Scientific Computing:
Solving Linear Systems

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Outline

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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 $x_3 = 0$. 
Consider a set of \(n\) vectors \(a_1, a_2, \cdots, a_n \in \mathbb{R}^m\) and form a matrix by putting these vectors as columns

\[
A = [a_1 \mid a_2 \mid \cdots \mid a_m] \in \mathbb{R}^{m,n}.
\]

I will denote matrices with bold capital letters, and sometimes write \(A = [m, n]\) to indicate dimensions.

The matrix-vector product is defined as a linear combination of the columns:

\[
b = Ax = x_1a_1 + x_2a_2 + \cdots + x_n a_n \in \mathbb{R}^m.
\]

The image \(\text{im}(A)\) or range \(\text{range}(A)\) of a matrix is the subspace of all linear combinations of its columns, i.e., the set of all \(b\)'s. It is also sometimes called the column space of the matrix.
The set of vectors $a_1, a_2, \cdots, a_n$ are **linearly independent** or form a **basis** for $\mathbb{R}^m$ if $b = Ax = 0$ implies that $x = 0$.

The **dimension** $r = \operatorname{dim} V$ of a vector (sub)space $V$ is the number of elements in a basis. This is a property of $V$ itself and not of the basis, for example,

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

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

$$b = x_1 a_1 + x_2 a_2 + \cdots + x_n a_n.$$ 

A simple and common basis for $\mathbb{R}^n$ is $\{e_1, \ldots, e_n\}$, where $e_k$ 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, $b \equiv x$. 

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

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

If $r = \min(m, n)$ then the matrix is of **full rank**.

The **nullspace** $\text{null}(A)$ or **kernel** $\text{ker}(A)$ of a matrix $A$ is the subspace of vectors $x$ for which

$$Ax = 0.$$

The dimension of the nullspace is called the **nullity** of the matrix.

For a basis $A$ the nullspace is $\text{null}(A) = \{0\}$ and the nullity is zero.
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:

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

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

\[
x \cdot y = x^* y = \sum_{i=1}^{n} \bar{x}_i y_i.
\]

Two vectors \( x \) and \( y \) are **orthogonal** if \( x \cdot y = 0 \).
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 $A \in \mathbb{R}^{m,n}$

$$\text{rank } A + \text{nullity } A = n.$$  

In addition to the range and kernel spaces of a matrix, two more important vector subspaces for a given matrix $A$ are the:

- **Row space** or **coimage** of a matrix is the column (image) space of its transpose, $\text{im } A^T$.  
  *Its dimension is also equal to the the rank.*

- **Left nullspace** or **cokernel** of a matrix is the nullspace or kernel of its transpose, $\text{ker } A^T$. 
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 $\mathbf{x} \in \mathbb{R}^3$ 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:

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

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

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

- 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 **matrix-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

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

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

\[ z = A(Bx) = Ay = (AB)x \]

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

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

- Matrix-matrix multiplication is **not commutative**, \( AB \neq BA \) in general.
A square matrix $A = [n, n]$ is **invertible or nonsingular** if there exists a **matrix inverse** $A^{-1} = B = [n, n]$ such that:

$$AB = BA = I,$$

where $I$ is the identity matrix (ones along diagonal, all the rest zeros).

The following statements are equivalent for $A \in \mathbb{R}^{n,n}$:

- $A$ is **invertible**.
- $A$ is **full-rank**, $\text{rank } A = n$.
- The columns and also the rows are linearly independent and form a **basis** for $\mathbb{R}^n$.
- The **determinant** is nonzero, $\det A \neq 0$.
- Zero is not an eigenvalue of $A$. 

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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).

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

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

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

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

$$AB = C \Rightarrow (A^{-1}A)B = A^{-1}C \Rightarrow \begin{cases} B = A^{-1}C \\ A = CB^{-1} \end{cases}$$
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 $\infty$-norm ($L^\infty$ or maximum norm), $\|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} |x_i|$  

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

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

\[
\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} \Rightarrow \|Ax\| \leq \|A\| \|x\|
\]

- The last bound holds for matrices as well, \(\|AB\| \leq \|A\| \|B\|\).

