ORF307 – Optimization

2. Solving linear systems in practice

Bartolomeo Stellato — Spring 2023

Today’s lecture

Solving linear systems in practice

- Matrices: definition, operations, special cases
- Linear systems solutions
- Solving linear systems

Matrices

Matrices

matrix of size $m \times n$

$$A = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix}$$

- A_{ij} is the i, j *element*
  (also called *entry* or *coefficient*)
- i is the row index, j the column index
- indices start at 1
  (when you code, at 0)
- vectors are like matrices with 1 column

Special matrices

$$I = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

Special matrices

- $A = 0$ (zero matrix): $A_{ij} = 0, \quad i = 1, \ldots, m,\ j = 1, \ldots, n$
- $A = I$ (identity matrix): $m = n$ with $A_{ii} = 1$ and $A_{ij} = 0$ for $i \neq j$

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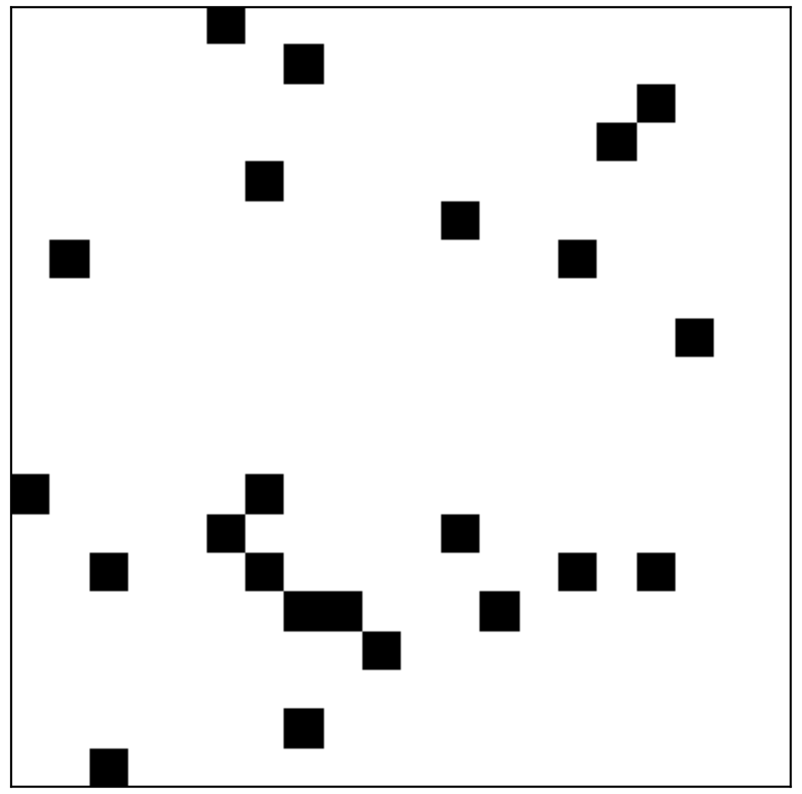
Sparse matrices (most entries are 0)



- Examples: 0 and I
- Can be stored and manipulated efficiently
- $\mathbf{nnz}(A)$ is the number of nonzero entries

Diagonal and triangular matrices

$$\begin{bmatrix} a_1 & & & & \\ & a_2 & & & \\ & & a_3 & & \\ & & & \ddots & \\ & & & & a_n \end{bmatrix}$$

diagonal matrix

- A square matrix $n \times n$
  with $A_{ij} = 0$ when $i \neq j$
- $\boxed{\mathbf{diag}(a_1, \ldots, a_n)}$ is the diagonal matrix
  with $A_{ii} = a_i$ for $i = 1, \ldots, n$

$$\mathbf{diag}(0.2, -3) = \begin{bmatrix} 0.2 & 0 \\ 0 & -3 \end{bmatrix}$$

Diagonal and triangular matrices

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lower triangular matrix

$A_{ij} = 0$ for $i < j$

$$\begin{bmatrix} -0.6 & 0 \\ 1.6 & -2 \end{bmatrix}$$

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lower triangular matrix

$A_{ij} = 0$ for $i < j$

$$\begin{bmatrix} -0.6 & 0 \\ 1.6 & -2 \end{bmatrix}$$

upper triangular matrix

$A_{ij} = 0$ for $i > j$

$$\begin{bmatrix} -0.2 & 0.3 \\ 0 & -1 \end{bmatrix}$$

Block matrices

Matrices whose entries are matrices

$n \times m$ matrix $A = \begin{bmatrix} B & C \\ D & E \end{bmatrix}$

where B, C, D, E are *submatrices* of *blocks* of A

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column representation

$$A = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix}$$

(a_i are m-vectors)

