Scientific Computing: Solving Linear Systems

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Outline

1. Linear Algebra Background
2. Conditioning of linear systems
3. Gauss elimination and LU factorization
4. Beyond GEM
   - Symmetric Positive-Definite Matrices
5. Overdetermined Linear Systems
6. Sparse Matrices
7. Conclusions

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Linear Spaces

- A **vector space** $\mathcal{V}$ is a set of elements called **vectors** $\mathbf{x} \in \mathcal{V}$ that may be multiplied by a **scalar** c and added, e.g.,

$$\mathbf{z} = \alpha \mathbf{x} + \beta \mathbf{y}$$

- I will denote scalars with lowercase letters and vectors with lowercase bold letters.
- Prominent examples of vector spaces are $\mathbb{R}^n$ (or more generally $\mathbb{C}^n$), but there are many others, for example, the set of polynomials in x.
- A **subspace** $\mathcal{V}' \subseteq \mathcal{V}$ of a vector space is a subset such that sums and multiples of elements of $\mathcal{V}'$ remain in $\mathcal{V}'$ (i.e., it is closed).
- An example is the set of vectors in $x \in \mathbb{R}^3$ such that $x_3 = 0$.

Image Space

- Consider a set of n vectors $\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n \in \mathbb{R}^m$ and form a **matrix** by putting these vectors as columns

$$\mathbf{A} = [\mathbf{a}_1 \,|\, \mathbf{a}_2 \,|\, \cdots \,|\, \mathbf{a}_m] \in \mathbb{R}^{m,n}.$$

- I will denote matrices with bold capital letters, and sometimes write $\mathbf{A} = [m, n]$ to indicate dimensions.
- The **matrix-vector product** is defined as a **linear combination** of the columns:

$$\mathbf{b} = \mathbf{A}\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + \cdots + x_n\mathbf{a}_n \in \mathbb{R}^m.$$

- The **image** $\operatorname{im}(\mathbf{A})$ or **range** $\operatorname{range}(\mathbf{A})$ of a matrix is the subspace of all linear combinations of its columns, i.e., the set of all $\mathbf{b}'s$.
  It is also sometimes called the **column space** of the matrix.

Dimension

- The set of vectors $\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n$ are **linearly independent** or form a **basis** for $\mathbb{R}^m$ if $\mathbf{b} = \mathbf{A}\mathbf{x} = \mathbf{0}$ implies that $\mathbf{x} = \mathbf{0}$.
- The **dimension** $r = \dim\mathcal{V}$ of a vector (sub)space $\mathcal{V}$ is the number of elements in a basis. This is a property of $\mathcal{V}$ itself and *not* of the basis, for example,

$$\dim \mathbb{R}^n = n$$

- Given a basis $\mathbf{A}$ for a vector space $\mathcal{V}$ of dimension n, every vector of $\mathbf{b} \in \mathcal{V}$ can be uniquely represented as the vector of coefficients $\mathbf{x}$ in that particular basis,

$$\mathbf{b} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + \cdots + x_n\mathbf{a}_n.$$

- A simple and common basis for $\mathbb{R}^n$ is $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$, where $\mathbf{e}_k$ has all components zero except for a single 1 in position k.
  With this choice of basis the coefficients are simply the entries in the vector, $\mathbf{b} \equiv \mathbf{x}$.

Kernel Space

- The dimension of the column space of a matrix is called the **rank** of the matrix $\mathbf{A} \in \mathbb{R}^{m,n}$,

$$r = \operatorname{rank} \mathbf{A} \leq \min(m, n).$$

- If $r = \min(m, n)$ then the matrix is of **full rank**.
- The **nullspace** null($\mathbf{A}$) or **kernel** ker($\mathbf{A}$) of a matrix $\mathbf{A}$ is the subspace of vectors $\mathbf{x}$ for which

$$\mathbf{A}\mathbf{x} = \mathbf{0}.$$

- The dimension of the nullspace is called the **nullity** of the matrix.
- For a basis $\mathbf{A}$ the nullspace is $\text{null}(\mathbf{A}) = \{\mathbf{0}\}$ and the nullity is zero.

Orthogonal Spaces

- An inner-product space is a vector space together with an **inner or dot product**, which must satisfy some properties.
- The standard dot-product in $\mathbb{R}^n$ is denoted with several different notations:

$$\mathbf{x} \cdot \mathbf{y} = (\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^{n} x_i y_i.$$

- For $\mathbb{C}^n$ we need to add complex conjugates (here $\star$ denotes a complex conjugate transpose, or **adjoint**),

$$\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^\star \mathbf{y} = \sum_{i=1}^{n} \bar{x}_i y_i.$$

- Two vectors $\mathbf{x}$ and $\mathbf{y}$ are **orthogonal** if $\mathbf{x} \cdot \mathbf{y} = 0$.

Part I of Fundamental Theorem

- One of the most important theorems in linear algebra is that the sum of rank and nullity is equal to the number of columns: For $\mathbf{A} \in \mathbb{R}^{m,n}$

$$\operatorname{rank} \mathbf{A} + \operatorname{nullity} \mathbf{A} = n.$$

- In addition to the range and kernel spaces of a matrix, two more important vector subspaces for a given matrix $\mathbf{A}$ are the:
    - **Row space** or **coimage** of a matrix is the column (image) space of its transpose, $\operatorname{im} \mathbf{A}^T$.
      Its dimension is also equal to the the rank.
    - **Left nullspace** or **cokernel** of a matrix is the nullspace or kernel of its transpose, $\ker \mathbf{A}^T$.

Part II of Fundamental Theorem

- The **orthogonal complement** $\mathcal{V}^{\perp}$ or orthogonal subspace of a subspace $\mathcal{V}$ is the set of all vectors that are orthogonal to every vector in $\mathcal{V}$.
- Let $\mathcal{V}$ be the set of vectors in $x \in \mathbb{R}^3$ such that $x_3 = 0$. Then $\mathcal{V}^{\perp}$ is the set of all vectors with $x_1 = x_2 = 0$.
- Second fundamental theorem in linear algebra:

$$\operatorname{im} \mathbf{A}^T = (\ker \mathbf{A})^{\perp}$$

$$\ker \mathbf{A}^T = (\operatorname{im} \mathbf{A})^{\perp}$$

Linear Transformation

- A function $L:\mathcal{V}\rightarrow\mathcal{W}$ mapping from a vector space $\mathcal{V}$ to a vector space $\mathcal{W}$ is a **linear function** or a **linear transformation** if

$$L(\alpha\mathbf{v})=\alpha L(\mathbf{v})\text{ and }L(\mathbf{v}_1+\mathbf{v}_2)=L(\mathbf{v}_1)+L(\mathbf{v}_2).$$

- Any linear transformation L can be represented as a multiplication by a matrix $\mathbf{L}$

$$L(\mathbf{v})=\mathbf{L}\mathbf{v}.$$

- For the common bases of $\mathcal{V}=\mathbb{R}^n$ and $\mathcal{W}=\mathbb{R}^m$, the product $\mathbf{w}=\mathbf{L}\mathbf{v}$ is simply the usual **matix-vector product**,

$$w_i=\sum_{k=1}^{n}L_{ik}v_k,$$

which is simply the dot-product between the i-th row of the matrix and the vector $\mathbf{v}$.