- Special cases of interest are:
  1. The 1-norm or **column sum norm**, \(\|A\|_1 = \max_j \sum_{i=1}^n |a_{ij}|\)
  2. The \(\infty\)-norm or **row sum norm**, \(\|A\|_\infty = \max_i \sum_{j=1}^n |a_{ij}|\)
  3. The 2-norm or **spectral norm**, \(\|A\|_2 = \sigma_1\) (largest singular value)
  4. The Euclidian or **Frobenius norm**, \(\|A\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2}\)

   (note this is not an induced norm)
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:

\[
\sum_{j=1}^{n} a_{ij} x_j = b_i, \quad i = 1, \ldots, m.
\]

- 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:

\[
Ax = b
\]

- Special case: Square invertible matrices, \( m = n \), \( \det A \neq 0 \):

\[
x = A^{-1}b.
\]

- The goal: Calculate solution \( x \) given data \( A, b \) in the most numerically stable and also efficient way.
Perturbations on right hand side (rhs) only:

\[ A(x + \delta x) = b + \delta b \quad \Rightarrow \quad b + A\delta x = b + \delta b \]

\[ \delta x = A^{-1}\delta b \quad \Rightarrow \quad \|\delta x\| \leq \|A^{-1}\| \|\delta b\| \]

Using the bounds

\[ \|b\| \leq \|A\| \|x\| \quad \Rightarrow \quad \|x\| \geq \|b\| / \|A\| \]

the relative error in the solution can be bounded by

\[ \frac{\|\delta x\|}{\|x\|} \leq \frac{\|A^{-1}\| \|\delta b\|}{\|b\| / \|A\|} = \kappa(A) \frac{\|\delta b\|}{\|b\|} \]

where the conditioning number \( \kappa(A) \) depends on the matrix norm used:

\[ \kappa(A) = \|A\| \|A^{-1}\| \geq 1. \]
The full derivation, not given here, estimates the uncertainty or perturbation in the solution:

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

The worst-case conditioning of the linear system is determined by \(\kappa(A)\).

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

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

Solving an ill-conditioned system, \(\kappa(A) \gg 1\) (e.g., \(\kappa = 10^{15}\!)\), should only be done if something special is known.

The conditioning number can only be estimated in practice since \(A^{-1}\) is not available (see MATLAB’s \(rcond\) function).
### GEM: Eliminating $x_1$

**Step 1:**

\[
\begin{bmatrix}
 a_{11} & a_{12} & a_{13} \\
 a_{21} & a_{22} & a_{23} \\
 a_{31} & a_{32} & a_{33}
\end{bmatrix}
\begin{bmatrix}
 x_1 \\
 x_2 \\
 x_3
\end{bmatrix} =
\begin{bmatrix}
 b_1 \\
 b_2 \\
 b_3
\end{bmatrix}
\]

- **Multiply first row by $\frac{a_{11}}{a_{21}}$**
- **Multiply second row by $\frac{a_{22}}{a_{32}}$**
- **Multiply third row by $\frac{a_{33}}{a_{33}}$$\frac{a_{34}}{a_{34}}$**

\[
\begin{bmatrix}
 a_{11} & a_{12} & a_{13} \\
 0 & a_{22} - a_{21} & a_{23} - a_{21} \cdot a_{13} \\
 0 & a_{32} - a_{31} \cdot a_{12} & a_{33} - a_{31} \cdot a_{13}
\end{bmatrix}
\begin{bmatrix}
 x_1 \\
 x_2 \\
 x_3
\end{bmatrix} =
\begin{bmatrix}
 b_1 \\
 b_2 - l_{21} \cdot b_1 \\
 b_3 - l_{31} \cdot b_1
\end{bmatrix}
\]
GEM: Eliminating $x_2$

\[
\begin{bmatrix}
  a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\
  0 & a_{22}^{(2)} & a_{23}^{(2)} \\
  0 & a_{32}^{(2)} & a_{33}^{(2)}
\end{bmatrix}
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix}
= \begin{bmatrix}
  \frac{b_1^{(2)}}{a_{11}^{(2)}} \\
  \frac{b_2^{(2)}}{a_{22}^{(2)}} \\
  \frac{b_3^{(2)}}{a_{33}^{(2)}}
\end{bmatrix}
\]

\[\text{done row!}\]

Multiply second row by $\frac{a_{32}^{(2)}}{a_{22}^{(2)}}$

Eliminate $x_2$

\[
\begin{bmatrix}
  a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\
  0 & a_{22}^{(2)} & a_{23}^{(2)} \\
  0 & 0 & a_{33}^{(3)}
\end{bmatrix}
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix}
= \begin{bmatrix}
  \frac{b_1^{(3)}}{a_{11}^{(3)}} \\
  \frac{b_2^{(3)}}{a_{22}^{(3)}} \\
  \frac{b_3^{(3)}}{a_{33}^{(3)}}
\end{bmatrix}
\]

