Deck 1: A Primer on Numerical Linear Algebra

Math 7870: Topics in Randomized Numerical Linear Algebra

Spring 2026

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Notation

Some consistent notation we'll use:

- Non-negative integers: $n, m, p, r \in \mathbb{N}_0$
- Index sets: $[n] = \{1, 2, \ldots, n\}$
- Vectors: $\boldsymbol{v} \in \mathbb{C}^n$ (often we'll specialize to $\mathbb{R}^n$ for notational simplicity)
- Matrices: $\boldsymbol{A} \in \mathbb{C}^{m \times n}$
- Slicing vectors: Given, $S \subset [n]$, then $\boldsymbol{v}_S \in \mathbb{C}^{|S|}$ is the S-sliced entries from $\boldsymbol{v}$
- Slicing matrices: Given, $S \subset [n]$, then $\boldsymbol{A}_{*S} \in \mathbb{C}^{m \times |S|}$ is the S-sliced columns from $\boldsymbol{A}$
- Row slices: $\boldsymbol{A}_{T*}$ for $T \subset [m]$. The matrix $\boldsymbol{A}_{TS}$ also makes sense.
- Matrix (conjugate) transpose/adjoint, determinant, trace: $\boldsymbol{A}^* \in \mathbb{C}^{n \times m}$, $\det(\boldsymbol{A})$, $\operatorname{tr}(\boldsymbol{A})$.
- Standard inner product on vectors: $\langle \boldsymbol{v}, \boldsymbol{w} \rangle = \boldsymbol{w}^* \boldsymbol{v} \in \mathbb{C}$.
- Vectors are orthogonal (in ℓ^2) if $\langle \boldsymbol{v}, \boldsymbol{w} \rangle = 0$.

only for m=n

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Some basic properties:

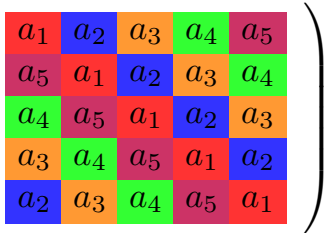
- 1-element slices produces entries: $S = \{i\}$ means $\boldsymbol{v}_S = v_i$. $T = \{j\}$ means $\boldsymbol{A}_{TS} = A_{ji}$.
- $|\det \boldsymbol{A}| = 1$ iff $\boldsymbol{A}$ has orthonormal columns. $(m = n)$
- Norms $\|\cdot\|$ on vectors or matrices are non-negative, order-1 positively homogeneous, convex functions with trivial zero level set. (Cf. the standard ℓ^p norm.)

Matrix classifications and structure

- Square/rectangular/wide/tall
- (skew-)Hermitian
- Unitary/orthogonal ($A^*A = I$, square / $A^TA = I$)
- Normal ($AA^* = A^*A$)
- Diagonalizable
- Sparse
- (Orthogonal) projectors ($P^2 = P$, and possibly $P = P^*$)
- Circulant

Matrix structure is very useful

E.g.: A matrix $\boldsymbol{A} \in \mathbb{C}^{n\times n}$ is *circulant* if it satisfies,



$$\boldsymbol{A} = \begin{pmatrix} a_1 & a_n & a_{n-1} & \cdots & a_2 \\ a_2 & a_1 & a_n & \cdots & a_3 \\ & \ddots & \ddots & \ddots & \\ & & & & \\ a_n & a_{n-1} & a_{n-2} & \cdots & a_1 \end{pmatrix}, \quad \text{i.e.:} \begin{cases} \boldsymbol{A}_{*,i+1} &= \boldsymbol{P}\boldsymbol{A}_{*,i}, \quad i \in [n-1] \\ \boldsymbol{A}_{*,1} &= \boldsymbol{P}\boldsymbol{A}_{*,n}. \end{cases}$$

where $\boldsymbol{P}$ is the down-shift permutation matrix:

$$\boldsymbol{P} = (\boldsymbol{e}_2 \;\; \boldsymbol{e}_2 \;\; \boldsymbol{e}_3 \;\; \ldots \;\; \boldsymbol{e}_n \;\; \boldsymbol{e}_1) = \begin{pmatrix} & & & & 1 \\ 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \end{pmatrix}, \qquad \boldsymbol{P}\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix} = \begin{pmatrix} v_n \\ v_1 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{pmatrix}$$

