

ORF522 – Linear and Nonlinear Optimization

6. Numerical linear algebra and simplex implementation

Ed Forum

- *What about pivoting rules vs complexity? “There exists pivoting rule...”*
For any pivoting rule, you can create an example for which it works badly. So there is no way to construct a pivoting rule that works in polynomial time for any example.
- *What is the complexity of each iteration?*
More of this today
- *What do you mean by “average complexity”?*
Average across problems encountered. More about it today...
- *Why don't we choose the "largest cost decrement" rule? My intuition was that with this rule we can guarantee finite termination (is that true?), and it also seems to be more efficient.*
It is less efficient in practice. You need to compute all the possible directions (solving a linear system) and check the largest decrement

Recap

An iteration of the simplex method

Initialization

- a basic feasible solution x
- a basis matrix $A_B = \begin{bmatrix} A_{B(1)} & \dots, A_{B(m)} \end{bmatrix}$

Iteration steps

1. Compute the reduced costs \bar{c}
 - Solve $A_B^T p = c_B$
 - $\bar{c} = c - A^T p$
2. If $\bar{c} \geq 0$, x **optimal. break**
3. Choose j such that $\bar{c}_j < 0$
4. Compute search direction d with $d_j = 1$ and $A_B d_B = -A_j$
5. If $d_B \geq 0$, the problem is **unbounded** and the optimal value is $-\infty$. **break**
6. Compute step length $\theta^* = \min_{\{i \in B \mid d_i < 0\}} \left(-\frac{x_i}{d_i} \right)$
7. Define y such that $y = x + \theta^* d$
8. Get new basis \bar{B} (i exits and j enters)

Today's agenda

[Chapter 3, Bertsimas and Tsitsiklis]

[Chapter 13, Nocedal and Wright]

[Chapter 8, Vanderbei]

- Numerical linear algebra
- Realistic simplex implementation
- Example
- Empirical complexity

Numerical linear algebra

Deeper look at complexity

Flop count

floating-point operations: one addition, subtraction, multiplication, division

Estimate complexity of an algorithm

- Express number of flops as a **function of problem dimensions**
- Simplify and keep only leading terms

Remarks

- Not accurate in modern computers (multicore, GPU, etc.)
- Still rough and widely-used estimate of complexity

Complexity

Basic examples

Vector operations ($x, y \in \mathbb{R}^n$)

- Inner product $x^T y$: $2n - 1$ flops
- Sum $x + y$ or scalar multiplication αx : n flops

Matrix-vector product ($y = Ax$ with $A \in \mathbb{R}^{m \times n}$)

- $m(2n - 1)$ flops
- $2N$ if A is sparse with N nonzero elements

Matrix-matrix product ($C = AB$ with $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$)

- $pm(2n - 1)$ flops
- Less if A and/or B are sparse

How do we solve linear systems in practice?

Idea

$$Ax = b$$

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

Example

5000 \times 5000 matrix A and a 5000-vector b

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

What's happening inside?

Complexity

Solving linear system

Execution time (cost) of solving $Ax = b$ with $A \in \mathbf{R}^{n \times n}$

General case $O(n^3)$

Much less if A structured (sparse, banded, Toeplitz, etc.)

You (almost) **never compute** A^{-1} explicitly!

- Numerically unstable (divisions)
- You lose structure

Easy linear systems

Diagonal matrix

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

Solution

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

Complexity

n flops

Easy linear systems

Lower triangular matrix

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

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

Complexity

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

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

Easy linear systems

Permutation matrices

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

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

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

Properties

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

Complexity

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

example

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


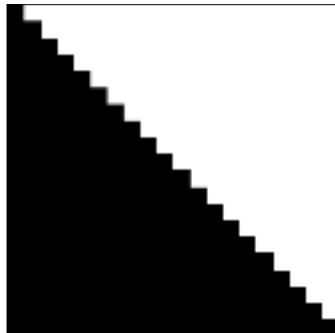
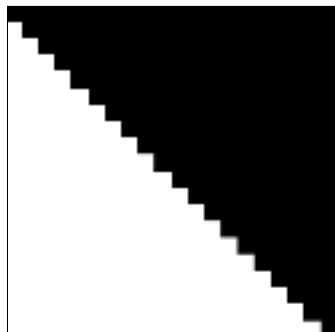