Matrix algebra

$$w_i = (\mathbf{Lv})_i = \sum_{k=1}^{n} L_{ik} v_k$$

- The composition of two linear transformations $\mathbf{A} = [m, p]$ and $\mathbf{B} = [p, n]$ is a **matrix-matrix product** $\mathbf{C} = \mathbf{AB} = [m, n]$:

$$\mathbf{z} = \mathbf{A}\left(\mathbf{Bx}\right) = \mathbf{Ay} = \left(\mathbf{AB}\right)\mathbf{x}$$

$$z_i = \sum_{k=1}^{n} A_{ik} y_k = \sum_{k=1}^{p} A_{ik} \sum_{j=1}^{n} B_{kj} x_j = \sum_{j=1}^{n} \left(\sum_{k=1}^{p} A_{ik} B_{kj} \right) x_j = \sum_{j=1}^{n} C_{ij} x_j$$

$$C_{ij} = \sum_{k=1}^{p} A_{lk} B_{kj}$$

- Matrix-matrix multiplication is **not commutative**, $\mathbf{AB} \neq \mathbf{BA}$ in general.

The Matrix Inverse

- A square matrix $\mathbf{A} = [n, n]$ is **invertible or nonsingular** if there exists a **matrix inverse** $\mathbf{A}^{-1} = \mathbf{B} = [n, n]$ such that:

  $$\mathbf{AB} = \mathbf{BA} = \mathbf{I},$$

  where $\mathbf{I}$ is the identity matrix (ones along diagonal, all the rest zeros).
- The following statements are equivalent for $\mathbf{A} \in \mathbb{R}^{n,n}$:
  - $\mathbf{A}$ is **invertible**.
  - $\mathbf{A}$ is **full-rank**, $\operatorname{rank} \mathbf{A} = n$.
  - The columns and also the rows are linearly independent and form a **basis** for $\mathbb{R}^n$.
  - The **determinant** is nonzero, $\det \mathbf{A} \neq 0$.
  - Zero is not an eigenvalue of $\mathbf{A}$.

Matrix Algebra

- Matrix-vector multiplication is just a special case of matrix-matrix multiplication. Note $\mathbf{x}^T\mathbf{y}$ is a scalar (dot product).

$$\mathbf{C}\left(\mathbf{A}+\mathbf{B}\right)=\mathbf{CA}+\mathbf{CB} \text{ and } \mathbf{ABC}=\left(\mathbf{AB}\right)\mathbf{C}=\mathbf{A}\left(\mathbf{BC}\right)$$

$$\left(\mathbf{A}^T\right)^T=\mathbf{A} \text{ and } \left(\mathbf{AB}\right)^T=\mathbf{B}^T\mathbf{A}^T$$

$$\left(\mathbf{A}^{-1}\right)^{-1}=\mathbf{A} \text{ and } \left(\mathbf{AB}\right)^{-1}=\mathbf{B}^{-1}\mathbf{A}^{-1} \text{ and } \left(\mathbf{A}^T\right)^{-1}=\left(\mathbf{A}^{-1}\right)^T$$

- Instead of **matrix division**, think of multiplication by an inverse:

$$\mathbf{AB}=\mathbf{C} \quad \Rightarrow \quad \left(\mathbf{A}^{-1}\mathbf{A}\right)\mathbf{B}=\mathbf{A}^{-1}\mathbf{C} \quad \Rightarrow \quad \begin{cases} \mathbf{B} & =\mathbf{A}^{-1}\mathbf{C} \\ \mathbf{A} & =\mathbf{CB}^{-1} \end{cases}$$

Vector norms

- Norms are the abstraction for the notion of a length or **magnitude**.
- For a vector $\mathbf{x} \in \mathbb{R}^n$, the p-norm is

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

and special cases of interest are:

1. The 1-norm (L^1 norm or Manhattan distance), $\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|$
2. The 2-norm (L^2 norm, **Euclidian distance**), $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x} \cdot \mathbf{x}} = \sqrt{\sum_{i=1}^{n} |x_i|^2}$
3. The ∞-norm (L^∞ or maximum norm), $\|\mathbf{x}\|_\infty = \max_{1 \le i \le n} |x_i|$

1. Note that all of these norms are inter-related in a finite-dimensional setting.

Matrix norms

- Matrix norm **induced** by a given vector norm:

$$\|\mathbf{A}\| = \sup_{\mathbf{x}\neq\mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|} \quad \Rightarrow \|\mathbf{A}\mathbf{x}\| \leq \|\mathbf{A}\| \, \|\mathbf{x}\|$$

- The last bound holds for matrices as well, $\|\mathbf{A}\mathbf{B}\| \leq \|\mathbf{A}\| \, \|\mathbf{B}\|$.
- Special cases of interest are:

1. The 1-norm or **column sum norm**, $\|\mathbf{A}\|_1 = \max_j \sum_{i=1}^{n} |a_{ij}|$
2. The ∞-norm or **row sum norm**, $\|\mathbf{A}\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$
3. The 2-norm or **spectral norm**, $\|\mathbf{A}\|_2 = \sigma_1$ (largest singular value)
4. The Euclidian or **Frobenius norm**, $\|\mathbf{A}\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2}$
   (note this is not an induced norm)

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Matrices and linear systems

- It is said that 70% or more of applied mathematics research involves solving systems of m linear equations for n unknowns:

$$\sum_{j=1}^{n} a_{ij}x_j = b_i, \quad i = 1, \cdots, m.$$

- Linear systems arise directly from **discrete models**, e.g., traffic flow in a city. Or, they may come through representing or more abstract **linear operators** in some finite basis (representation).
  Common abstraction:

$$\mathbf{Ax} = \mathbf{b}$$

- Special case: Square invertible matrices, $m = n$, $\det \mathbf{A} \neq 0$:

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

- The goal: Calculate solution $\mathbf{x}$ given data $\mathbf{A}, \mathbf{b}$ in the most numerically stable and also efficient way.

