ORF307 – Optimization

3. Least squares

Bartolomeo Stellato — Spring 2024

Ed Forum

- Why do we need docker? Can we use Colab instead?

The docker image has all the packages installed, including jupyterlab and the right tools to export notebooks to pdf. Once you start docker, you have everything you need in the images we specifically designed for this class. We used Colab in the past and students had several issues exporting the notebooks (plots are cut between pages, some equations are not readable, etc). Also, Colab automatically disconnects/shuts down if you do not use it and you lose your data. ***You can use colab at your own risk.*** *If submissions are not readable, we will discard points.* ***It is your responsibility to have readable submissions.***

- Irina's office hours moved from Monday 2pm-3:30pm to Monday 3:30pm-5pm

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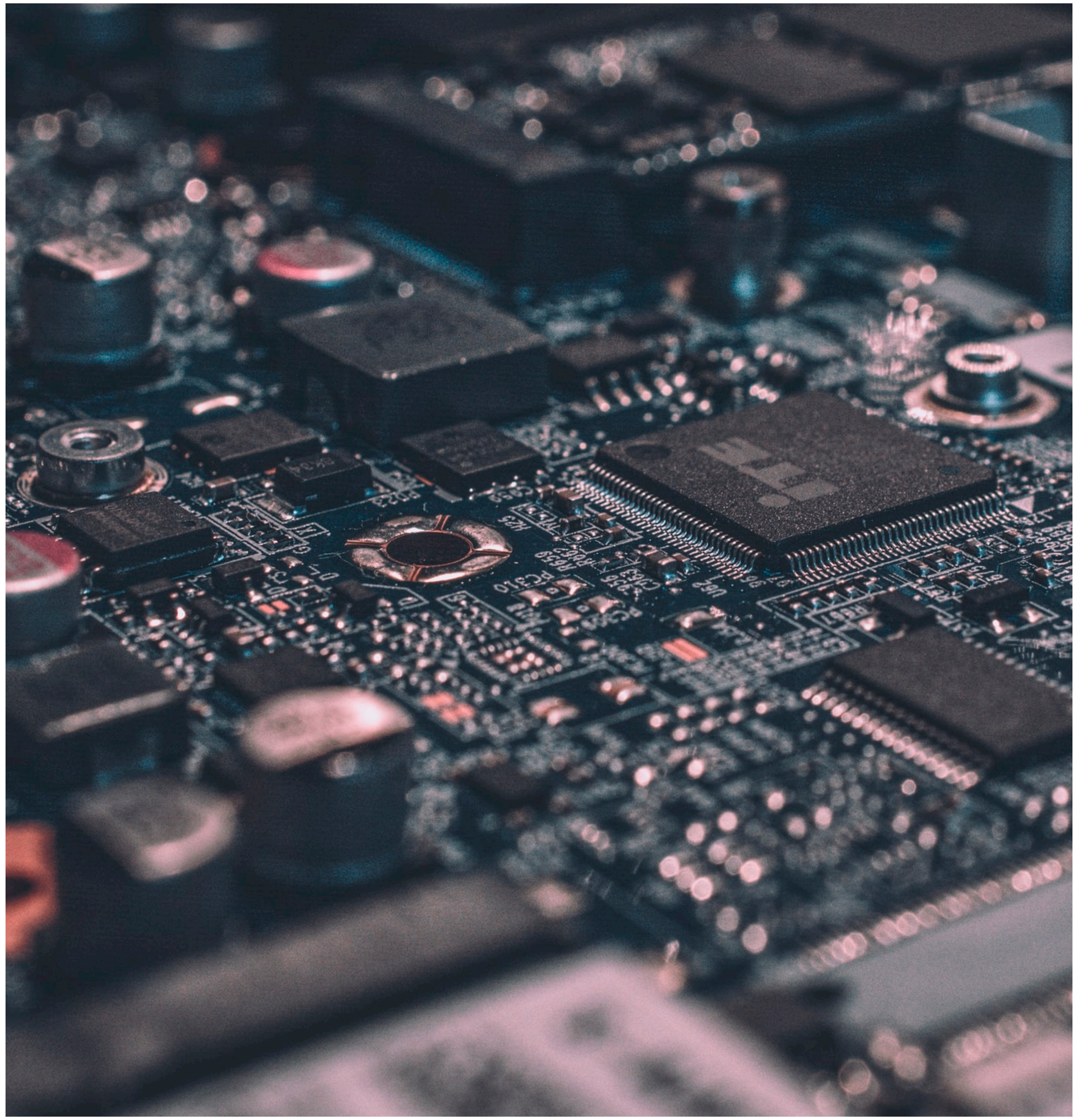
- I was confused about Ax=b and PLUx=b solving for x. How does PLUx=b get to x=…?

- How does the factor-solve procedure actually help us in real applications? —> We will see this today!

