. p_k depends on all previous p_i , $j \le k$.
- Algorithm builds an orthonormal basis for $\mathcal{K}(b, A, k)$ via modified Gram-Schmidt (Arnoldi) in each iteration.
- Matlab commands:

```
>> pcg(A,b);
>> gmres(A,b);
```

+ many other arguments and options possible

- Multigrid is an iterative method tailored for discretizations of elliptic PDEs (primarily).
- Solves PDE on different grid sizes N, N/2, N/4, ... and uses differences between numerical solutions to eliminate coarse scale errors.
- Uses simple stationary methods (e.g. Jacobi) to eliminiate fine scale errors.
- Highly efficient.

Computational costs

To achieve a certain given accuracy, the costs can be divided as $computational\ cost = cost/iteration\ \times\ \#\ iterations\ needed.$

Cost/iteration

We suppose $A \in \mathbb{R}^{N \times N}$ is sparse with O(N) non-zero elements. (Typical for PDE discretizations.) Then

Stationary methods

$$Mx_{k+1} = Tx_k + b,$$
 $A = M - T.$

Since A sparse, then so is M and T, and the cost of Tx_k is O(N). If also Mx = f can be solved in O(N) time (as it can for Jacobi and Gauss–Seidel), then cost/iteration is O(N).

Search methods
 Main cost is the matrix-vector mulitply Ap_k which costs O(N).

Conclusion: Cost/iteration is O(N). This is true for any sparsity pattern with O(N) non-zero elements, not just banded matrices.

Convergence rate

• For the methods discussed one can derive convergence estimates of the type, that if $A\mathbf{x}^* = \mathbf{b}$, then

$$||\boldsymbol{x}_k - \boldsymbol{x}^*|| \le C\beta^k ||\boldsymbol{x}_0 - \boldsymbol{x}^*||,$$

for some norm, constant C and $0 < \beta < 1$ called the convergence rate. It depends on A and on the method.

• Smaller β gives faster convergence. Often $\beta = 1 - \delta$ with $\delta \ll 1$ however.

Convergence rate

Stationary methods

We can write the stationary methods in concise form as

$$x_{k+1} = Rx_k + c,$$
 $R = M^{-1}T,$ $c = M^{-1}b.$

• Since $\mathbf{x}^* = R\mathbf{x}^* + \mathbf{c}$ we get

$$\mathbf{x}_k - \mathbf{x}^* = R\mathbf{x}_{k-1} + \mathbf{c} - R\mathbf{x}^* - \mathbf{c} = R(\mathbf{x}_{k-1} - \mathbf{x}^*) = R^k(\mathbf{x}_0 - \mathbf{x}^*)$$

And therefore,

$$||\mathbf{x}_k - \mathbf{x}^*|| \le ||R^k|| ||\mathbf{x}_0 - \mathbf{x}^*||.$$

Finally, if R can be diagonalized, then

$$||R^k|| \le \rho(R)^k$$

where $\rho(R)$ is the spectral radius of R.

- We conclude that one can take $\beta = \rho(R)$, if R can be diagonalized.
- In stationary methods, the convergence rate thus depends on the structure of *M* and *T* in a complicated way.

Convergence rate

Search methods

- In search methods β depends on the condition number κ of the matrix A.
- For steepest descent,

$$\beta = 1 - \frac{1}{\kappa}.$$

For conjugate gradient,

$$eta = 1 - rac{1}{\sqrt{\kappa}} \qquad \Big(ext{ which is } < 1 - rac{1}{\kappa} ext{ for } \kappa ext{ large} \Big)$$

 Well-conditioned matrices A give faster convergence for search methods.

Convergence rate vs # iterations needed

Suppose we want an error $\leq \varepsilon$ and $\beta = 1 - \delta$ with $0 < \delta \ll 1$. How many iterations are then needed?

