

Numerical Methods I

Non-Square and Sparse Linear Systems

Aleksandar Donev

*Courant Institute, NYU*¹

donev@courant.nyu.edu

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Outline

Homework 1 is due tomorrow, Friday Sept. 19th:

go through instructions in class.

Homework 2 (linear systems) is posted online.

1 Overdetermined Linear Systems

2 Sparse Matrices

3 Iterative Methods

4 Conclusions

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

- The most appropriate algorithm really depends on the properties of the matrix \mathbf{A} :
 - General **dense matrices**, where the entries in \mathbf{A} are mostly non-zero and nothing special is known: Use LU factorization.
 - **Symmetric** ($a_{ij} = a_{ji}$) and also **positive-definite** matrices.
 - General **sparse matrices**, where only a small fraction of $a_{ij} \neq 0$.
 - Special **structured sparse matrices**, arising from specific physical properties of the underlying system.
- It is also important to consider **how many times** a linear system with the same or related matrix or right hand side needs to be solved.

Non-Square Matrices

- In the case of **over-determined** (more equations than unknowns) or **under-determined** (more unknowns than equations), the solution to linear systems in general becomes **non-unique**.
- One must first define what is meant by a solution, and the common definition is to use a **least-squares formulation**:

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{Ax} - \mathbf{b}\| = \arg \min_{\mathbf{x} \in \mathbb{R}^n} \Phi(\mathbf{x})$$

where the choice of the L_2 norm leads to:

$$\Phi(\mathbf{x}) = (\mathbf{Ax} - \mathbf{b})^T (\mathbf{Ax} - \mathbf{b}).$$

- Over-determined systems, $m > n$, can be thought of as **fitting a linear model (linear regression)**:
The unknowns \mathbf{x} are the coefficients in the fit, the input data is in \mathbf{A} (one column per measurement), and the output data (observables) are in \mathbf{b} .

Normal Equations

- It can be shown that the least-squares solution satisfies:

$$\nabla \Phi(\mathbf{x}) = \mathbf{A}^T [2(\mathbf{A}\mathbf{x} - \mathbf{b})] = \mathbf{0} \text{ (critical point)}$$

- This gives the square linear system of **normal equations**

$$(\mathbf{A}^T \mathbf{A}) \mathbf{x}^* = \mathbf{A}^T \mathbf{b}.$$

- If \mathbf{A} is of full rank, $\text{rank}(\mathbf{A}) = n$, it can be shown that $\mathbf{A}^T \mathbf{A}$ is positive definite, and Cholesky factorization can be used to solve the normal equations.
- Multiplying \mathbf{A}^T ($n \times m$) and \mathbf{A} ($m \times n$) takes n^2 dot-products of length m , so $O(mn^2)$ operations

Problems with the normal equations

$$(\mathbf{A}^T \mathbf{A}) \mathbf{x}^* = \mathbf{A}^T \mathbf{b}.$$

- The conditioning number of the normal equations is

$$\kappa(\mathbf{A}^T \mathbf{A}) = [\kappa(\mathbf{A})]^2$$

- Furthermore, roundoff can cause $\mathbf{A}^T \mathbf{A}$ to no longer appear as positive-definite and the Cholesky factorization will fail.
- If the normal equations are ill-conditioned, another approach is needed.

The QR factorization

- For nonsquare or ill-conditioned matrices of **full-rank** $r = n \leq m$, the LU factorization can be replaced by the QR factorization:

$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

$$[m \times n] = [m \times n][n \times n]$$

where \mathbf{Q} has **orthogonal columns**, $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}_n$, and \mathbf{R} is a **non-singular upper triangular** matrix.

- Observe that orthogonal / unitary matrices are **well-conditioned** ($\kappa_2 = 1$), so the QR factorization is numerically better (but also more expensive!) than the LU factorization.
- For matrices **not of full rank** there are modified QR factorizations but **the SVD decomposition is better** (next class).
- In MATLAB, the QR factorization can be computed using `qr` (with column pivoting).