Note: let ω be an nth root of $\underline{1}$: $\omega^n = \underline{1}$

$\omega = e^{2\pi i j/n}$ for some $j \in [n]$.

$$\underline{v} = \begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix} \qquad \underline{\underline{A}}\,\underline{v} = \begin{pmatrix} a_1 & a_n & \cdots & a_2 \\ a_2 & a_1 & \cdots & a_3 \\ \cdot & & & \\ \cdot & & & \end{pmatrix} \begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix}$$

$$= \begin{pmatrix} a_1 + a_n\omega + a_{n-1}\omega^2 + \cdots + a_2\omega^{n-1} \\ a_2 + a_1\omega + a_n\omega^2 + \cdots + a_3\omega^{n-1} \\ \vdots \end{pmatrix}$$

$\omega^n = 1 \iff \omega^n = \omega^0$ $\qquad \omega^k = \omega^{(k \bmod n)}$

$\omega^{n-1} = \omega^{-1}$

$$= \begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix} \left[a_1 + a_n\omega + a_{n-1}\omega^2 + \cdots + a_2\omega^{n-1}\right]$$

NB: $\underline{v}$ for different ω are linearly indep.

$\Rightarrow \underline{v}_j = \underline{v}$ for $\omega = (e^{2\pi i j/n})$

$\Rightarrow \{v_1 \dots v_n\}$: eigenvectors of $\underline{\underline{A}}$

$$\underbrace{\begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix}}$$: eigenvector matrix of $\underline{\underline{A}}$

Discrete FT matrix

$\Rightarrow$ A is diagonalizable by a DFT (!!)

Matrix structure is very useful

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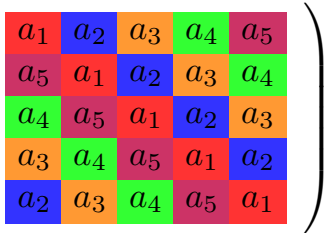

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The punchline: circulant matrices are diagonalizable by the discrete Fourier transform!
(Why is this useful...?)

Why focus on linear algebra?

The canonical reasons:

- Solving linear systems
- Vector manipulation (e.g., orthogonalizing, identifying subspaces)
- Constructing operators: projectors, discretization of differential operators

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Some less obvious reasons:

- Compression, dimension reduction
- High-order optimization schemes
- Low-rank approximations
- Training for AI/LLM/neural architectures

There are "classical" applications where linear algebra is known to be useful (physics-based modeling, classical statistics, computer vision/animation).

But it's quite hard to undersell the importance of (numerical) linear algebra in modern computational applications (data science/analysis, machine learning, language models).

Computational building blocks

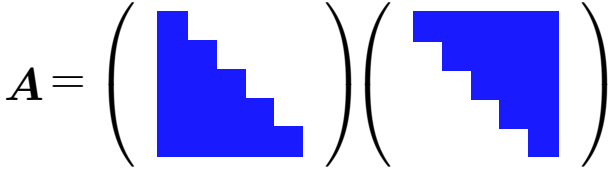
Linear algebra (LA), roughly, studies the mathematics of objects in linear (sub)spaces, which include operators.
(i.e., vectors, matrices, and linear-type operations involving these)

Numerical linear algebra (NLA), roughly, studies computational methods/algorithms that one actually uses to accomplish some linear algebraic operations.
(e.g., computing the determinant of a matrix)

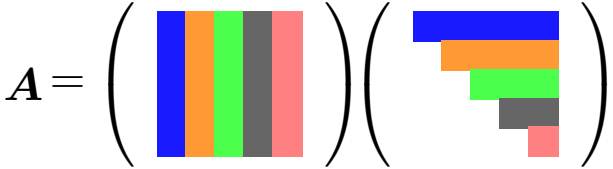
The core, classical components of NLA are matrix decompositions.