$$P \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$



$$P^{-1} \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

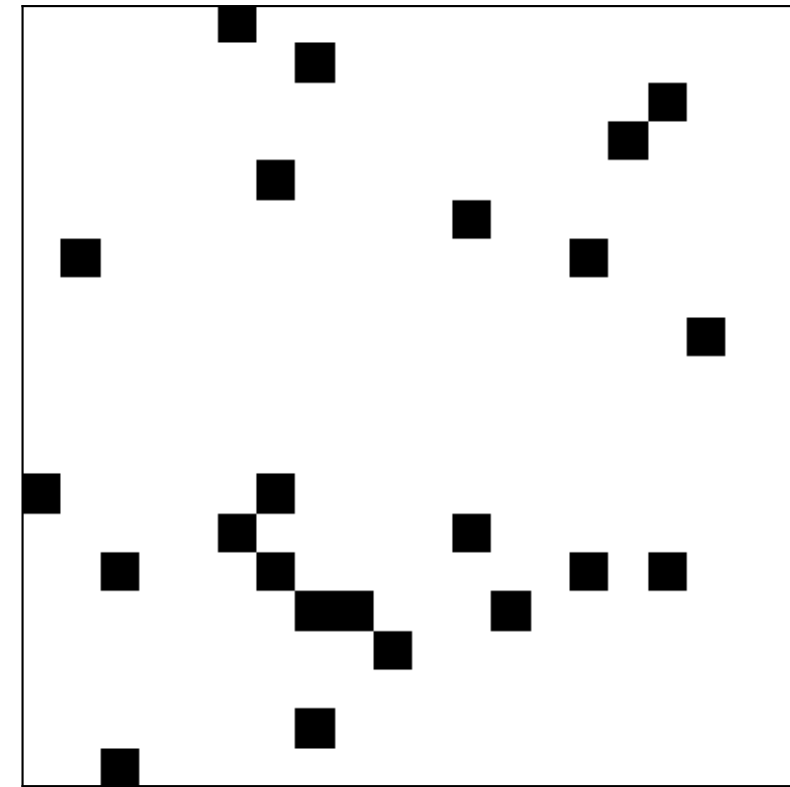
Summary of easy linear systems

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

Sparse matrices

Most **real-world problems** are sparse

A matrix A is **sparse** if the majority of its elements is 0



typically $< 15\%$ nonzeros

Efficient representations

- Triplet format: (i, j, x_{ij})
- Compressed Sparse Column format: (i, x_{ij}) and p_j
- Compressed Sparse Row format: (j, x_{ij}) and p_i

How do we solve linear systems in practice?

$$Ax = b$$

Any idea?

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:

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

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

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

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

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 right-hand side m -vectors b_i

$$Ax = b_1 \quad Ax = b_2 \quad \dots \quad Ax = b_d$$

Factorization-caching procedure

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

Solve many “at the price of one”

(Sparse) LU factorization

Every nonsingular matrix A can be factored as

$$A = P_r L U P_c \longrightarrow P_r^T A P_c^T = L U$$

P_r, P_c permutation, L lower triangular, U upper triangular

Permutations

- Reorder rows P_r and columns P_c of A to (heuristically) get **sparser** L, U
- P_r, P_c depend on sparsity pattern and values of A

Cost

- If A dense, typically $O(n^3)$ but usually much less
- It depends on the number of nonzeros in A , sparsity pattern, etc.

(Sparse) LU solution

$$Ax = b, \quad \Rightarrow \quad P_r L U P_c x = b$$

Iterations

1. *Permutation*: Solve $P_r z_1 = b$ (0 flops)
2. *Forward substitution*: Solve $L z_2 = z_1$ (n^2 flops)
3. *Backward substitution*: Solve $U z_3 = z_2$ (n^2 flops)
4. *Permutation*: Solve $P_c x = z_3$ (0 flops)

Cost

Factor + Solve $\sim O(n^3)$

Just solve (prefactored) $\sim O(n^2)$

(Sparse) Cholesky factorization

Every positive definite matrix A can be factored as

$$A = P L L^T P^T \longrightarrow P^T A P = L L^T$$

P permutation, L lower triangular

Permutations

- Reorder rows/cols of A with P to (heuristically) get **sparser** L
- P depends only on sparsity pattern of A (unlike LU factorization)
- If A is dense, we can set $P = I$

Cost

- If A dense, typically $O(n^3)$ but usually much less
- It depends on the number of nonzeros in A , sparsity pattern, etc.
- Typically 50% faster than LU (need to find only one matrix)

(Sparse) Cholesky solution

$$Ax = b, \quad \Rightarrow \quad PLL^T P^T x = b$$

Iterations

1. *Permutation*: Solve $Pz_1 = b$ (0 flops)
2. *Forward substitution*: Solve $Lz_2 = z_1$ (n^2 flops)
3. *Backward substitution*: Solve $L^T z_3 = z_2$ (n^2 flops)
4. *Permutation*: Solve $P^T x = z_3$ (0 flops)

Cost

Factor + Solve $\sim O(n^3)$

Just solve (prefactored) $\sim O(n^2)$

“Realistic” simplex implementation

Complexity of a single simplex iteration

1. Compute the reduced costs \bar{c}
 - Solve $A_B^T p = c_B$
 - $\bar{c} = c - A^T p$
2. If $\bar{c} \geq 0$, x **optimal. break**
3. Choose j such that $\bar{c}_j < 0$
4. Compute search direction d with $d_j = 1$ and $A_B d_B = -A_j$
5. If $d_B \geq 0$, the problem is **unbounded** and the optimal value is $-\infty$. **break**
6. Compute step length $\theta^* = \min_{\{i \in B \mid d_i < 0\}} \left(-\frac{x_i}{d_i} \right)$
7. Define y such that $y = x + \theta^* d$
8. Get new basis \bar{B} (i exits and j enters)

Bottleneck
“same” two linear systems

Linear system solutions

Very similar linear systems

$$\begin{aligned} A_B^T p &= c_B \\ A_B d_B &= -A_j \end{aligned}$$

LU factorization
 $O(n^3)$ flops

$$A_B = P_r L U P_c$$

Easy linear systems

$O(n^2)$ flops

$$\begin{aligned} P_c^T U^T L^T P_r^T p &= c_B \\ P_r L U P_c d_B &= -A_j c_B \end{aligned}$$

Factorization is expensive

Do we need to recompute it at every iteration?