Solving Linear Systems via QR factorization

$$(\mathbf{A}^T \mathbf{A}) \mathbf{x}^* = \mathbf{A}^T \mathbf{b} \text{ where } \mathbf{A} = \mathbf{Q} \mathbf{R}$$

- Observe that \mathbf{R} is the Cholesky factor of the matrix in the normal equations:

$$\mathbf{A}^T \mathbf{A} = \mathbf{R}^T (\mathbf{Q}^T \mathbf{Q}) \mathbf{R} = \mathbf{R}^T \mathbf{R}$$

$$(\mathbf{R}^T \mathbf{R}) \mathbf{x}^* = (\mathbf{R}^T \mathbf{Q}^T) \mathbf{b} \Rightarrow \mathbf{x}^* = \mathbf{R}^{-1} (\mathbf{Q}^T \mathbf{b})$$

which amounts to solving a triangular system with matrix \mathbf{R} .

- This calculation turns out to be much **more numerically stable** against roundoff than forming the normal equations (and has similar cost).

Undetermined Linear Systems

- Sometimes the solution to the least-squares is still **not unique**:
 - **Under-determined** systems (not enough equations to fix all unknowns)
 - Singular systems, i.e., \mathbf{A} that is **not of full rank** (use SVD):
Any solution to $\mathbf{Ax}_0 = \mathbf{0}$ can be added to \mathbf{x} without changing the left hand side!
- Additional condition: Choose the \mathbf{x}^* that has **minimal Euclidean norm**, i.e., use a least-squares definition:

$$\min_{\mathbf{Ax}=\mathbf{b}} \|\mathbf{x}\|_2,$$

although more recently of great importance are solutions that minimize the L_1 norm (**compressed sensing**).

- For **under-determined full-rank** systems, $r = m \leq n$, one does a QR factorization of $\mathbf{A}^T = \tilde{\mathbf{Q}}\tilde{\mathbf{R}}$ and the least-squares solution is

$$\mathbf{x}^* = \tilde{\mathbf{Q}} \left(\tilde{\mathbf{R}}^{-T} \mathbf{b} \right)$$

Practice: Derive the above formula.

Computing the QR Factorization

- Assume that

$$\exists \mathbf{x} \text{ s.t. } \mathbf{b} = \mathbf{A}\mathbf{x}, \text{ that is, } \mathbf{b} \in \text{range}(\mathbf{A})$$

$$\mathbf{b} = \mathbf{Q}(\mathbf{R}\mathbf{x}) = \mathbf{Q}\mathbf{y} \Rightarrow \mathbf{x} = \mathbf{R}^{-1}\mathbf{y}$$

showing that the columns of \mathbf{Q} form an **orthonormal basis** for the range of \mathbf{A} (linear subspace spanned by the columns of \mathbf{A}).

- The QR factorization is thus closely-related to the **orthogonalization** of a set of n vectors (columns) $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\}$ in \mathbb{R}^m .
- Classical approach is the **Gram-Schmidt method**: To make a vector \mathbf{b} orthogonal to \mathbf{a} do:

$$\tilde{\mathbf{b}} = \mathbf{b} - (\mathbf{b} \cdot \mathbf{a}) \frac{\mathbf{a}}{(\mathbf{a} \cdot \mathbf{a})}$$

Practice: Verify that $\tilde{\mathbf{b}} \cdot \mathbf{a} = 0$

- Repeat this in sequence: Start with $\tilde{\mathbf{a}}_1 = \mathbf{a}_1$, then make $\tilde{\mathbf{a}}_2$ orthogonal to $\tilde{\mathbf{a}}_1 = \mathbf{a}_1$, then make $\tilde{\mathbf{a}}_3$ orthogonal to $\text{span}(\tilde{\mathbf{a}}_1, \tilde{\mathbf{a}}_2) = \text{span}(\mathbf{a}_1, \mathbf{a}_2)$.