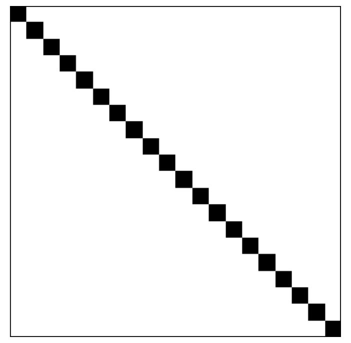
Recap

Flop counts

- Computers store real numbers in **floating-point format**
- Basic arithmetic operations (addition, multiplication, etc…) are called **floating point operations (flops)**
- **Algorithm complexity**: total number of flops needed as function of dimensions
- **Execution time** $\approx$ (flops)/(computer speed) *[Very grossly approximated]*
- Modern computers can go at 1 Gflop/sec (10^9 flops/sec)



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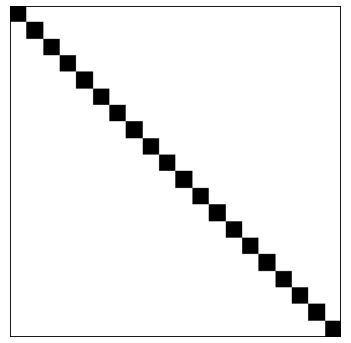
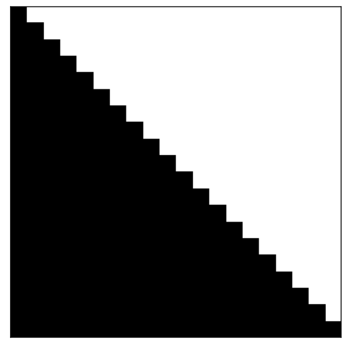
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2

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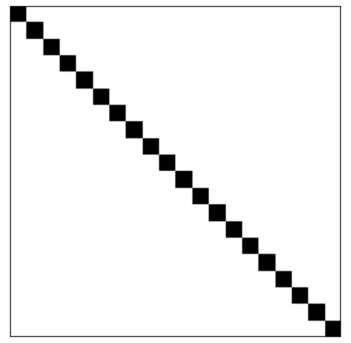
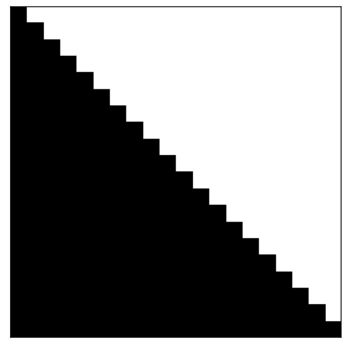
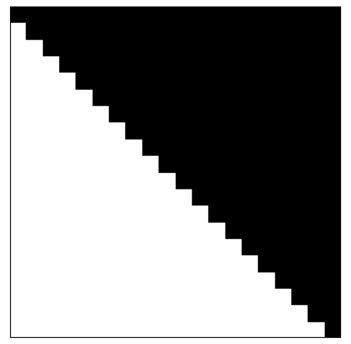
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2
	**upper triangular** $A_{ij} = 0$ for $i > j$	backward substitution	n^2

Summary of easy linear systems

$Ax = b$

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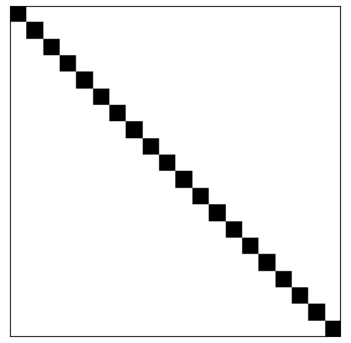
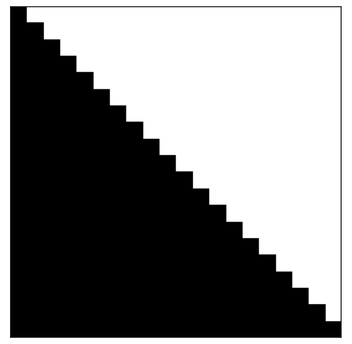
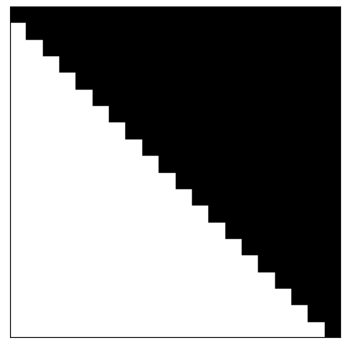
	**diagonal** $A = \mathbf{diag}(a_1, \ldots, a_n)$	$x_i = b_i / a_i$	n
	**lower triangular** $A_{ij} = 0$ for $i < j$	forward substitution	n^2
	**upper triangular** $A_{ij} = 0$ for $i > j$	backward substitution	n^2
	permutation $P_{ij} = 1$ if $j = \pi_i$ else 0	inverse permutation	0

$Px = \tilde{x}$

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

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

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

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

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

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

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

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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Factorization-caching procedure

1. Factor $A = A_1, \ldots, A_k$ **only once** (expensive)
2. Solve all linear systems using **the same factorization** (cheap)

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Solve many "at the price of one"