• We need to find the number of iterations $m\ddot{i}$ 2/2such that

$$||\boldsymbol{x}_m - \boldsymbol{x}^*|| \leq C\beta^m \underbrace{||\boldsymbol{x}_0 - \boldsymbol{x}^*||}_{\boldsymbol{a}_2} \leq \varepsilon.$$

This will be satisfied when

$$m \ln(\beta) \leq \ln\left(\frac{\varepsilon}{Ce_0}\right) \quad \Rightarrow \quad m |\ln(\beta)| \geq \left|\ln\left(\frac{\varepsilon}{Ce_0}\right)\right| \quad \Rightarrow \quad m \geq \frac{D}{|\ln(\beta)|},$$

where $D = |\ln(\varepsilon/(Ce_0))|$ only depends on e_0 and ε .

• Since $\delta \ll 1$,

$$ln(\beta) = ln(1 - \delta) \approx -\delta.$$

Consequently, we need, roughly,

$$m \approx \frac{D}{\delta}$$
 iterations.

• Small δ means more iterations m needed. Precise number also depends on initial error e_0 and tolerance ε .

Computational costs

In summary, to achieve a certain given accuracy, we have ${\it computational\ cost} = {\it cost/iteration}\ \times\ \# \ iterations\ needed.$

• Assuming that the number of non-zero entries in A is O(N), then

$$Cost = O(Nm) = O(N/\delta),$$

where *m* is the number iterations needed and $\beta = 1 - \delta$.

• For stationary methods $\beta = \rho(R)$, so $\delta = 1 - \rho(R)$. This gives

$$Cost=O\left(\frac{N}{1-\rho(R)}\right).$$

• For steepest descent, $\delta = 1/\kappa$. This gives

$$Cost=O(N\kappa)$$
.

• For conjugate gradient, $\delta = 1/\sqrt{\kappa}$. This gives

Cost=
$$O(N\sqrt{\kappa})$$
.

(Also true for GMRES when A close to normal.)

Costs of solving Poisson equation

Consider a finite difference discretization of

$$-\Delta u = f$$
,

in *d* dimensions. This leads to a matrix equation

$$Au = f, \qquad A \in \mathbb{R}^{N \times N}.$$

Suppose discretization has n grid points in each coordinate direction. For direct methods we saw before that

Dimension	Unknowns (N)	Bandwidth (p)	Cost ($\sim Np^2$)
1	n	1	<i>O</i> (<i>n</i>)
2	n ²	n	$O(n^4)$
3	n ³	n ²	$O(n^7)$

Remark: Direct methods can sometimes be improved if problem is highly structured (square, constant coefficients, ...). E.g. d=2 can be solved in $O(n^3)$ i ¿½or even $O(n^2 \log n)$ time.

Costs of solving Poisson equation

For iterative methods we have when Ax = b comes from a finite difference discretization of Poisson:

- For Jacobi, Gauss–Seidel: $\rho(R) \sim 1 1/n^2$ (Can be derived from discretization.)
- Condition number $\kappa \sim h^{-2}$, where h = O(1/n), for all d. (We derived this in one dimension when we talked about elliptic equations.)
- Multigrid (MG): $\beta \leq \beta_0 < 1$ independent of N.

	δ	$m\sim 1/\delta$	$cost (Nm = n^d m)$
Jacobi	1/ <i>n</i> ²	n ²	n ^{d+2}
Gauss-Seidel	1/ <i>n</i> ²	n ²	n ^{d+2}
SD	$1/\kappa \sim 1/n^2$	n ²	n ^{d+2}
CG	$1/\sqrt{\kappa}\sim 1/n$	n	n ^{d+1}
GMRES	$1/\sqrt{\kappa}\sim 1/n$	n	n^{d+1}
Multigrid	O(1)	1	n ^d

Costs of solving Poisson equation

In summary, we have the following costs for solving the Poisson equation with finite differences in 1D, 2D and 3D.

