Applied Mathematics 205

Unit 2. Numerical Linear Algebra

Lecturer: Petr Karnakov

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Motivation

- Scientific Computing relies on Numerical Linear Algebra
- We often reformulate problems as $Ax = b$
- Examples from Unit 1:
    - interpolation (Vandermonde matrix) and linear least squares (normal equations) are naturally expressed as linear systems
    - Gauss–Newton method involves approximating a nonlinear problem with a sequence of linear systems
- We will see more applications of linear systems (Numerical Calculus, Optimization, Eigenvalue problems)

Motivation

- The goal of this Unit is to cover:
  - concepts from linear algebra relevant for Scientific Computing
  - stable and efficient algorithms for solving $Ax = b$
  - algorithms for computing factorizations of A

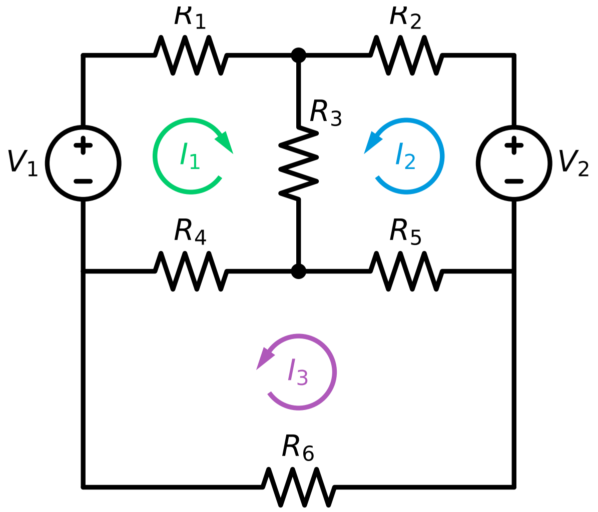
  that are useful in many practical contexts (LU, QR)
- First, we discuss some practical cases where $Ax = b$ arises directly in mathematical modeling of physical systems

Example: Electric Circuits

- Linear systems describe circuits consisting of voltage sources and resistors
  - Ohm's law: Voltage drop V due to current I through a resistor R is

$$V = IR$$

  - Kirchoff's law: Directed sum of the voltages around any closed loop is zero



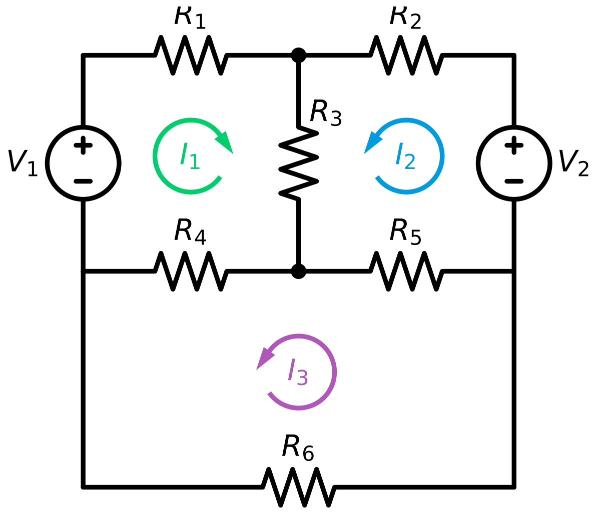
Example: Electric Circuits

- The circuit has three loops
  - Loop 1

    $R_1 I_1 + R_3(I_1 + I_2) + R_4(I_1 + I_3) = V_1$
  - Loop 2

    $R_2 I_2 + R_3(I_1 + I_2) + R_5(I_2 - I_3) = V_2$
  - Loop 3

    $R_5(I_3 - I_2) + R_4(I_3 + I_1) + R_6 I_3 = 0$



Example: Electric Circuits

- We obtain a linear system for unknown currents I_1, I_2, I_3

$$\begin{bmatrix} R_1 + R_3 + R_4 & R_3 & R_4 \\ R_3 & R_2 + R_3 + R_5 & -R_5 \\ R_4 & -R_5 & R_4 + R_5 + R_6 \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ I_3 \end{bmatrix} = \begin{bmatrix} V_1 \\ V_2 \\ 0 \end{bmatrix}$$

- Note that the matrix is
  - symmetric, i.e. $a_{ij} = a_{ji}$
  - strictly diagonally dominant, i.e. $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$ (assuming $R_k > 0$)
- Circuit simulators solve large linear systems of this type

Example: Electric Circuits

- Another linear system corresponds to unknown resistances R_i, $i = 1, \dots, 6$

$$\begin{bmatrix} I_1 & 0 & I_1 + I_2 & I_1 & 0 & 0 \\ 0 & I_2 & I_2 & 0 & -I_3 & 0 \\ 0 & 0 & 0 & I_1 + I_3 & -I_2 & I_3 \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \\ R_6 \end{bmatrix} = \begin{bmatrix} V_1 \\ V_2 \\ 0 \end{bmatrix}$$

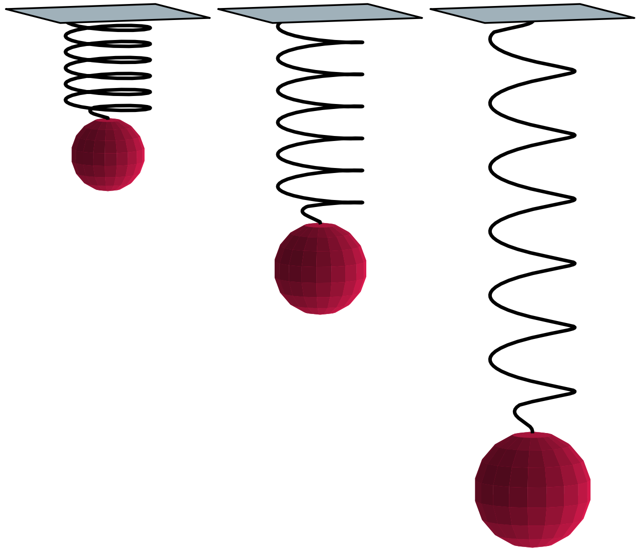
- Note that the matrix has full rank (assuming $I_k \neq 0$)
- The system is underdetermined: 3 equations for 6 unknowns

Example: Structural Analysis

- Common in structural analysis is to use a linear relationship between force and displacement, Hooke's law
- Simplest case is the Hookean spring law

$$F = kx$$

  - k: spring constant (stiffness)
  - F: applied load
  - x: spring extension (displacement)



Example: Structural Analysis

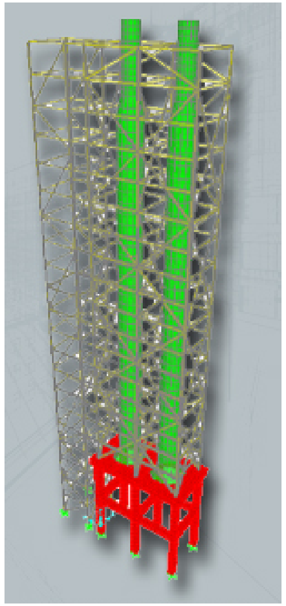
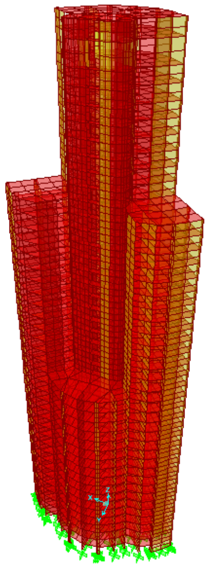
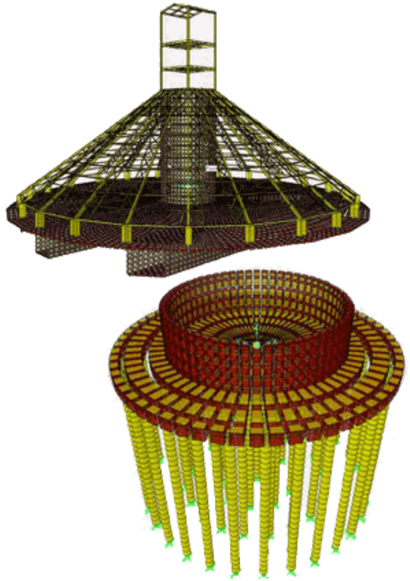
- This relationship can be generalized to structural systems in 2D and 3D, which yields a linear system of the form

$$Kx = F$$

  - $K \in \mathbb{R}^{n \times n}$: “stiffness matrix”
  - $F \in \mathbb{R}^{n}$: “load vector”
  - $x \in \mathbb{R}^{n}$: “displacement vector”

Example: Structural Analysis

- It is common engineering practice to use Hooke's law to simulate complex structures, which leads to large linear systems

(from SAP2000, structural analysis software)

Example: Economics

- Leontief awarded Nobel Prize in Economics in 1973 for developing a linear input/output model for production/consumption of goods
- Consider an economy in which n goods are produced and consumed
  - $A \in \mathbb{R}^{n \times n}$: a_{ij} represents
    the amount of good j required to produce a unit of good i
  - $x \in \mathbb{R}^n$: x_i is number of units of good i produced
  - $d \in \mathbb{R}^n$: d_i is consumer demand for good i
- In general $a_{ii} = 0$, and A may be sparse

Example: Economics

- The total amount of x_i produced is given by the sum of consumer demand d_i and the amount of x_i required to produce each x_j

$$x_i = \underbrace{a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n}_{\text{production of other goods}} + d_i$$

- Hence $x = Ax + d$ or,

$$(\mathrm{I} - A)x = d$$

- Solve for x to determine the required amount of production of each good
- If we consider many goods (e.g. an entire economy), then we get a large linear system
- Can be used to predict the effect of disruptions in the supply chain

Summary

- Matrix computations are very common
- Numerical Linear Algebra provides us with a toolbox
  for performing these computations in an efficient and stable manner
- In most cases, we can use these tools as a black box,
  but it's important to understand what they do
  - pick the right algorithm for a given situation
    (e.g. exploit structure of a problem: symmetry, sparsity, etc)
  - understand how and when the algorithm fail

Preliminaries

Preliminaries

- In this section we will focus on linear systems

$$Ax = b$$

with matrix $A \in \mathbb{R}^{n\times n}$, unknown vector $x \in \mathbb{R}^n$
and the right-hand side vector $b \in \mathbb{R}^n$

- Recall that it is often helpful to think of matrix multiplication as a linear combination of the columns of A, where x_j are the coefficients
- That is, we have

$$Ax = \sum_{j=1}^{n} x_j a_{(:,j)}$$

where $a_{(:,j)} \in \mathbb{R}^n$ is the j-th column of A and x_j are scalars

Preliminaries

- This can be displayed schematically as

$$Ax = \left[\begin{array}{c|c|c|c} \\ a_{(:,1)} & a_{(:,2)} & \cdots & a_{(:,n)} \\ \\ \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} =$$

$$= \; x_1 \begin{bmatrix} \\ a_{(:,1)} \\ \\ \end{bmatrix} + \cdots + \; x_n \begin{bmatrix} \\ a_{(:,n)} \\ \\ \end{bmatrix}$$

Preliminaries

- We therefore interpret $Ax = b$ as:
  "x is the vector of coordinates of b in the basis of columns of A"
- Often this is a more helpful point of view than conventional interpretation of "dot-product of matrix row with vector"
- Now we see that $Ax = b$ has a solution if

$$b \in \mathrm{span}\{a_{(:,1)}, a_{(:,2)}, \cdots, a_{(:,n)}\}$$

  (this holds even for a non-square A)
- Denote

$$\mathrm{image}(A) = \mathrm{span}\{a_{(:,1)}, a_{(:,2)}, \cdots, a_{(:,n)}\}$$

Preliminaries

Existence and Uniqueness

- If $b \in \text{image}(A)$, then solution $x \in \mathbb{R}^n$ exists
  - if solution x exists and the columns $\{a_{(:,1)}, a_{(:,2)}, \cdots, a_{(:,n)}\}$ are linearly independent, then x is unique
    (if x and y are both solutions, then $A(x-y) = 0$, therefore $x = y$)
  - if x is a solution and $z \neq 0$ is such that $Az = 0$,
    then also $A(x + \gamma z) = b$ for any $\gamma \in \mathbb{R}$,
    so there are infinitely many solutions
- If $b \notin \text{image}(A)$ then $Ax = b$ has no solution

Preliminaries

- The inverse map $A^{-1}\colon \mathbb{R}^n \to \mathbb{R}^n$ is well-defined if and only if $Ax = b$ has unique solution for any $b \in \mathbb{R}^n$
- The inverse matrix $A^{-1} \in \mathbb{R}^{n\times n}$ such that $AA^{-1} = A^{-1}A = I$ exists if any of the following equivalent conditions are satisfied
  - $\det(A) \neq 0$
  - $\mathrm{rank}(A) = n$
  - $Az \neq 0$ for any $z \neq 0$ (null space of A is $\{0\}$)
- A is nonsingular if A^{-1} exists, and then $x = A^{-1}b \in \mathbb{R}^n$
- A is singular if A^{-1} does not exist

Norms

- A norm $\|\cdot\| : V \to \mathbb{R}$ is a function on a vector space V that satisfies
  - positive definiteness, $\|x\| \geq 0$ and $\|x\| = 0 \implies x = 0$
  - absolute homogeneity, $\|\gamma x\| = |\gamma|\|x\|$, for $\gamma \in \mathbb{R}$
  - triangle inequality, $\|x + y\| \leq \|x\| + \|y\|$

Norms

- The triangle inequality implies another helpful inequality: the "reverse triangle inequality"

$$\big|\|x\| - \|y\|\big| \leq \|x - y\|$$

- Proof:

$$\|x\| = \|(x-y) + y\| \leq \|x - y\| + \|y\| \implies \|x\| - \|y\| \leq \|x - y\|$$

$$\|y\| = \|(y-x) + x\| \leq \|y - x\| + \|x\| \implies \|y\| - \|x\| \leq \|x - y\|$$

- Therefore $\big|\|x\| - \|y\|\big| \leq \|x - y\|$

Vector Norms

- Let's now introduce some common norms on $\mathbb{R}^n$
- Most common norm is the Euclidean norm (or 2-norm):

$$\|x\|_2 = \sqrt{\textstyle\sum_{j=1}^{n} x_j^2}$$

- 2-norm is special case of the p-norm for any $p \geq 1$:

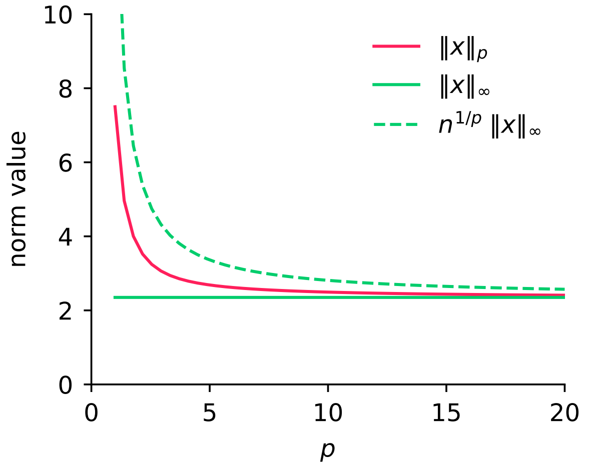
$$\|x\|_p = \left(\textstyle\sum_{j=1}^{n} |x_j|^p\right)^{1/p}$$

- Condition $p \geq 1$ is required for the triangle inequality
- Norm $\|x\|_p$ approaches $\|x\|_\infty$ as $p \to \infty$

$$\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$$

Example: Limit of p-norm

- See [examples/unit2/norm_inf.py]
- For vector $x = (1.2, 0.5, -0.1, 2.3, -1.05, -2.35)^T \in \mathbb{R}^6$
- $\|x\|_\infty = 2.35$ (component of x with the largest magnitude)
- Norm $\|x\|_p$ approaches $\|x\|_\infty$ as $p \to \infty$
- Bounds: $\|x\|_\infty \leq \|x\|_p \leq n^{1/p}\|x\|_\infty$



Vector Norms

- We generally use whichever norm is most convenient/appropriate for a given problem, e.g. 2-norm for least-squares analysis
- Different norms give different (but related) measures of size
- An important fact is:

  All norms on a finite dimensional space (such as $\mathbb{R}^n$) are equivalent

Vector Norms

- That is, let $\|\cdot\|_a$ and $\|\cdot\|_b$ be two norms on a finite dimensional space V, then $\exists\ c_1, c_2 > 0$ such that for any $x \in V$

$$c_1\|x\|_a \leq \|x\|_b \leq c_2\|x\|_a$$

- Also, from above we have $\frac{1}{c_2}\|x\|_b \leq \|x\|_a \leq \frac{1}{c_1}\|x\|_b$
- Hence if we can derive an inequality in one norm on V, it applies (after appropriate scaling) in any other norm as well

Vector Norms

- Norm $\|x\|_2$ bounds norm $\|x\|_1$

$$\|x\|_2 \le \|x\|_1 \le \sqrt{n}\|x\|_2$$

- Proof of $\|x\|_2 \le \|x\|_1$

$$\|x\|_1^2 = \left(\sum_{i=1}^n |x_i|\right)^2 = \left(\sum_{i=1}^n |x_i|\right)\left(\sum_{j=1}^n |x_j|\right) =$$
$$= \sum_{i=1}^n \sum_{j=1}^n |x_i|\,|x_j| \ge \sum_{i=1}^n |x_i|\,|x_i| = \sum_{i=1}^n |x_i|^2 = \|x\|_2^2$$

- Proof of $\|x\|_1 \le \sqrt{n}\|x\|_2$. The Cauchy-Schwarz inequality

$$\sum_{i=1}^n a_i b_i \le \left(\sum_{i=1}^n a_i^2\right)^{1/2}\left(\sum_{i=1}^n b_i^2\right)^{1/2}$$

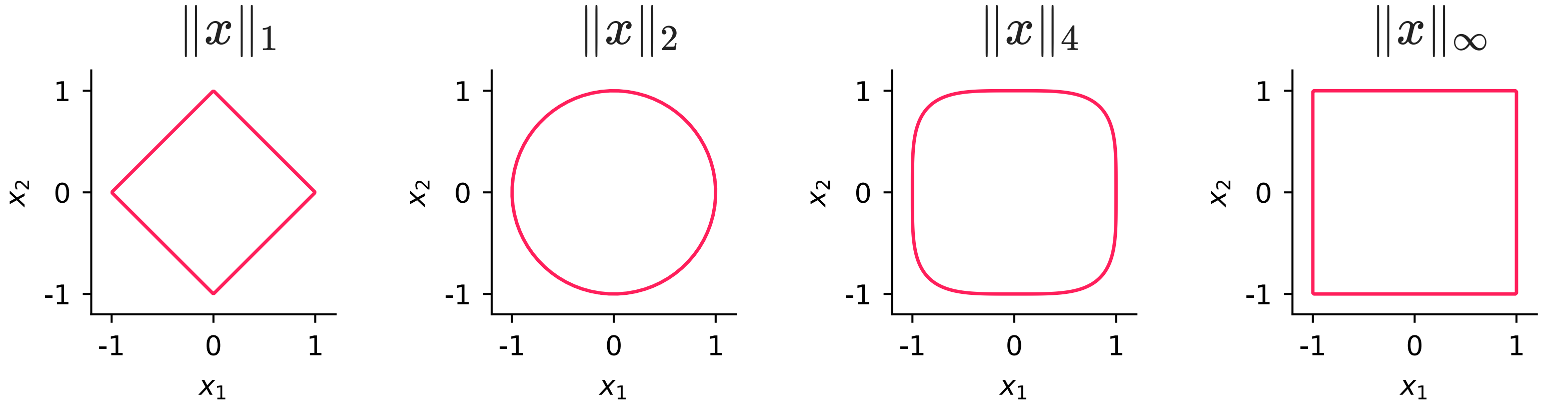
with $a_i = 1$ and $b_i = |x_i|$ gives

$$\|x\|_1 = \sum_{i=1}^n 1\,|x_i| \le \left(\sum_{i=1}^n 1^2\right)^{1/2}\left(\sum_{i=1}^n |x_i|^2\right)^{1/2} = \sqrt{n}\,\|x\|_2$$

Vector Norms

- Each norm produces a different unit circle

$$\{x \in \mathbb{R}^2 : \|x\|_p = 1\}$$



- Norm $\|x\|_p$ approaches $\|x\|_\infty$ as $p \to \infty$
- Commonly used norms are $\|x\|_1$, $\|x\|_2$, and $\|x\|_\infty$

Matrix Norms

- There are many ways to define norms on matrices
- For example, the Frobenius norm is defined as

$$\|A\|_F = \left(\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2}$$

- If we think of A as a vector in $\mathbb{R}^{n^2}$,
  then Frobenius is equivalent to the vector 2-norm of A

Matrix Norms

- Matrix norms induced by vector norms are most useful
- Here, matrix p-norm is induced by vector p-norm

$$\|A\|_p = \max_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p} = \max_{\|x\|_p = 1} \|Ax\|_p$$

- This definition implies the useful property

$$\|Ax\|_p \leq \|A\|_p \|x\|_p$$

since

$$\|Ax\|_p = \frac{\|Ax\|_p}{\|x\|_p} \|x\|_p \leq \left(\max_{v \neq 0} \frac{\|Av\|_p}{\|v\|_p} \right) \|x\|_p = \|A\|_p \|x\|_p$$

Matrix Norms

- The 1-norm and ∞-norm can be calculated straightforwardly:

$$\|A\|_1 = \max_{1\le j\le n} \|a_{(:,j)}\|_1 \qquad \text{(max column sum)}$$

$$\|A\|_\infty = \max_{1\le i\le n} \|a_{(i,:)}\|_1 \qquad \text{(max row sum)}$$

- Later we will see how to compute the 2-norm of a matrix

Example: Matrix Norm Using Monte Carlo

- How to compute the matrix norm induced by a "black box" vector norm?
- One approach is the Monte-Carlo method
  that solves problems using repeated random sampling
- Recall the definition of a matrix norm induced by vector norm

$$\|A\| = \max_{x \neq 0} \frac{\|Ax\|}{\|x\|}$$

- See [examples/unit2/norm_monte_carlo.py]
- Warning: Common norms can be computed with more efficient methods!

Condition Number

- Recall from Unit 0 that the condition number of $A \in \mathbb{R}^{n\times n}$ is defined as

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

- The value of $\kappa(A)$ depends on which norm we use
- `numpy.linalg.cond` computes the condition number for various norms
- If A is a singular square matrix, then by convention $\kappa(A) = \infty$

Residual

- Recall that the residual $r(x) = b - Ax$
  was crucial in least-squares problems
- It is also crucial in assessing the accuracy
  of a proposed solution ($\hat{x}$) to a linear system $Ax = b$
- Key point: The residual $r(\hat{x})$ is straightforward to compute,
  while the error $\Delta x = x - \hat{x}$ is not (without knowing the exact solution)

Residual

- We have that $\|\Delta x\| = \|x - \hat{x}\| = 0$ if and only if $\|r(\hat{x})\| = 0$
- However, small residual doesn't necessarily imply small $\|\Delta x\|$
- Observe that

$$\|\Delta x\| = \|x - \hat{x}\| = \|A^{-1}(b - A\hat{x})\| = \|A^{-1} r(\hat{x})\| \le \|A^{-1}\| \|r(\hat{x})\|$$

Hence

$$\frac{\|\Delta x\|}{\|\hat{x}\|} \le \frac{\|A^{-1}\| \|r(\hat{x})\|}{\|\hat{x}\|} = \frac{\|A\| \|A^{-1}\| \|r(\hat{x})\|}{\|A\| \|\hat{x}\|} = \kappa(A) \frac{\|r(\hat{x})\|}{\|A\| \|\hat{x}\|} \qquad (*)$$

Residual

- Define the relative residual as

$$\frac{\|r(\hat{x})\|}{\|A\|\|\hat{x}\|}$$

- Then our inequality $(*)$ states that
"relative error is bounded by condition number times the relative residual"
- This is just like our condition number relationship from Unit 0:

$$\kappa(A) \geq \frac{\|\Delta x\|/\|x\|}{\|\Delta b\|/\|b\|}, \qquad \text{i.e.} \qquad \frac{\|\Delta x\|}{\|x\|} \leq \kappa(A)\frac{\|\Delta b\|}{\|b\|} \qquad (**)$$

- The reason $(*)$ and $(**)$ are related is that
the residual measures the input pertubation (Δb) in $Ax = b$
- To see this, let's consider $Ax = b$ to be a map $b \in \mathbb{R}^n \to x \in \mathbb{R}^n$

Residual

- Then we can consider $\hat{x}$ to be the exact solution for some perturbed input $\hat{b} = b + \Delta b$

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

- The residual associated with $\hat{x}$ is

$$r(\hat{x}) = b - A\hat{x} = b - \hat{b} = -\Delta b$$

  i.e. $\|r(\hat{x})\| = \|\Delta b\|$
- In general, a (backward) stable algorithm gives us the exact solution to a slightly perturbed problem, i.e. a small residual
- This is a reasonable expectation for a stable algorithm: rounding error doesn't accumulate, so effective input perturbation is small

Example: Residual vs. Error

- From Heath's book (Example 2.8)
- Consider a 2×2 example to clearly demonstrate the difference between residual and error

$$Ax = \begin{bmatrix} 0.913 & 0.659 \\ 0.457 & 0.330 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.254 \\ 0.127 \end{bmatrix} = b$$

- The exact solution is given by $x = [1, -1]^T$
- Suppose we compute two different approximate solutions

$$\hat{x}^{(1)} = \begin{bmatrix} -0.0827 \\ 0.5 \end{bmatrix}, \qquad \hat{x}^{(2)} = \begin{bmatrix} 0.999 \\ -1.001 \end{bmatrix}$$

Example: Residual vs. Error

- Then,

$$\|r(\hat{x}^{(1)})\|_1 = 2.1 \times 10^{-4}, \qquad \|r(\hat{x}^{(2)})\|_1 = 2.4 \times 10^{-2}$$

- but

$$\|x - \hat{x}^{(1)}\|_1 = 2.58, \qquad \|x - \hat{x}^{(2)}\|_1 = 0.002$$

- In this case, $\hat{x}^{(2)}$ is better solution, but has larger residual!
- This is possible here because $\kappa(A) = 1.25 \times 10^4$ is quite large (relative error $\leq 1.25 \times 10^4 \times$ relative residual)

Solving $Ax = b$

Solving $Ax = b$

- Familiar idea for solving $Ax = b$ is to use Gaussian elimination to transform $Ax = b$ to a triangular system
- What is a triangular system?
  - upper triangular $U \in \mathbb{R}^{n\times n}$

$$u_{ij} = 0 \text{ for } i > j$$

$$U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

  - lower triangular $L \in \mathbb{R}^{n\times n}$

$$\ell_{ij} = 0 \text{ for } i < j$$

$$L = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix}$$

- Question: Why triangular?
- Answer: Because triangular systems are easy to solve!

Solving $Ax = b$

- For an upper-triangular system $Ux = b$, we can use backward substitution

$$\begin{aligned}
x_n &= b_n / u_{nn} \\
x_{n-1} &= (b_{n-1} - u_{n-1,n} x_n) / u_{n-1,n-1} \\
\ldots \\
x_j &= \left(b_j - \textstyle\sum_{k=j+1}^{n} u_{jk} x_k \right) / u_{jj}
\end{aligned}$$

Solving $Ax = b$

- For a lower triangular system $Lx = b$, we can use forward substitution

$$\begin{aligned} x_1 &= b_1/\ell_{11} \\ x_2 &= (b_2 - \ell_{21}x_1)/\ell_{22} \\ &\ldots \\ x_j &= \left(b_j - \textstyle\sum_{k=1}^{j-1} \ell_{jk}x_k\right)/\ell_{jj} \end{aligned}$$

Asymptotic Notation

- To simplify the cost estimation for an algorithm, we analyze its asymptotic behavior as the size of the problem increases ($n \to \infty$)
- Notation $f(n) \sim g(n)$ refers to asymptotic equivalence

$$\lim_{n\to\infty} \frac{f(n)}{g(n)} = 1$$

- Notation $f(n) = \mathcal{O}(g(n))$ refers to an asymptotic upper bound

$$|f(n)| \leq M|g(n)|$$

  for all $n \geq N$, where $M > 0$ and $N > 0$
- If $f(n) \sim g(n)$, then $f(n) = \mathcal{O}(g(n))$. The opposite is not true!
- We prefer "$\sim$" since it indicates the scaling factor of the leading term
- For example, if $f(n) = n^2/4 + n$, then $f(n) = \mathcal{O}(n^2)$, whereas $f(n) \sim n^2/4$

Solving $Ax = b$

- Backward (and forward) substitution
  can be implemented with a double nested loop
- It requires just one pass through the matrix!
- The computational work is dominated by evaluating the sum

$$\sum_{k=1}^{j-1} \ell_{jk} x_k \quad j = 1, \ldots, n$$

  which takes $j - 1$ additions and multiplications for each j
- So the total number of floating point operations is asymptotically

$$2 \sum_{j=1}^{n} j = \frac{2n(n+1)}{2} \sim n^2$$

Solving $Ax = b$

- How can we transform $Ax = b$ to a triangular system?
- Observation: If we multiply $Ax = b$ by a nonsingular matrix M, then the new system $MAx = Mb$ has the same solution
- We can devise a sequence of matrices

$$M_1, M_2, \ldots, M_{n-1}$$

  such that $M = M_{n-1} \ldots M_1$ and $U = MA$ is upper triangular
- Gaussian elimination provides such a sequence and gives the transformed system $Ux = Mb$