LL^T (Cholesky) Factorization

Every positive definite matrix A can be factored as

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L lower triangular

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Procedure

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

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Complexity

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

LL^T (Cholesky) Solution

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

$x = (L^T)^{-1} L^{-1} b$

1. $\boxed{x_1} = L^{-1} b$

$\hookrightarrow L x_1 = b$

2. $x = (L^T)^{-1} x_1$

$\hookrightarrow L^T x = x_1$

Iterations

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

LL^T (Cholesky) Solution

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Iterations

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Complexity

- Factor + solve: $(1/3)n^3 + 2n^2 \approx (1/3)n^3$ (for large n)
- Just solve (prefactored): $2n^2$

Today's lecture

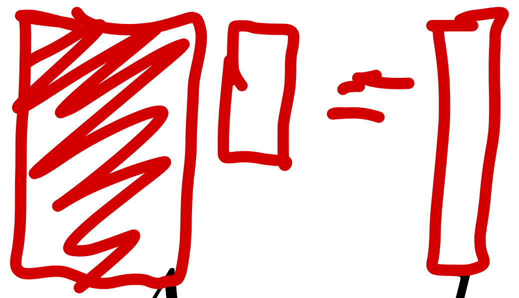
Least squares

- Least squares optimization
- Gram matrix
- Solving least squares
- Example

Least squares optimization

Solving overdetermined linear systems

You have an *overdetermined* $m \times n$ linear system (m > n)



$$Ax = b$$

(with tall A)

Solving overdetermined linear systems

You have an *overdetermined* $m \times n$ linear system (m > n)

$$Ax = b$$

(with tall A)

$x_1 = 1/2$
$x_2 = +1/2$ ←

$$\begin{cases} 2x_1 = 1 \\ -x_1 + x_2 = 0 \\ 2x_2 = -1 \end{cases}$$

example

Typically no solution

$$\begin{bmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Least squares problem

residual vector

$$r = Ax - b$$

$\longrightarrow$

Goal: make it as small as possible

minimize $\quad \|r\|$

Least squares problem

residual vector

$$r = Ax - b$$

$\longrightarrow$

Goal: make it as small as possible

minimize $\quad \|r\|$

Least squares problem

minimize $\quad \|Ax - b\|_2^2$

- x is the *decision variable*
- $\|Ax - b\|_2^2$ is the *objective function*

Least squares solution

$$\text{minimize} \quad \|Ax - b\|_2^2$$

Least squares solution

$$\text{minimize} \quad \|Ax - b\|_2^2$$

$x^\star$ is a *solution* of least squares problem if

optimality condition

$$\|Ax^\star - b\|^2 \leq \|Ax - b\|^2, \quad \text{for any } n\text{-vector } x$$

Least squares solution

minimize $\quad \|Ax - b\|_2^2$

$x^\star$ is a *solution* of least squares problem if

optimality condition $\quad \|Ax^\star - b\|^2 \leq \|Ax - b\|^2, \quad$ for any n-vector x

$x^\star$ need not (and usually does not) satisfy $Ax^\star = b$

What happens if $x^\star$ does satisfy $Ax^\star = b$?

Column interpretation

$$A = \Big[a_1, \ldots, a_n\Big], \qquad a_1, \ldots, a_n \text{ are columns of } A$$

Goal: find a linear combination of the columns of A that is closest to b

$$\|Ax - b\|^2 = \|(x_1 a_1 + \cdots + x_n a_n) - b\|^2$$

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$$\|Ax - b\|^2 = \|(x_1 a_1 + \cdots + x_n a_n) - b\|^2$$

If $x^\star$ is a solution of the least squares problem, the m-vector

$$Ax^\star = x_1^\star a_1 + \cdots + x_n^\star a_n$$

is the closest to b among all linear combinations of the columns of A

$r = Ax - b$

Row interpretation

$$A = \begin{bmatrix} \tilde{a}_1^T \\ \vdots \\ \tilde{a}_m^T \end{bmatrix}, \qquad \tilde{a}_1^T, \ldots, \tilde{a}_m^T \text{ are rows of } A$$

The residual components are $r_i = \tilde{a}_i^T x - b_i$

$\|r\|_2 = \sqrt{r^T r}$

$\|r\|_2^2 = r^T r = r_1^2 + r_2^2 \dots r_m^2$

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Goal minimize sum of squares of the residuals

$$\|Ax - b\|^2 = (\tilde{a}_1^T x - b_1)^2 + \cdots + (\tilde{a}_m^T x - b_m)^2$$

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Comparison

- Solving $Ax = b$ forces all residuals to be zero
- Least squares attempts to make them small

Example

$$\overset{A}{\begin{bmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{bmatrix}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \overset{b}{\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}}$$