Stability analysis

Perturbations on **right hand side** (rhs) only:

$$\mathbf{A}\left(\mathbf{x}+\delta\mathbf{x}\right)=\mathbf{b}+\delta\mathbf{b} \quad \Rightarrow \mathbf{b}+\mathbf{A}\delta\mathbf{x}=\mathbf{b}+\delta\mathbf{b}$$

$$\delta\mathbf{x}=\mathbf{A}^{-1}\delta\mathbf{b} \quad \Rightarrow \left\|\delta\mathbf{x}\right\|\leq\left\|\mathbf{A}^{-1}\right\|\left\|\delta\mathbf{b}\right\|$$

Using the bounds

$$\left\|\mathbf{b}\right\|\leq\left\|\mathbf{A}\right\|\left\|\mathbf{x}\right\| \quad \Rightarrow \left\|\mathbf{x}\right\|\geq\left\|\mathbf{b}\right\|/\left\|\mathbf{A}\right\|$$

the relative error in the solution can be bounded by

$$\frac{\left\|\delta\mathbf{x}\right\|}{\left\|\mathbf{x}\right\|}\leq\frac{\left\|\mathbf{A}^{-1}\right\|\left\|\delta\mathbf{b}\right\|}{\left\|\mathbf{x}\right\|}\leq\frac{\left\|\mathbf{A}^{-1}\right\|\left\|\delta\mathbf{b}\right\|}{\left\|\mathbf{b}\right\|/\left\|\mathbf{A}\right\|}=\kappa(\mathbf{A})\frac{\left\|\delta\mathbf{b}\right\|}{\left\|\mathbf{b}\right\|}$$

where the **conditioning number** $\kappa(\mathbf{A})$ depends on the matrix norm used:

$$\kappa(\mathbf{A})=\left\|\mathbf{A}\right\|\left\|\mathbf{A}^{-1}\right\|\geq 1.$$

Conditioning Number

- The full derivation, not given here, estimates the uncertainty or perturbation in the solution:

$$\frac{\|\delta \mathbf{x}\|}{\|\mathbf{x}\|} \leq \frac{\kappa(\mathbf{A})}{1 - \kappa(\mathbf{A})\frac{\|\delta \mathbf{A}\|}{\|\mathbf{A}\|}} \left(\frac{\|\delta \mathbf{b}\|}{\|\mathbf{b}\|} + \frac{\|\delta \mathbf{A}\|}{\|\mathbf{A}\|} \right).$$

  The **worst-case conditioning** of the linear system is determined by $\kappa(\mathbf{A})$.

- Best possible error with rounding unit $u \approx 10^{-16}$:

$$\frac{\|\delta \mathbf{x}\|_\infty}{\|\mathbf{x}\|_\infty} \lesssim 2u\kappa(\mathbf{A}),$$

- Solving an ill-conditioned system, $\kappa(\mathbf{A}) \gg 1$ (e.g., $\kappa = 10^{15}!$) , should only be done if something special is known.
- The conditioning number can only be **estimated** in practice since $\mathbf{A}^{-1}$ is not available (see MATLAB's *rcond* function).

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GEM: Eliminating x_1

Step 1: $Ax = b$

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \end{bmatrix} \begin{array}{l} \leftarrow \text{Multiply FIRST row by} \\ \leftarrow l_{21} = \dfrac{a_{21}^{(1)}}{a_{11}^{(1)}} \\ \leftarrow l_{31} = \dfrac{a_{31}^{(1)}}{a_{11}^{(1)}} \end{array}$$

$\Downarrow$ Eliminate x_1

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ 0 = a_{21}^{(1)} - l_{21} \cdot a_{11} & a_{22}^{(1)} - l_{21} \cdot a_{12}^{(1)} & a_{23}^{(1)} - l_{21} \cdot a_{13}^{(1)} \\ 0 & a_{32}^{(1)} - l_{31} \cdot a_{12}^{(1)} & a_{33}^{(1)} - l_{31} \cdot a_{13}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 - l_{21} \cdot b_1 \\ b_3 - l_{31} \cdot b_1 \end{bmatrix}$$

GEM: Eliminating x_2

Step 2:

$$\left[\begin{array}{c|cc} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ \hline 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ \hline 0 & a_{32}^{(2)} & a_{33}^{(2)} \end{array}\right] \left[\begin{array}{c} x_1 \\ \hline x_2 \\ \hline x_3 \end{array}\right] = \left[\begin{array}{c} b_1^{(2)} \\ \hline b_2^{(2)} \\ \hline b_3^{(3)} \end{array}\right]$$

done row!

← Multiply second row by

← $l_{32} = \frac{a_{32}^{(2)}}{a_{22}^{(2)}}$

$\Downarrow$ Eliminate x_2

$$\left[\begin{array}{c|c|c} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ \hline 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ \hline 0 & 0 & a_{33}^{(3)} \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \end{array}\right] = \left[\begin{array}{c} b_1^{(3)} \\ \hline b_2^{(3)} \\ \hline b_3^{(3)} \end{array}\right]$$

Upper triangular system

← Solve $x_3 = \frac{b_3^{(3)}}{a_{33}^{(3)}}$

GEM: Backward substitution

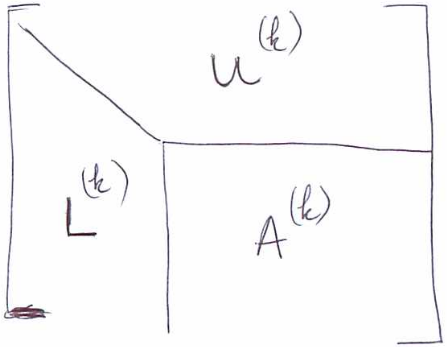
Eliminate x_3 entirely →

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} \\ 0 & a_{22}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1^{(3)} - a_{13}^{(1)} x_3 \\ b_2^{(3)} - a_{23}^{(2)} x_3 \end{bmatrix} = \tilde{b}$$

↑ solve for $x_2 = \dfrac{\tilde{b}}{a_{22}^{(2)}}$, then x_1, and done!