LU Factorization

- We will show shortly that if $MA = U$, then $L = M^{-1}$ is lower triangular
- Therefore, we obtain that the matrix factorizes into

$$A = M^{-1}U = LU$$

  a product of lower (L) and upper (U) triangular matrices
- This is the LU factorization of A

LU Factorization

- LU factorization is a common way of solving linear systems!
- Once a factorization $A = LU$ is known, the system

$$LUx = b$$

  is solved in two steps
  - lower triangular: $Ly = b$
  - upper triangular: $Ux = y$

LU Factorization

- Next question: How can we find $M_1, M_2, \cdots, M_{n-1}$?
- We need to be able to annihilate selected entries of A below the diagonal in order to obtain an upper-triangular matrix
- To do this, we use elementary elimination matrices
- Let L_j denote j-th elimination matrix
- From now on, we denote them L_j rather than M_j since elimination matrices are lower triangular

LU Factorization

- Here we describe how to proceed from step $j-1$ to step j
- Let $X = L_{j-1}L_{j-2}\cdots L_1 A$ denote the matrix at the start of step j, and $x_{(:,k)} \in \mathbb{R}^n$ denote column k of X

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1,j-1} & x_{1j} & x_{1,j+1} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & x_{j-1,j-1} & x_{j-1,j} & x_{j-1,j+1} & \cdots & x_{j-1,n} \\ 0 & \cdots & 0 & x_{jj} & x_{j,j+1} & \cdots & x_{jn} \\ 0 & \cdots & 0 & x_{j+1,j} & x_{j+1,j+1} & \cdots & x_{j+1,n} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & x_{nj} & x_{n,j+1} & \cdots & x_{nn} \end{bmatrix}$$

LU Factorization

- We are looking for a matrix L_j such that multiplication $L_j X$
  - eliminates elements below the diagonal in $x_{(:,j)}$
  - does not modify columns $x_{(:,k)}$ for $k = 1, \dots, j-1$
- Let's define L_j such that

$$L_j x_{(:,j)} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -x_{j+1,j}/x_{jj} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -x_{nj}/x_{jj} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_{1j} \\ \vdots \\ x_{jj} \\ x_{j+1,j} \\ \vdots \\ x_{nj} \end{bmatrix} = \begin{bmatrix} x_{1j} \\ \vdots \\ x_{jj} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

LU Factorization

- For brevity, we denote $\ell_{ij} = x_{ij}/x_{jj}$ and define

$$L_j = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -\ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -\ell_{nj} & 0 & \cdots & 1 \end{bmatrix}$$

LU Factorization

- Using elementary elimination matrices, we can reduce A to an upper triangular form, one column at a time
- Schematically, for a 4×4 matrix, we have

$$\underset{A}{\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}} \xrightarrow{L_1} \underset{L_1 A}{\begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix}} \xrightarrow{L_2} \underset{L_2 L_1 A}{\begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{bmatrix}}$$

- Key point: L_j does not modify columns $1, \ldots, j-1$ of $L_{j-1} L_{j-2} \cdots L_1 A$

LU Factorization

- After $n-1$ steps, we obtain an upper triangular matrix

$$U = L_{n-1} \cdots L_2 L_1 A = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix}$$

LU Factorization

- We have $L_{n-1} \cdots L_2 L_1 A = U$
- To form a factorization $A = LU$,
  we need $L = (L_{n-1} \cdots L_2 L_1)^{-1} = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$
- First observation:
  L_j^{-1} is obtained by negating the subdiagonal elements of L_j

$$L_j = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -\ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -\ell_{nj} & 0 & \cdots & 1 \end{bmatrix} \qquad L_j^{-1} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & \ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \ell_{nj} & 0 & \cdots & 1 \end{bmatrix}$$

LU Factorization

- $L_j L_j^{-1} = I$ can be verified directly by multiplication
- Intuitive explanation
  - multiplication $L_j v$ subtracts a scaled component v_j
  - so the inverse should add it back (v_j itself is unchanged)

$$L_j \begin{bmatrix} v_1 \\ \vdots \\ v_j \\ v_{j+1} \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} v_1 \\ \vdots \\ v_j \\ v_{j+1} - \ell_{j+1,j} v_j \\ \vdots \\ v_n - \ell_{nj} v_j \end{bmatrix} \qquad L_j^{-1} \begin{bmatrix} v_1 \\ \vdots \\ v_j \\ v_{j+1} \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} v_1 \\ \vdots \\ v_j \\ v_{j+1} + \ell_{j+1,j} v_j \\ \vdots \\ v_n + \ell_{nj} v_j \end{bmatrix}$$

LU Factorization

- Second observation: consider $L_{j-1}^{-1} L_j^{-1}$

$$\underbrace{\begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & \ell_{j,j-1} & 1 & 0 & \cdots & 0 \\ 0 & \cdots & \ell_{j+1,j-1} & 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \ell_{n,j-1} & 0 & 0 & \cdots & 1 \end{bmatrix}}_{L_{j-1}^{-1}} \underbrace{\begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \ell_{nj} & 0 & \cdots & 1 \end{bmatrix}}_{L_j^{-1}} = \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & \ell_{j,j-1} & 1 & 0 & \cdots & 0 \\ 0 & \cdots & \ell_{j+1,j-1} & \ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \ell_{n,j-1} & \ell_{nj} & 0 & \cdots & 1 \end{bmatrix}$$

LU Factorization

- Therefore, by generalizing to all $n-1$ matrices

$$L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{n1} & \ell_{n2} & \cdots & \ell_{n,n-1} & 1 \end{bmatrix}$$

- So we simply collect the subdiagonal terms from all steps of factorization

LU Factorization

- Therefore, basic LU factorization algorithm is

```
1: $U = A, L = \mathrm{I}$
2: **for** $j = 1 : n-1$ **do**
3:     **for** $i = j+1 : n$ **do**
4:         $\ell_{ij} = u_{ij}/u_{jj}$
5:         **for** $k = j : n$ **do**
6:             $u_{ik} = u_{ik} - \ell_{ij} u_{jk}$
7:         **end for**
8:     **end for**
9: **end for**
```

- Note that the entries of U are updated each iteration so at the start of step j, $U = L_{j-1} L_{j-2} \cdots L_1 A$
- Here line 4 comes straight from the definition $\ell_{ij} = \frac{u_{ij}}{u_{jj}}$

LU Factorization

- Line 6 accounts for the effect of L_j on columns $k = j, \ldots, n$ of U
- For $k = j : n$ we have

$$L_j u_{(:,k)} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -\ell_{j+1,j} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -\ell_{nj} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{1k} \\ \vdots \\ u_{jk} \\ u_{j+1,k} \\ \vdots \\ u_{nk} \end{bmatrix} = \begin{bmatrix} u_{1k} \\ \vdots \\ u_{jk} \\ u_{j+1,k} - \ell_{j+1,j} u_{jk} \\ \vdots \\ u_{nk} - \ell_{nj} u_{jk} \end{bmatrix}$$

- The right hand side is the updated k-th column of U, which is computed in line 6

LU Factorization

- LU factorization involves a triple nested loop, hence $\mathcal{O}(n^3)$ operations
- Careful operation counting shows LU factorization requires
  - $\sim \frac{1}{3}n^3$ additions
  - $\sim \frac{1}{3}n^3$ multiplications
- Therefore $\sim \frac{2}{3}n^3$ operations in total

Solving Linear Systems Using LU

- To solve $Ax = b$, we perform the following three steps:
  - Step 1: Factorize A into $A = LU$: $\sim \frac{2}{3}n^3$
  - Step 2: Solve $Ly = b$ by forward substitution: $\sim n^2$
  - Step 3: Solve $Ux = y$ by backward substitution: $\sim n^2$
- The total work, dominated by Step 1, is $\sim \frac{2}{3}n^3$

Solving Linear Systems Using LU

- An alternative approach would be to first compute A^{-1} and evaluate $x = A^{-1}b$, but this is a bad idea!
- Question: How would we compute A^{-1}?

Solving Linear Systems Using LU

- Answer: Let $a^{\text{inv}}_{(:,k)}$ denote the k-th column of A^{-1}, then $a^{\text{inv}}_{(:,k)}$ must satisfy

$$Aa^{\text{inv}}_{(:,k)} = e_k$$

  where e_k is the k-th basis vector
- Therefore, inverting matrix A reduces to solving $Ax = b$ for n various b
- We first factorize $A = LU$, then forward/backward substitute for

$$LUa^{\text{inv}}_{(:,k)} = e_k, \quad k = 1, \ldots, n$$

Solving Linear Systems Using LU

- Solving linear systems using A^{-1} is inefficient!
  - one pair of substitutions requires $\sim 2n^2$ operations
  - n pairs of substitutions require $\sim 2n^3$ operations
  - evaluating $A^{-1}b$ takes $\sim 2n^2$ operations
    (as many as one pair of substitutions)
- A rule of thumb in Numerical Linear Algebra:
  It is rarely a good idea to compute A^{-1} explicitly

Solving Linear Systems Using LU

- Another case where LU factorization is very helpful is if we want to solve $Ax = b_i$ for several different right-hand sides b_i, $i = 1, \ldots, k$
- We incur the $\sim \frac{2}{3}n^3$ cost only once, and then each subsequent pair of forward/backward substitutions costs only $\sim 2n^2$
- Makes a huge difference if n is large!

Stability of Gaussian Elimination

- There is a problem with the LU algorithm presented above
- Consider the matrix

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

- A is nonsingular, well-conditioned ($\kappa(A) \approx 2.62$)
  but LU factorization fails at first step (division by zero)

Stability of Gaussian Elimination

- LU factorization doesn't fail for

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$$

but we get

$$L = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1 - 10^{20} \end{bmatrix}$$

Stability of Gaussian Elimination

- Let's suppose that $-10^{20} \in \mathbb{F}$ (a floating point number) and that $\text{round}(1 - 10^{20}) = -10^{20}$
- Then in finite precision arithmetic we get

$$\widetilde{L} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \qquad \widetilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$$

Stability of Gaussian Elimination

- Hence due to rounding error we obtain

$$\widetilde{L}\widetilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 0 \end{bmatrix}$$

  which is not close to

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$$

- Then, for example, let $b = [3, 3]^T$
  - using $\widetilde{L}\widetilde{U}$, we get $\tilde{x} = [3, 3]^T$
  - true answer is $x = [0, 3]^T$
- The relative error is large
  even though the problem is well-conditioned

Stability of Gaussian Elimination

- In this example, standard Gaussian elimination yields a large residual
- Or equivalently, it yields the exact solution to a problem corresponding to a large input perturbation: $\Delta b = [0, 3]^T$
- So the algorithm is unstable!
- In this case the cause of the large error in x is numerical instability, not ill-conditioning
- To stabilize Gaussian elimination, we need to permute rows, i.e. perform pivoting

Pivoting

- Recall the Gaussian elimination process

$$\begin{bmatrix} * & * & * & * \\ & x_{jj} & * & * \\ & * & * & * \\ & * & * & * \end{bmatrix} \longrightarrow \begin{bmatrix} * & * & * & * \\ & x_{jj} & * & * \\ & 0 & * & * \\ & 0 & * & * \end{bmatrix}$$

- But we could just as easily do

$$\begin{bmatrix} * & * & * & * \\ & * & * & * \\ & x_{ij} & * & * \\ & * & * & * \end{bmatrix} \longrightarrow \begin{bmatrix} * & * & * & * \\ & 0 & * & * \\ & x_{ij} & * & * \\ & 0 & * & * \end{bmatrix}$$

Partial Pivoting

- The entry x_{ij} is called the pivot, and flexibility in choosing the pivot is essential otherwise we can't deal with:

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

- Choosing the pivot as the largest element in column j improves numerical stability. This is called partial pivoting
- Full pivoting additionally permutes the columns and looks for the largest over $\mathcal{O}(n^2)$ elements, which is costly and only marginally beneficial for stability
- This ensures that each ℓ_{ij} entry — which acts as a multiplier in the LU factorization process — satisfies $|\ell_{ij}| \leq 1$

Partial Pivoting

- To maintain the triangular LU structure,
  we permute rows by premultiplying by permutation matrices

$$\underset{\text{pivot selection}}{\begin{bmatrix} * & * & * & * \\ & * & * & * \\ & * & * & * \\ & x_{ij} & * & * \end{bmatrix}} \xrightarrow{P_1} \underset{\text{row swap}}{\begin{bmatrix} * & * & * & * \\ & x_{ij} & * & * \\ & * & * & * \\ & * & * & * \end{bmatrix}} \xrightarrow{L_1} \begin{bmatrix} * & * & * & * \\ & x_{ij} & * & * \\ & 0 & * & * \\ & 0 & * & * \end{bmatrix}$$

- In this case

$$P_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

and each P_j is obtained by swapping two rows of I

Partial Pivoting

- Therefore, with partial pivoting we obtain

$$L_{n-1}P_{n-1}\cdots L_2P_2L_1P_1A = U$$

- It can be shown (we omit the details here, see Trefethen & Bau) that this can be rewritten as

$$PA = LU$$

  where $P = P_{n-1}\cdots P_2P_1$. Note that L is not the same as without pivoting
- Theorem: Gaussian elimination with partial pivoting produces nonsingular factors L and U if and only if A is nonsingular

Partial Pivoting

- Pseudocode for LU factorization with partial pivoting (new code is highlighted):

```
1: $U = A$, $L = \mathrm{I}$, $P = \mathrm{I}$
2: for $j = 1 : n - 1$ do
3:     Select $i (\geq j)$ that maximizes $|u_{ij}|$
4:     Swap rows of $U$: $u_{(j,j:n)} \leftrightarrow u_{(i,j:n)}$
5:     Swap rows of $L$: $\ell_{(j,1:j-1)} \leftrightarrow \ell_{(i,1:j-1)}$
6:     Swap rows of $P$: $p_{(j,:)} \leftrightarrow p_{(i,:)}$
7:     for $i = j + 1 : n$ do
8:         $\ell_{ij} = u_{ij}/u_{jj}$
9:         for $k = j : n$ do
10:            $u_{ik} = u_{ik} - \ell_{ij} u_{jk}$
11:        end for
12:    end for
13: end for
```

- Again this requires $\sim \frac{2}{3}n^3$ floating point operations

Partial Pivoting: Solve $Ax = b$

- To solve $Ax = b$ using the factorization $PA = LU$
  - Multiply through by P to obtain $PAx = LUx = Pb$
  - Solve $Ly = Pb$ using forward substitution
  - Then solve $Ux = y$ using back substitution