Upper triangular system

Solve $x_3 = \frac{b_3^{(3)}}{a_{33}^{(3)}}$
GEM: Backward substitution

Eliminate $x_3$ entirely:

\[
\begin{bmatrix}
  a_{11} & a_{12} \\
  0 & a_{22}
\end{bmatrix}
\begin{bmatrix}
  x_1 \\
  x_2
\end{bmatrix} =
\begin{bmatrix}
  b_1^{(3)} - a_{13} x_3 \\
  b_2^{(3)} - a_{23} x_3
\end{bmatrix}
\]

Solve for $x_2 = \frac{\tilde{b}_2}{a_{22}}$, then $x_1$, and done!

Idea: Store the multipliers in the lower triangle of $A$.

Matrix at Step $k$:

\[
\begin{bmatrix}
  L^{(k)} & U^{(k)}
\end{bmatrix}
\]

Example: Step 2
GEM as an \textit{LU} factorization tool

We have actually \textbf{factorized} \textbf{A} as

\[
A = LU,
\]

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

\textbf{GEM} is thus essentially the same as the \textit{LU} \textbf{factorization method}. 
Sample MATLAB code (for learning purposes only, not real computing!):

```matlab
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)

\[ A \times = b \]

\[
\begin{bmatrix}
1 & 1 & 3 \\
2 & 2 & 2 \\
3 & 6 & 4
\end{bmatrix}
\begin{bmatrix}
1 \\
1 \\
1
\end{bmatrix}
=
\begin{bmatrix}
5 \\
6 \\
13
\end{bmatrix}
\Rightarrow
\begin{bmatrix}
1 & 1 & 3 \\
0 & -4 & 0 \\
3 & 3 & -5
\end{bmatrix}
\begin{bmatrix}
1 & 1 & 3 \\
3 & 1 & 3 \\
2 & 0 & 1
\end{bmatrix}
\]

Observe PERTMUTED

\[ LU = A \]
Partial (row) pivoting permutes the rows (equations) of $A$ in order to ensure sufficiently large pivots and thus numerical stability:

$$PA = LU$$

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 and LU factorization

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!
Once an $LU$ factorization is available, solving a linear system is simple:

$$Ax = LUx = L(Ux) = Ly = b$$

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**

$$Ux = y.$$ 

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

$$A = \tilde{L}U = (P^T L) U.$$
In MATLAB, the **backslash operator** (see help on `mldivide`)

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

solves the linear system \( Ax = b \) 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):

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

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

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

\[
L = \\
0.1429 \quad 1.0000 \quad 0 \\
0.5714 \quad 0.5000 \quad 1.0000 \\
1.0000 \quad 0 \quad 0 \\
\]

\[
U = \\
7.0000 \quad 8.0000 \quad 0 \\
0 \quad 0.8571 \quad 3.0000 \\
0 \quad 0 \quad 4.5000 \\
\]

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

>> y = L \ b;

>> x = U \ y; \ x'
\[
ans = \\
-2.5556 \quad 2.1111 \quad 0.1111
\]
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 $A$ the factorization can be reused.
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 $x$ and $b$ to be the natural units $x_0$ and $b_0$.
- Rescaling the unknowns and the equations is generally a good idea even if not necessary:
  \[ x = D_x \tilde{x} = \text{Diag} \{ x_0 \} \tilde{x} \text{ and } b = D_b \tilde{b} = \text{Diag} \{ b_0 \} \tilde{b}. \]
  \[ Ax = AD_x \tilde{x} = D_b \tilde{b} \Rightarrow (D_b^{-1} AD_x) \tilde{x} = \tilde{b} \]
- The rescaled matrix $\tilde{A} = D_b^{-1} AD_x$ should have a better conditioning.
- Also note that reordering the variables from most important to least important may also help.
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.
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. $\forall x \neq 0$, $x^T Ax > 0$, i.e., the quadratic form defined by the matrix $A$ is convex.
3. There exists a \textit{unique} lower triangular $L$, $L_{ii} > 0$, 
$$A = LL^T,$$

termed the \textbf{Cholesky factorization} of $A$ (symmetric $LU$ factorization).

4. For Hermitian complex matrices just replace transposes with adjoints (conjugate transpose), e.g., $A^T \rightarrow A^*$ (or $A^H$ in the book).
The MATLAB built-in function

$$R = \text{chol}(A)$$

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.
- Solving linear systems is as for \(LU\) factorization, replacing \(U\) with \(L^T\).
- 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

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

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 $\text{linsolve}$ instead of backslash if you know (for sure!) something about your matrix.
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**:

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

where the choice of the \(L_2\) norm leads to:

\[
\Phi(x) = (Ax - b)^T (Ax - b).
\]

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 \(b\).
It can be shown that the least-squares solution satisfies:

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

This gives the square linear system of normal equations

$$(A^T A) x^* = A^T b.$$ 

If $A$ is of full rank, $\text{rank}(A) = n$, it can be shown that $A^T A$ is positive definite, and Cholesky factorization can be used to solve the normal equations.

Multiplying $A^T$ ($n \times m$) and $A$ ($m \times n$) takes $n^2$ dot-products of length $m$, so $O(mn^2)$ operations.
Problems with the normal equations

\[(A^T A) \ x^* = A^T b.\]

- The conditioning number of the normal equations is
  \[\kappa (A^T A) = [\kappa (A)]^2\]

- Furthermore, roundoff can cause \(A^T A\) to no longer appear as positive-definite and the Cholesky factorization will fail.

- If the normal equations are ill-conditioned, another approach is needed.
For nonsquare or ill-conditioned matrices of full-rank $r = n \leq m$, the $LU$ factorization can be replaced by the $QR$ factorization:

$$A = QR$$

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

where $Q$ has orthogonal columns, $Q^TQ = I_n$, 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

\[
(A^T A) \; x^* = A^T b \quad \text{where} \quad A = QR
\]

- Observe that \( R \) is the Cholesky factor of the matrix in the normal equations:

\[
A^T A = R^T (Q^T Q) R = R^T R
\]

\[
(R^T R) \; x^* = (R^T Q^T) \; b \quad \Rightarrow \quad x^* = R^{-1} (Q^T b)
\]

which amounts to solving a triangular system with matrix \( R \).

- This calculation turns out to be much more numerically stable against roundoff than forming the normal equations (and has similar cost).
The QR factorization is closely-related to the orthogonalization of a set of $n$ vectors (columns) $\{a_1, a_2, \ldots, a_n\}$ in $\mathbb{R}^m$, which is a common problem in numerical computing.

Classical approach is the **Gram-Schmidt method**: To make a vector $b$ orthogonal to $a$ do:

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

Repeat this in sequence: Start with $\tilde{a}_1 = a_1$, then make $\tilde{a}_2$ orthogonal to $\tilde{a}_1 = a_1$, then make $\tilde{a}_3$ orthogonal to span $(\tilde{a}_1, \tilde{a}_2) = \text{span} (a_1, a_2)$:

$$\tilde{a}_1 = a_1$$

$$\tilde{a}_2 = a_2 - (a_2 \cdot a_1) \frac{a_1}{(a_1 \cdot a_1)}$$

$$\tilde{a}_3 = a_3 - (a_3 \cdot a_1) \frac{a_1}{(a_1 \cdot a_1)} - (a_3 \cdot a_2) \frac{a_2}{(a_2 \cdot a_2)}$$
More efficient formula (standard Gram-Schmidt):

\[
\tilde{a}_{k+1} = a_{k+1} - \sum_{j=1}^{k} (a_{k+1} \cdot q_j) q_j, \quad q_{k+1} = \frac{\tilde{a}_{k+1}}{\|\tilde{a}_{k+1}\|},
\]

with cost \(\approx 2mn^2\) FLOPS but is not numerically stable against roundoff errors (loss of orthogonality).

A numerically stable alternative is the modified Gram-Schmidt, in which each orthogonalization is carried against each of the already-computed basis vectors.

As we saw in previous lecture, a small rearrangement of mathematically-equivalent approaches can produce a much more robust numerical method.
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

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

- 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

\[ A = \begin{bmatrix}
  2 & 0 & 0 & 0 \\
  0 & 4 & 0 & 0 \\
  0 & 0 & 3 & 0 \\
  1 & 2 & 3 & 4
\end{bmatrix} \]

**Sparse matrix**

**Directed Graph representation:**

- Nodes are variables (vertices) or equations
- Arcs (edges) are the non-zero terms

**Undirected graph for symmetric matrices**
Sparse matrices in MATLAB

\[
\begin{align*}
\text{>> } &\ A = \text{sparse}([1\ 2\ 2\ 4\ 4], [3\ 1\ 4\ 2\ 3], 1:5) \\
A &= \\
&\quad (2,1) \quad 2 \\
&\quad (4,2) \quad 4 \\
&\quad (1,3) \quad 1 \\
&\quad (4,3) \quad 5 \\
&\quad (2,4) \quad 3
\end{align*}
\]

\[
\text{>> } \text{nnz}(A) \ % \ Number \ of \ non\text{-}zeros \\
\text{ans} &= 5
\]

\[
\text{>> } \text{whos} \ A \\
A &\quad 4x4 \quad 120 \ double \quad \text{sparse}
\]

\[
\text{>> } A = \text{sparse}([], [], [], 4, 4, 5); \ % \ Pre\text{-}allocate \ memory \\
\text{>> } A(2,1)=2; \ A(4,2)=4; \ A(1,3)=1; \ A(4,3)=5; \ A(2,4)=3;
\]
Sparse matrix factorization