IDEA: Store the multipliers in the lower triangle of A:

Matrix at Step k:

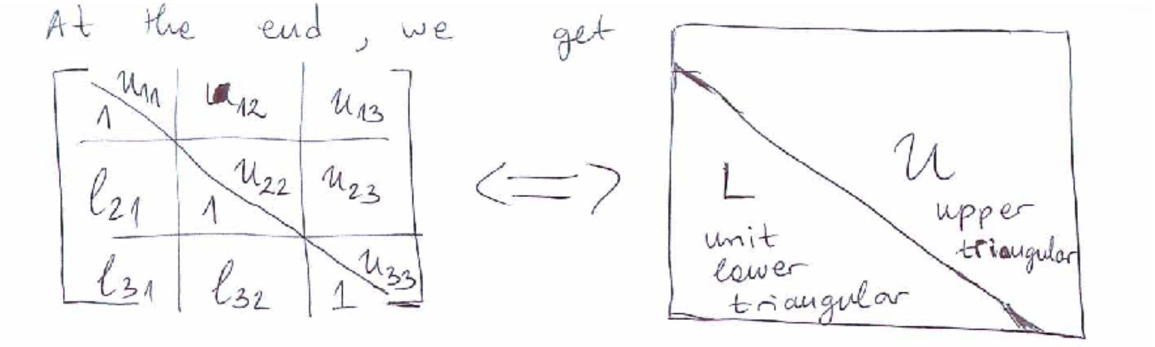


$$\left[\begin{array}{c|cc} u_{11} & u_{12} & u_{13} \\ \hline l_{21} & a_{22}^{(2)} & a_{23}^{(2)} \\ l_{31} & a_{32}^{(2)} & a_{33}^{(2)} \end{array}\right]$$

Example step 2

3

GEM as an *LU* factorization tool



At the end, we get

$$\begin{bmatrix} 1 \setminus u_{11} & u_{12} & u_{13} \\ l_{21} & 1 \setminus u_{22} & u_{23} \\ l_{31} & l_{32} & 1 \setminus u_{33} \end{bmatrix} \Longleftrightarrow$$

- We have actually **factorized A** as

$$\mathbf{A} = \mathbf{LU},$$

L is **unit lower triangular** ($l_{ii} = 1$ on diagonal), and **U** is **upper triangular**.

- GEM is thus essentially the same as the *LU* **factorization method**.

GEM in MATLAB

```
% Sample MATLAB code (for learning purposes only, not
 function A = MyLU(A)
% LU factorization in-place (overwrite A)
 [n,m]=size(A);
 if (n ~= m); error('Matrix not square'); end
 for k=1:(n-1) % For variable x(k)
    % Calculate multipliers in column k:
    A((k+1):n,k) = A((k+1):n,k) / A(k,k);
    % Note: Pivot element A(k,k) assumed nonzero!
    for j=(k+1):n
       % Eliminate variable x(k):
       A((k+1):n,j) = A((k+1):n,j) - ...
          A((k+1):n,k) * A(k,j);
    end
end
end
```

Pivoting

Zero diagonal entries (pivots) pose a problem → PIVOTING (swapping rows and columns)

$$A x = b$$

$$\begin{bmatrix} 1 & 1 & 3 \\ 2 & 2 & 2 \\ 3 & 6 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 6 \\ 13 \end{bmatrix} \Rightarrow \left[\begin{array}{c|cc} 1 & 1 & 3 \\ \hline 2 & \mathbf{0} & -4 \\ 3 & 3 & -5 \end{array}\right]$$

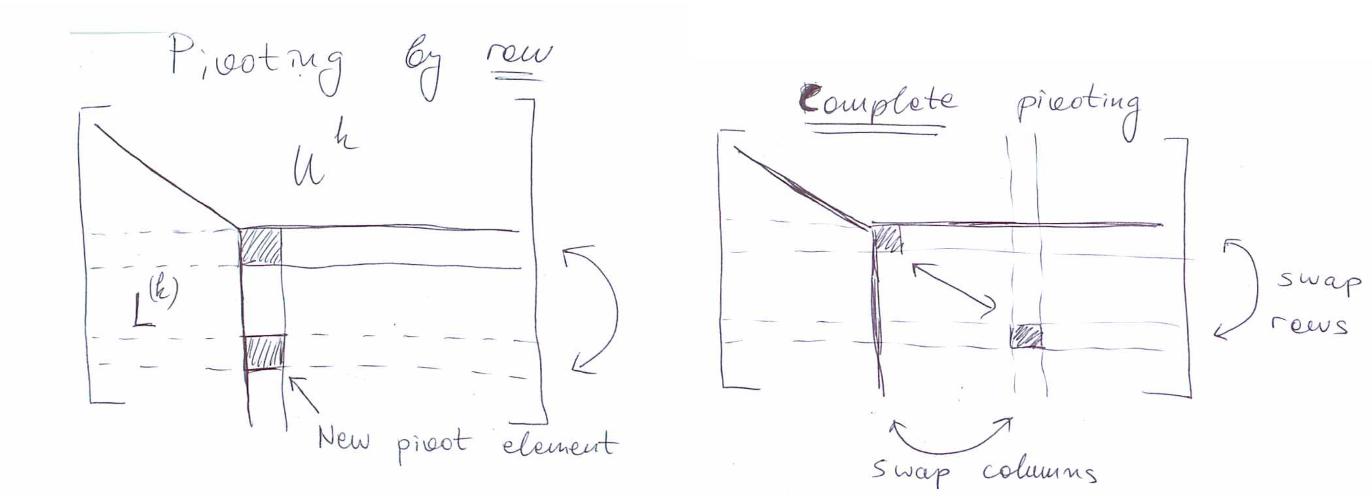
$$\left[\begin{array}{c|cc} 1 & 1 & 3 \\ \hline 3 & \textcircled{3} & -5 \\ 2 & 0 & -4 \end{array}\right] \Rightarrow \left[\begin{array}{c|c|c} {}_{1}{}^{1} & 1 & 3 \\ \hline 3 & {}_{1}{}^{3} & -5 \\ \hline 2 & 0 & {}_{1}{}^{-4} \end{array}\right]$$

OBSERVE

$$\underline{\underline{LU = \overset{\text{PERMUTED}}{A}}}$$

4

Pivoting during LU factorization



- **Partial (row) pivoting** permutes the rows (equations) of **A** in order to ensure sufficiently large pivots and thus numerical stability:

$$\mathbf{PA} = \mathbf{LU}$$

- Here **P** is a **permutation matrix**, meaning a matrix obtained by permuting rows and/or columns of the identity matrix.
- **Complete pivoting** also permutes columns, **PAQ = LU**.