Partial Pivoting in Python

- Python's `scipy.linalg.lu` function can do LU factorization with pivoting

```
>>> import numpy as np
>>> import scipy.linalg
>>> A=np.random.rand(4, 4)
>>> (P,L,U) = scipy.linalg.lu(A)
>>> A
array([[0.48657354, 0.72177328, 0.89725033, 0.10555858],
       [0.19356039, 0.21192135, 0.001038  , 0.20308355],
       [0.04709362, 0.82519218, 0.29700521, 0.85089909],
       [0.35533098, 0.30291277, 0.98852909, 0.7303831 ]])
>>> P
array([[1., 0., 0., 0.],
       [0., 0., 0., 1.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.]])
>>> L
array([[ 1.        ,  0.        ,  0.        ,  0.        ],
       [ 0.09678623,  1.        ,  0.        ,  0.        ],
       [ 0.73027189, -0.29679299,  1.        ,  0.        ],
       [ 0.39780295, -0.09956144, -0.8465861 ,  1.        ]])
>>> U
array([[0.48657354, 0.72177328, 0.89725033, 0.10555858],
       [0.        , 0.75533446, 0.21016373, 0.84068247],
       [0.        , 0.        , 0.39566752, 0.9028053 ],
       [0.        , 0.        , 0.        , 1.00909401]])
```

Stability of Gaussian Elimination

- Numerical stability of Gaussian Elimination has been an important research topic since the 1940s
- Major figure in this field: James H. Wilkinson (England, 1919–1986)
- Showed that for $Ax = b$ with $A \in \mathbb{R}^{n \times n}$:
    - Gaussian elimination without partial pivoting is numerically unstable
      (as we've already seen)
    - Gaussian elimination with partial pivoting satisfies

$$\frac{\|r\|}{\|A\|\|x\|} \leq 2^{n-1} n^2 \epsilon_{\text{mach}}$$

Stability of Gaussian Elimination

- That is, pathological cases exist where the relative residual $\frac{\|r\|}{\|A\|\|x\|}$ grows exponentially with n due to rounding error
- Worst case behavior of Gaussian Elimination with partial pivoting is explosive instability but such pathological cases are extremely rare!
- In over 50 years of Scientific Computation, instability has only been encountered due to deliberate construction of pathological cases
- In practice, Gaussian elimination is stable in the sense that it produces a small relative residual

Stability of Gaussian Elimination

- In practice, we typically obtain

$$\frac{\|r\|}{\|A\|\|x\|} \lesssim n\epsilon_{\text{mach}}$$

  i.e. grows only linearly with n, and is scaled by ϵ_{mach}

- Combining this result with our inequality $(*)$:

$$\frac{\|\Delta x\|}{\|x\|} \leq \kappa(A)\frac{\|r\|}{\|A\|\|x\|}$$

  implies that in practice Gaussian elimination gives small error for well-conditioned problems!

Cholesky Factorization

Cholesky Factorization

- Suppose that matrix $A \in \mathbb{R}^{n\times n}$ is
  - symmetric: $A^T = A$
  - positive definite: for any $x \neq 0$, $x^T A x > 0$
- Then the matrix can be represented as

$$A = LL^T$$

  known as Cholesky factorization,
  where $L \in \mathbb{R}^{n\times n}$ is a lower triangular matrix
- In general, any matrix of the form BB^T
  is symmetric and positive definite for any nonsingular $B \in \mathbb{R}^{n\times n}$

Cholesky Factorization

- Matrix L is found directly from equation

$$A = LL^T$$

- Consider the 3×3 case

$$\begin{bmatrix} a_{11} & * & * \\ a_{21} & a_{22} & * \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11}^2 & * & * \\ \ell_{11}\ell_{21} & \ell_{21}^2 + \ell_{22}^2 & * \\ \ell_{11}\ell_{31} & \ell_{21}\ell_{31} + \ell_{22}\ell_{32} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{bmatrix}$$

- Equate components starting with the first column

$$\begin{array}{l|l|l} \ell_{11} = \sqrt{a_{11}} & & \\ \ell_{21} = a_{21}/\ell_{11} & \ell_{22} = \sqrt{a_{22} - \ell_{21}^2} & \\ \ell_{31} = a_{31}/\ell_{11} & \ell_{32} = (a_{32} - \ell_{21}\ell_{31})/\ell_{22} & \ell_{33} = \sqrt{a_{33} - \ell_{31}^2 - \ell_{32}^2} \end{array}$$

Cholesky Factorization

- The same approach is generalized to the $n \times n$ case

```
1:  $L = 0$
2:  $\ell_{ij} = a_{ij}$ for $i = 1, \ldots, n, j = 1, \ldots, i$
3:  for $j = 1 : n$ do
4:      $\ell_{jj} = \sqrt{\ell_{jj}}$
5:      for $i = j + 1 : n$ do
6:          $\ell_{ij} = \ell_{ij} / \ell_{jj}$
7:      end for
8:      for $k = j + 1 : n$ do
9:          for $i = k : n$ do
10:             $\ell_{ik} = \ell_{ik} - \ell_{ij}\ell_{kj}$
11:         end for
12:     end for
13: end for
```

Cholesky Factorization

- Notes on Cholesky factorization
  - Cholesky factorization is numerically stable and does not require pivoting
  - Operation count: $\sim \frac{1}{3}n^3$ operations in total, i.e. about half as many as Gaussian elimination
  - Only need to store L, so uses less memory than LU. Can be done in-place, overwriting matrix A
- See [examples/unit2/cholesky.py]

Performance Metrics

Performance Metrics

- There are various metrics for software performance
  - performance (FLOP/s): floating point operations per second
  - time to solution
  - scaling efficiency (for parallel computing)
- High Performance Computing studies and develops efficient implementations of numerical algorithms
- Naive Python implementations (e.g. using for-loops) are typically slow
- Modules such as NumPy rely on faster implementations (e.g. written in C)
- Example of performance measurements for Cholesky factorization
  - Python [examples/unit2/cholesky_time.py]
  - C++ [examples/unit2/cholesky_time.cpp]

Sparse Matrices

- In applications, we often encounter sparse matrices
- Common example: discretizations of partial differential equations
- The term sparse matrix typically means that the number of non-zero elements is comparable to the number of rows or columns (e.g. $n \times n$ matrix with $\mathcal{O}(n)$ non-zeros)
- It is advantageous to store and operate only on non-zero elements
- Positions of non-zero elements of a sparse matrix form its sparsity pattern
- Matrices that are not sparse are called dense matrices

Sparse Matrices

- Dense matrices are typically stored as two-dimensional arrays
- Sparse matrices benefit from special data structures and algorithms for computational efficiency
- Example from Unit 1 (constructing a spline)
  - a tridiagonal matrix is stored as three one-dimensional arrays
  - the linear system is solved using the TDMA algorithm
- Standard algorithms (e.g. LU or Cholesky factorization) can be directly applied to sparse matrices. However, new non-zero elements will appear
- These new non-zero elements are called the fill-in.
  Fill-in can be reduced by permuting rows and columns of the matrix
- `scipy.sparse` implements sparse linear algebra

Sparse Matrices: Data Structures

- Coordinate format (COO):
  Arrays: `data`, `row`, `col`
  Element `data[k]` is in row `row[k]` and column `col[k]`
- Compressed Sparse Row (CSR):
  Arrays: `data`, `indices`, `indptr`
  Row `i` contains elements `data[indptr[i]:indptr[i+1]]`
  in columns `indices[indptr[i]:indptr[i+1]]`
- Compressed Sparse Column (CSC):
  Arrays: `data`, `indices`, `indptr`
  Column `j` contains elements `data[indptr[j]:indptr[j+1]]`
  in rows `indices[indptr[j]:indptr[j+1]]`

Example: Sparse Matrix

$$\begin{bmatrix} a & b & b & b & b \\ 0 & c & 0 & 0 & 0 \\ 0 & 0 & c & 0 & 0 \\ 0 & 0 & 0 & c & 0 \end{bmatrix}$$

- Coordinate format (COO):
  `data` $= (a, b, b, b, b, c, c, c)$
  `row` $= (0, 0, 0, 0, 0, 1, 2, 3)$
  `col` $= (0, 1, 2, 3, 4, 1, 2, 3)$
  (assume zero-based indexing)
- See [examples/unit2/sparse.py]

- Compressed Sparse Row (CSR):
  `data` $= (a, b, b, b, b, c, c, c)$
  `indices` $= (0, 1, 2, 3, 4, 1, 2, 3)$
  `indptr` $= (0, 5, 6, 7, 8)$
- Compressed Sparse Column (CSC)
  `data` $= (a, b, c, b, c, b, c, b)$
  `indices` $= (0, 0, 1, 0, 2, 0, 3, 0)$
  `indptr` $= (0, 1, 3, 5, 7, 8)$

QR Factorization

- A square matrix $Q \in \mathbb{R}^{n \times n}$ is called orthogonal if its columns and rows are orthonormal vectors
- Equivalently, $Q^T Q = QQ^T = \mathrm{I}$
- Orthogonal matrices preserve the Euclidean norm of a vector

$$\|Qv\|_2^2 = v^T Q^T Qv = v^T v = \|v\|_2^2$$

- Geometrically, orthogonal matrices correspond to reflection or rotation
- Orthogonal matrices are very important in scientific computing, norm-preservation implies no amplification of numerical error!

QR Factorization

- The full QR factorization of matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$ has the form

$$A = QR$$

  where
  - $Q \in \mathbb{R}^{m \times m}$ is orthogonal
  - $R = \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} \in \mathbb{R}^{m \times n}$
  - $\hat{R} \in \mathbb{R}^{n \times n}$ is upper-triangular
- QR is used for solving overdetermined linear least-squares problems
- QR can be used for solving square systems, but requires twice as many operations as Gaussian elimination

QR Factorization

- Consider the 2-norm of the least-squares residual

$$\|r(x)\|_2^2 = \|b - Ax\|_2^2 = \left\| b - Q \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} x \right\|_2^2 =$$

$$= \left\| Q^T \left(b - Q \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} x \right) \right\|_2^2 = \left\| Q^T b - \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} x \right\|_2^2$$

- Denote $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = Q^T b$ with $c_1 \in \mathbb{R}^n, c_2 \in \mathbb{R}^{m-n}$, so that

$$\|r(x)\|_2^2 = \left\| \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} - \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} x \right\|_2^2 = \left\| \begin{bmatrix} c_1 - \hat{R}x \\ c_2 \end{bmatrix} \right\|_2^2 = \|c_1 - \hat{R}x\|_2^2 + \|c_2\|_2^2$$

QR Factorization

- Question: How do we choose x to minimize $\|r(x)\|_2$?

$$\|r(x)\|_2^2 = \|c_1 - \hat{R}x\|_2^2 + \|c_2\|_2^2$$

where $A = Q\begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}$ and $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = Q^T b$

- Answer: Only the first term depends on x. Try setting the first term to zero, i.e. solve the $n \times n$ triangular system

$$\hat{R}x = c_1$$

- This is what `numpy.linalg.lstsq()` does
- Also, this implies that $\min_{x \in \mathbb{R}^n} \|r(x)\|_2 = \|c_2\|_2$

QR Factorization

- Recall that solving linear least-squares via the normal equations requires solving a system with the matrix A^TA
- But using the normal equations directly is problematic since

$$\kappa(A^TA) = \kappa(A)^2$$

  (with $\kappa(A)$ for rectangular A defined using SVD, to be covered soon)
- The QR approach avoids this condition-squaring effect and is much more numerically stable!

QR Factorization

- How do we compute the QR factorization?
- There are three main methods
  - Gram–Schmidt orthogonalization
  - Householder triangularization
  - Givens rotations

Gram–Schmidt Orthogonalization

- Suppose $A \in \mathbb{R}^{m \times n}$, $m \geq n$
- One way to picture the QR factorization is to construct a sequence of orthonormal vectors $q_1, q_2, \ldots$ such that

$$\text{span}\{q_1, q_2, \ldots, q_j\} = \text{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j)}\}, \quad j = 1, \ldots, n$$

- We seek coefficients r_{ij} such that

$$\begin{aligned} a_{(:,1)} &= r_{11} q_1 \\ a_{(:,2)} &= r_{12} q_1 + r_{22} q_2 \\ &\ldots \\ a_{(:,n)} &= r_{1n} q_1 + r_{2n} q_2 + \ldots + r_{nn} q_n \end{aligned}$$

- This can be done via the Gram–Schmidt process

Gram–Schmidt Orthogonalization

- In matrix form we have:

$$\left[\begin{array}{c|c|c|c} a_{(:,1)} & a_{(:,2)} & \cdots & a_{(:,n)} \end{array}\right] = \left[\begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array}\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}$$

- This gives $A = \hat{Q}\hat{R}$ for $\hat{Q} \in \mathbb{R}^{m\times n}$, $\hat{R} \in \mathbb{R}^{n\times n}$
- This is called the reduced QR factorization of A, which is different from the full QR factorization: Q is non-square
- Note that for $m > n$, $\hat{Q}^T\hat{Q} = \mathrm{I}$, but $\hat{Q}\hat{Q}^T \neq \mathrm{I}$

Full vs Reduced QR Factorization

- To obtain the full QR factorization defined earlier

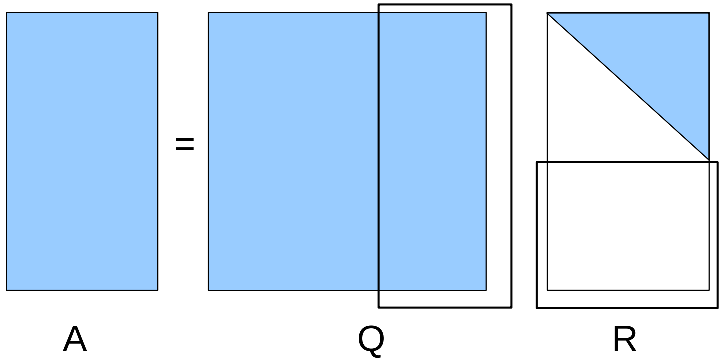
$$A = QR$$

  - append $\hat{Q}$ by $m - n$ arbitrary columns
    that are linearly independent with columns of $\hat{Q}$
  - apply the Gram–Schmidt process to obtain an orthogonal $Q \in \mathbb{R}^{m\times m}$

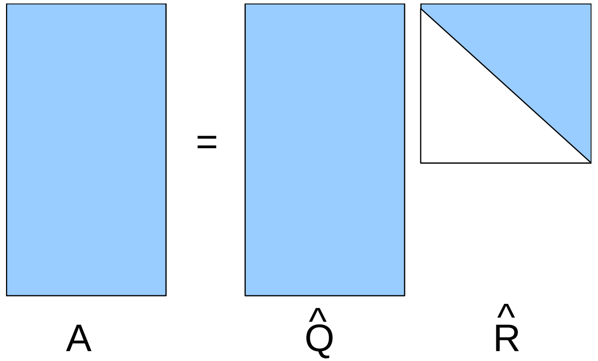
- We also need to append $\hat{R}$ with zero rows to obtain $R = \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} \in \mathbb{R}^{m\times n}$

  so that the new arbitrary columns in Q do not affect the product

Full vs Reduced QR Factorization



Full QR



Reduced QR

Full vs Reduced QR Factorization

- Exercise: Show that the linear least-squares solution is given by

$$\hat{R}x = \hat{Q}^T b$$

  by plugging $A = \hat{Q}\hat{R}$ into the normal equations
- This is equivalent to the least-squares result
  we showed earlier using the full QR factorization, since $c_1 = \hat{Q}^T b$