Least squares problem

Compute x to minimize

$$\|Ax - b\|^2 = (2x_1 - 1)^2 + (-x_1 + x_2)^2 + (2x_2 + 1)^2$$

Example

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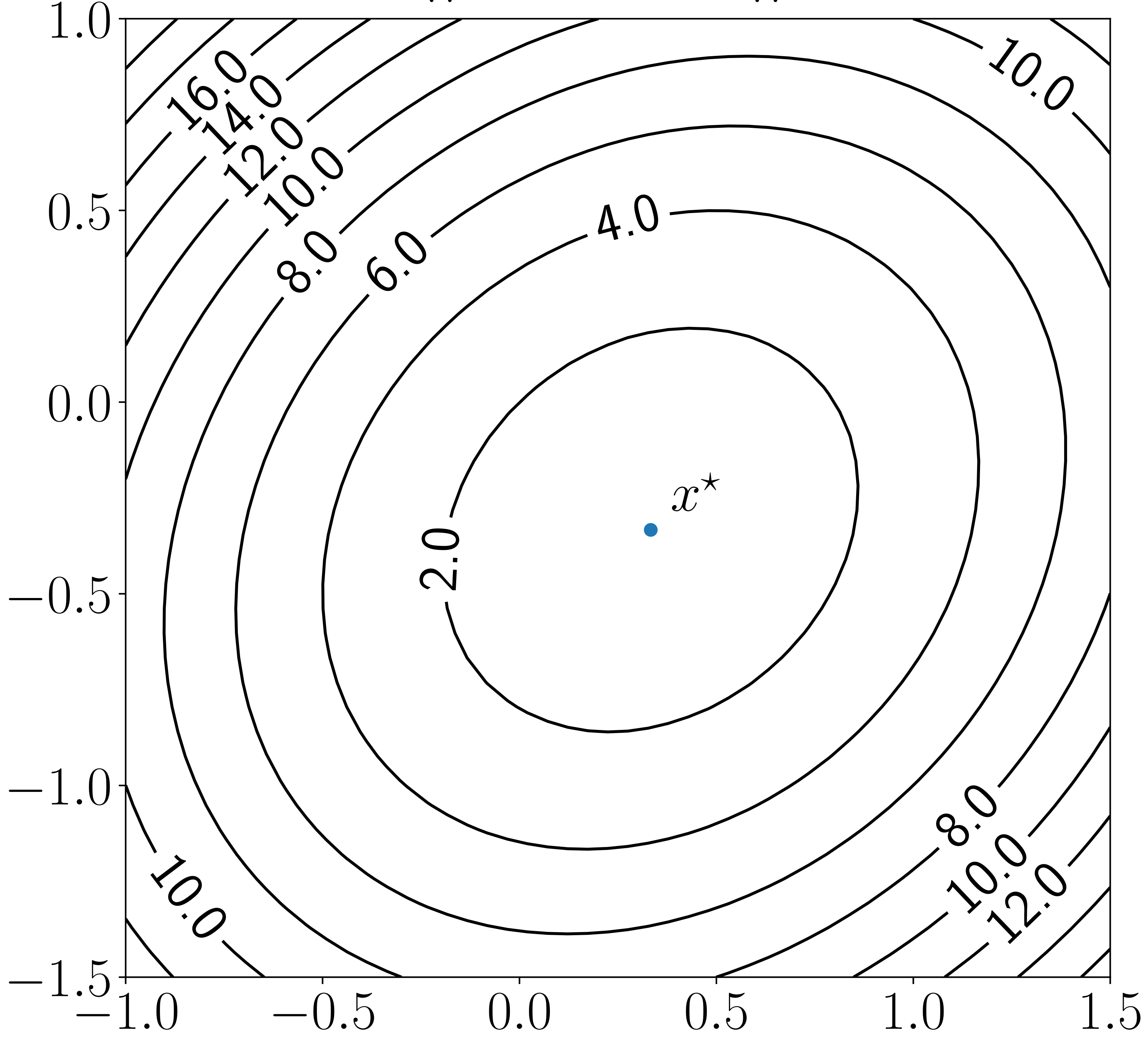
$\|Ax - b\|^2$