Modified Gram-Schmidt Orthogonalization

- More efficient formula (**standard Gram-Schmidt**):

$$\tilde{\mathbf{a}}_{k+1} = \mathbf{a}_{k+1} - \sum_{j=1}^k (\mathbf{a}_{k+1} \cdot \mathbf{q}_j) \mathbf{q}_j, \quad \mathbf{q}_{k+1} = \frac{\tilde{\mathbf{a}}_{k+1}}{\|\tilde{\mathbf{a}}_{k+1}\|},$$

with cost $\sim mn^2$ FLOPS.

- A mathematically-equivalent but numerically much superior **against roundoff error** is the **modified Gram-Schmidt**, in which each **orthogonalization** is carried in sequence and **repeated** against each of the already-computed basis vectors:

Start with $\tilde{\mathbf{a}}_1 = \mathbf{a}_1$, then make $\tilde{\mathbf{a}}_2$ orthogonal to $\tilde{\mathbf{a}}_1$, then make $\tilde{\mathbf{a}}_3$ orthogonal to $\tilde{\mathbf{a}}_1$ and **then make the result orthogonal to $\tilde{\mathbf{a}}_2$** .

- The modified procedure is **twice more expensive**, $\sim 2mn^2$ FLOPS, but usually **worth it**.
- Pivoting** is strictly necessary for matrices not of full rank but it can also improve stability in general.

Sparse Matrices

- A matrix where a substantial fraction of the entries are zero is called a **sparse matrix**. The difference with **dense matrices** is that only the nonzero entries are stored in computer memory.
- Exploiting sparsity is important for **large matrices** (what is large depends on the computer).
- The structure of a sparse matrix refers to the set of indices i, j such that $a_{ij} > 0$, and is visualized in MATLAB using `spy`.
- The structure of sparse matrices comes from the nature of the problem, e.g., in an inter-city road transportation problem it corresponds to the pairs of cities connected by a road.
- In fact, just counting the number of nonzero elements is not enough: the **sparsity structure** is the most important property that determines the best method.

Banded Matrices

- **Banded matrices** are a very special but common type of sparse matrix, e.g., **tridiagonal matrices**

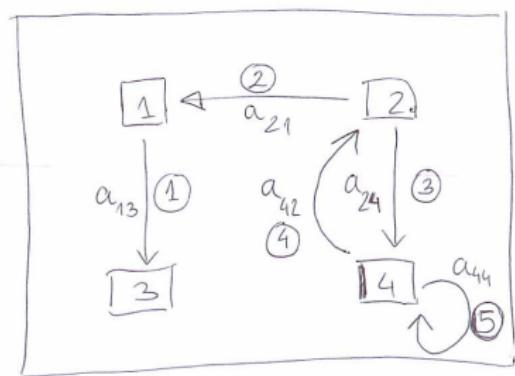
$$\begin{bmatrix} a_1 & c_1 & & \mathbf{0} \\ b_2 & a_2 & \ddots & \\ \ddots & \ddots & c_{n-1} & \\ \mathbf{0} & & b_n & a_n \end{bmatrix}$$

- There exist special techniques for banded matrices that are much faster than the general case, e.g, only $8n$ FLOPS and no additional memory for tridiagonal matrices.
- A general matrix should be considered sparse if it has sufficiently many zeros that exploiting that fact is advantageous: usually only the case for **large matrices** (what is large?)!

Sparse Matrices

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 5 \end{bmatrix} \quad \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} \quad \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix}$$

Sparse matrix



← DIRECTED
Graph
representation :

→ NODES (VERTICES) are variables
or equations

→ ARCS (EDGES) are
the non-zeros

UNDIRECTED GRAPH FOR
SYMMETRIC MATRICES

①

Fill-In

- There are general techniques for dealing with sparse matrices such as **sparse LU factorization**. How well they work depends on the structure of the matrix.
- When factorizing sparse matrices, the factors, e.g., **L** and **U**, can be much less sparse than **A**: **fill-in**.
- Pivoting (**reordering** of variables and equations) has a dual, sometimes conflicting goal:
 - ① Reduce fill-in, i.e., **improve memory use**.
 - ② Reduce roundoff error, i.e., **improve stability**. Typically some **threshold pivoting** is used only when needed.
- For many sparse matrices there is a large fill-in and **iterative methods** are required.