```matlab
>> 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 and columns
>> PBP = B(p,p); spy(PBP);
>> [L,U,P] = lu(PBP); spy(L);
```
The MATLAB function *spy* shows where the nonzeros are as a plot.
Fill-in (generation of lots of nonzeros) is large for a random sparse matrix

\[
\begin{align*}
\text{nz} &= 3552 \\
\text{L for random matrix B} \\
\text{nz} &= 3617 \\
\text{U for random matrix B}
\end{align*}
\]
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**.
In iterative methods the core computation is **iterative matrix-vector multiplication** starting from an **initial guess** $x^{(0)}$.

Prototype is the **linear recursion**:

$$x^{(k+1)} = Bx^{(k)} + f,$$

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 $x = A^{-1}b$ is a **stationary point** of the iteration:

$$x = Bx + f \quad \Rightarrow \quad A^{-1}b = BA^{-1}b + f$$

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

For example, this fixed-point iteration is an iterative method:

$$x^{(k+1)} = (I - A)x^{(k)} + b$$
For this method to be **stable**, and thus **convergent**, the error $e^{(k)} = x^{(k)} - x$ must decrease:

$$e^{(k+1)} = x^{(k+1)} - x = Bx^{(k)} + f - x = B\left(x + e^{(k)}\right) + (I - B)x - x = Be^{(k)}$$

We saw that the error propagates from iteration to iteration as

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

When does this converge? Taking norms,

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

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

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

A. Donev (Courant Institute)
Theorem: The simple iterative method converges iff the spectral radius of the iteration matrix is less than unity:

$$\rho(B) < 1.$$ 

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

$$\rho(A) = \max_\lambda |\lambda| \leq \|A\|$$

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:

$$\rho(A) = \lim_{k \to \infty} \|A^k\|^{1/k}$$
The iterations of an iterative method can be terminated when:

1. The **residual** becomes small,
   \[ \| r^{(k)} \| = \| A x^{(k)} - b \| \leq \varepsilon \| b \| \]
   This is good for well-conditioned systems.

2. The solution \( x^{(k)} \) stops changing, i.e., the **increment** becomes small,
   \[ [1 - \rho(B)] \| e^{(k)} \| \leq \| x^{(k+1)} - x^{(k)} \| \leq \varepsilon \| b \|, \]
   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**.
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 \( Ax = b \) as:

\[ x = (I - A)x + b \]

Fixed-point iteration gives the consistent iterative method

\[ x^{(k+1)} = (I - A)x^{(k)} + b \]
Preconditioning

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

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

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

\[ \mathbf{P}^{-1} \approx A^{-1} \]

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:

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

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

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

- In practice, we solve linear systems with the matrix \( P \) instead of inverting it:

\[ Px^{(k+1)} = (P - A) x^{(k)} + b = Px^{(k)} + r^{(k)}, \]

where \( r^{(k)} = b - Ax^{(k)} \) is the residual vector.

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

\[ x^{(k+1)} = x^{(k)} + P^{-1}r^{(k)}. \]

- Note that convergence will be faster if we have a good initial guess \( x^{(0)} \).
The conditioning of a linear system $Ax = b$ is determined by the condition number

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

Gauss elimination can be used to solve general square linear systems and also produces a factorization $A = LU$.

Partial pivoting is often necessary to ensure numerical stability during GEM and leads to $PA = LU$ or $A = \tilde{LU}$.

MATLAB has excellent linear solvers based on well-known public domain libraries like LAPACK. Use them!
For symmetric positive definite matrices the Cholesky factorization $A = LL^T$ 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.