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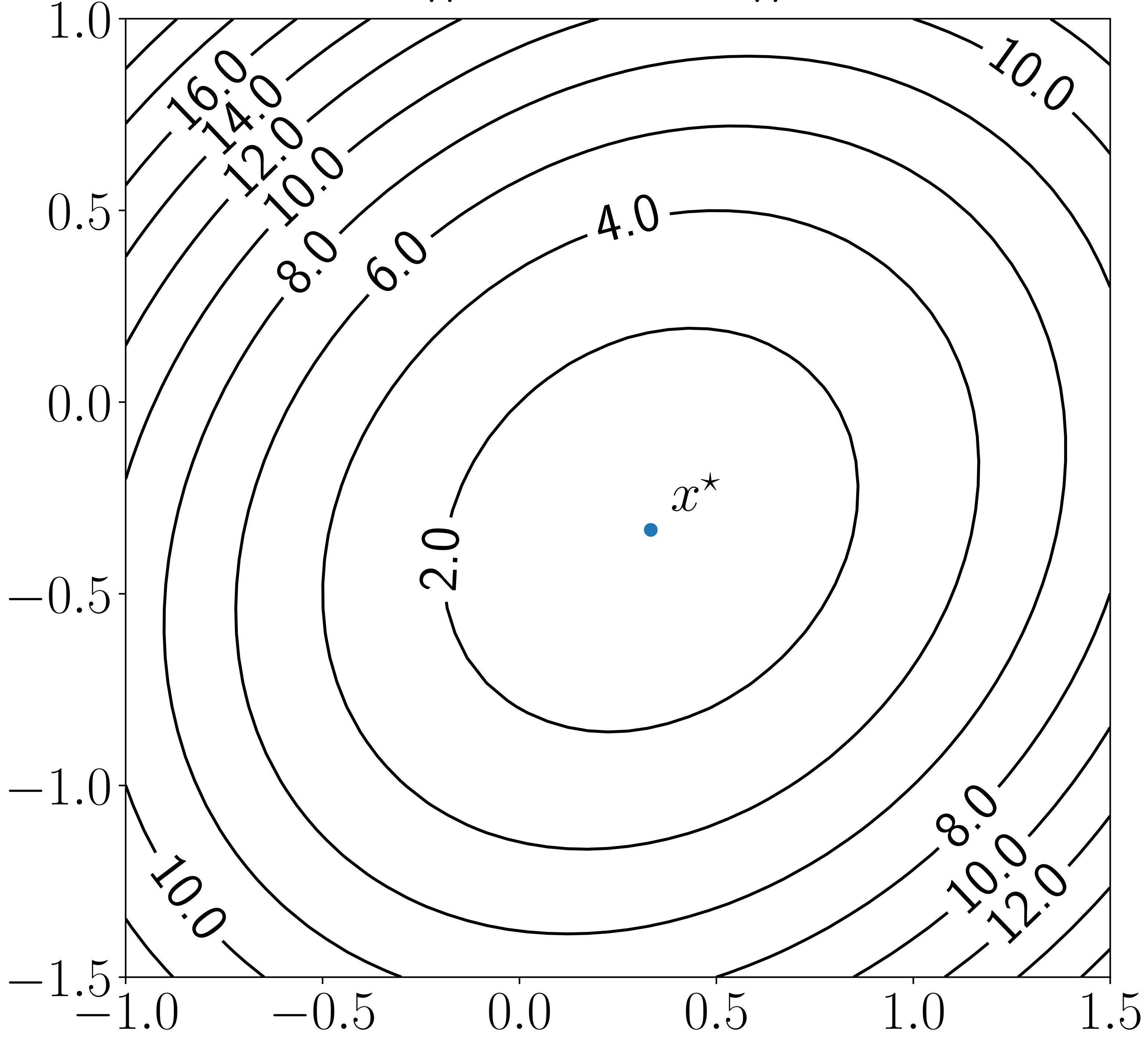

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Solution $x^\star = (1/3, -1/3)$ (via calculus)

Interpretations

- $\|Ax^\star - b\|^2 = 2/3$ smallest possible value of $\|Ax - b\|^2$
- $Ax^\star = (2/3, -2/3, -2/3)$ is the linear combination of columns of A closest to b

Gram matrix

Gram matrix

$\boxed{m \geq n}$

Given an $m \times n$ matrix A with columns $a_1, \ldots, a_n$

$(A^T A)_{12} = a_1^T a_2$

the **Gram matrix** of A is

$$\underset{\in \mathbb{R}^{n \times n}}{A^T A} = \begin{array}{c c} & \begin{array}{cccc} & 2 & & \end{array} \\ \begin{array}{c} 1 \\ \\ \\ \\ \end{array} & \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \ldots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \ldots & a_2^T a_n \\ \vdots & \vdots & \ddots & \vdots \\ a_n^T a_1 & a_n^T a_2 & \ldots & a_n^T a_n \end{bmatrix} \end{array}$$

Very useful in least squares problems

Gram matrix

Invertibility

A has linearly independent columns if and only if $A^T A$ is invertible

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We show that $Ax = 0 \iff A^T A x = 0$

$\Rightarrow$ if $Ax = 0$ then we can write

$$A^T A x = A^T \underbrace{(Ax)}_{0} = A^T 0 = 0$$

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We show that $Ax = 0 \iff A^T Ax = 0$

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$$A^T Ax = A^T(Ax) = A^T 0 = 0$$

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

$\Leftarrow$ if $A^T Ax = 0$ then we can write

$$0 = x^T 0 = x^T(A^T Ax) = x^T A^T \underbrace{Ax}_{v} = \|Ax\|^2$$

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$$0 = x^T 0 = x^T(A^T Ax) = x^T A^T Ax = \|Ax\|^2$$

which implies that $Ax = 0$ (definition of norm) $\blacksquare$

Positive (semi)definiteness of Gram matrix

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

Positive semidefinite (always)

$$x^T A^T A x = \underbrace{(Ax)}_{v}^T \underbrace{(Ax)}_{v} = \|Ax\|^2 \geq 0, \qquad \text{for any } n\text{-vector } x$$

Positive (semi)definiteness of Gram matrix

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If the columns of A are linearly independent, then

$Ax \neq 0$ for any $x \neq 0$

Positive (semi)definiteness of Gram matrix

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Proof

If the columns of A are linearly independent, then

$Ax \neq 0$ for any $x \neq 0$

Therefore, $x^T A^T A x = \|Ax\|^2 > 0$ (definition of norm) ■

Solving least squares problems

Main assumption

Least squares problem

$$\text{minimize} \quad \|Ax - b\|_2^2$$

A has **linearly independent columns**

True in most practical examples such as data fitting (next lecture)