np.bmat

Block matrices

Matrices whose entries are matrices

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column representation

$$A = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix}$$

(a_i are m-vectors)

row representation

$$A = \begin{bmatrix} b_1^T \\ b_2^T \\ \vdots \\ b_n^T \end{bmatrix}$$

(b_i are n-~~row~~ vectors)

Matrix operations

transpose

A *transpose* of a matrix A is denoted as A^T where

$$(A^T)_{ij} = A_{ji}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

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addition (just like vectors)

$$(A + B)_{ij} = A_{ij} + B_{ij}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

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scalar multiplication (just like vectors)

$$(\alpha A)_{ij} = \alpha A_{ij}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

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Many properties

$$(A^T)^T = A, \qquad A + B = B + A, \qquad \alpha(A + B) = \alpha A + \alpha B$$

Matrix-vector multiplication

dot product

A matrix-vector product of an $m \times n$ matrix A and a n-vector x is denoted as

$$y = Ax, \qquad \text{where} \quad y_i = A_{i1}x_1 + \cdots + A_{in}x_n, \quad i = 1, \ldots, m$$

$$\begin{bmatrix} 0 & 2 & -1 \\ -2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 3 \\ -4 \end{bmatrix}$$

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row interpretation

$$y_i = b_i^T x$$

where $b_1^T, \ldots, b_m^T$ are rows of A

example $A1$

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column interpretation

$$y = x_1 a_1 + \ldots x_n a_n$$

where $a_1, \ldots, a_n$ are the columns of A

example $Ae_j = a_j$

Return matrix — portfolio vector

R is the $T \times n$ matrix of **asset returns**

$$R = \begin{array}{cc} \begin{array}{cccc} \text{AAPL} & \text{GOOG} & \text{MMM} & \text{AMZN} \end{array} & \\ \begin{bmatrix} 0.00219 & 0.0006 & -0.00113 & 0.00202 \\ 0.00744 & -0.00894 & -0.00019 & -0.00468 \\ 0.01488 & -0.00215 & 0.00433 & -0.00407 \end{bmatrix} & \begin{array}{l} \text{Mar 1, 2016} \\ \text{Mar 2, 2016} \\ \text{Mar 3, 2016} \end{array} \end{array}$$

$$R_{ti} = \frac{p_{ti}^{\text{final}} - p_{ti}^{\text{initial}}}{p_{ti}^{\text{initial}}}$$

Return matrix — portfolio vector

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\end{array}
$$

constant investment w

↓

Rw is the vector of portfolio returns over periods $1, \ldots, T$

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$$R_{ti} = \frac{p_{ti}^{\text{final}} - p_{ti}^{\text{initial}}}{p_{ti}^{\text{initial}}}$$

constant investment w

$\downarrow$

Rw is the vector of portfolio returns over periods $1, \ldots, T$

example $w = (0.4, 0.3, -0.2, 0.5)$ $\qquad$ $Rw = (0.00213, -0.00201, 0.00241)$

Symmetric positive semidefinite matrices

symmetric matrix

$A^T = A$

positive semidefinite matrix

$x^T Ax \geq 0$ for any $x \in \mathbf{R}^n$

positive definite matrix

$x^T Ax > 0$ for any $x \neq 0$

Symmetric positive semidefinite matrices

example

$$A = \begin{bmatrix} 2 & 6 \\ 6 & 20 \end{bmatrix}$$

symmetric matrix

$A^T = A$

positive semidefinite matrix

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positive definite matrix

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Symmetric positive semidefinite matrices