Matrix decompositions/factorizations

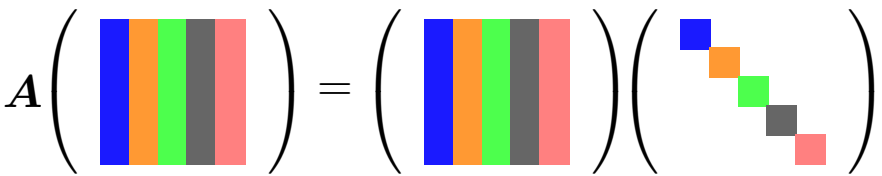
(LU factorization)



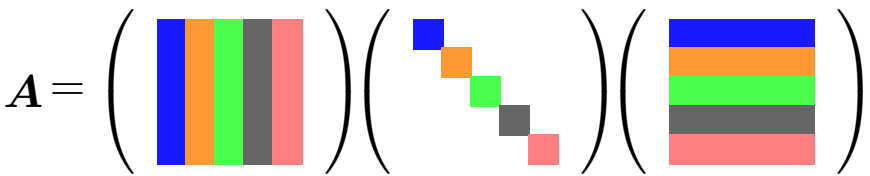
(QR factorization)



(Eigenvalue decomposition)



(Singular value decomposition)



(P)LU

Given $\boldsymbol{A} \in \mathbb{C}^{m \times n}$, its LU decomposition is,

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}, \qquad \boldsymbol{L} \in \mathbb{C}^{m \times p}, \qquad \boldsymbol{U} \in \mathbb{C}^{p \times n}, \qquad p = \min\{m, n\},$$

where $\boldsymbol{L}$ is *lower triangular*, and $\boldsymbol{U}$ is *upper triangular*.

The LU decomposition need not exist for an arbitrary matrix $\boldsymbol{A}$.
(It exists iff $\det \boldsymbol{A}_{[q],[q]} \neq 0$ for all $q \in [p]$.)

$$\underline{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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A more general LU-type decomposition is the *pivoted* LU decomposition. This is one of the decompositions:

$$\begin{aligned}
\boldsymbol{A}\boldsymbol{P}_2 &= \boldsymbol{L}\boldsymbol{U}, & & \boldsymbol{P}_2 \in \mathbb{C}^{n\times n},\\
\boldsymbol{P}_1\boldsymbol{A} &= \boldsymbol{L}\boldsymbol{U}, & \boldsymbol{P}_1 \in \mathbb{C}^{m\times m}, & \\
\boldsymbol{P}_1\boldsymbol{A}\boldsymbol{P}_2 &= \boldsymbol{L}\boldsymbol{U}, & \boldsymbol{P}_1 \in \mathbb{C}^{m\times m}, & \boldsymbol{P}_2 \in \mathbb{C}^{n\times n},
\end{aligned}$$

where both $\boldsymbol{P}_1$ and $\boldsymbol{P}_2$ are row and column *permutation* matrices, respectively.
(A permutation matrix is a unitary matrix, where each row/colunn is a cardinal unit vector.)

Pivoted LU decompositions exist for any matrix.

(P)LU – in practice and uses

The computation of the LU decomposition is "easy": it's Gaussian elimination.
(This is actually how the direct computation is done on a computer.)

The permutations are chosen iteratively so that elements in pivot locations have as large a magnitude as possible.

The most popular pivoting strategy is row(-only) pivoting.

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Why compute an LU decomposition?