$r_i = \tilde{a}_i^T x - b_i$

Calculus derivation

$$f(x) = \|Ax - b\|^2 = \sum_{i=1}^{m} \left(\overbrace{\sum_{j=1}^{n} A_{ij} x_j - b_i}^{r_i} \right)^2$$

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$$\nabla f(x^\star)_k = \frac{\partial f}{\partial x_k}(x^\star) = 0,$$

for $k = 1, \ldots, n$

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$$\frac{\partial f}{\partial x_k}(x) = 2 \sum_{i=1}^{m} \left(\overbrace{\sum_{j=1}^{n} A_{ij} x_j - b_i}^{r_i = (Ax-b)_i} \right) (A_{ik})$$

$$= 2 \sum_{i=1}^{m} (A^T)_{ki} \overbrace{(Ax - b)_i}^{r_i}$$

$$= 2(A^T(Ax - b))_k$$

Calculus derivation in vector form

$(Ax)^T Ax - (Ax)^T b$
$- b^T(Ax) + b^T b$

$$f(x) = \|Ax - b\|^2 = (Ax-b)^T(Ax-b) = x^T \underbrace{A^T A}_{M} x - 2\underbrace{(A^T b)}_{q}{}^T x + b^T b$$

$\rightarrow \nabla_x (q^T x) = q$

$\rightarrow \nabla_x (x^T M x) = 2Mx$

SYMMETRIC

Calculus derivation in vector form

$$f(x) = \|Ax - b\|^2 = (Ax - b)^T(Ax - b) = x^T A^T A x - 2(A^T b)^T x + b^T b$$

$$\nabla f(x^\star) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x^\star) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x^\star) \end{bmatrix} = 2A^T A x^\star - 2A^T b = 2A^T(Ax^\star - b) = 0$$

Calculus derivation in vector form

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normal equations

$$(A^T A)x^\star = A^T b$$

Calculus derivation in vector form

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normal equations

$n \times n$
square
linear system $\longrightarrow$ $(A^T A) x^\star = A^T b$

Optimality

For $x^\star$ such that $A^T A x^\star = A^T b$, we have

$\|v+e\|^2 = (v+e)^T(v+e) = \|v\|^2 + \|e\|^2$
$+ 2v^Te$

Optimality

For $x^\star$ such that $A^TAx^\star = A^Tb$, we have

$$
\begin{aligned}
\|Ax-b\|^2 &= \|(Ax - Ax^\star) + (Ax^\star - b)\|^2 \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(A(x-x^\star))^T(Ax^\star - b) \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(x-x^\star)^TA^T(Ax^\star - b) \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star - b\|^2
\end{aligned}
$$

Optimality

For $x^\star$ such that $A^TAx^\star = A^Tb$, we have

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\underbrace{\|Ax-b\|^2}_{f(x)} &= \|(Ax-Ax^\star)+(Ax^\star-b)\|^2 \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star-b\|^2 + 2(A(x-x^\star))^T(Ax^\star-b) \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star-b\|^2 + 2(x-x^\star)^T A^T(Ax^\star-b) \\
&= \|A(x-x^\star)\|^2 + \underbrace{\|Ax^\star-b\|^2}_{f(x^\star)}
\end{aligned}
$$

$$(A^T(Ax^\star-b)=0)$$

Optimality

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\begin{aligned}
\|Ax-b\|^2 &= \|(Ax - Ax^\star) + (Ax^\star - b)\|^2 \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(A(x-x^\star))^T(Ax^\star - b) \\
&= \|A(x-x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(x-x^\star)^T A^T(Ax^\star - b) \\
&= \underbrace{\|A(x-x^\star)\|^2}_{\geq 0} + \|Ax^\star - b\|^2
\end{aligned}
$$

$$(A^T(Ax^\star - b) = 0)$$

Therefore, for any x, we have

$$\|Ax-b\|^2 \geq \|Ax^\star - b\|^2$$

Optimality

For $x^\star$ such that $A^T A x^\star = A^T b$, we have

$$\begin{aligned}
\|Ax - b\|^2 &= \|(Ax - Ax^\star) + (Ax^\star - b)\|^2 \\
&= \|A(x - x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(A(x - x^\star))^T(Ax^\star - b) \\
&= \|A(x - x^\star)\|^2 + \|Ax^\star - b\|^2 + 2(x - x^\star)^T A^T(Ax^\star - b) \\
&= \underbrace{\|A(x - x^\star)\|^2}_{=0} + \|Ax^\star - b\|^2
\end{aligned}$$

$$(A^T(Ax^\star - b) = 0)$$

Therefore, for any x, we have

$$\|Ax - b\|^2 \geq \|Ax^\star - b\|^2$$

If equality holds, $A\overbrace{(x - x^\star)}^{v} = 0 \Rightarrow x = x^\star$
since columns of A are linearly independent