Basis update

Index update

- j enters (x_j becomes θ^*)
- $i = B(\ell)$ exists (x_i becomes 0)



Basis matrix change

$$A_{\bar{B}} = A_B + (A_j - A_i)e_\ell^T$$

Example

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$B = \{4, 1, 6\} \rightarrow \bar{B} = \{4, 1, 2\}$$

- 2 enters
- $6 = B(3)$ exists

$$A_{\bar{B}} = \begin{matrix} & A_B & & A_2 e_3^T & & A_6 e_3^T \\ \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 2 & 1 \end{bmatrix} & + & \begin{bmatrix} 0 & 0 & 2 \\ 0 & 0 & 1 \\ 0 & 0 & 2 \end{bmatrix} & - & \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} & = & \begin{bmatrix} 1 & 1 & 2 \\ 0 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix} \end{matrix}$$

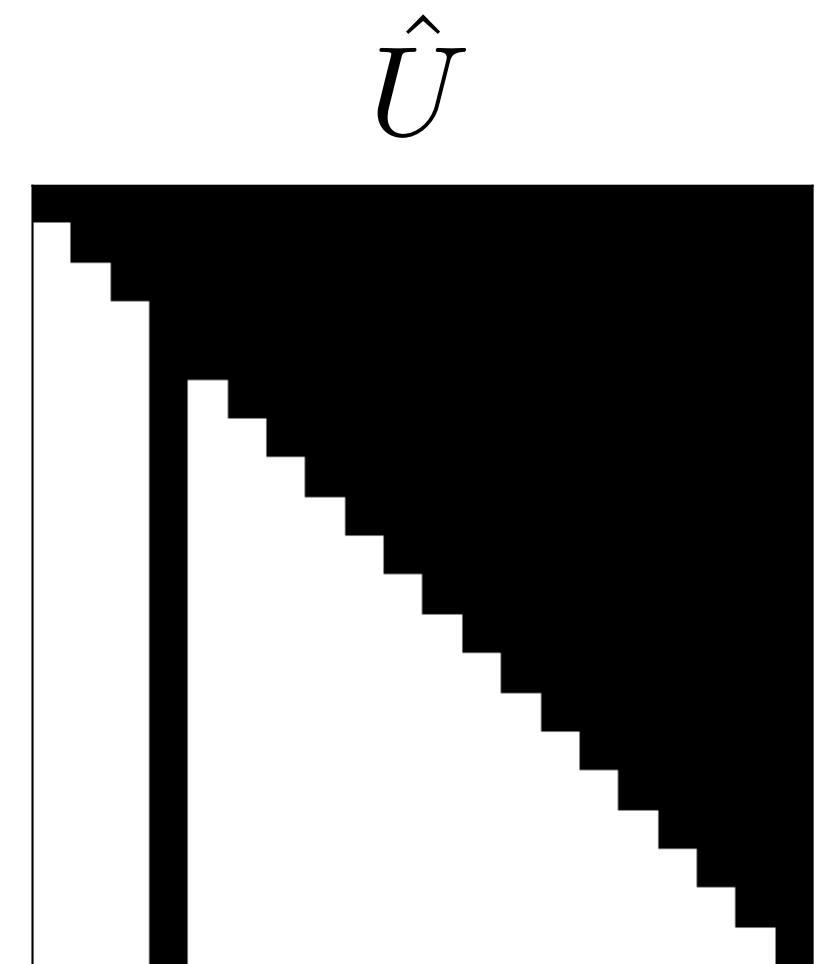
Basis update

Rank-1 update

$$A_{\bar{B}} = A_B + (A_j - A_i)e_\ell^T$$

Forrest-Tomlin update $O(m^2)$

- **Given:** $A_B = LU$
- **Goal:** compute $A_{\bar{B}} = LR\bar{U}$ (same L , lower tri. R , upper tri. \bar{U})
 1. $L^{-1}A_{\bar{B}} = U + (L^{-1}A_j - Ue_\ell)e_\ell^T = \hat{U}$
 2. LU factorization $\hat{U} = R\bar{U}$ via **elimination** ($O(m^2)$)



Remarks

- Implemented in modern sparse solvers
- Accumulates errors (we need to refactor B from scratch once in a while)
- Many more algorithms: Block-LU, Bartels-Golub-Reid, etc.