Gauss Elimination Method (GEM)

- GEM is a **general** method for **dense matrices** and is commonly used.
- Implementing GEM efficiently and stably is difficult and we will not discuss it here, since others have done it for you!
- The **LAPACK** public-domain library is the main repository for excellent implementations of dense linear solvers.
- MATLAB uses a highly-optimized variant of GEM by default, mostly based on LAPACK.
- MATLAB does have **specialized solvers** for special cases of matrices, so always look at the help pages!

Solving linear systems

- Once an *LU* factorization is available, solving a linear system is simple:

$$\mathbf{Ax} = \mathbf{LUx} = \mathbf{L}\left(\mathbf{Ux}\right) = \mathbf{Ly} = \mathbf{b}$$

  so solve for **y** using **forward substitution**.
  This was implicitly done in the example above by overwriting **b** to become **y** during the factorization.

- Then, solve for **x** using **backward substitution**

$$\mathbf{Ux} = \mathbf{y}.$$

- If row pivoting is necessary, the same applies but **L** or **U** may be permuted upper/lower triangular matrices,

$$\mathbf{A} = \widetilde{\mathbf{L}}\mathbf{U} = \left(\mathbf{P}^T\mathbf{L}\right)\mathbf{U}.$$

In MATLAB

- In MATLAB, the **backslash operator** (see help on *mldivide*)

$$x = A \backslash b \approx A^{-1} b,$$

  solves the linear system $\mathbf{Ax} = \mathbf{b}$ using the LAPACK library.
  Never use matrix inverse to do this, even if written as such on paper.

- Doing $x = A \backslash b$ is **equivalent** to performing an LU factorization and doing two **triangular solves** (backward and forward substitution):

$$[\tilde{L}, U] = lu(A)$$
$$y = \tilde{L} \backslash b$$
$$x = U \backslash y$$

- This is a carefully implemented **backward stable** pivoted LU factorization, meaning that the returned solution is as accurate as the conditioning number allows.

GEM Matlab example (1)

```
>> A = [ 1    2    3 ;  4    5    6 ;  7    8    0 ];
>> b=[2 1 -1]';

>> x=A^(-1)*b; x' % Don't do this!
ans =     -2.5556    2.1111    0.1111

>> x = A\b; x' % Do this instead
ans =    -2.5556    2.1111    0.1111

>> linsolve(A,b)' % Even more control
ans =     -2.5556    2.1111    0.1111
```

GEM Matlab example (2)

```
>> [L,U] = lu(A) % Even better if resolving

L =     0.1429    1.0000         0
        0.5714    0.5000    1.0000
        1.0000         0         0
U =     7.0000    8.0000         0
             0    0.8571    3.0000
             0         0    4.5000

>> norm(L*U-A,inf)
ans =      0

>> y = L\b;
>> x = U\y; x'
ans =   -2.5556    2.1111    0.1111
```

Backwards Stability

- Even though we cannot get $\mathbf{x}$ correctly for ill-conditioned linear systems, we can still get an (not *the* one!) $\mathbf{x}$ that is a solution of the equation to almost machine precision.
- This sort of **backward stability** means that there is a problem nearby the original problem such that the answer we compute $\hat{\mathbf{x}}$ is the solution of that "perturbed" problem,

$(x+\delta x)$ ← Forward stability

$$(\mathbf{A}+\delta\mathbf{A})\,\hat{\mathbf{x}} = \mathbf{b}+\delta\mathbf{b}. \quad \leftarrow$$

Do this!

- A backwards stable method gives a **residual** $\mathbf{r}=\mathbf{A}\mathbf{x}-\mathbf{b}$ that is zero to within the rounding unit $u \approx 10^{-16}$,

compute this always

$$\left\{ \frac{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|}{\|\mathbf{b}\|} \sim \frac{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|}{\|\mathbf{A}\mathbf{x}\|} \sim u, \right.$$

But cond. $K \approx 10^{16}$ tough

- Observe that the conditioning number of the matrix does not enter here, it can be large!

Backwards Stability contd.

- Gaussian elimination with partial pivoting is almost always backwards stable in practice, but one can always check the residual after computing the answer (**always good practice** to confirm you solved the problem you thought you solved!)
- Specifically, if we compute the LU factorization we are guaranteed that

$$\mathbf{A} + \delta\mathbf{A} = \mathbf{LU} \quad \text{where} \quad \frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} \leq Cu$$

  where C is some modest constant that depends *polynomially* on the number of unknowns (not exponentially).
- Complete pivoting is rarely used in practice because it is expensive, even though it will give better guarantees.

Cost estimates for GEM

- For forward or backward substitution, at step k there are $\sim (n-k)$ multiplications and subtractions, plus a few divisions.
  The total over all n steps is
  $$\sum_{k=1}^{n} (n-k) = \frac{n(n-1)}{2} \approx \frac{n^2}{2}$$
  subtractions and multiplications, giving a total of $O(n^2)$ **floating-point operations** (FLOPs).
- The LU factorization itself costs a lot more, $O(n^3)$,
  $$\text{FLOPS} \approx \frac{2n^3}{3},$$
  and the triangular solves are negligible for large systems.
- When many linear systems need to be solved with the same $\mathbf{A}$ the **factorization can be reused**.

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Matrix Rescaling and Reordering

- Pivoting is not always sufficient to ensure lack of roundoff problems. In particular, **large variations** among the entries in **A should be avoided**.
- This can usually be remedied by changing the physical units for $\mathbf{x}$ and $\mathbf{b}$ to be the **natural units** $\mathbf{x}_0$ and $\mathbf{b}_0$.
- **Rescaling** the unknowns and the equations is generally a good idea even if not necessary:

$$\mathbf{x} = \mathbf{D}_x \tilde{\mathbf{x}} = \text{Diag}\left\{\mathbf{x}_0\right\} \tilde{\mathbf{x}} \text{ and } \mathbf{b} = \mathbf{D}_b \tilde{\mathbf{b}} = \text{Diag}\left\{\mathbf{b}_0\right\} \tilde{\mathbf{b}}.$$

$$\mathbf{A}\mathbf{x} = \mathbf{A}\mathbf{D}_x \tilde{\mathbf{x}} = \mathbf{D}_b \tilde{\mathbf{b}} \quad \Rightarrow \quad \left(\mathbf{D}_b^{-1}\mathbf{A}\mathbf{D}_x\right) \tilde{\mathbf{x}} = \tilde{\mathbf{b}}$$

- The **rescaled matrix** $\widetilde{\mathbf{A}} = \mathbf{D}_b^{-1}\mathbf{A}\mathbf{D}_x$ should have a better conditioning.
- Also note that **reordering the variables** from most important to least important may also help.