Dimension	Direct method	Jacobi/GS/SD	CG/GMRES	MG
1	n	n ³	n ²	n
2	n ⁴	n ⁴	n ³	n ²
3	n ⁷	n ⁵	n ⁴	n ³

- Little or no gain from iterative methods in 1D, compared to direct methods.
- Large gains in 3D.
- Unclear gains in 2D.
- Multigrid superior to the other methods.
- Jacobi/GS/SD not competetive. Mostly used as components in Multigrid or as "preconditioners".

Preconditioning

For CG and GMRES the convergence rate is in general

$$\beta = 1 - \frac{1}{\sqrt{\kappa}} \quad \Rightarrow \quad m \sim \sqrt{\kappa}.$$

Slow convergence therefore for ill-conditioned matrices.

- Preconditioning can be used to lower κ .
- Idea:

Replace $A\mathbf{x} = \mathbf{b}$ by equivalent system $M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$, where

- (a) $\kappa(M^{-1}A)$ smaller than $\kappa(A)$
- (b) Mx = y is easy to solve

Then iterate with CG/GMRES on $M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$ instead of $A\mathbf{x} = \mathbf{b}$.

- \Rightarrow Faster convergence.
- Note that (a) and (b) are conflicting goals. Best for (a) is to take M=A, which gives $\kappa=1$, but then (b) is not satisfied. Best for (b) is to take M=I, but then κ does not change. Find good trade-off!

Preconditioning

The preconditioner *M* can be quite simple and still help. Some examples:

- M = diagonal part of A (similar to one step with Jacobi, with $x_0 = 0$).
- Multiple steps with Jacobi or Gauss-Seidel.
- Incomplete LU- or Cholesky factorizations.
- Good choice highly problem dependent.

Preconditioned Conjugate Gradient (PCG)

- Need extra trick to precondition conjugate gradient since $M^{-1}A$ is in general not symmetric positive definite (SPD) even if both M and A are.
- Let M be SPD and set $C = M^{1/2}$, i.e. an SPD matrix such that $C^2 = M$. (Such C exists.)
- Then $C^{-1}AC^{-1}$ is also SPD and since

$$A\mathbf{x} = \mathbf{b} \quad \Rightarrow \quad C^{-1}AC^{-1}C\mathbf{x} = C^{-1}\mathbf{b}$$

we can apply conjugate gradient to the SPD system

$$C^{-1}AC^{-1}\tilde{\mathbf{x}}=\tilde{\mathbf{b}}, \qquad C\mathbf{x}=\tilde{\mathbf{x}}, \quad C\tilde{\mathbf{b}}=\mathbf{b},$$

instead.

• This only changes CG very little in the end. (Main change: In each iteration an additional system $M\mathbf{z}_k = \mathbf{r}_k$ must be solved.)

Incomplete LU/Cholesky factorization

- Perform standard LU/Cholesky (via gaussian elimination) but let elements of L and U be zero whenever corresponding element of A is zero ($\ell_{j,k} = u_{j,k} = 0$ if $a_{j,k} = 0$).
- Gives approximate factors \tilde{L} and \tilde{U} with $\tilde{L}\tilde{U}\approx A$ for LU and $\tilde{L}\tilde{L}^T\approx A$ for Cholesky.
- In Matlab: [L,U]=ilu(A) and L=ichol(A)
- Cost = O(N) if there is a fixed number of non-zeros in each row and column.
- Use $M = \tilde{L}\tilde{U}$ and $M = \tilde{L}\tilde{L}^T$ as preconditioners. Then $M\mathbf{x} = \mathbf{y}$ can easily be solved in O(N) time.
- In Matlab, call pcg and gmres as

```
>> pcg(A,b,tol,maxiter,M); (if M is preconditioner)
>> pcg(A,b,tol,maxiter,L,L'); (if LL<sup>T</sup> is preconditioner)
>> gmres(A,b,tol,maxiter,M); (if M is preconditioner)
>> gmres(A,b,tol,maxiter,L,U); (if LU is preconditioner)
```