Full vs. Reduced QR Factorization

- By default, **`numpy.linalg.qr()`** does reduced QR factorization

```
>>> import numpy as np
>>> np.random.seed(2022)
>>> a = np.random.random((4,2))
>>> a
array([[0.00935861, 0.49905781],
       [0.11338369, 0.04997402],
       [0.68540759, 0.48698807],
       [0.89765723, 0.64745207]])
>>> (q, r) = np.linalg.qr(a)
>>> q
array([[-0.00824455,  0.99789386],
       [-0.09988626, -0.06374317],
       [-0.60381526, -0.01057732],
       [-0.79079826,  0.00572413]])
>>> r
array([[-1.13512797, -0.81516102],
       [ 0.        ,  0.4933763 ]])
```

- Supplying **`mode="complete"`** gives complete QR factorization

```
>>> import numpy as np
>>> np.random.seed(2022)
>>> a = np.random.random((4,2))
>>> a
array([[0.00935861, 0.49905781],
       [0.11338369, 0.04997402],
       [0.68540759, 0.48698807],
       [0.89765723, 0.64745207]])
>>> (q, r) = np.linalg.qr(a, mode="complete")
>>> q
array([[-0.00824455,  0.99789386, -0.02953283, -0.
       [-0.09988626, -0.06374317, -0.61111959, -0.
       [-0.60381526, -0.01057732,  0.66414863, -0.
       [-0.79079826,  0.00572413, -0.42961291,  0.
>>> r
array([[-1.13512797, -0.81516102],
       [ 0.        ,  0.4933763 ],
       [ 0.        ,  0.        ],
       [ 0.        ,  0.        ]])
```

Gram–Schmidt Orthogonalization

- Returning to the Gram–Schmidt process, how do we compute the q_i, $i = 1, \ldots, n$?
- In the j-th step, find a unit vector $q_j \in \operatorname{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j)}\}$ that is orthogonal to $\operatorname{span}\{q_1, q_n, \ldots, q_{j-1}\}$
- We set

$$v_j = a_{(:,j)} - \sum_{i=1}^{j-1} (q_i^T a_{(:,j)}) q_i$$

  and then set $q_j = v_j / \|v_j\|_2$
- Exercise: Verify that q_j satisfies the requirements
- We can now determine the required values of r_{ij}

Gram–Schmidt Orthogonalization

- From the equations $A = \hat{Q}\hat{R}$, for $j = 1, \ldots, n$

$$q_j = \frac{a_{(:,j)} - \sum_{i=1}^{j-1} r_{ij} q_i}{r_{jj}}$$

- From the Gram–Schmidt process, for $j = 1, \ldots, n$

$$q_j = \frac{a_{(:,j)} - \sum_{i=1}^{j-1} (q_i^T a_{(:,j)}) q_i}{\|a_{(:,j)} - \sum_{i=1}^{j-1} (q_i^T a_{(:,j)}) q_i\|_2}$$

- Both expressions have the same structure, by matching the terms

$$\begin{aligned} r_{ij} &= q_i^T a_{(:,j)} \qquad (i \neq j) \\ |r_{jj}| &= \|a_{(:,j)} - \textstyle\sum_{i=1}^{j-1} r_{ij} q_i\|_2 \end{aligned}$$

- The sign of r_{jj} is not determined uniquely, so we can choose $r_{jj} > 0$

Classical Gram–Schmidt Process

- The resulting algorithm is referred to as the classical Gram–Schmidt (CGS) method

```
1: for $j = 1 : n$ do
2:     $v_j = a_{(:,j)}$
3:     for $i = 1 : j - 1$ do
4:         $r_{ij} = q_i^T a_{(:,j)}$
5:         $v_j = v_j - r_{ij} q_i$
6:     end for
7:     $r_{jj} = \|v_j\|_2$
8:     $q_j = v_j / r_{jj}$
9: end for
```

Gram–Schmidt Orthogonalization

- The only way the Gram–Schmidt process can fail is if $|r_{jj}| = \|v_j\|_2 = 0$ for some j
- This can only happen if $a_{(:,j)} = \sum_{i=1}^{j-1} r_{ij} q_i$ for some j, i.e. if $a_{(:,j)} \in \operatorname{span}\{q_1, q_n, \ldots, q_{j-1}\} = \operatorname{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j-1)}\}$
- This means that columns of A are linearly dependent
- Therefore, Gram–Schmidt fails $\implies$ columns of A linearly dependent

Gram–Schmidt Orthogonalization

- Therefore, if columns of A are linearly independent, then the Gram–Schmidt succeeds
- The only non-uniqueness in the Gram–Schmidt process was in the sign of r_{ii}, therefore $\hat{Q}\hat{R}$ is unique under the requirement that all $r_{ii} > 0$
- This proves the following

  Theorem: Every $A \in \mathbb{R}^{m\times n}(m \geq n)$ of full rank has a unique reduced QR factorization $A = \hat{Q}\hat{R}$ with $r_{ii} > 0$

Gram–Schmidt Orthogonalization

- Theorem: Every $A \in \mathbb{R}^{m\times n} (m \geq n)$ has a full QR factorization
- Case 1: A has full rank
  - we compute the reduced QR factorization from above
  - to make Q square we pad $\hat{Q}$ with $m - n$ arbitrary orthonormal columns
  - we also pad $\hat{R}$ with $m - n$ zero rows to get R
- Case 2: A does not have full rank
  - at some point in computing the reduced QR factorization, we encounter $\|v_j\|_2 = 0$
  - at this point we pick an arbitrary unit q_j orthogonal to $\text{span}\{q_1, q_2, \ldots, q_{j-1}\}$ and then proceed as in Case 1

Modified Gram–Schmidt Process

- The classical Gram–Schmidt process is numerically unstable!
  (sensitive to rounding error, orthogonality of the q_j degrades)
- The algorithm can be reformulated to give
  the modified Gram–Schmidt process,
  which is numerically more robust
- Key idea: when each new q_j is computed,
  orthogonalize each remaining column of A against it

Modified Gram–Schmidt Process

- Applying this idea results in the modified Gram–Schmidt (MGS) method

```
1:  for $i = 1 : n$ do
2:      $v_i = a_{(:,i)}$
3:  end for
4:  for $i = 1 : n$ do
5:      $r_{ii} = \|v_i\|_2$
6:      $q_i = v_i / r_{ii}$
7:      for $j = i + 1 : n$ do
8:          $r_{ij} = q_i^T v_j$
9:          $v_j = v_j - r_{ij} q_i$
10:     end for
11: end for
```

Modified Gram–Schmidt Process

- Key difference between MGS and CGS
  - In CGS we compute orthogonalization coefficients r_{ij} using the original column $a_{(:,j)}$
  - In MGS we remove components of $a_{(:,j)}$ in span$\{q_1, q_2, \ldots, q_{i-1}\}$ before computing r_{ij}
- This makes no difference mathematically:
  In exact arithmetic components in span$\{q_1, q_2, \ldots, q_{i-1}\}$ are annihilated by q_i^T
- But in practice it reduces degradation of orthogonality of the q_j and improves the numerical stability of MGS over CGS

Operation Count

- MGS is dominated by the innermost loop (lines 8 and 9):

$$r_{ij} = q_i^T v_j$$
$$v_j = v_j - r_{ij} q_i$$

- The first requires m multiplications, $m - 1$ additions;
  the second requires m multiplications, m subtractions
- Therefore, each innermost iteration takes $\sim 4m$ operations
- The rotal number of operations is asymptotically

$$\sum_{i=1}^{n} \sum_{j=i+1}^{n} 4m \sim 4m \sum_{i=1}^{n} i \sim 2mn^2$$

Alternative QR Factorization Methods

- The QR factorization can also be computed using
  - Householder triangularization
  - Givens rotations
- Both methods apply a sequence of orthogonal matrices

$$Q_1, Q_2, Q_3, \dots$$

  that successively remove terms below the diagonal (similar to the LU factorization)

Householder Triangularization

Householder Triangularization

- We will now discuss the Householder triangularization which is more numerically stable and more efficient than Gram–Schmidt
- Unlike Gram–Schmidt, it will not guarantee that the orthonormal basis at each step will span the same subspaces as columns of A

$$\operatorname{span}\{a_{(:,1)}\}, \quad \operatorname{span}\{a_{(:,1)}, a_{(:,2)}\}, \quad \dots$$

  which may be important for some applications
- Method used by `scipy.linalg.qr()` calling `dgeqrf()` from LAPACK
- Introduced by Alston Householder (1904–1993, USA)

Householder Triangularization

- Idea: Apply a succession of orthogonal matrices $Q_k \in \mathbb{R}^{m \times m}$ to A to compute an upper triangular matrix R

$$R = Q_n \cdots Q_2 Q_1 A$$

- That will result in the full QR factorization

$$A = QR$$

since $Q = Q_1^T Q_2^T \ldots Q_n^T$ is a square matrix

Householder Triangularization

- In 1958, Householder proposed a way to choose Q_k to introduce zeros below the diagonal in column k while preserving the previous columns

$$\underbrace{\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}}_{A} \xrightarrow{Q_1} \underbrace{\begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & * & * \\ 0 & * & * \\ 0 & * & * \end{bmatrix}}_{Q_1 A} \xrightarrow{Q_2} \underbrace{\begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \\ 0 & 0 & * \\ 0 & 0 & * \end{bmatrix}}_{Q_2 Q_1 A} \xrightarrow{Q_3} \underbrace{\begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{Q_3 Q_2 Q_1 A}$$

- This is achieved by Householder reflectors

Householder Reflectors

- We choose

$$Q_k = \begin{bmatrix} \mathrm{I}_{k-1} & 0 \\ 0 & F \end{bmatrix}$$

  - $\mathrm{I}_{k-1} \in \mathbb{R}^{(k-1)\times(k-1)}$
  - $F \in \mathbb{R}^{(m-k+1)\times(m-k+1)}$ is a Householder reflector
- The I_{k-1} block ensures the first $k-1$ rows are unchanged
- F is an orthogonal matrix that operates on the bottom $m-k+1$ rows
- If F is orthogonal, then Q_k is orthogonal

Householder Reflectors

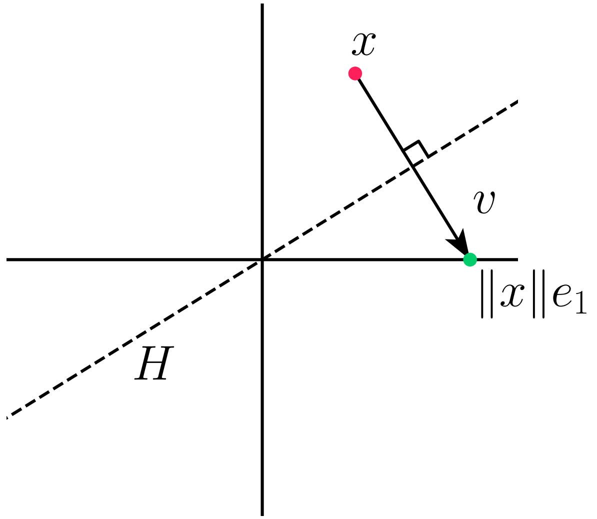
- Let $x \in \mathbb{R}^{m-k+1}$ denote elements $k, \dots, m$ of the k-th column in the current matrix $Q_{k-1} \dots Q_1 A$
- We have two requirements for F
  1. F is orthogonal, in particular $\|Fx\|_2 = \|x\|_2$
  2. only the first element of Fx is non-zero
- Therefore, we must have

$$Fx = F \begin{bmatrix} * \\ * \\ \vdots \\ * \end{bmatrix} = \begin{bmatrix} \|x\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\|_2 e_1$$

- Question: How can we achieve this?

Householder Reflectors

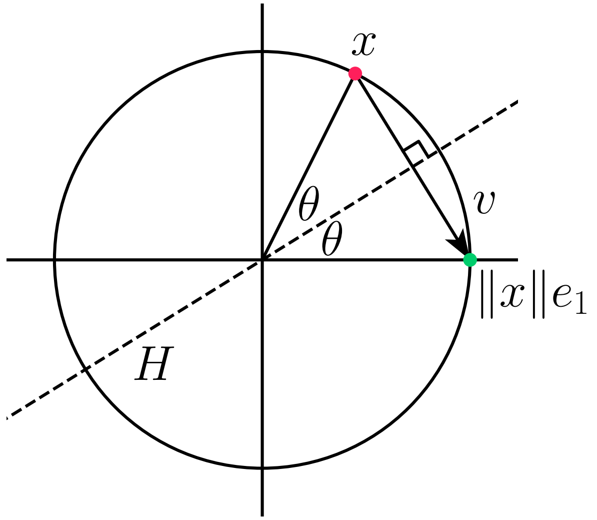
- We can see geometrically that this can be achieved by reflection across a hyperplane H



- Here H is the hyperplane orthogonal to $v = \|x\|e_1 - x$, and the key point is that H passes through the origin 0

Householder Reflectors

- H passes through the origin because x and $\|x\|e_1$ both belong to the hypersphere with radius $\|x\|_2$ centered at the origin



- Also analytically, since $(x + \|x\|e_1)/2 \in H$, we have $0 \in H \iff (\|x\|e_1 - x) \cdot (x + \|x\|e_1) = \|x\|^2 - x \cdot x = 0$

Householder Reflectors

- Next, we need to determine the matrix F which maps x to $\|x\|_2 e_1$
- F is closely related to the orthogonal projection of x onto H, since that projection takes us "half way" from x to $\|x\|_2 e_1$
- Hence we first consider orthogonal projection onto H, and subsequently derive F

Householder Reflectors

- The orthogonal projection of vector a onto vector b is given by

$$\frac{(a \cdot b)}{\|b\|^2} b$$

since $\left(a - \frac{(a\cdot b)}{\|b\|^2} b\right) \cdot b = a \cdot b - \frac{(a\cdot b)}{\|b\|^2} b \cdot b = 0$

- In the matrix form

$$\frac{(a \cdot b)}{\|b\|^2} b = \frac{1}{b^T b}(a^T b)b = \frac{1}{b^T b} b(b^T a) = \left(\frac{1}{b^T b} b b^T\right) a$$