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example

$$A = \begin{bmatrix} 2 & 6 \\ 6 & 20 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 6 \\ 6 & 20 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2x_1 + 6x_2 \\ 6x_1 + 20x_2 \end{bmatrix}$$

$$= 2x_1^2 + 12x_1x_2 + 20x_2^2$$

$$= 2(x_1 + 3x_2)^2 + 2x_2^2$$

sum of squares

Matrix multiplication

matrix product

A matrix product of an $m \times p$ matrix A and a $p \times n$ matrix B is

$$C = AB, \qquad \text{where} \quad C_{ij} = A_{i1}B_{1j} + \cdots + A_{ip}B_{pj}, \quad i = 1, \ldots, m, j = 1, \ldots, n$$

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$m \times n$

(move along ith row of A and jth column of B)

$$\begin{bmatrix} -1.5 & 3 & 2 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 0 & -2 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 3.5 & -4.5 \\ -1 & 1 \end{bmatrix}$$

Complexity

Given $m \times n$ matrix A

- Matrix addition, scalar-matrix multiplication: mn flops
- Matrix-vector multiplication: $m(2n-1) \approx 2mn$ flops
- Matrix-matrix multiplication: $(mn)(2p-1) \approx 2mnp$ flops (inner product of p vectors)

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Questions

- How many flops does it take to multiply two 1000×1000 matrices?
- How long does it take on a computer?

Linear systems solutions

Linear systems of equations

Given an $m \times n$ matrix A and a m-vector b, find a n-vectors x such that

$$Ax = b$$

Linear systems of equations

Given an $m \times n$ matrix A and a m-vector b, find a n-vectors x such that

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typical scenarios

underdetermined
(wide)

$$m < n$$

$$\begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$$

infinite
solutions

Linear systems of equations

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infinite
solutions

square

$$m = n$$

$$\begin{bmatrix} * & * \\ * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$$

unique
solution

Linear systems of equations

Given an $m \times n$ matrix A and a m-vector b, find a n-vectors x such that

$$Ax = b$$

typical scenarios

underdetermined (wide)	square	overdetermined (tall)
$m < n$	$m = n$	$m > n$
$\begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$	$\begin{bmatrix} * & * \\ * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$	$\begin{bmatrix} * & * \\ * & * \\ * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} * \\ * \\ * \end{bmatrix}$
infinite solutions	unique solution	no solution

Linear systems of equations

Given an $m \times n$ matrix A and a m-vector b, find a n-vectors x such that

$$Ax = b$$

typical scenarios

underdetermined (wide)

$m < n$

$$\begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$$

infinite solutions

square

$m = n$

$$\begin{bmatrix} * & * \\ * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$$

unique solution

most common

overdetermined (tall)

$m > n$

$$\begin{bmatrix} * & * \\ * & * \\ * & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} * \\ * \\ * \end{bmatrix}$$

no solution

Solving square linear systems

Given an $n \times n$ matrix A and a n-vector b, find a n-vector x such that

$$Ax = b$$

Solving square linear systems

Given an $n \times n$ matrix A and a n-vector b, find a n-vector x such that

$$Ax = b \longrightarrow A^{-1}Ax = A^{-1}b$$

Solving square linear systems

Given an $n \times n$ matrix A and a n-vector b, find a n-vector x such that

$$Ax = b \longrightarrow A^{-1}Ax = A^{-1}b \longrightarrow x = \underbrace{A^{-1}}_{\text{inverse}}b$$

Solving square linear systems

Given an $n \times n$ matrix A and a n-vector b, find a n-vector x such that

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When does it work?

Solving square linear systems

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When does it work?

$$\downarrow$$

A must be invertible

- Columns of A are linearly independent
- Rows of A are linearly independent
- Columns/rows form a **basis** of $\mathbf{R}^n$

Solving linear systems

How do we solve linear systems in practice?

$$Ax = b$$

Idea

- compute A^{-1}
- multiply $A^{-1}b$

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Example

5000×5000 matrix A and a 5000-vector b

- Solve by computing A^{-1}
- Solve with `numpy.linalg.solve`

How do we solve linear systems in practice?

$$Ax = b$$

Idea

- compute A^{-1}
- multiply $A^{-1}b$

Example

5000×5000 matrix A and a 5000-vector b

- Solve by computing A^{-1}
- Solve with `numpy.linalg.solve`

What's happening inside?