- This is how invertible linear systems are solved: $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \longrightarrow \boldsymbol{x} = \boldsymbol{U}^{-1}\boldsymbol{L}^{-1}\boldsymbol{P}^{*}\boldsymbol{b}$.
- This is how "simultaneous" systems are solved (and how matrix inverses are computed).
- This is how determinants are computed: $\det \boldsymbol{A} = (\det \boldsymbol{P}^{*}_{1})(\det \boldsymbol{L})(\det \boldsymbol{U})$.
- This is how (quasi-optimal) low-rank approximations are built. ("skeletonization", "empirical interpolation")
- If $\boldsymbol{A}$ is Hermitian and positive-definite, then its LU decomposition ($\boldsymbol{U} = \boldsymbol{L}^{*}$) is called the *Cholesky decomposition*, which is quite useful when working with these classes of matrices.

QR

Given $\boldsymbol{A} \in \mathbb{C}^{m \times n}$, its QR decomposition is,

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}, \qquad \boldsymbol{Q} \in \mathbb{C}^{m \times m}, \qquad \boldsymbol{R} \in \mathbb{C}^{m \times n},$$

where $\boldsymbol{Q}$ is unitary ($\boldsymbol{Q}^*\boldsymbol{Q} = \boldsymbol{I}_m$), and $\boldsymbol{R}$ is upper triangular.

There is also an "economical"/"thin" QR decomposition, mainly useful when $m > n$, which truncates columns of $\boldsymbol{Q}$ corresponding to all-zero rows of $\boldsymbol{R}$.

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There's also a (column-)pivoted version of QR:

$$\boldsymbol{A}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{R}, \qquad \boldsymbol{P} \in \mathbb{C}^{m \times m},$$

where $\boldsymbol{P}$ is chosen to ensure that the diagonal elements of $\boldsymbol{R}$ are non-decreasing.

increasing

QR – in practice and uses

Explicit computation of the QR decomposition is "just" orthogonalizing the column vectors of $\boldsymbol{A}$. Gram-Schmidt orthogonalization can do this – but this is a numerically unstable procedure.

"Modified" Gram-Schmidt fixes the instability, but is not really used in practice: there are procedures that employ a sequence of *unitary* transforms to compute the QR decomposition:

- Householder reflectors
- Givens rotations

This is how any modern implementation of the QR decomposition works in practice.

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Why compute a QR decomposition?

- To orthogonalize vectors and/or compute orthogonal projection matrices
- This is how one could solve invertible linear systems: $\boldsymbol{Ax} = \boldsymbol{b} \longrightarrow \boldsymbol{x} = \boldsymbol{R}^{-1}\boldsymbol{Q}^*\boldsymbol{b}$.
- This is how one solves (linear) least squares problems: $\boldsymbol{Ax} = \boldsymbol{b} \longrightarrow \boldsymbol{x} = \boldsymbol{R}^{-1}(\boldsymbol{Q}_{*,[n]})^*\boldsymbol{b}$.
- This is a core ingredient in computing eigenvalues (!).

Eigenvalue decompositions

Given $\boldsymbol{A} \in \mathbb{C}^{n \times n}$, its eigenvalue decomposition is given by,

$$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{-1}, \qquad \boldsymbol{V}, \boldsymbol{\Lambda} \in \mathbb{C}^{n \times n},$$

where $\boldsymbol{\Lambda}$ is a diagonal matrix. The diagonal elements of $\boldsymbol{\Lambda}$ are the *eigenvalues* of $\boldsymbol{A}$, and the columns of $\boldsymbol{V}$ are the corresponding *eigenvectors* of $\boldsymbol{A}$.

Square matrices having an eigenvalue decomposition are *diagonalizable*. Not all square matrices are diagonalizable. (But "most" are.)

Diagonalizable matrices are "just" diagonal matrices, when the mapping $\boldsymbol{A}$ is represented in the right coordinate system.

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There is a special class of matrices for which even more is true: $\boldsymbol{A}$ is normal if $\boldsymbol{A}\boldsymbol{A}^* = \boldsymbol{A}^*\boldsymbol{A}$. A matrix is normal iff it's *unitarily diagonalizable*, i.e., is diagonalizable with $\boldsymbol{V}$ a unitary matrix.

Normal matrices are diagonal matrices, when the input/output coordinates are simply rotated/reflected.
(For example, Hermitian and skew-Hermitian matrices are normal.)