- Therefore, the matrix $\frac{1}{b^T b} b b^T$ orthogonally projects onto b

Householder Reflectors

- We have that $\frac{1}{v^T v} v v^T$ orthogonally projects onto v
- Then, the following matrix

$$P_H = \mathrm{I} - \frac{vv^T}{v^T v}$$

orthogonally projects onto H as it satisfies

  - $P_H x \in H$

    since $v^T P_H x = v^T x - v^T \frac{vv^T}{v^T v} x = v^T x - \frac{v^T v}{v^T v} v^T x = 0$
  - $x - P_H x$ is orthogonal to H

    since $x - P_H x = x - x + \frac{vv^T}{v^T v} x = \frac{v^T x}{v^T v} v$ is proportional to v

Householder Reflectors

- But recall that F should reflect across H rather than project onto H

$$P_H = \mathrm{I} - \frac{vv^T}{v^T v}$$

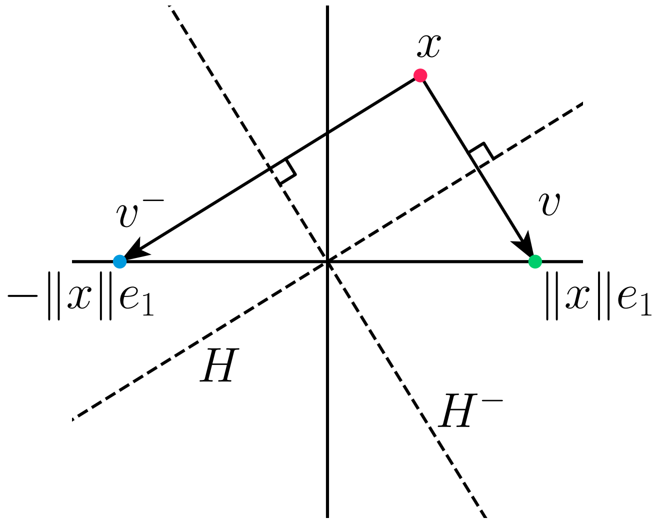
- We obtain F by going "twice as far" in the direction of v compared to P_H

$$F = \mathrm{I} - 2\frac{vv^T}{v^T v}$$

- Exercise: Show that F is an orthogonal matrix, i.e. that $F^T F = \mathrm{I}$

Householder Reflectors

- In fact, there are two Householder reflectors that we can choose from



- Which one is better?

Householder Reflectors

- If x and $\|x\|_2 e_1$ (or x and $-\|x\|_2 e_1$) are close, we could obtain loss of precision due to cancellation when computing $v = \|x\|e_1 - x$ (or $v = -\|x\|e_1 - x$)
- To ensure x and its reflection are well separated we should choose the reflection to be

$$-\operatorname{sign}(x_1)\|x\|_2 e_1$$

- Therefore, we want to have $v = -\operatorname{sign}(x_1)\|x\|_2 e_1 - x$
- Since the sign of v does not affect F, we scale v by -1 to get

$$v = \operatorname{sign}(x_1)\|x\|_2 e_1 + x$$

Householder Reflectors

- Let's compare the two options for v in the potentially problematic case when $x \approx \|x\|_2 e_1$, i.e. when $x_1 \approx \|x\|_2$
  - $v_{\text{bad}} = \|x\|_2 e_1 - x$
  - $v_{\text{good}} = \text{sign}(x_1)\|x\|_2 e_1 + x$
- The corresponding norms are

$$\|v_{\text{bad}}\|_2^2 = \Big\| \|x\|_2 e_1 - x \Big\|_2^2 \approx 0$$

$$\begin{aligned}
\|v_{\text{good}}\|_2^2 &= \Big\| \text{sign}(x_1)\|x\|_2 e_1 + x \Big\|_2^2 \\
&= (\text{sign}(x_1)\|x\|_2 + x_1)^2 + \|x_{(2:m-k+1)}\|_2^2 \\
&= (\text{sign}(x_1)\|x\|_2 + \text{sign}(x_1)|x_1|)^2 + \|x_{(2:m-k+1)}\|_2^2 \\
&= (\|x\|_2 + |x_1|)^2 + \|x_{(2:m-k+1)}\|_2^2 \approx (2\|x\|_2)^2
\end{aligned}$$

Householder Reflectors

- Recall that v is computed from two vectors of magnitude $\|x\|_2$
- The argument above shows that with v_{bad} we can get $\|v\|_2 \ll \|x\|_2$ leading to loss of precision due to cancellation
- In contrast, with v_{good} we always have $\|v_{\text{good}}\|_2 \geq \|x\|_2$, which rules out loss of precision due to cancellation

Householder Triangularization

- We can now write out the Householder algorithm

```
1: **for** $k = 1 : n$ **do**
2:     $x = a_{(k:m,k)}$
3:     $v_k = \text{sign}(x_1)\|x\|_2 e_1 + x$
4:     $v_k = v_k / \|v_k\|_2$
5:     $a_{(k:m,k:n)} = a_{(k:m,k:n)} - 2v_k(v_k^T a_{(k:m,k:n)})$
6: **end for**
```

- It overwrites A with R and stores $v_1, \ldots, v_n$
- Note that we do not divide by $v_k^T v_k$ in line 5 since we normalize v_k in line 4
- Householder algorithm requires $\sim 2mn^2 - \frac{2}{3}n^3$ operations (while Gram–Schmidt requires $2mn^2$)

Householder Triangularization

- Note that we do not explicitly form Q
- We can use the vectors $v_1, \ldots, v_n$ to compute Q in a post-processing step
- Recall that

$$Q_k = \begin{bmatrix} \mathrm{I} & 0 \\ 0 & F \end{bmatrix}$$

  and $Q = (Q_n \cdots Q_2 Q_1)^T = Q_1^T Q_2^T \cdots Q_n^T$
- Also, the Householder reflectors are symmetric (see the definition of F), so $Q = Q_1^T Q_2^T \cdots Q_n^T = Q_1 Q_2 \cdots Q_n$ and
- Note that each Q_k is involutory (i.e. $Q_k^{-1} = Q_k$)
  but in general this does not hold for the product ($Q^{-1} \neq Q$)

Householder Triangularization

- For any y, we can evaluate $Qy = Q_1 Q_2 \cdots Q_n y$ using the v_k

```
1: for $k = n : -1 : 1$ do
2:     $y_{(k:m)} = y_{(k:m)} - 2v_k(v_k^T y_{(k:m)})$
3: end for
```

- Question: How can we use this to form the matrix Q?

Householder Triangularization

- Answer: Compute Q from Qe_i, $i = 1, \dots, m$ since Q consists of columns Qe_i
- Similarly, compute the reduced $\hat{Q}$ from Qe_i, $i = 1, \dots, n$
- However, often not necessary to form Q or $\hat{Q}$ explicitly, e.g. to solve the least-squares problem $Ax \simeq b$, we only need the product $Q^T b$ and the matrix R
- Note that the product $Q^T b = Q_n \cdots Q_2 Q_1 b$ can be evaluated as

```
1: for $k = 1 : n$ do
2:     $b_{(k:m)} = b_{(k:m)} - 2v_k(v_k^T b_{(k:m)})$
3: end for
```

Givens Rotations

Givens Rotations

- Another method of QR-factorization is based on Givens rotation matrix

$$G(i,j,\theta) = \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & c & \dots & -s & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & s & \dots & c & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

which is defined for $i < j$ and $\theta \in \mathbb{R}$ as an $m \times m$ matrix with elements

$$\begin{aligned} g_{ii} &= c, \qquad g_{jj} = c, \qquad g_{ij} = -s, \qquad g_{ji} = s \\ g_{kk} &= 1 \quad \text{for } k \neq i, j, \qquad g_{kl} = 0 \quad \text{otherwise} \end{aligned}$$

where $c = \cos\theta$ and $s = \sin\theta$

Givens Rotations

- A Givens rotation matrix applies a rotation within the space spanned by the i-th and j-th coordinates
- Named after James W. Givens, Jr. (1910–1993, USA)

Effect of a Givens rotation

- Consider a rectangular matrix $A \in \mathbb{R}^{m \times n}$ where $m \geq n$
- Suppose that a_1 and a_2 are in the i-th and j-th positions in a particular column of A. Assume that $a_1^2 + a_2^2 \neq 0$
- Restricting to just i-th and j-th dimensions, a Givens rotation $G(i, j, \theta)$ for a particular angle θ can be chosen so that

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \alpha \\ 0 \end{pmatrix}$$

  where α is non-zero, and the j-th component is eliminated

Stable computation

- Since the length is preserved, $\alpha = \sqrt{a_1^2 + a_2^2}$
- We could compute

$$c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}, \qquad s = \frac{-a_2}{\sqrt{a_1^2 + a_2^2}}$$

  but this is susceptible to underflow/overflow if α is very small
- A better procedure is
  - if $|a_1| > |a_2|$, set $t = \tan\theta = a_2/a_1$ and then $c = \frac{1}{\sqrt{1+t^2}}, s = -ct$
  - if $|a_2| \geq |a_1|$, set $t = \cot\theta = a_1/a_2$ and then $s = \frac{-1}{\sqrt{1+t^2}}, c = -st$

Givens rotation algorithm

- The following algorithm performs the full QR-factorization of a matrix $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ using Givens rotations

```
1: $R = A, Q = I$
2: for $k = 1 : n$ do
3:     for $j = m : k + 1$ do
4:         Construct $G = G(j-1, j, \theta)$ to eliminate $a_{jk}$
5:         $R = GR$
6:         $Q = QG^T$
7:     end for
8: end for
```

Advantages of Givens Rotations

- In general, for dense matrices, Givens rotations are not as efficient as the other two approaches (Gram–Schmidt and Householder)
- However, they are advantageous for sparse matrices,
  since non-zero elements can be eliminated one-by-one
  without affecting other rows

Advantages of Givens Rotations

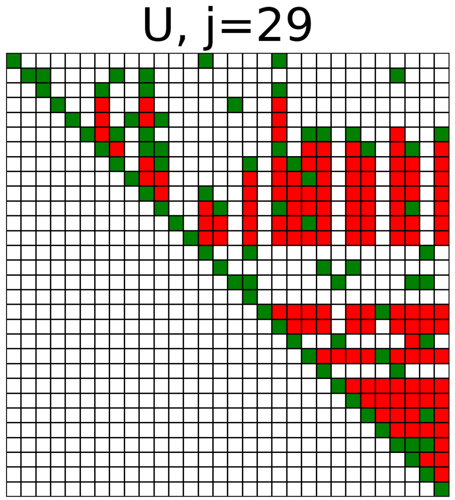
- Also, Givens rotations of different rows can be done concurrently
- Consider the 6×6 matrix

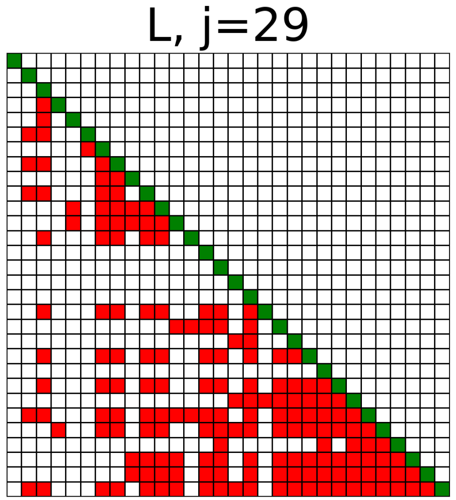
$$\begin{bmatrix} * & * & * & * & * & * \\ 5 & * & * & * & * & * \\ 4 & 6 & * & * & * & * \\ \boxed{3} & 5 & 7 & * & * & * \\ 2 & 4 & 6 & 8 & * & * \\ 1 & \boxed{3} & 5 & 7 & 9 & * \end{bmatrix}$$

- Each number denotes the step when that element can be eliminated
- For example, on step 3, elements $(4, 1)$ and $(6, 2)$ can be eliminated concurrently using $G(3, 4, \cdot)$ and $G(5, 6, \cdot)$ since they operate on different rows

Example: Sparsity Patterns

- Positions of non-zero elements of a sparse matrix form its sparsity pattern
- Transformations of the matrix may introduce new non-zero elements
- These new non-zero elements are called the fill-in
- See [examples/unit2/sparse_pattern.py]

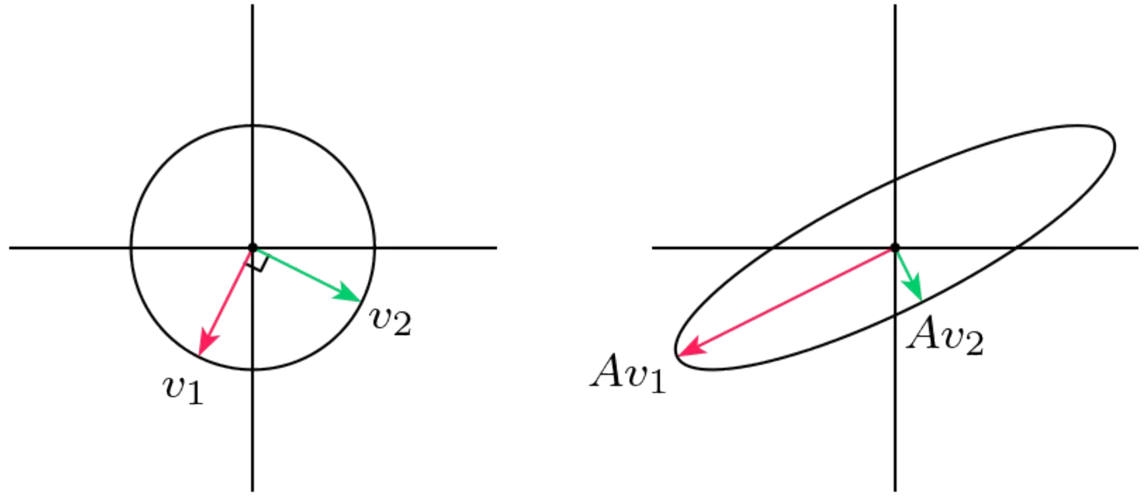




Singular Value Decomposition

Singular Value Decomposition

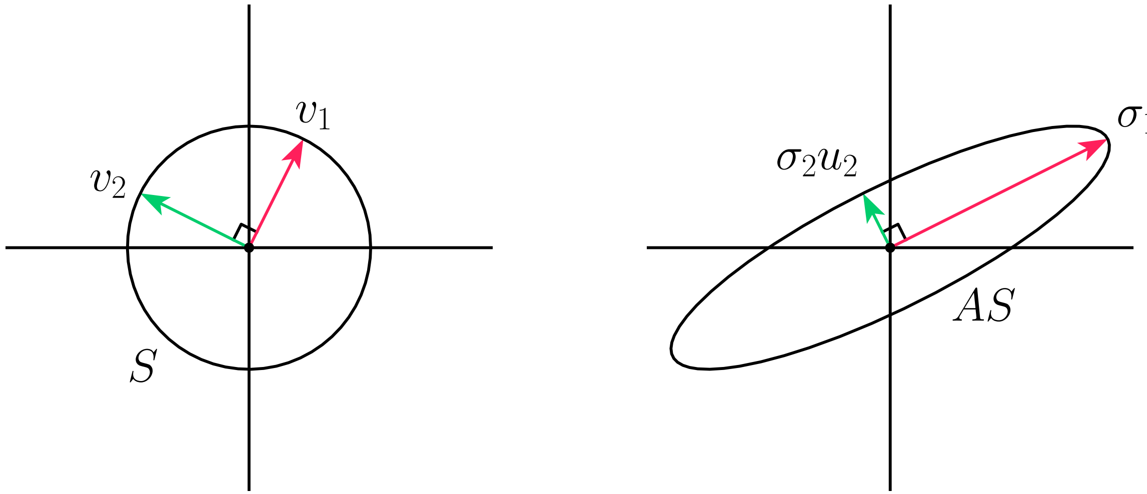
- How does a matrix deform the space?
- Example of $A = \begin{bmatrix} 1 & 1.5 \\ 0 & 1 \end{bmatrix}$ mapping the unit circle to an ellipse