Realistic (revised) simplex method

Initialization

- a basic feasible solution x
- a basis matrix $A_B = \begin{bmatrix} A_{B(1)} & \dots, A_{B(m)} \end{bmatrix}$

Iteration steps

Per-iteration cost $O(m^2)$

1. Compute the reduced costs \bar{c}
 - Solve $A_B^T p = c_B$ ($O(m^2)$)
 - $\bar{c} = c - A^T p$
2. If $\bar{c} \geq 0$, x **optimal. break**
3. Choose j such that $\bar{c}_j < 0$
4. Compute search direction. d with $d_j = 1$ and $A_B d_B = -A_j$ ($O(m^2)$)
5. If $d_B \geq 0$, the problem is **unbounded** and the optimal value is $-\infty$. **break**
6. Compute step length $\theta^* = \min_{\{i \in B \mid d_i < 0\}} \left(-\frac{x_i}{d_i} \right)$
7. Define y such that $y = x + \theta^* d$
8. Get new basis $A_{\bar{B}} = A_B + (A_j - A_i)e_\ell^T$
rank-1 factor update (i exits and j enters) ($O(m^2)$)

Example

Example

Inequality form

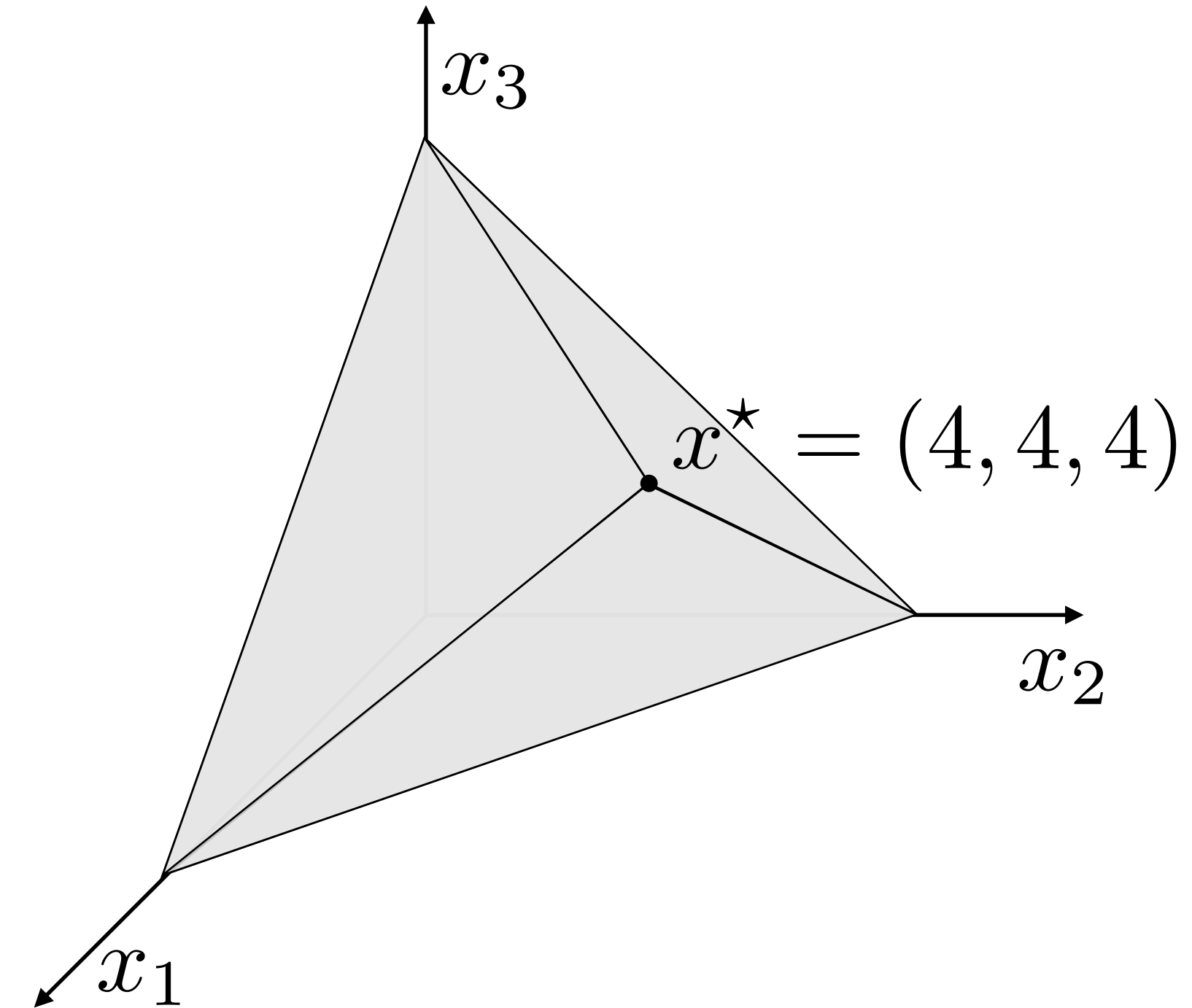
$$\text{minimize} \quad -10x_1 - 12x_2 - 12x_3$$

$$\text{subject to} \quad x_1 + 2x_2 + 2x_3 \leq 20$$

$$2x_1 + x_2 + 2x_3 \leq 20$$

$$2x_1 + 2x_2 + x_3 \leq 20$$

$$x_1, x_2, x_3 \geq 0$$



Standard form

$$\text{minimize} \quad -10x_1 - 12x_2 - 12x_3$$

$$\text{subject to} \quad \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} 20 \\ 20 \\ 20 \end{bmatrix}$$

$$x \geq 0$$

Example

Start

$$\begin{array}{ll}\text{minimize} & c^T x \\ \text{subject to} & Ax = b \\ & x \geq 0\end{array}$$