Sparse matrices in MATLAB

```
>> A = sparse( [1 2 2 4 4], [3 1 4 2 3], 1:5 )
A =
(2,1)      2
(4,2)      4
(1,3)      1
(4,3)      5
(2,4)      3
>> nnz(A)
ans =      5
>> whos A
  A            4x4            120    double    sparse
>> A = sparse( [],[],[],4,4,5); % Pre-allocate memory
>> A(2,1)=2; A(4,2)=4; A(1,3)=1; A(4,3)=5; A(2,4)=3;
```

Sparse matrix factorization

```
>> B=sprand(4,4,0.25); % Density of 25%
>> full(B)
```

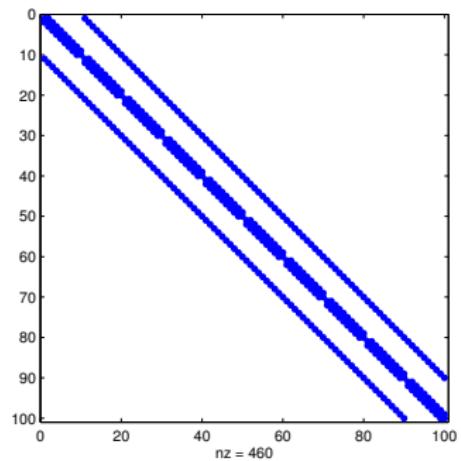
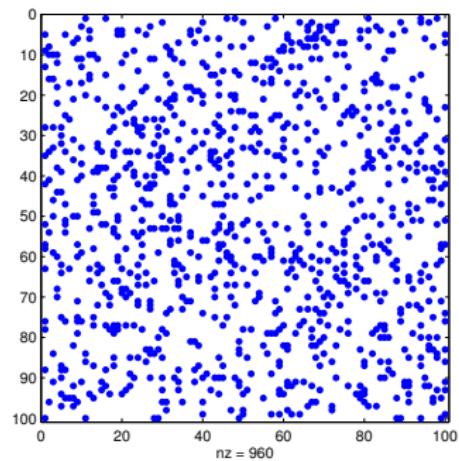
ans =

0	0	0	0.7655
0	0.7952	0	0
0	0.1869	0	0
0.4898	0	0	0

```
>> B=sprand(100,100,0.1); spy(B)
>> X=gallery('poisson',10); spy(X)
>> [L,U,P]=lu(B); spy(L)
>> p = symrcm(B); % Symmetric Reverse Cuthill-McKee or
>> PBP=B(p,p); spy(PBP);
>> [L,U,P]=lu(PBP); spy(L);
```

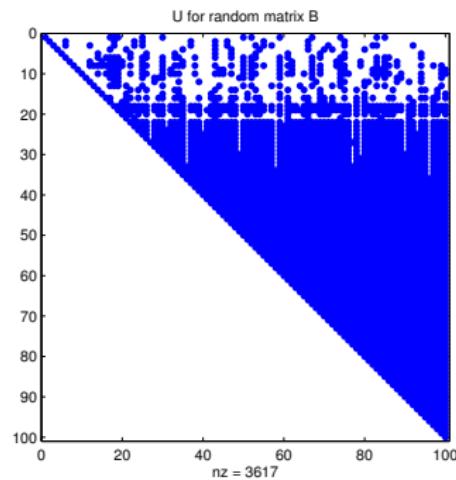
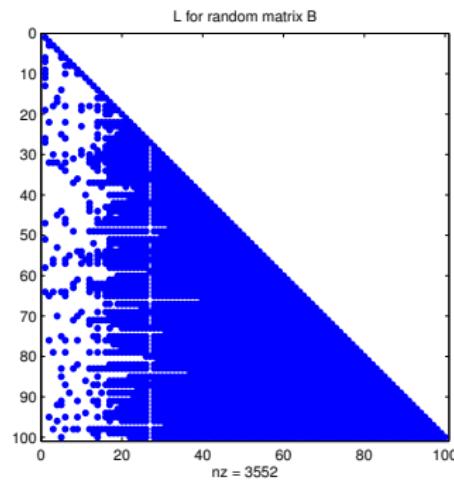
Random matrix **B** and structured matrix **X**