Easy linear systems

Diagonal matrix

$$\begin{bmatrix} A_{11} & & \\ & \ddots & \\ & & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} \longrightarrow \begin{aligned} A_{11}x_1 &= b_1 \\ A_{22}x_2 &= b_2 \\ &\vdots \\ A_{nn}x_n &= b_n \end{aligned}$$

Easy linear systems

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Solution

$$x = A^{-1}b = (b_1/A_{11}, \ldots, b_n/A_{nn})$$

Easy linear systems

Diagonal matrix

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Solution

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Complexity

n flops

Easy linear systems

Lower triangular matrix

$$\begin{bmatrix} A_{11} & & & \\ A_{21} & A_{22} & & \\ \vdots & & \ddots & \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \longrightarrow \begin{aligned} A_{11}\boxed{x_1} &= b_1 \\ A_{21}x_1 + A_{22}\underline{x_2} &= b_2 \\ &\vdots \\ A_{n1}x_1 + A_{n2}x_2 + \dots A_{nn}x_n &= b_n \end{aligned}$$

Easy linear systems

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Solution: "forward substitution"

- First equation: $x_1 = b_1/A_{11}$
- Second equation: $x_2 = (b_2 - A_{21}x_1)/A_{22}$
- Repeat to get $x_3, \dots, x_n$

$\sum_{i=1}^{n} 2i - 1 = 2\left(\sum_{i=1}^{n} i\right) - n =$

$= 2\frac{n(n+1)}{2} - n = n^2 + n - n = n^2$

Easy linear systems

Lower triangular matrix

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Complexity

- First equation: 1 flop (division)
- Second equation: 3 flops
- ith step needs $2i - 1$ flops

$$1 + 3 + \dots + (2n - 1) = n^2 \text{ flops}$$

Easy linear systems

Upper triangular matrix

$$\begin{bmatrix} A_{11} & \dots & A_{n-1,n} & A_{1n} \\ & \ddots & & \vdots \\ & & A_{n-1,n-1} & A_{n-1,n} \\ & & & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \longrightarrow \begin{aligned} A_{11}x_1 + \cdots + A_{1,n-1}x_{n-1} + A_{1n}x_n &= b_1 \\ &\vdots \\ A_{n-1,n-1}x_{n-1} + A_{n-1,n}x_n &= b_{n-1} \\ A_{nn}x_n &= b_n \end{aligned}$$

Easy linear systems

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Solution: **“**backward substitution”

- Last equation: $x_n = b_n / A_{nn}$
- Second to last equation:
  $x_{n-1} = (b_{n-1} - A_{n-1,n}x_n)/A_{n-1,n-1}$
- Repeat to get $x_{n-2}, \ldots, x_1$

Easy linear systems

Upper triangular matrix

$$\begin{bmatrix} A_{11} & \dots & A_{n-1,n} & A_{1n} \\ & \ddots & & \vdots \\ & & A_{n-1,n-1} & A_{n-1,n} \\ & & & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \longrightarrow \begin{aligned} A_{11}x_1 + \cdots + A_{1,n-1}x_{n-1} + A_{1n}x_n &= b_1 \\ &\vdots \\ A_{n-1,n-1}x_{n-1} + A_{n-1,n}x_n &= b_{n-1} \\ A_{nn}x_n &= b_n \end{aligned}$$

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  $x_{n-1} = (b_{n-1} - A_{n-1,n}x_n)/A_{n-1,n-1}$
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Complexity

- Last equation: 1 flop (division)
- Second to last equation: 3 flops
- ith step needs $2i - 1$ flops

$1 + 3 + \cdots + (2n - 1) = n^2$ flops

Easy linear systems

Permutation matrices

$\pi = (\pi_1, \ldots, \pi_n)$ is a permutation of $(1, 2, \ldots, n)$

A $n \times n$ permutation matrix P,
permutes the vector x

$$Px = (x_{\pi_1}, \ldots, x_{\pi_n})$$

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example

$$\pi = (2, 3, 1)$$

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}_{P} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$

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Properties

- $P_{ij} = \begin{cases} 1 & j = \pi_i \\ 0 & \text{otherwise} \end{cases}$
- $P^{-1} = P^T$ (inverse permutation)

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Complexity

Solve $Px = b$: 0 flops (no operations)

example

$$\pi = (2, 3, 1)$$

$$\begin{array}{c} P \\ \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \end{array} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$