Solving normal equations

$$(A^T A)x^\star = A^T b$$

Solving normal equations

$$(A^T A)x^\star = A^T b$$

Inversion

$$x^\star = (A^T A)^{-1} A^T b$$

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Inversion

$$x^\star = (A^T A)^{-1} A^T b$$

$\longrightarrow$

Pseudo-inverse

$$A^\dagger = (A^T A)^{-1} A^T$$

Solving normal equations

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Inversion

$$x^\star = (A^T A)^{-1} A^T b$$

$\longrightarrow$

Pseudo-inverse

$$A^\dagger = (A^T A)^{-1} A^T$$

Factor-solve method

A has linearly independent columns

$\downarrow$

$A^T A$ is **symmetric positive-definite**

Solving normal equations

$$(A^T A)x^\star = A^T b$$

Inversion

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Factor-solve method

A has linearly independent columns

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$A^T A$ is **symmetric positive-definite**

$\longrightarrow$

Cholesky factorization

$$A^T A = LL^T$$

Solving normal equations

$$(A^TA)x^\star = A^Tb$$

Inversion

$$x^\star = (A^TA)^{-1}A^Tb$$

$\longrightarrow$

Pseudo-inverse

$$A^\dagger = (A^TA)^{-1}A^T$$

Factor-solve method

A has linearly independent columns

$\downarrow$

A^TA is **symmetric positive-definite**

$\longrightarrow$

Cholesky factorization

$$A^TA = LL^T$$

Which method is faster?

Solving normal equations with Cholesky

1. Form linear system $A^T Ax = A^T b$
    - Form $M = A^T A$ ($2mn^2$ flops)
    - Form $q = A^T b$: ($2mn$ flops)

Solving normal equations with Cholesky

$A^TA \in \mathbb{R}^{n \times n}$

1. Form linear system $A^TAx = A^Tb$
   - Form $M = A^TA$ ($2mn^2$ flops)
   - Form $q = A^Tb$: ($2mn$ flops)

2. Factor $M = LL^T$ ($(1/3)n^3$ flops)

Solving normal equations with Cholesky

1. Form linear system $A^T Ax = A^T b$
   - Form $M = A^T A$ ($2mn^2$ flops)
   - Form $q = A^T b$: ($2mn$ flops)

2. Factor $M = LL^T$ ($(1/3)n^3$ flops)

3. Solve $LL^T x = q$ ($2n^2$ flops)
   (with forward/backward substitution)

Solving normal equations with Cholesky

1. Form linear system $A^TAx = A^Tb$
   - Form $M = A^TA$ ($2mn^2$ flops)
   - Form $q = A^Tb$: ($2mn$ flops)
2. Factor $M = LL^T$ ($(1/3)n^3$ flops)
3. Solve $LL^Tx = q$ ($2n^2$ flops)
   (with forward/backward substitution)

Complexity

- Factor + solve: $2mn^2 + 2mn + (1/3)n^3 + 2n^2 \approx 2mn^2$
- Solve given a new b (prefactored): $2mn + 2n^2 \approx 2mn$

Example

Optimal advertising

m demographic groups
we want to advertise to

v^{des} is the m-vector
of desired views/impressions

Optimal advertising

m demographic groups
we want to advertise to

$\longrightarrow$

v^{des} is the m-vector
of desired views/impressions

n advertising channels
(web publishers, radio, print, etc.)

$\longrightarrow$

s is the n-vector
of purchases

Optimal advertising

m demographic groups
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(web publishers, radio, print, etc.) → s is the n-vector
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$m \times n$ matrix A gives
demographic reach of channels → A_{ij} is the number of views
for group i and dollar spent
on channel j $(1000/\$)$

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Views across demographic groups

$$v = As$$

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Views across demographic groups