The MATLAB function *spy* shows where the nonzeros are as a plot



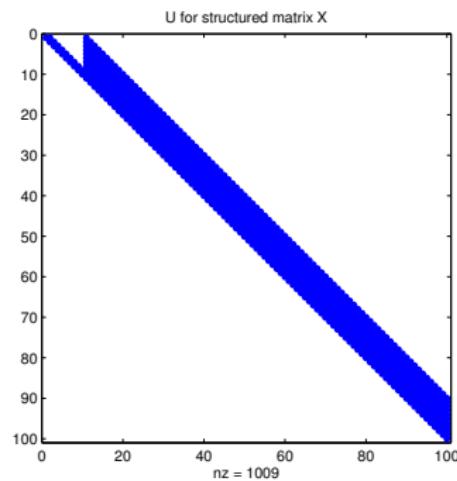
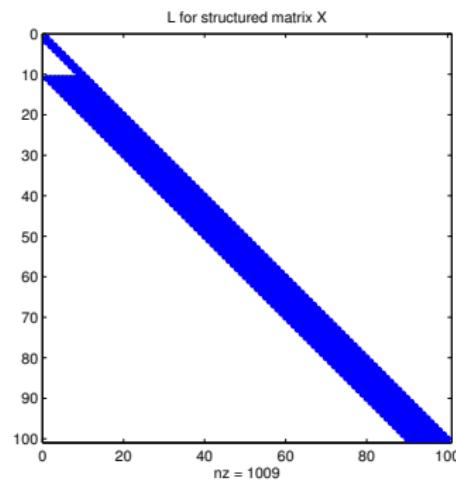
LU factors of random matrix B

Fill-in (generation of lots of nonzeros) is large for a random sparse matrix



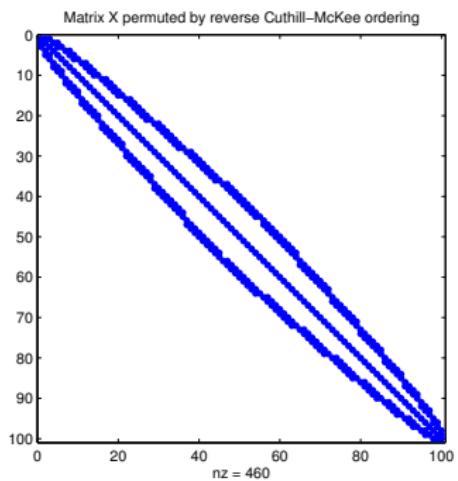
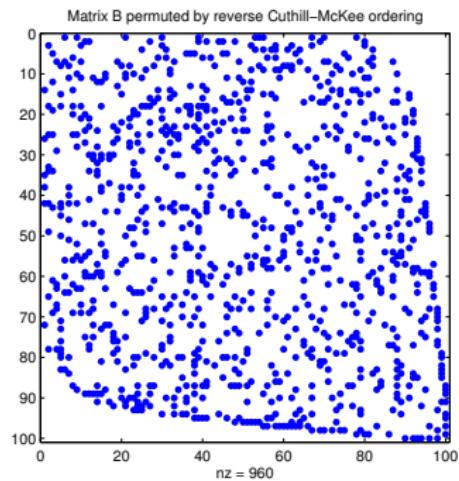
LU factors of structured matrix X

Fill-in is much smaller for the sparse matrix but still non-negligible.