Efficiency of Solution

Cost of GE

$O(n^3)$

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

- The most appropriate algorithm really depends on the properties of the matrix **A**:
  - General **dense matrices**, where the entries in **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.

Positive-Definite Matrices

- A real symmetric matrix **A** is positive definite iff (if and only if):
  1. All of its eigenvalues are real (follows from symmetry) and positive.
  2. $\forall x \neq \mathbf{0}$, $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$, i.e., the quadratic form defined by the matrix **A** is convex.

     $(x, Ax) > 0 \quad \forall x \neq 0$
  3. There exists a *unique* lower triangular **L**, $L_{ii} > 0$,

     $U = L^T$

     $$\mathbf{A} = \mathbf{L}\mathbf{L}^T,$$

     L does not necessarily have 1's on diagonal

     LU

     termed the **Cholesky factorization** of **A** (symmetric *LU* factorization).

1. For Hermitian complex matrices just replace transposes with adjoints (conjugate transpose), e.g., $\mathbf{A}^T \rightarrow \mathbf{A}^\star$ (or $\mathbf{A}^H$ in the book).

Cholesky Factorization

- The MATLAB built in function

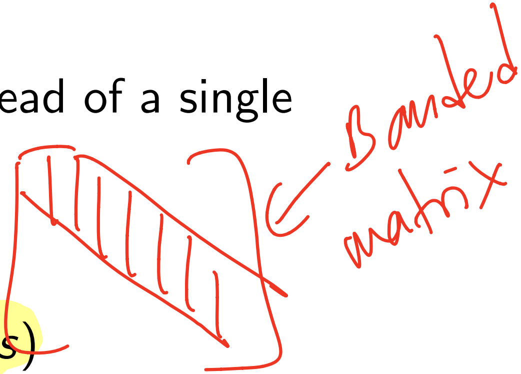
$$\underbrace{L^T =}\, R = chol(A)$$

  gives the Cholesky factorization and is a good way to **test for positive-definiteness**.
- The cost of a Cholesky factorization is about half the cost of *LU* factorization, $n^3/3$ FLOPS. L'
- Solving linear systems is as for *LU* factorization, replacing $\underline{\mathbf{U}}$ with $\underline{\mathbf{L}^T}$.
- For Hermitian/symmetric matrices with positive diagonals MATLAB tries a Cholesky factorization first, *before* resorting to *LU* factorization with pivoting.

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 **B** instead of a single right-hand side vector **b**.
- The MATLAB function

$$X = linsolve(A, B, opts)$$



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.

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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**.

$Ax=b$

- One must first define what is meant by a solution, and the common definition is to use a **least-squares formulation**:

$$\mathbf{x}^\star = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{A}\mathbf{x}-\mathbf{b}\|^{2}_{L_2} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \Phi(\mathbf{x})$$

$\|r\|^2 = r^T r$

where the choice of the L_2 norm leads to:

$A=[m \times n]$

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

$[1\times N][N\times 1] = [1\times 1]$

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

Normal Equations

$\frac{d}{dx}(ax-b)^2 = 2a(ax-b)$

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

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

Cholesky $O(n^3)$

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

$A^T(Ax) = A^T b$

$$\left(\mathbf{A}^T\mathbf{A}\right)\mathbf{x}^\star = \mathbf{A}^T\mathbf{b}.$$

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

square linear system

- If $\mathbf{A}$ is of full rank, $\text{rank}\left(\mathbf{A}\right) = n$, 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

$O(m^3)$

$O(m^2 n)$

$m > n$

$m >> n$ in practice

Problems with the normal equations

$O(mn^2) >> O(n^3)$

so overall cost is $O(mn^2)$

$$\left(\mathbf{A}^T\mathbf{A}\right)\mathbf{x}^\star = \mathbf{A}^T\mathbf{b}.$$

- The conditioning number of the normal equations is

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

- 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:

$$\mathbf{A} = \mathbf{QR}$$

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

$Rx = b$

easy $O(n^2)$

  where **Q** has **orthogonal columns**, $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_n$, and **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

$$\left(\mathbf{A}^T\mathbf{A}\right)\mathbf{x}^\star = \mathbf{A}^T\mathbf{b} \text{ where } \mathbf{A} = \mathbf{QR}$$

$$A^T = R^T Q^T$$

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

$$\mathbf{A}^T\mathbf{A} = \mathbf{R}^T \overset{I}{\overset{\|}{\left(\mathbf{Q}^T\mathbf{Q}\right)}} \mathbf{R} = \mathbf{R}^T\mathbf{R}$$

$$\boxed{Rx^\star = Q^T b}$$

$$\underbrace{R^{-T}\left(\mathbf{R}^T\mathbf{R}\right)}_{I}\mathbf{x}^\star = \underbrace{R^{-T}\left(\mathbf{R}^T\right.}_{I}\left.\mathbf{Q}^T\right)\mathbf{b} \quad\Rightarrow\quad \mathbf{x}^\star = \mathbf{R}^{-1}\left(\mathbf{Q}^T\mathbf{b}\right)$$

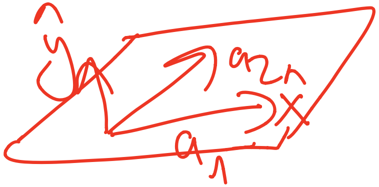
which amounts to solving a triangular system with matrix $\mathbf{R}$.