Eigenvalue decompositions – in practice and uses

Computing eigenvalues/eigenvectors is a big (+ difficult) business.

When $\boldsymbol{A}$ is normal, the business is not too bad. (Roughly speaking, the spectrum can be computed from $\boldsymbol{A}$ through a well-conditioned operation.)

The so-called "non-symmetric" eigenvalue problem is really hard – computing eigenvalues can be "arbitrarily difficult".

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Here's a vague sense of how QR is used to compute eigenvalues:

- Suppose we knew $\boldsymbol{V}$.
- Compute $\boldsymbol{V} = \boldsymbol{QR}$.
- How could we compute the spectrum of $\boldsymbol{Q}^*\boldsymbol{AQ}$?

$$A = V \Lambda V^{-1}$$
$$= Q R \Lambda R^{-1} Q^*$$

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Why compute eigenvalues?

- Transforming a complicated matrix to a diagonal makes it easy to understand what the matrix is "doing".
- When $\boldsymbol{A}$ is Hermitian and positive-definite, the spectrum tells us a *lot* about how to perform compression and low-rank approximation.
- We can compute singular values....

An interlude: Hermitian positive (semi)-definite matrices

Hermitian matrices $\boldsymbol{A} \in \mathbb{C}^{n\times n}$ that are *positive semi-definite*, i.e., $\boldsymbol{x}^*\boldsymbol{A}\boldsymbol{x} \geqslant \boldsymbol{0}$ for all $\boldsymbol{x}$, are so important that they deserve their own discussion.

The standard abbreviation for these matrices is "SPD". An SPD matrix $\boldsymbol{A}$ has n real eigenvalues:

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n \geqslant 0.$$

These eigenvalues are informative about $\boldsymbol{A}$: $\|\boldsymbol{A}\|_2 = \lambda_1$, and $\boldsymbol{A}$ is singular iff $\lambda_n = 0$.

SPD matrices are ubiquitous, with the simplest examples being covariance matrices, (graph) Laplacian matrices, kernel matrices, Gram matrices, ...

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The cone of Hermitian matrices has a useful partial ordering, the *Loewner order*:

$$\boldsymbol{A} \preceq \boldsymbol{B} \quad \Longleftrightarrow \quad \boldsymbol{B} - \boldsymbol{A} \text{ is SPD}$$

This ordering plays a nice role in matrix functional analysis: A sensible way to define a matrix function is through its spectral decomposition:

$$f : \mathbb{R} \to \mathbb{R}, \quad \boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^*, \quad f(\boldsymbol{A}) := \boldsymbol{U} f(\boldsymbol{\Lambda}) \boldsymbol{U}^* \quad (f(\boldsymbol{\Lambda}) \text{ diagonal, componentwise evaluation}).$$

An interesting question: are there *operator monotone* functions on SPD matrices?
I.e., if $\boldsymbol{A}, \boldsymbol{B} \succeq \boldsymbol{0}$ and $\boldsymbol{A} \preceq \boldsymbol{B}$, is $f(\boldsymbol{A}) \preceq f(\boldsymbol{B})$?

SVD

Given $\boldsymbol{A} \in \mathbb{C}^{m \times n}$, its singular value decomposition (SVD) is,

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^*, \qquad \boldsymbol{U} \in \mathbb{C}^{m \times m}, \qquad \boldsymbol{\Sigma} \in \mathbb{R}^{m \times n}, \qquad \boldsymbol{V} \in \mathbb{C}^{n \times n},$$

where both $\boldsymbol{U}$ and $\boldsymbol{V}$ are unitary, and $\boldsymbol{\Sigma}$ is diagonal with its non-negative entries arranged in non-increasing order.

The diagonal elements of $\boldsymbol{\Sigma}$ are the *singular values*, $\sigma_1, \sigma_2, \ldots, \sigma_p$, with $p = \min\{m, n\}$.