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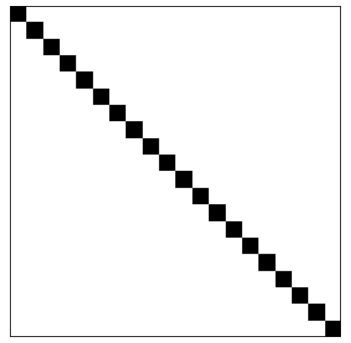
Summary of easy linear systems

		method	flops
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n

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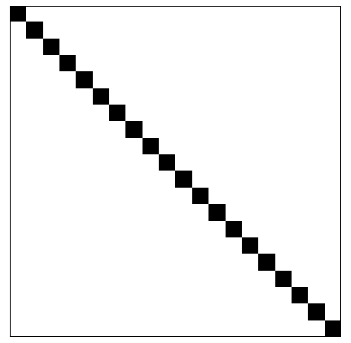
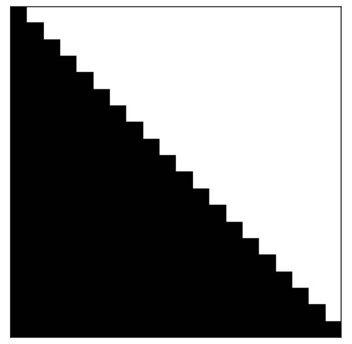
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2

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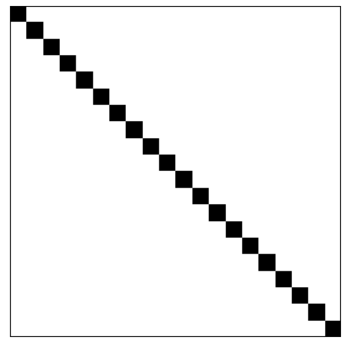
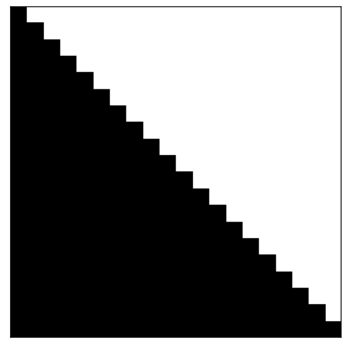
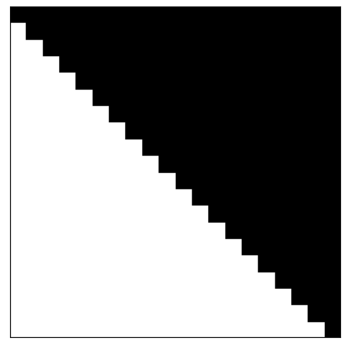
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2
	**upper triangular** $A_{ij} = 0$ for $i > j$	backward substitution	n^2

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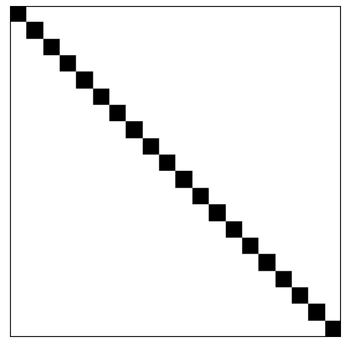
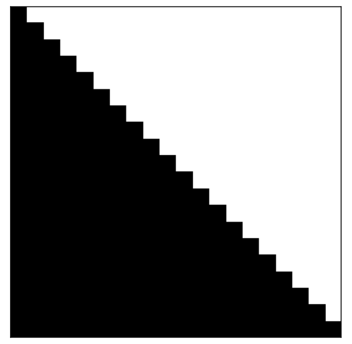
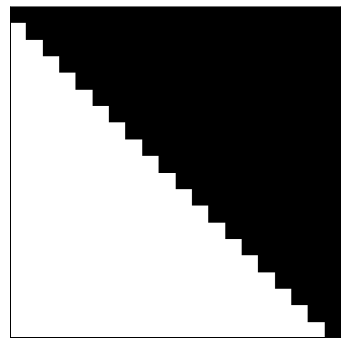
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2
	**upper triangular** $A_{ij} = 0$ for $i > j$	backward substitution	n^2
	permutation $P_{ij} = 1$ if $j = \pi_i$ else 0	inverse permutation	0

How do we solve linear systems in practice?

$$Ax = b$$

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We know how to solve special ones

Let’s use that!