$$v = As$$

Goal

$$\text{minimize} \quad \|As - v^{\text{des}}\|^2$$

Optimal advertising

Results

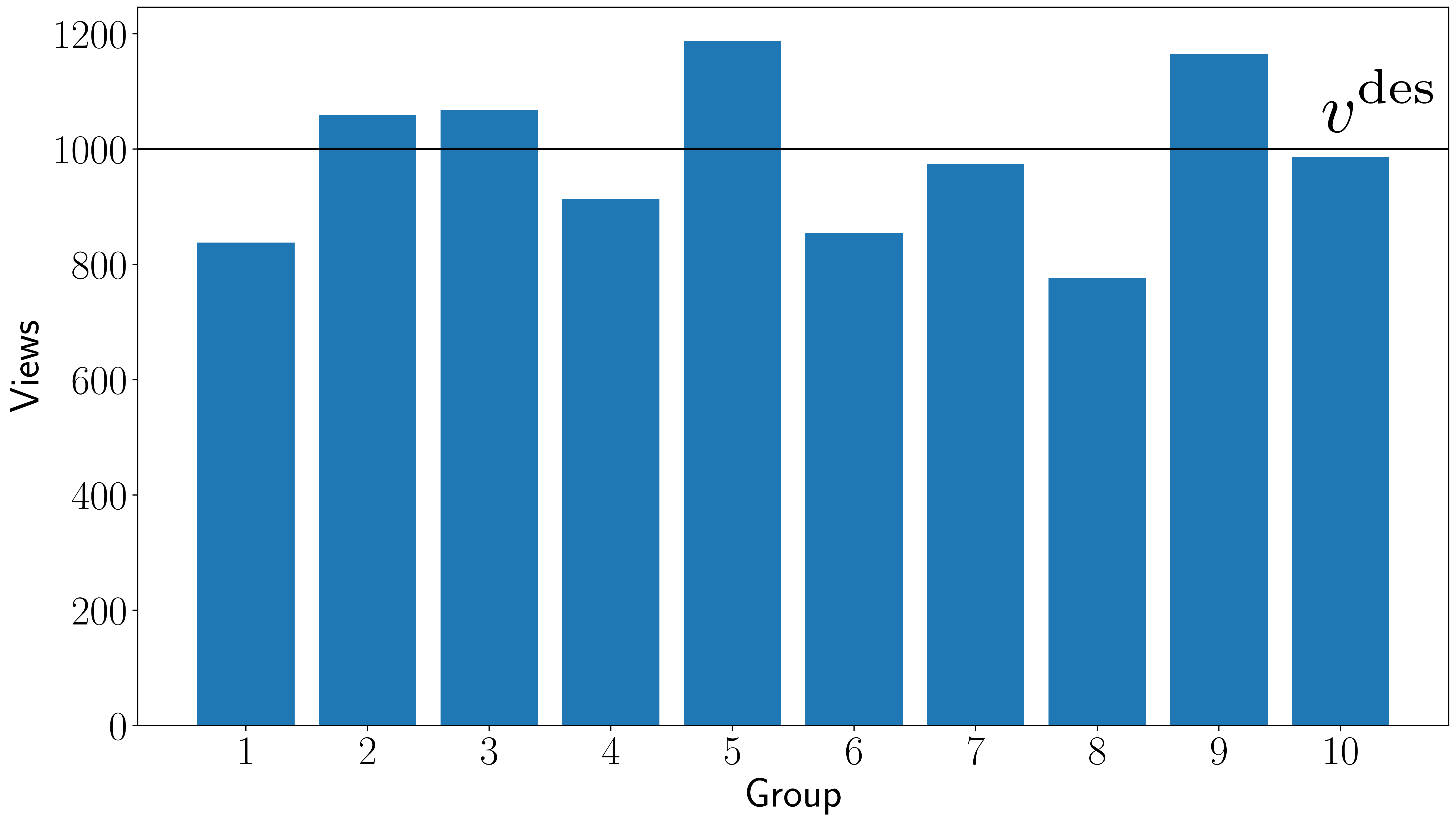
$m = 10$ groups, $n = 3$ channels

desired views vector $v^{\text{des}} = (10^3)\mathbf{1}$

minimize $\quad \|As - v^{\text{des}}\|^2$

$\downarrow$

optimal spending $s^\star = (62, 100, 1443)$



Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

$$\text{minimize} \quad \|As - v^{\text{des}}\|^2$$

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\mathrm{des}}\|^2$

Pseudoinverse

Time: 263 sec

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\text{des}}\|^2$

First solve

desired views $v^{\text{des},1} = (10^3)\mathbf{1}$

1. Form linear system $Mx = q$
   where $M = A^T A, q = A^T b$
2. Factor $M = LL^T$
3. Solve $LL^T x = q$

Pseudoinverse

Time: 263 sec

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\mathrm{des}}\|^2$

First solve

desired views $v^{\mathrm{des},1} = (10^3)\mathbf{1}$

1. Form linear system $Mx = q$
   where $M = A^T A, q = A^T b$
2. Factor $M = LL^T$
3. Solve $LL^T x = q$

Pseudoinverse

Time: 263 sec

Complexity

$2mn^2$

Time: 9 sec

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\mathrm{des}}\|^2$

Pseudoinverse

Time: 263 sec

First solve

desired views $v^{\mathrm{des},1} = (10^3)\mathbf{1}$

1. Form linear system $Mx = q$
   where $M = A^T A, q = A^T b$
2. Factor $M = LL^T$
3. Solve $LL^T x = q$

Complexity

$2mn^2$

Time: 9 sec

Second solve

desired views $v^{\mathrm{des},2} = 500\mathbf{1}$

1. Form $q = A^T b$
2. Solve $LL^T x = q$

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\mathrm{des}}\|^2$

Pseudoinverse

Time: 263 sec

First solve

desired views $v^{\mathrm{des},1} = (10^3)\mathbf{1}$

1. Form linear system $Mx = q$ where $M = A^T A, q = A^T b$
2. Factor $M = LL^T$
3. Solve $LL^T x = q$

Complexity

$2mn^2$

Time: 9 sec

Second solve

desired views $v^{\mathrm{des},2} = 500\mathbf{1}$

1. Form $q = A^T b$
2. Solve $LL^T x = q$

Complexity

$2mn$

Time: 0.37 sec

Least squares

Today, we learned to:

- **Define and recognize** least squares problems
- **Solve** least squares problems using Cholesky factorization
- **Understand** the benefits of reusing factorizations

References

- S. Boyd, L. Vandenberghe: Introduction to Applied Linear Algebra – Vectors, Matrices, and Least Squares
  - Chapter 12: least squares

Next lecture

- Least squares and data fitting