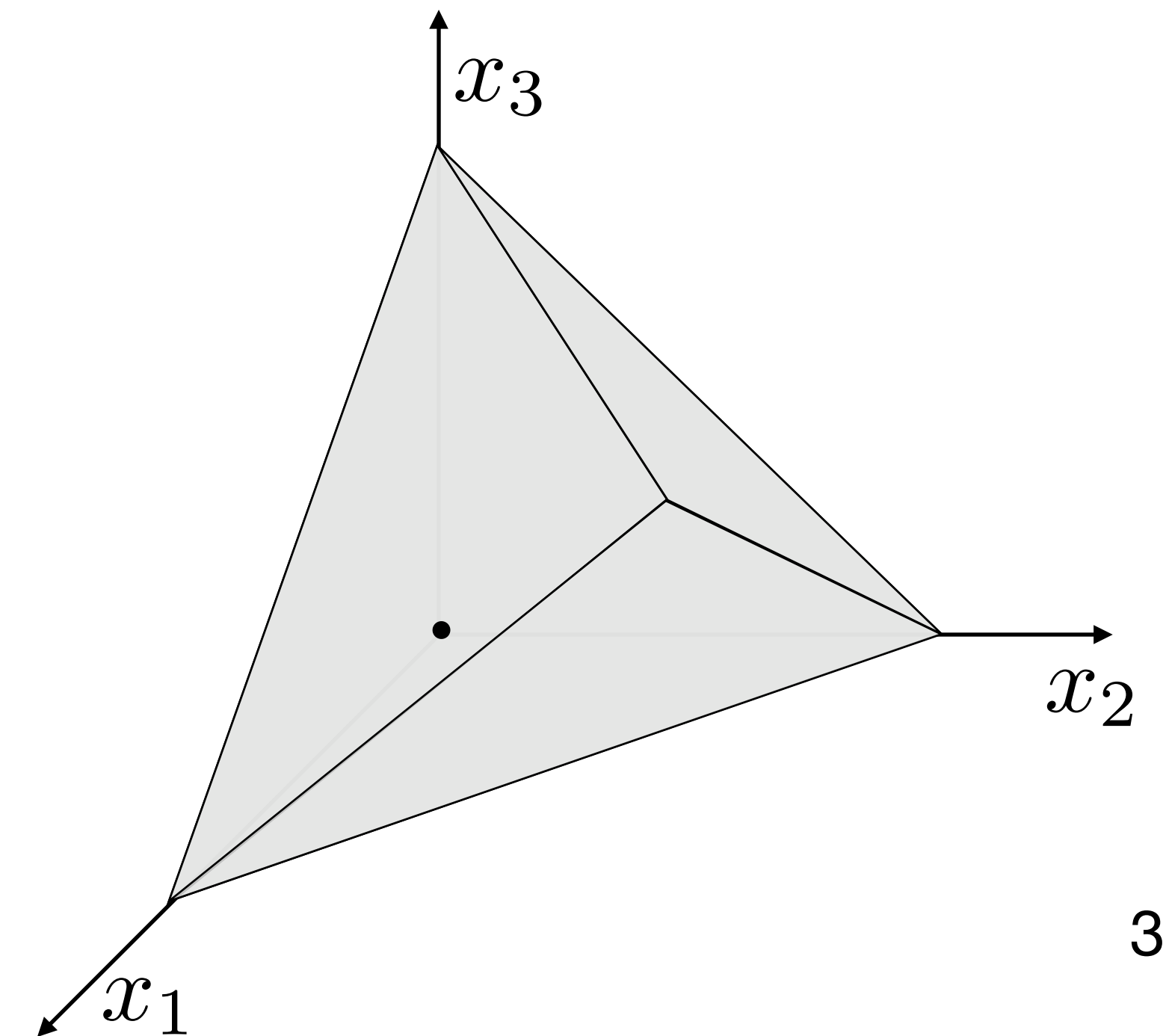
$$c = (-10, -12, -12, 0, 0, 0)$$

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$b = (20, 20, 20)$$

Initialize

$$x = (0, 0, 0, 20, 20, 20) \quad A_B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Example