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

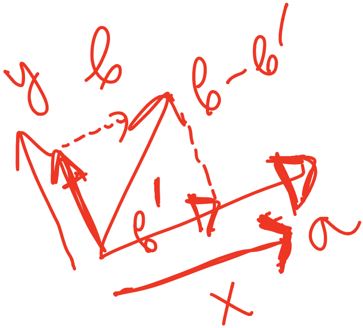
Computing the QR Factorization

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

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



- 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 span $(\tilde{\mathbf{a}}_1, \tilde{\mathbf{a}}_2) =$ span $(\mathbf{a}_1, \mathbf{a}_2)$:



$$\tilde{\mathbf{a}}_1 = \mathbf{a}_1$$

$$\tilde{\mathbf{a}}_2 = \mathbf{a}_2 - (\mathbf{a}_2 \cdot \mathbf{a}_1) \frac{\mathbf{a}_1}{(\mathbf{a}_1 \cdot \mathbf{a}_1)}$$

$$\tilde{\mathbf{a}}_3 = \mathbf{a}_3 - (\mathbf{a}_3 \cdot \mathbf{a}_1) \frac{\mathbf{a}_1}{(\mathbf{a}_1 \cdot \mathbf{a}_1)} - (\mathbf{a}_3 \cdot \mathbf{a}_2) \frac{\mathbf{a}_2}{(\mathbf{a}_2 \cdot \mathbf{a}_2)}$$

$$x = \frac{a}{\|a\|_2}$$

Gram-Schmidt Orthogonalization

- More efficient formula (**standard Gram-Schmidt**): $O\left(mn^2\right)$

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

  with cost $\approx 2mn^2$ FLOPS but is **not numerically stable** against roundoff errors (**loss of orthogonality**).
- In the standard method we make each vector orthogonal to all previous vectors. A **numerically stable** alternative is the **modified Gram-Schmidt**, in which we take each vector and modify all following vectors (not previous ones) to be orthogonal to it (so the sum above becomes $\sum_{j=k+1}^{m}$).
- As we saw in previous lecture, a small rearrangement of mathematically-equivalent approaches can produce a much more robust numerical method.

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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**

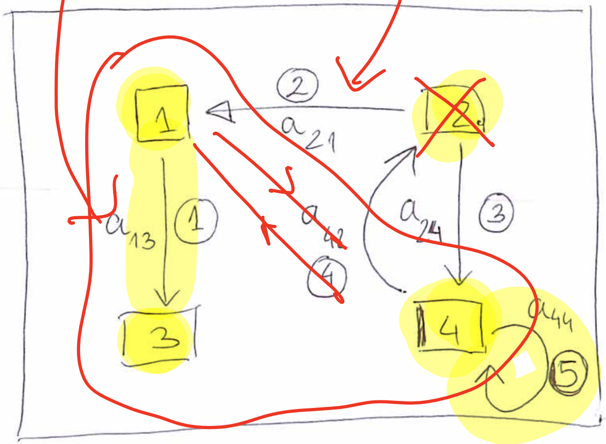
$$\begin{bmatrix} a_1 & c_1 & & \mathbf{0} \\ b_2 & a_2 & \ddots & \\ & \ddots & \ddots & c_{n-1} \\ \mathbf{0} & & b_n & a_n \end{bmatrix}$$

- 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

$$A = \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 0 & 1 & 0 \\ 2 & 2 & 0 & 0 & 3 \\ 3 & 0 & 0 & 0 & 0 \\ 4 & 0 & 4 & 0 & 5 \end{array}$$

Sparse matrix



Directed Graph representation:

→ Nodes (vertices) are variables or equations

→ Arcs (edges) are the non-zeros

Undirected graph for symmetric matrices ①

Sparse matrices in MATLAB

```
>> A = sparse( [1 2 2 4 4], [3 1 4 2 3], 1:5 )
```

[1,2,3,4,5]

```
A =
   (2,1)        2
   (4,2)        4
   (1,3)        1
   (4,3)        5
   (2,4)        3
>> nnz(A) % Number of non-zeros
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

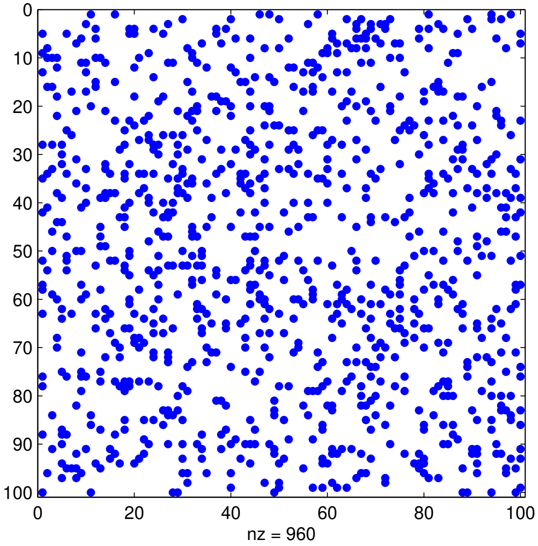
random matrix has NO structure

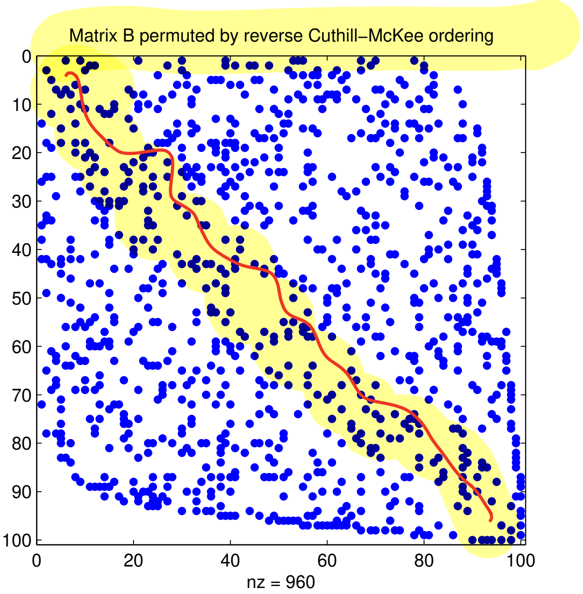
```
>> B=sprand(4,4,0.25); % Density of 25%
>> full(B)
ans =
         0         0         0    0.7655
         0    0.7952         0         0
         0    0.1869         0         0
    0.4898         0         0         0