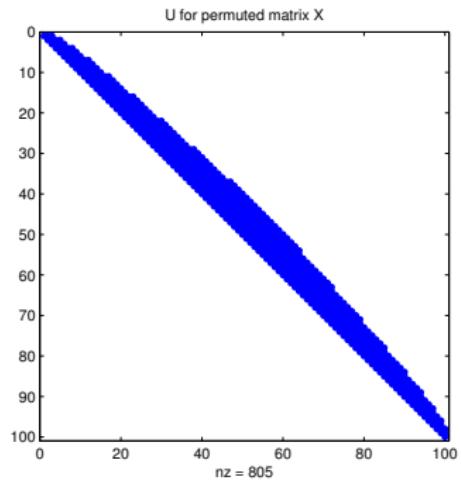
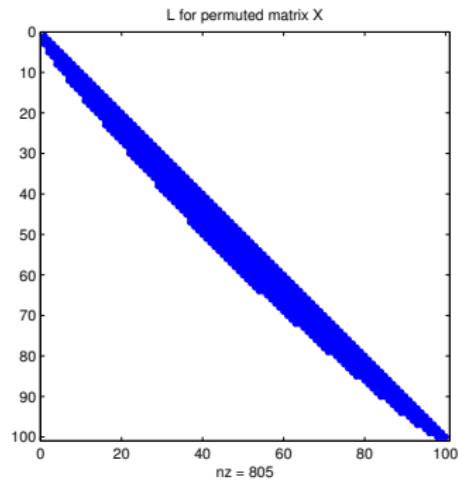
Matrix reordering

Matrix reordering cannot do much for the random matrix \mathbf{B} , but it can help for structured ones!



Reducing fill-in by reordering \mathbf{X}

Fill-in was reduced by about 20% (from 1000 nonzeros to 800) by the reordering for the structured \mathbf{X} , but does not help much for \mathbf{B} .
The actual numbers are different for different classes of matrices!



Importance of Sparse Matrix Structure

- Important to remember: While there are general techniques for dealing with sparse matrices that help greatly, it all depends on the structure (origin) of the matrix.
- Pivoting has a dual, sometimes conflicting goal:
 - ① Reduce fill-in, i.e., **improve memory use**: *Still active subject of research!*
 - ② Reduce roundoff error, i.e., **improve stability**. Typically some **threshold pivoting** is used only when needed.
- Pivoting for symmetric non-positive definite matrices is trickier: One can permute the diagonal entries only to **preserve symmetry**, but small diagonal entries require special treatment.
- For many sparse matrices **iterative methods** (briefly covered next lecture) are required to large fill-in.

Why iterative methods?

- Direct solvers are great for dense matrices and can be made to avoid roundoff errors to a large degree. They can also be implemented very well on modern machines.
- **Fill-in** is a major problem for certain sparse matrices and leads to extreme memory requirements (e.g., three-d).
- Some matrices appearing in practice are **too large** to even be represented explicitly (e.g., the Google matrix).
- Often linear systems only need to be **solved approximately**, for example, the linear system itself may be a linear approximation to a nonlinear problem.
- Direct solvers are much harder to implement and use on (massively) **parallel computers**.

Stationary Linear Iterative Methods of First Order

- In iterative methods the core computation is **iterative matrix-vector multiplication** starting from an **initial guess** $\mathbf{x}^{(0)}$.
- Prototype is the **linear recursion**:

$$\mathbf{x}^{(k+1)} = \mathbf{B}\mathbf{x}^{(k)} + \mathbf{f},$$

where \mathbf{B} is an **iteration matrix** somehow related to \mathbf{A} .

- For this method to be **consistent**, we must have that the actual solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ is a **stationary point** of the iteration:

$$\mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{f} \quad \Rightarrow \quad \mathbf{A}^{-1}\mathbf{b} = \mathbf{B}\mathbf{A}^{-1}\mathbf{b} + \mathbf{f}$$

$$\mathbf{f} = \mathbf{A}^{-1}\mathbf{b} - \mathbf{B}\mathbf{A}^{-1}\mathbf{b} = (\mathbf{I} - \mathbf{B})\mathbf{x}$$