- In general, a matrix does not preserve orthogonality and length

Singular Value Decomposition

- However, orthogonal v_1 and v_2 can be chosen such that $Av_1 = \sigma_1 u_1$ and $Av_2 = \sigma_2 u_2$ are orthogonal



where $\sigma_1 \geq \sigma_2 \geq 0$ and $\|u_1\| = \|u_2\| = 1$

Singular Value Decomposition

- To obtain a Singular Value Decomposition (SVD) of a matrix $A \in \mathbb{R}^{m \times n}$, we are looking for orthonormal vectors v_i such that

$$Av_i = \sigma_i u_i, \quad i = 1, \ldots, n$$

where vectors u_i are also orthonormal and $\sigma_i \in \mathbb{R},\ \sigma_i \geq 0$

- In the matrix form, we get

$$AV = \hat{U}\hat{\Sigma}$$

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \left[\begin{array}{c|c|c} v_1 & \cdots & v_n \end{array}\right] = \left[\begin{array}{c|c|c} u_1 & \cdots & u_n \end{array}\right] \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix}$$

Singular Value Decomposition

- Matrices in $AV = \hat{U}\hat{\Sigma}$ are
  - $A \in \mathbb{R}^{m \times n}$ is a general matrix
  - $V \in \mathbb{R}^{n \times n}$ with orthonormal columns
  - $\hat{\Sigma} \in \mathbb{R}^{n \times n}$ is diagonal with non-negative, real entries
  - $\hat{U} \in \mathbb{R}^{m \times n}$ with orthonormal columns
- Therefore V is an orthogonal matrix ($V^T V = V V^T = \mathrm{I}$) and we have the following decomposition called the reduced SVD

$$A = \hat{U}\hat{\Sigma}V^T$$

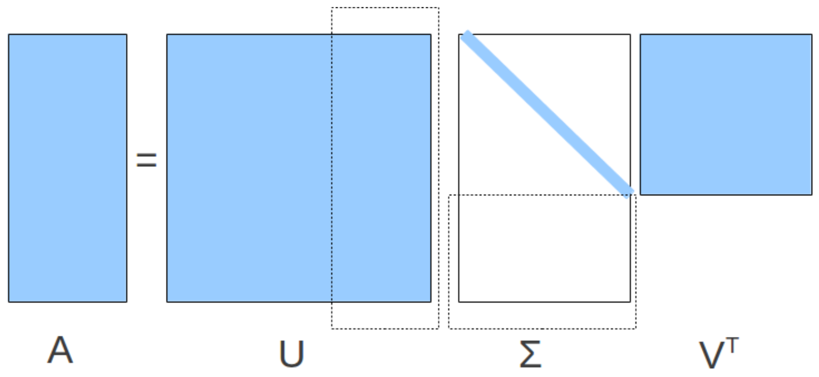
  - $\sigma_1, \sigma_2, \ldots, \sigma_n \geq 0$ are singular values (typically $\sigma_1 \geq \sigma_2 \geq \ldots$)
  - $u_1, u_2, \ldots, u_n$ are left singular vectors (columns of $\hat{U}$)
  - $v_1, v_2, \ldots, v_n$ are right singular vectors (rows of V^T)

Singular Value Decomposition

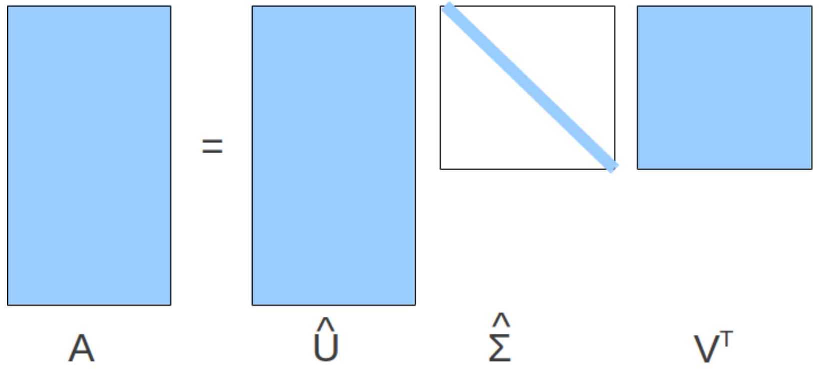
- Just as with QR factorization, we can pad the columns of $\hat{U}$ with $m - n$ arbitrary orthonormal vectors to obtain an orthogonal $U \in \mathbb{R}^{m\times m}$
- We then need to "silence" these arbitrary columns by adding rows of zeros to $\hat{\Sigma} \in \mathbb{R}^{n\times n}$ to obtain $\Sigma \in \mathbb{R}^{m\times n}$
- This gives the full SVD for $A \in \mathbb{R}^{m\times n}$

$$A = U\Sigma V^T$$

Full vs Reduced SVD



Full SVD



Reduced SVD

Singular Value Decomposition

- Theorem: Every matrix $A \in \mathbb{R}^{m \times n}$ has a full singular value decomposition. Furthermore:
  - singular values σ_i are uniquely determined
  - if A is square and σ_j are distinct, then u_i and v_i are uniquely determined up to sign
- Proof is outside of the scope of the course

Singular Value Decomposition

- This theorem justifies the statement:
  the image of the unit hypersphere under any $m \times n$ matrix is a hyperellipse
- Consider $A = U\Sigma V^T$ (full SVD) applied to the unit sphere $S \subset \mathbb{R}^n$:
  - the orthogonal map V^T preserves S
  - Σ stretches S into a hyperellipse aligned with the canonical axes e_j
  - U rotates or reflects the hyperellipse without changing its shape

SVD in Python

- `numpy.linalg.svd()` computes the full SVD by default

```
>>> import numpy as np
>>> np.random.seed(2022)
>>> a=np.random.random((4,2))
>>> a
array([[0.00935861, 0.49905781],
       [0.11338369, 0.04997402],
       [0.68540759, 0.48698807],
       [0.89765723, 0.64745207]])
>>> (u, s, v) = np.linalg.svd(a)
>>> u
array([[-0.22570503,  0.97206861, -0.02953283, -0.0571636
       [-0.08357767, -0.08399541, -0.61111959, -0.7826189
       [-0.58696968, -0.14202585,  0.66414863, -0.4406833
       [-0.77300621, -0.16690133, -0.42961291,  0.4359335
>>> s
array([1.42929716, 0.39183261])
>>> v
array([[-0.77506396, -0.63188279],
       [-0.63188279,  0.77506396]])
```

- with `full_matrices=0` it computes the reduced SVD

```
>>> import numpy as np
>>> np.random.seed(2022)
>>> a = np.random.random((4,2))
>>> a
array([[0.00935861, 0.49905781],
       [0.11338369, 0.04997402],
       [0.68540759, 0.48698807],
       [0.89765723, 0.64745207]])
>>> (u, s, v) = np.linalg.svd(a, full_matrices
>>> u
array([[-0.22570503,  0.97206861],
       [-0.08357767, -0.08399541],
       [-0.58696968, -0.14202585],
       [-0.77300621, -0.16690133]])
>>> s
array([1.42929716, 0.39183261])
>>> v
array([[-0.77506396, -0.63188279],
       [-0.63188279,  0.77506396]])
```

Matrix Properties via the SVD

- Let r denote the number of nonzero singular values, so that

$$\sigma_1 \geq \sigma_2 > \cdots \geq \sigma_r > 0, \quad \sigma_{r+1} = \ldots = \sigma_n = 0$$

- Property: $r = \mathrm{rank}(A)$
- Proof: In the full SVD $A = U\Sigma V^T$, matrices U and V^T have full rank, so multiplication by them preserves rank, leading to $\mathrm{rank}(A) = \mathrm{rank}(\Sigma) = r$
- Property: $\mathrm{image}(A) = \mathrm{span}\{u_1, \ldots, u_r\}$ and $\mathrm{null}(A) = \mathrm{span}\{v_{r+1}, \ldots, v_n\}$
- Proof: This follows from $A = U\Sigma V^T$ and

$$\begin{aligned} \mathrm{image}(\Sigma) &= \mathrm{span}\{e_1, \ldots, e_r\} \in \mathbb{R}^m \\ \mathrm{null}(\Sigma) &= \mathrm{span}\{e_{r+1}, \ldots, e_n\} \in \mathbb{R}^n \end{aligned}$$

Matrix Properties via the SVD

- Property: $\|A\|_2 = \sigma_1$
- Proof: By definition $\|A\|_2 = \max_{\|v\|_2=1} \|Av\|_2 = \max_{\|v\|_2=1} \|U\Sigma V^T v\|_2$. Orthogonal matrices preserve the norm, $\|A\|_2 = \max_{\|v\|_2=1} \|\Sigma v\|_2 = \sigma_1$
- Property: Singular values of A are the square roots of the eigenvalues of $A^T A$ or AA^T
- Proof: $A^T A = (U\Sigma V^T)^T (U\Sigma V^T) = V\Sigma U^T U\Sigma V^T = V(\Sigma^T\Sigma)V^T$
  Therefore, $(A^T A)V = V(\Sigma^T\Sigma)$, or $(A^T A)v_{(:,j)} = \sigma_j^2 v_{(:,j)}$
  (Analogous for AA^T)

Matrix Properties via the SVD

- The pseudoinverse A^+ can be defined more generally in terms of the SVD
- Define pseudoinverse of a scalar $\sigma \in \mathbb{R}$ to be
  $\sigma^+ = 1/\sigma$ if $\sigma \neq 0$ and $\sigma^+ = 0$ if $\sigma = 0$
- Define pseudoinverse $\Sigma^+ \in \mathbb{R}^{n\times m}$ of a diagonal matrix $\Sigma \in \mathbb{R}^{m\times n}$ as its transpose after taking scalar pseudoinverse of each element
- Define pseudoinverse of $A \in \mathbb{R}^{m\times n}$ as

$$A^+ = V\Sigma^+U^T$$

- Note: A^+ exists for any matrix A, and it covers our previous definitions of pseudoinverse

Matrix Properties via the SVD

- We generalize the condition number to rectangular matrices via the definition

$$\kappa(A) = \|A\| \|A^+\|$$

- Property: The 2-norm condition number is given by

$$\kappa(A) = \sigma_{\max}/\sigma_{\min}$$

- Proof: $\|A\|_2 = \sigma_{\max}$ as shown before.
  The largest singular value of A^+ is $1/\sigma_{\min}$ so $\|A^+\|_2 = 1/\sigma_{\min}$

Matrix Properties via the SVD

- These results indicate the importance of the SVD, both theoretical and as a computational tool
- Algorithms for calculating the SVD are outside scope of this course
- SVD requires $\sim 4mn^2 - \frac{4}{3}n^3$ operations
- For more details on algorithms, see Trefethen & Bau, or Golub & van Loan

Low-Rank Approximation via the SVD

- One of the most useful properties of the SVD is that it allows us to obtain an optimal low-rank approximation to A
- We can recast SVD as

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^T$$

- Follows from writing Σ as a sum of r matrices Σ_j, where $\Sigma_j = \mathrm{diag}(0, \ldots, 0, \sigma_j, 0, \ldots, 0)$
- Each $u_j v_j^T$ is a rank one matrix: each column is a scaled version of u_j

Low-Rank Approximation via the SVD

- Theorem: For any index $\nu = 0, \ldots, r$ the matrix

$$A_\nu = \sum_{j=1}^{\nu} \sigma_j u_j v_j^T$$

satisfies

$$\|A - A_\nu\|_2 = \inf_{B \in \mathbb{R}^{m \times n},\ \mathrm{rank}(B) \leq \nu} \|A - B\|_2 = \sigma_{\nu+1}$$

- That is
  - A_ν is the closest rank ν matrix to A, measured in the 2-norm
  - The error in A_ν is given by the first omitted singular value

Low-Rank Approximation via the SVD

- A similar result holds in the Frobenius norm:

$$\|A - A_\nu\|_F = \inf_{B \in \mathbb{R}^{m\times n},\ \operatorname{rank}(B)\le\nu} \|A - B\|_F = \sqrt{\sigma_{\nu+1}^2 + \cdots + \sigma_r^2}$$

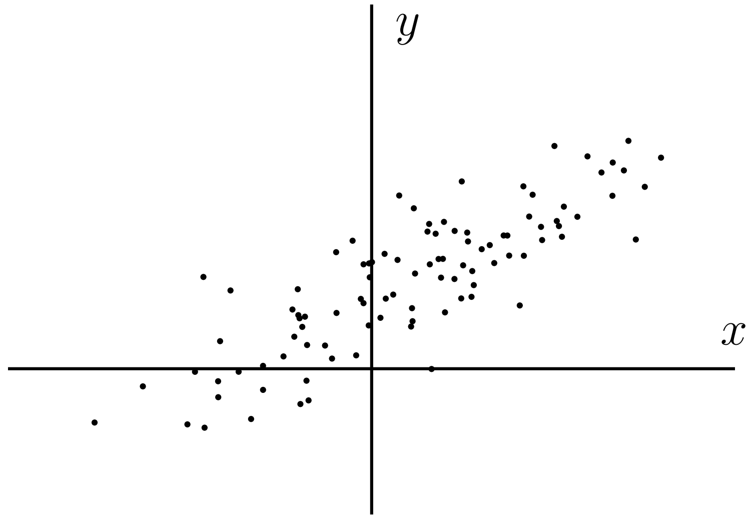
Low-Rank Approximation via the SVD

- These theorems indicate that the SVD is an effective way to compress data encapsulated by a matrix!
- For example, A can represent an image
- If singular values of A decay rapidly, we can approximate A with few rank one matrices
- For each rank one matrix $\sigma_j u_j v_j$, we only need to store $m + n + 1$ numbers: $\sigma_j,\ u_j,\ v_j$