Iteration 1

Current point

$$x = (0, 0, 0, 20, 20, 20)$$

$$c^T x = 0$$

Basis: $\{4, 5, 6\}$

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

$$c = (-10, -12, -12, 0, 0, 0)$$

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$b = (20, 20, 20)$$

Reduced costs $\bar{c} = c$

$$\text{Solve } A_B^T p = c_B \Rightarrow p = c_B = 0$$

$$\bar{c} = c - A^T p = c$$

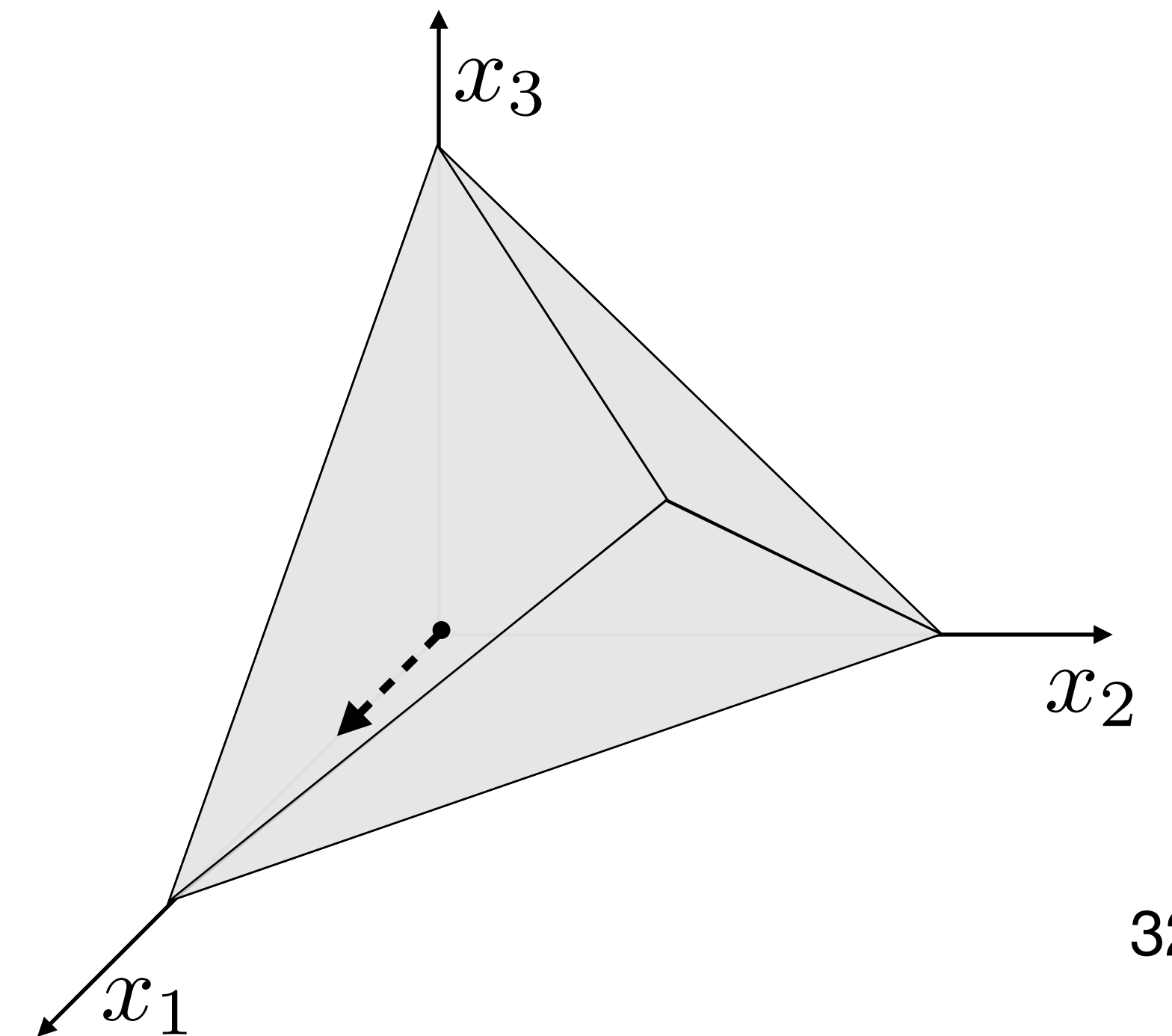
Direction $d = (1, 0, 0, -1, -2, -2), \quad j = 1$

$$\text{Solve } A_B d_B = -A_j \Rightarrow d_B = (-1, -2, -2)$$

Step $\theta^* = 10, \quad i = 5$

$$\theta^* = \min_{\{i | d_i < 0\}} (-x_i / d_i) = \min\{20, 10, 10\}$$

$$\text{New } x \leftarrow x + \theta^* d = (10, 0, 0, 10, 0, 0)$$



Example

Iteration 2

Current point

$$x = (10, 0, 0, 10, 0, 0)$$

$$c^T x = -100$$

$$\text{Basis: } \{4, 1, 6\}$$

$$A_B = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 2 & 1 \end{bmatrix}$$