The factor-solve method for solving $Ax = b$

1. **Factor** A as a product of simple matrices:

$$A = A_1 A_2 \cdots A_k, \longrightarrow A_1 A_2, \ldots A_k x = b$$

(A_i diagonal, upper/lower triangular, permutation, etc)

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$$A_2 \underbrace{A_3 \dots A_k x}_{x_2} = x_1$$

$\vdots$

(A_i diagonal, upper/lower triangular, permutation, etc)

2. **Compute** $x = A^{-1}b = A_k^{-1} \cdots A_2^{-1} \boxed{A_1^{-1} b}$
   by solving k "easy" systems

$$\longrightarrow \quad \begin{aligned} A_1 x_1 &= b \\ A_2 x_2 &= x_1 \\ &\vdots \\ A_k x &= x_{k-1} \end{aligned}$$

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Note: step 2 is much cheaper than step 1

Multiple right-hand sides

You now have factored A and you want to solve d linear systems with different righ-hand side m-vectors b_i

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1. Factor $A = A_1, \dots, A_k$ **only once** (expensive)
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Solve many “at the price of one”

LU Factorization

Every invertible matrix A can be factored as

$$A = PLU \longrightarrow P^T A = LU$$

P permutation, L lower triangular, U upper triangular

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- One of infinite possible combinations of P, L, U

Complexity

- $(2/3)n^3$ flops
- Less if A has special structure (sparse, diagonal, etc)

LU **Solution**

$$Ax = b, \quad \Rightarrow \quad PLUx = b$$

Iterations

1. *Permutation*: Solve $Px_1 = b$ (0 flops)
2. *Forward substitution*: Solve $Lx_2 = x_1$ (n^2 flops)
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Complexity

- Factor + solve: $(2/3)n^3 + 2n^2 \approx (2/3)n^3$ (for large n)
- Just solve (prefactored): $2n^2$

LL^T (Cholesky) Factorization

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- One of infinite possible choices of L

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L lower triangular

Procedure

- Works only on **symmetric with positive definite** matrices
- No need to permute as in LU
- One of infinite possible choices of L

Complexity

- $(1/3)n^3$ flops (half of LU decomposition)
- Less if A has special structure (sparse, diagonal, etc)

LL^T (Cholesky) Solution

$$Ax = b, \quad \Rightarrow \quad LL^T x = b$$

Iterations

1. *Forward substitution*: Solve $Lx_1 = b$ (n^2 flops)
2. *Backward substitution*: Solve $L^T x = x_1$ (n^2 flops)

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$$Ax = b, \quad \Rightarrow \quad LL^T x = b$$

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What complexity really means?