Principal Component Analysis

Principal Component Analysis

- Consider a dataset of $(x_i, y_i) \in \mathbb{R}^2$ for $i = 1, \ldots, m$



- There is a strong correlation between x and y
- This means that we can describe most of the data with just one feature
- This is done by Principal Component Analysis (PCA)

Principal Component Analysis

- The new axis should maximize variance of the data
- Consider the empirical covariance matrix

$$M = \begin{bmatrix} \mathrm{Var}(x) & \mathrm{Cov}(x,y) \\ \mathrm{Cov}(x,y) & \mathrm{Var}(y) \end{bmatrix}$$

- In terms of the samples (x_i, y_i)

$$M = \frac{1}{m} \begin{bmatrix} \sum_{i=1}^{m} (x_i - \bar{x})^2 & \sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y}) \\ \sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y}) & \sum_{i=1}^{m} (y_i - \bar{y})^2 \end{bmatrix}$$

where $\bar{x} = \sum_{i=1}^{m} x_i$ and $\bar{y} = \sum_{i=1}^{m} y_i$ are the empirical means

Principal Component Analysis

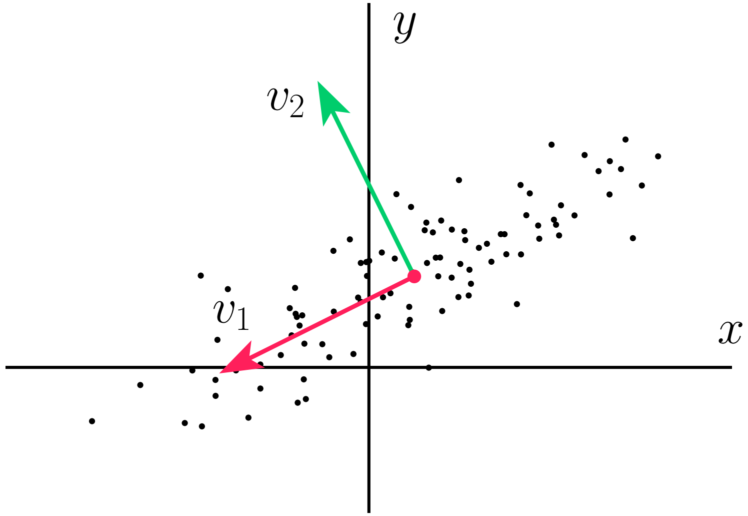
- M is a symmetric positive-definite matrix
- Variance in the direction $v \in \mathbb{R}^2$ is given by $v^T M v$
- $v^T M v$ is maximized if v is the eigenvector of M corresponding to the largest eigenvalue
- Define a matrix $A \in \mathbb{R}^{m \times 2}$

$$A = \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ x_2 - \bar{x} & y_2 - \bar{y} \\ \vdots & \vdots \\ x_m - \bar{x} & y_m - \bar{y} \end{bmatrix}$$

- Then $M = \frac{1}{m} A^T A$

Principal Component Analysis

- From the full SVD $A = U\Sigma V^T$,
  the columns of V are the eigenvectors of $M = \frac{1}{m}A^T A$
- Define the new axes along v_1 and v_2

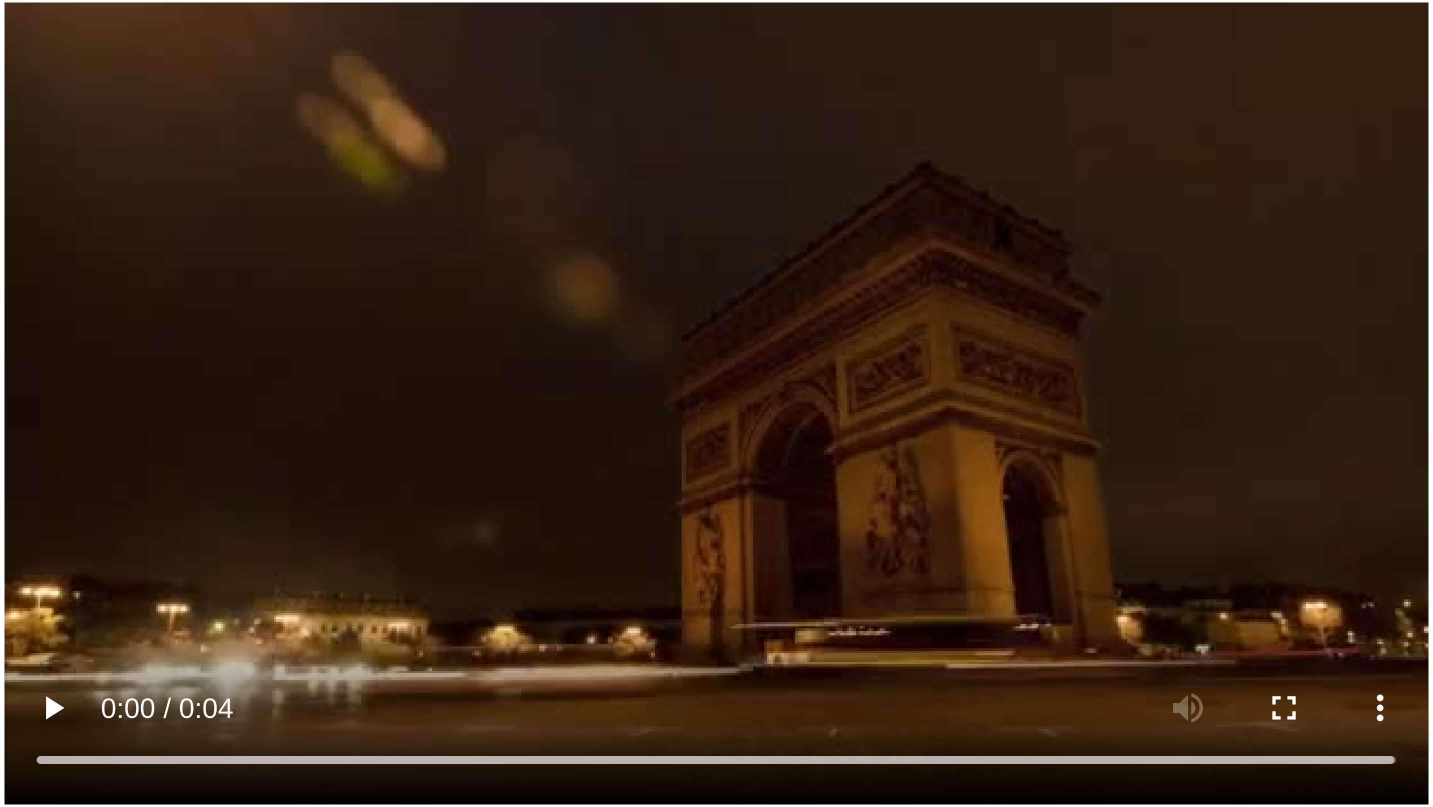


- See [examples/unit2/pca.py]

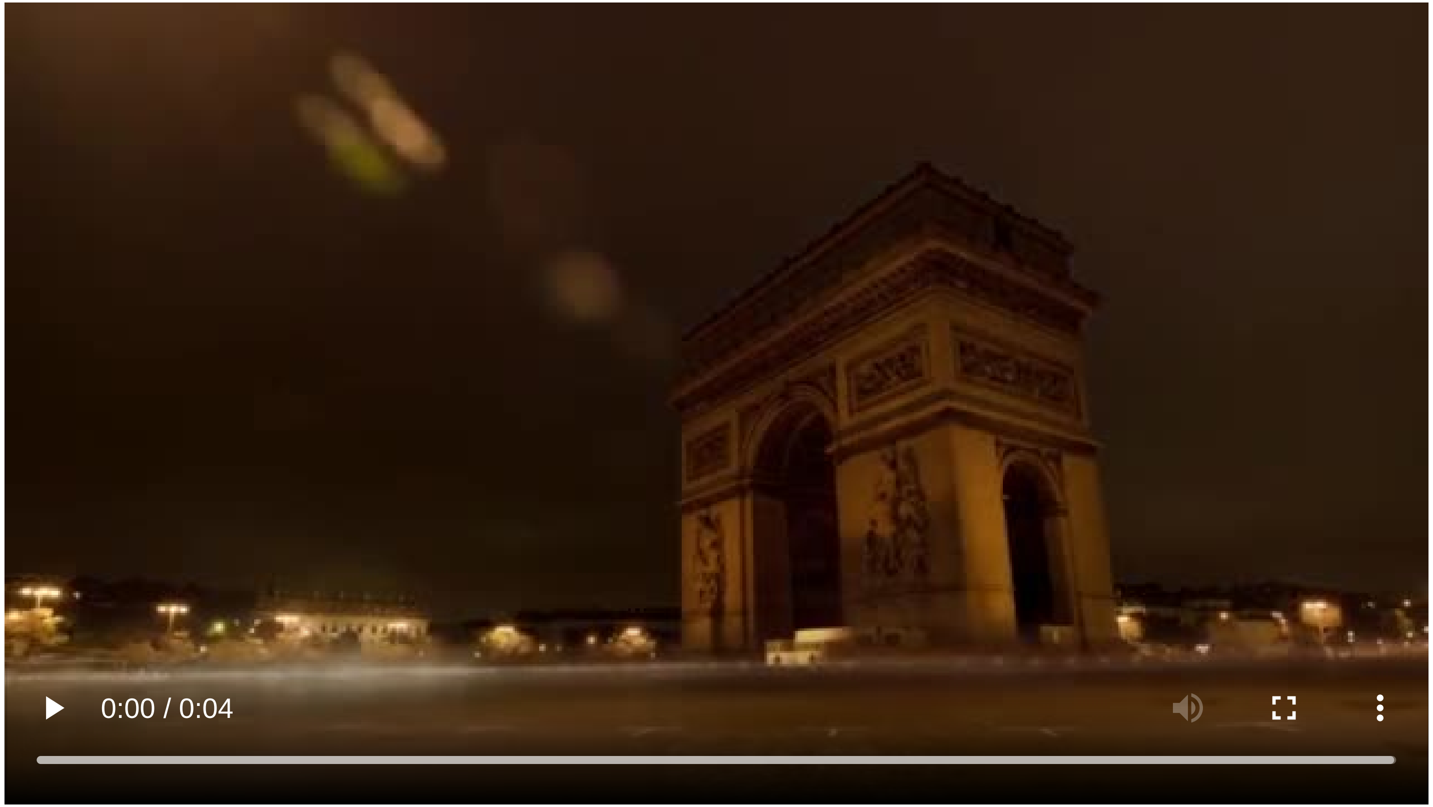
Example: Video Reconstruction

- Three videos
  - Paris https://www.pexels.com/video/852352
  - Vietnam https://www.youtube.com/watch?v=OiqSsE0B-Rc
  - Sunrise https://www.pexels.com/video/855646
- PCA applied to frames of the videos

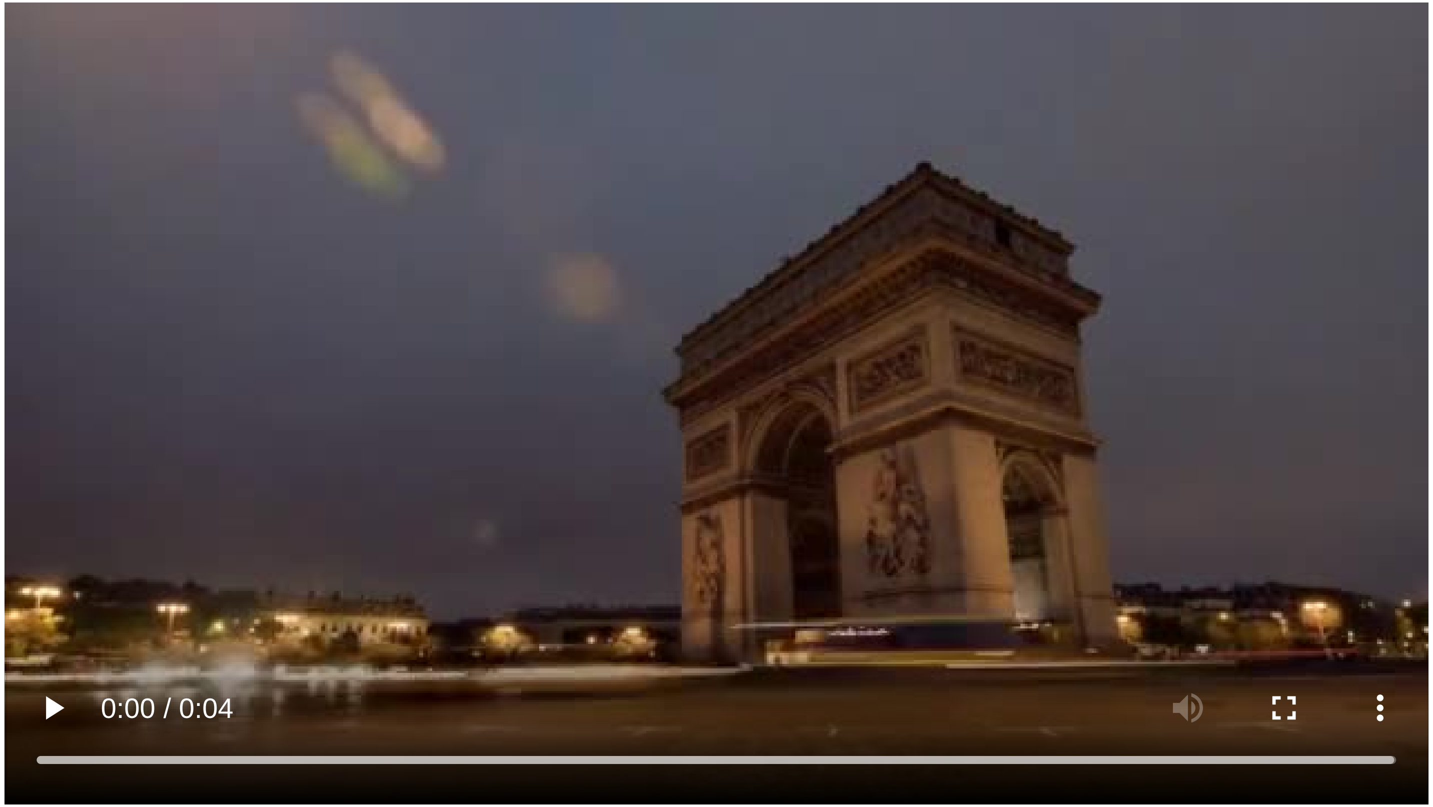
Paris, original



Paris, only first three



Paris, without first three



Vietnam, original

Vietnam, only first three

Vietnam, without first three

Sunrise, original

Sunrise, only first three

Sunrise, without first three