- For this method to be **stable**, and thus **convergent**, the error $\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}$ must decrease:

$$\mathbf{e}^{(k+1)} = \mathbf{x}^{(k+1)} - \mathbf{x} = \mathbf{B}\mathbf{x}^{(k)} + \mathbf{f} - \mathbf{x} = \mathbf{B}(\mathbf{x} + \mathbf{e}^{(k)}) + (\mathbf{I} - \mathbf{B})\mathbf{x} - \mathbf{x} = \mathbf{B}\mathbf{e}^{(k)}$$

Convergence of simple iterative methods

- We saw that the error propagates from iteration to iteration as

$$\mathbf{e}^{(k)} = \mathbf{B}^k \mathbf{e}^{(0)}.$$

- When does this converge? Taking norms,

$$\|\mathbf{e}^{(k)}\| \leq \|\mathbf{B}\|^k \|\mathbf{e}^{(0)}\|$$

which means that $\|\mathbf{B}\| < 1$ is a **sufficient condition** for convergence.

- More precisely, $\lim_{k \rightarrow \infty} \mathbf{e}^{(k)} = \mathbf{0}$ for any $\mathbf{e}^{(0)}$ iff $\mathbf{B}^k \rightarrow \mathbf{0}$.
- Theorem: The method converges iff the **spectral radius** of the iteration matrix is less than unity:

$$\rho(\mathbf{B}) < 1.$$

Spectral Radius

- The **spectral radius** $\rho(\mathbf{A})$ of a matrix \mathbf{A} can be thought of as the smallest consistent matrix norm

$$\rho(\mathbf{A}) = \max_{\lambda} |\lambda| \leq \|\mathbf{A}\|$$

- The spectral radius often **determines convergence of iterative schemes** for linear systems and eigenvalues and even methods for solving PDEs because it estimates the asymptotic rate of error propagation:

$$\rho(\mathbf{A}) = \lim_{k \rightarrow \infty} \|\mathbf{A}^k\|^{1/k}$$

Termination

- The iterations of an iterative method can be terminated when:
 - ➊ The **residual** becomes small,

$$\| \mathbf{r}^{(k)} \| \leq \varepsilon \| \mathbf{b} \|$$

This is good for well-conditioned systems.

- ➋ The solution $\mathbf{x}^{(k)}$ stops changing, i.e., the **increment** becomes small,

$$[1 - \rho(\mathbf{B})] \| \mathbf{e}^{(k)} \| \leq \| \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} \| \leq \varepsilon \| \mathbf{b} \|,$$

which can be seen to be good if convergence is rapid, $\rho(\mathbf{B}) \ll 1$.

- Usually a careful **combination** of the two strategies is employed along with some **safeguards**.

Fixed-Point Iteration

- A naive but often successful method for solving

$$x = f(x)$$

is the **fixed-point iteration**

$$x_{n+1} = f(x_n).$$

- In the case of a linear system, consider rewriting $\mathbf{Ax} = \mathbf{b}$ as:

$$\mathbf{x} = (\mathbf{I} - \mathbf{A})\mathbf{x} + \mathbf{b}$$

- Fixed-point iteration gives the consistent iterative method

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{(k)} + \mathbf{b}$$

Preconditioning

- The above method is consistent but it may not converge or may converge very slowly

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \mathbf{A}) \mathbf{x}^{(k)} + \mathbf{b}.$$

- As a way to speed it up, consider having a **good approximate solver**

$$\mathbf{P}^{-1} \approx \mathbf{A}^{-1}$$

called the **preconditioner** (\mathbf{P} is the preconditioning matrix), and transform

$$\mathbf{P}^{-1} \mathbf{A} \mathbf{x} = \mathbf{P}^{-1} \mathbf{b}$$

- Now apply fixed-point iteration to this modified system:

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \mathbf{P}^{-1} \mathbf{A}) \mathbf{x}^{(k)} + \mathbf{P}^{-1} \mathbf{b},$$

which now has an iteration matrix $\mathbf{I} - \mathbf{P}^{-1} \mathbf{A} \approx \mathbf{0}$, which means more **rapid convergence**.