The columns of $\boldsymbol{U}$ and $\boldsymbol{V}$ are the left- and right-singular vectors of $\boldsymbol{A}$, respectively.

Sometimes, the SVD is *truncated* to remove unnecessary columns/rows from $\boldsymbol{U}/\boldsymbol{V}^*$, e.g., those corresponding to zero singluar values.

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Generally, singular values and eigenvalues are unrelated.
E.g., a matrix can have all zero eigenvalues but some non-zero singular values.

Similarly, singular vectors and eigenvectors are generally unrelated.
The SVD and the eigenvalue decomposition of $\boldsymbol{A}$ coincide iff $\boldsymbol{A}$ is Hermitian and positive semi-definite.

SVD – in practice and uses

The SVD is computed through an eigenvalue decomposition of the (normal!) matrix $\boldsymbol{A}^*\boldsymbol{A}$:

$$\boldsymbol{A}\boldsymbol{A}^* = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^*, \qquad \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^2, \qquad \boldsymbol{V}^* = \boldsymbol{\Sigma}^{-1}\boldsymbol{U}^*\boldsymbol{A}$$

For simplicity, we've assumed above that $\boldsymbol{\Sigma}$ is invertible. ($\boldsymbol{\Sigma}$ is invertible iff $\boldsymbol{A}$ has full rank.)

Therefore: computing eigenvalues of Hermitian matrices is sufficient to allow us to compute the SVD.

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Therefore: computing eigenvalues of Hermitian matrices is sufficient to allow us to compute the SVD.

Why compute the SVD?

- The SVD tells you "almost everything" you need to know about a matrix: its (co)range/(co)kernel, its rank, its norm for any unitarily invariant norm.
- One can solve linear systems, solve least-squares problems, compute determinants, determine matrix rank, etc.
- Truncated SVDs are *optimal* low-rank approximations of $\boldsymbol{A}$ in any unitarily invariant norm, and norms of sequence of truncated singular value are corresponding low-rank approximation errors.

Software and implementation

The core routines for computing essentially everything we've discussed is standardized through existing, nearly bulletproof software:

- (BLAS) Basic linear algebra subroutines: low-level addition/subtraction of vectors, scalar multiplication, matrix-vector and matrix-matrix multiplication.
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This is all great: what's the problem?

All of the above is *dense* linear algebra: matrices are stored and manipulated as explicit arrays, where each array entry is explicitly stored and arithmetically exercised.

Modern practice and bottlenecks

The problem: We always want our hammer to smack bigger, tougher nails.

Using these established routines:

- For $n \times n$ matrices, matmat multiplications have $\mathcal{O}(n^3)$ complexity, matvecs are $\mathcal{O}(n^2)$.
- For $\boldsymbol{A} \in \mathbb{C}^{m \times n}$, $m \geqslant n$, computing its LU, QR, or SVD factorizations requires $\mathcal{O}(mn^2)$ effort, with $\mathcal{O}(mn)$ memory.
- For $\boldsymbol{A} \in \mathbb{C}^{n \times n}$, solving a corresponding linear system requires $\mathcal{O}(n^3)$ effort, and $\mathcal{O}(n^2)$ memory.

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For context:

- Datasets often feature $m, n \sim 10^6$.
- ML architectures routinely have 10^6 parameters. (We need to compute matvecs with these parameters, store/use gradients, or maybe even Hessians?)
- In physics-based models, we'd *love* to routinely solve linear systems with $n \gg 10^{10}$.
- Even if matrices/vectors are *sparse* and you can get away with storing them with reasonable memory requirements, many intermediate NLA quantities are dense.
- In general, matrices/vectors do not have special structure/sparsity that we can exploit.

This is the problem: the scale of modern problems defy naive usage of dense NLA procedures.

The potential, pitfalls, and promise of *randomized* NLA

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It is here where *randomized* methods hold promise:

- I can get "close" to the answer by randomly approximating the problem
- I can get "part" of the answer by randomly compressing the problem
- Randomness entails some possibility of failure

The foundation of randomized NLA methods is laid in probability and statistics....