>> B=sprand(100,100,0.1); spy(B)
>> [L,U,P]=lu(B); spy(L)
>> p = symrcm(B); % Permutation to reorder the rows an
>> PBP=B(p,p); spy(PBP);
>> [L,U,P]=lu(PBP); spy(L);
```

[1,2,3,4,5) reshuffled [1,5,3,2,4]

Random matrix **B**

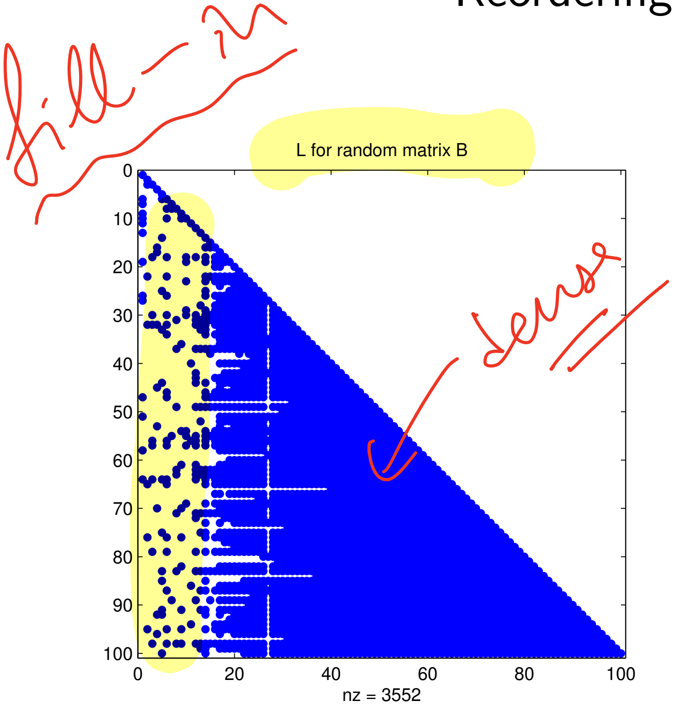
The MATLAB function *spy* shows where the nonzeros are (left), and what reordering does (right)

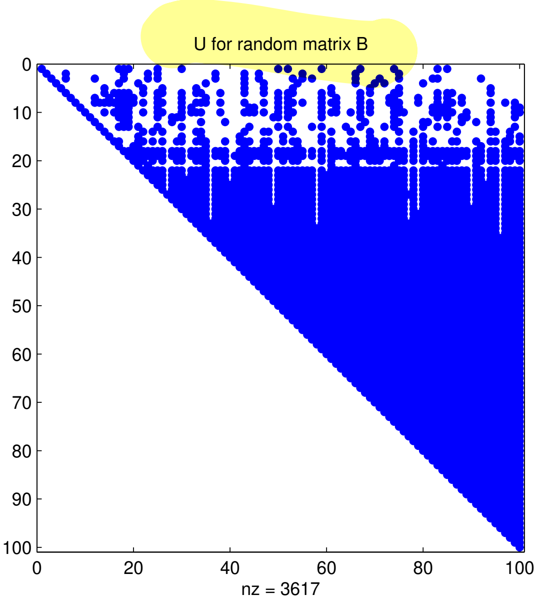




LU factors of random matrix **B**

Fill-in (generation of lots of nonzeros) is large for a random sparse matrix. Reordering helps only a bit.





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.

Why iterative methods?

- Direct solvers are great for dense matrices and are implemented very well on modern machines.
- **Fill-in** is a major problem for certain sparse matrices and leads to extreme memory requirements.
- 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

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

$Ax=b$

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

where **B** is an **iteration matrix** somehow related to **A** (many different choices/algorithms exist).

- 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:

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

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

Simple Fixed-Point Iteration

$$B = I - A$$

- If we just pick a matrix **B**, in general we cannot easily figure out what **f** needs to be since this requires knowing the solution we are after,

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

- But what if we choose $\mathbf{I} - \mathbf{B} = \mathbf{A}$? Then we get

$$\mathbf{f} = \mathbf{A}\cancel{\mathbf{A}}^{-1}\mathbf{b} = \mathbf{b} \qquad x^{k+1} = x^{k} + \underbrace{(b - Ax^{k})}_{r^{k}}$$

which we know.

- This leads us to this **fixed-point iteration** is an iterative method:

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

Krylov methods

$$x^{k+1} = Ax^{(k)} + (b - x^{(k)})$$

Side-note: 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 $\mathbf{A}\mathbf{x} = \mathbf{b}$ as:

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

- Fixed-point iteration gives the consistent iterative method

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

  which is the same as we already derived differently.

Convergence of simple iterative methods

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

$$\underline{\underline{\mathbf{e}^{(k+1)}}} = \mathbf{x}^{(k+1)} - \mathbf{x} = \underline{\mathbf{B}\mathbf{x}^{(k)} + \mathbf{f}} - \mathbf{x} = \mathbf{B}\left(\overset{\overset{x^k}{\|}}{\mathbf{x} + \mathbf{e}^{(k)}}\right) + (\mathbf{I} - \mathbf{B})\,\mathbf{x} - \mathbf{x} = \underline{\underline{\mathbf{B}\mathbf{e}^{(k)}}}$$

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

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

$$e^k = B^k e^{(0)}$$

- When does this converge? Taking norms,

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

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

- More precisely, $\lim_{k\to\infty} \mathbf{e}^{(k)} = \mathbf{0}$ for any $\mathbf{e}^{(0)}$ iff $\mathbf{B}^k \to \mathbf{0}$.

Spectral Radius

- Theorem: The simple iterative method converges iff the **spectral radius** of the iteration matrix is less than unity:

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

- 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:

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

Termination

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

     $$\left\|\mathbf{r}^{(k)}\right\| = \left\|\mathbf{A}\mathbf{x}^{(k)} - \mathbf{b}\right\| \leq \varepsilon \left\|\mathbf{b}\right\|$$

     This is good for well-conditioned systems.
  2. The solution $\mathbf{x}^{(k)}$ stops changing, i.e., the **increment** becomes small,

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

     which can be shown to be good if convergence is rapid.
- Usually a careful **combination** of the two strategies is employed along with some **safeguards**.

Preconditioning

- The fixed-point iteration 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:

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

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

Preconditioned Iteration

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

- In practice, we solve linear systems with the matrix **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** $\mathbf{x}^{(0)}$.

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Conclusions/Summary

- The conditioning of a linear system $\mathbf{Ax} = \mathbf{b}$ is determined by the condition number

$$\kappa(\mathbf{A}) = \|\mathbf{A}\| \left\|\mathbf{A}^{-1}\right\| \geq 1$$

- Gauss elimination can be used to solve general square linear systems and also produces a factorization $\mathbf{A} = \mathbf{LU}$.
- Partial pivoting is often necessary to ensure numerical stability during GEM and leads to $\mathbf{PA} = \mathbf{LU}$ or $\mathbf{A} = \widetilde{\mathbf{L}}\mathbf{U}$.
- MATLAB has excellent linear solvers based on well-known public domain libraries like LAPACK. Use them!

Conclusions/Summary

- For symmetric positive definite matrices the Cholesky factorization $\mathbf{A} = \mathbf{L}\mathbf{L}^T$ is preferred and does not require pivoting.
- The *QR* factorization is a numerically-stable method for solving **full-rank non-square systems**.
- **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.