Preconditioned Iteration

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \mathbf{P}^{-1} \mathbf{A}) \mathbf{x}^{(k)} + \mathbf{P}^{-1} \mathbf{b}$$

- In practice, we solve linear systems with the matrix \mathbf{P} instead of inverting it:

$$\mathbf{P}\mathbf{x}^{(k+1)} = (\mathbf{P} - \mathbf{A})\mathbf{x}^{(k)} + \mathbf{b} = \mathbf{P}\mathbf{x}^{(k)} + \mathbf{r}^{(k)},$$

where $\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(k)}$ is the **residual vector**.

- Finally, we obtain the usual form of a **preconditioned stationary iterative solver**

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{P}^{-1} \mathbf{r}^{(k)}.$$

- Note that convergence will be faster if we have a **good initial guess** $\mathbf{x}^{(0)}$.

Some Standard Examples

$$\text{Splitting: } \mathbf{A} = \mathbf{L}_A + \mathbf{U}_A + \mathbf{D}$$

- Since diagonal systems are trivial to solve, we can use the **Jacobi method**

$$\mathbf{P} = \mathbf{D}.$$

- Or since triangular systems are easy to solve by forward/backward substitution, we can use **Gauss-Seidel method**

$$\mathbf{P} = \mathbf{L}_A + \mathbf{D}.$$

- Both of these converge for strictly **diagonally-dominant matrices**.
- Gauss-Seidel converges for **positive-definite matrices** (maybe slowly though!).

A Good Preconditioner

- Note that the matrix \mathbf{A} is only used when calculating the residual through the **matrix-vector product** $\mathbf{Ax}^{(k)}$.
- We must be able to do a **direct** linear solver for the preconditioner

$$\mathbf{P}(\Delta \mathbf{x}) = \mathbf{r}^{(k)},$$

so it must be in some sense simpler to deal with than \mathbf{A} .

- Preconditioning is all about a **balance between fewer iterations to convergence and larger cost per iteration**.
- Making good preconditioners is in many ways an art and very **problem-specific**:

The goal is to make $\mathbf{P}^{-1}\mathbf{A}$ as close to being a normal (diagonalizable) matrix with **clustered eigenvalues** as possible.

In the Real World

- Some general preconditioning strategies have been designed, for example, **incomplete LU factorization** (MATLAB's *cholinc*).
- There are many **more-sophisticated iterative methods** (non-stationary, higher-order, etc) but most have the same **basic structure**:

At each iteration, solve a preconditioning linear system, do a matrix-vector calculation, and a convergence test.

- For positive-(semi)definite matrices the **Preconditioned Conjugate Gradient** method is good (MATLAB's *pcg*).
- For certain types of matrices specialized methods have been designed, such as **multigrid methods** for linear systems on large grids (PDE solvers in Numerical Methods II).

Special Matrices in MATLAB

- MATLAB recognizes (i.e., tests for) some special matrices automatically: banded, permuted lower/upper triangular, symmetric, Hessenberg, but **not** sparse.
- In MATLAB one may specify a matrix \mathbf{B} instead of a single right-hand side vector \mathbf{b} .
- The MATLAB function

$$X = \text{linsolve}(A, B, \text{opts})$$

allows one to specify certain properties that speed up the solution (triangular, upper Hessenberg, symmetric, positive definite, none), and also estimates the condition number along the way.

- Use *linsolve* instead of backslash if you know (for sure!) something about your matrix.

Conclusions/Summary

- The QR factorization is a numerically-stable method for solving **full-rank non-square systems**.
- For **rank-deficient** matrices the singular value decomposition (**SVD**) is best, discussed in later lectures.
- **Sparse matrices** deserve special treatment but the details depend on the specific field of application.
- In particular, special sparse **matrix reordering** methods or iterative systems are often required.
- When **sparse direct methods** fail due to memory or other requirements, **iterative methods** are used instead.
- Convergence of iterative methods depends strongly on the matrix, and a good **preconditioner** is often required.
- There are **good libraries for iterative methods** as well (but you must supply your own preconditioner!).