$$c = (-10, -12, -12, 0, 0, 0)$$

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$b = (20, 20, 20)$$

Reduced costs $\bar{c} = (0, -7, -2, 0, 5, 0)$

Solve $A_B^T p = c_B \Rightarrow p = (0, -5, 0)$

$$\bar{c} = c - A^T p = (0, -7, -2, 0, 5, 0)$$

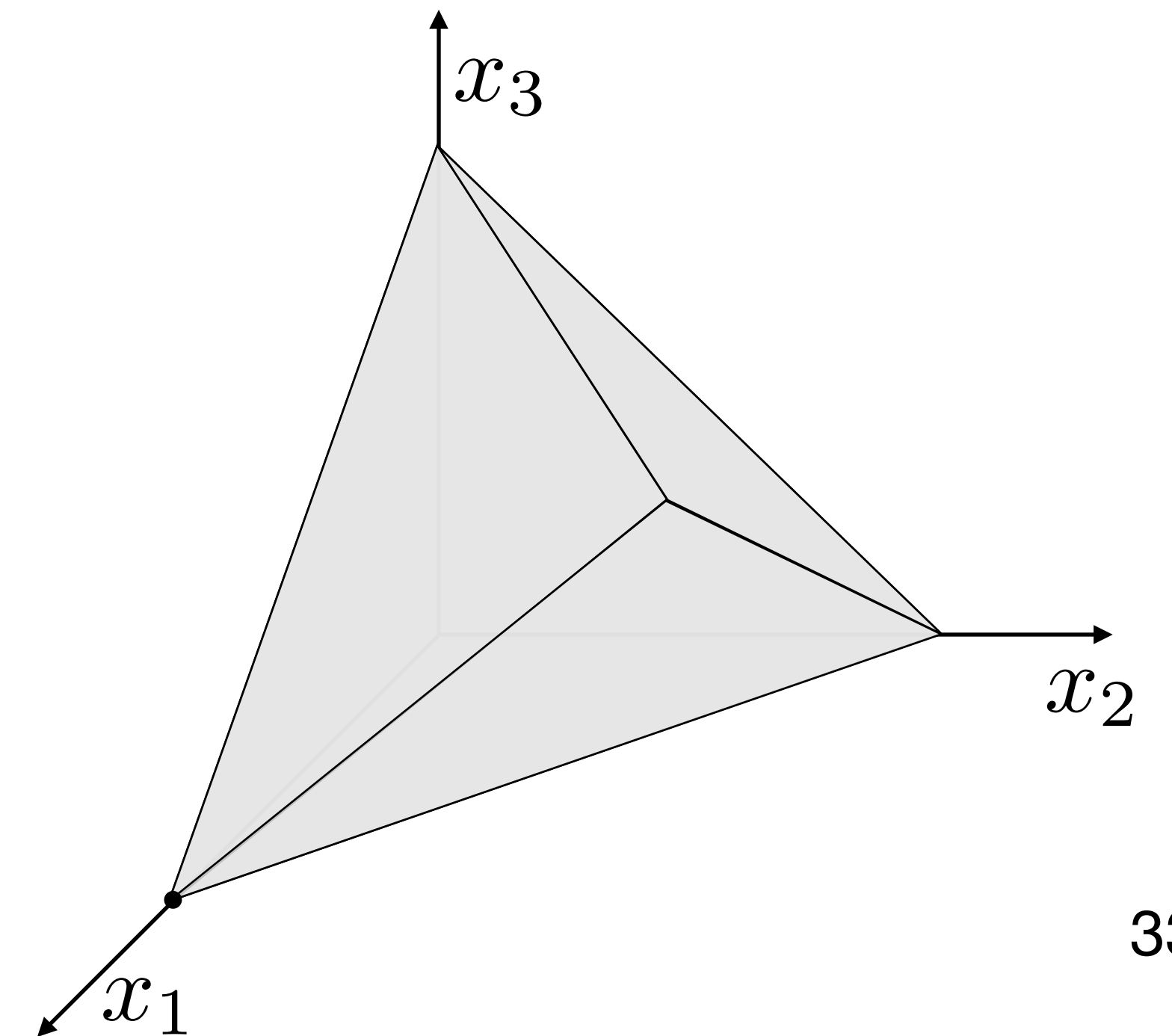
Direction $d = (-0.5, 1, 0, -1.5, 0, -1), \quad j = 2$