Example

Large matrix $n \times n$ matrix A with $n = 10,000$

Factor + solve: $(2/3)n^3$

Just solve: $2n^2$

$\longrightarrow$ Gains: $\dfrac{(2/3)n^3}{2n^2} = (1/3)n \approx 3,333$ times

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$\longrightarrow$

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3 **thousand times!**

Something that takes 1 second $\longrightarrow$ ≈ 1 hour

Linear system example

Polynomial interpolation

Given a cubic polynomial

$$p(x) = c_1 + c_2 x + c_3 x^2 + c_4 x^3$$

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Equivalent linear system

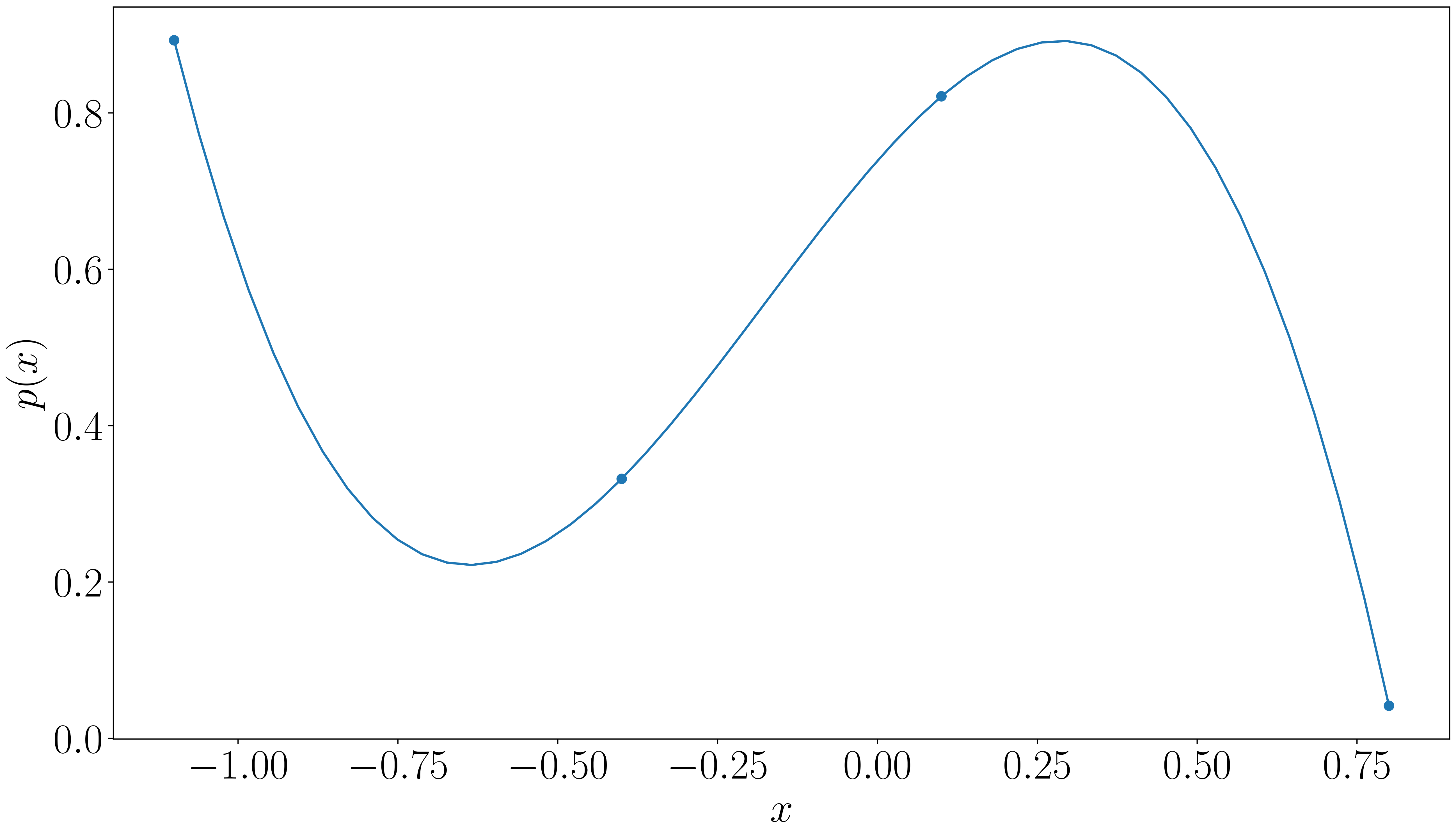
$$Ac = b$$

$$\begin{bmatrix} 1 & -1.1 & (-1.1)^2 & (-1.1)^3 \\ 1 & -0.4 & (-0.4)^2 & (-0.4)^3 \\ 1 & 0.1 & (0.1)^2 & (0.1)^3 \\ 1 & 0.8 & (0.8)^2 & (0.8)^3 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

Polynomial interpolation

Plot

$$p(x) = c_1 + c_2 x + c_3 x^2 + c_4 x^3 \qquad c = (0.74, 0.93, -0.89, -1.70)$$



Solving linear systems in practice

Today, we learned to:

- **Avoid** computing inverses
- **Solve** linear systems using the factor-solve method
- **Understand** the complexity of solving linear systems
  (useful to build optimization algorithms!)

References

- S. Boyd, L. Vandenberghe: Introduction to Applied Linear Algebra – Vectors, Matrices, and Least Squares
  - Chaptrer 6: matrices
  - Chapter 10: matrix multiplication
  - Chapter 11: matrix inverses/solving linear systems

Next lecture

- Solve optimization problems: least squares