Solve $A_B d_B = -A_j \Rightarrow d_B = (-1.5, -0.5, -1)$

Step $\theta^* = 0, \quad i = 6$

$$\theta^* = \min_{\{i|d_i < 0\}} (-x_i/d_i) = \min\{6.66, 20, 0\}$$

New $x \leftarrow x + \theta^* d = (10, 0, 0, 10, 0, 0)$



Example

Iteration 3

Current point

$$x = (10, 0, 0, 10, 0, 0)$$

$$c^T x = -100$$

$$\text{Basis: } \{4, 1, 2\}$$

$$A_B = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$$

$$c = (-10, -12, -12, 0, 0, 0)$$

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$b = (20, 20, 20)$$

Reduced costs $\bar{c} = (0, 0, -9, 0, -2, 7)$

Solve $A_B^T p = c_B \Rightarrow p = (0, 2, -7)$

$$\bar{c} = c - A^T p = (0, 0, -9, 0, -2, 7)$$

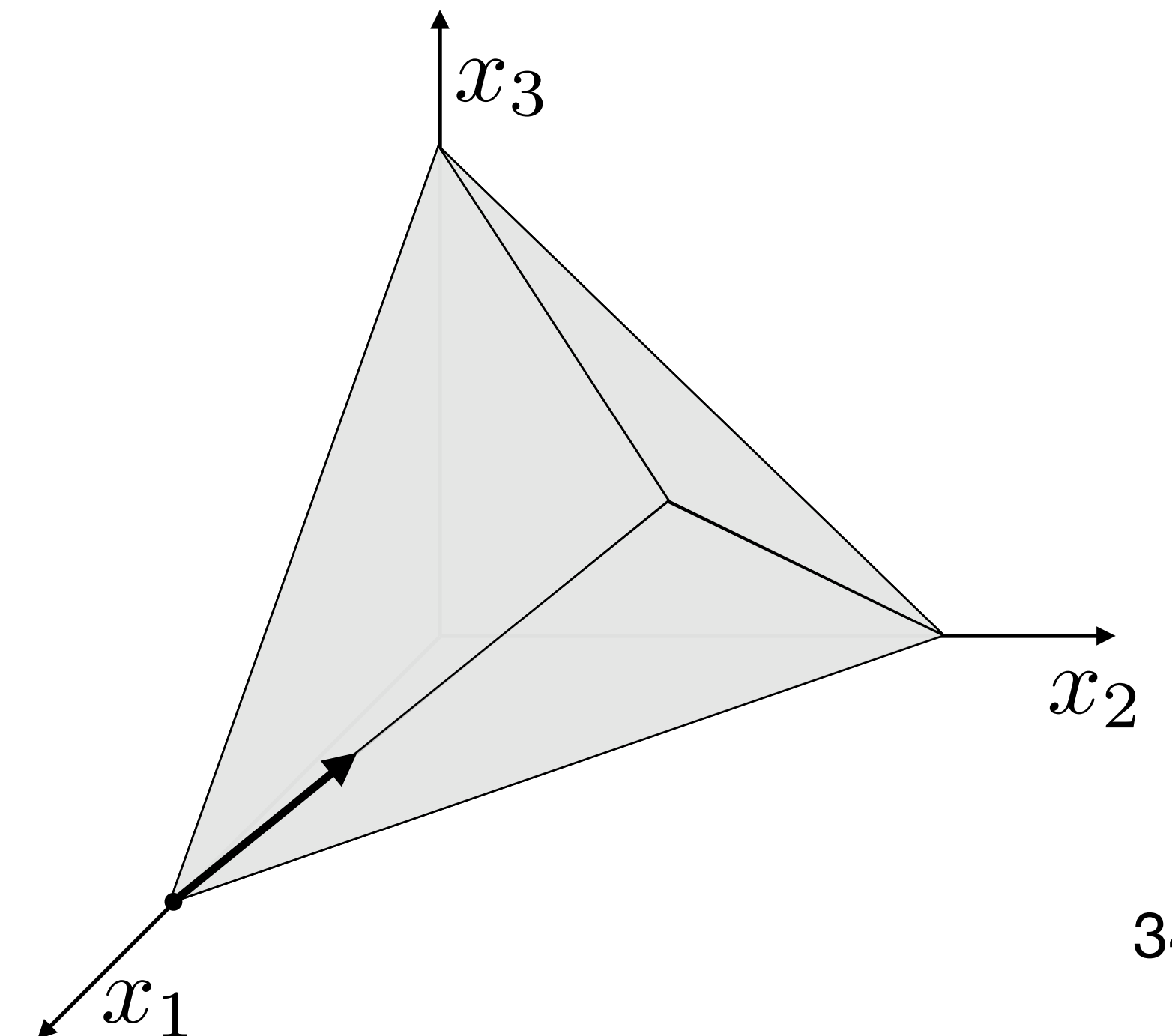
Direction $d = (-1.5, 1, 1, -2.5, 0, 0), \quad j = 3$

Solve $A_B d_B = -A_j \Rightarrow d_B = (-2.5, -1.5, 1)$

Step $\theta^* = 4, \quad i = 4$

$$\theta^* = \min_{\{i | d_i < 0\}} (-x_i / d_i) = \min\{4, 6.67\}$$

New $x \leftarrow x + \theta^* d = (4, 4, 4, 0, 0, 0)$



Example

Iteration 4

Current point

$$x = (4, 4, 4, 0, 0, 0)$$

$$c^T x = -136$$

Basis: $\{3, 1, 2\}$

$$A_B = \begin{bmatrix} 2 & 1 & 2 \\ 2 & 2 & 1 \\ 1 & 2 & 2 \end{bmatrix}$$

$$c = (-10, -12, -12, 0, 0, 0)$$

$$A = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 1 & 2 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$b = (20, 20, 20)$$

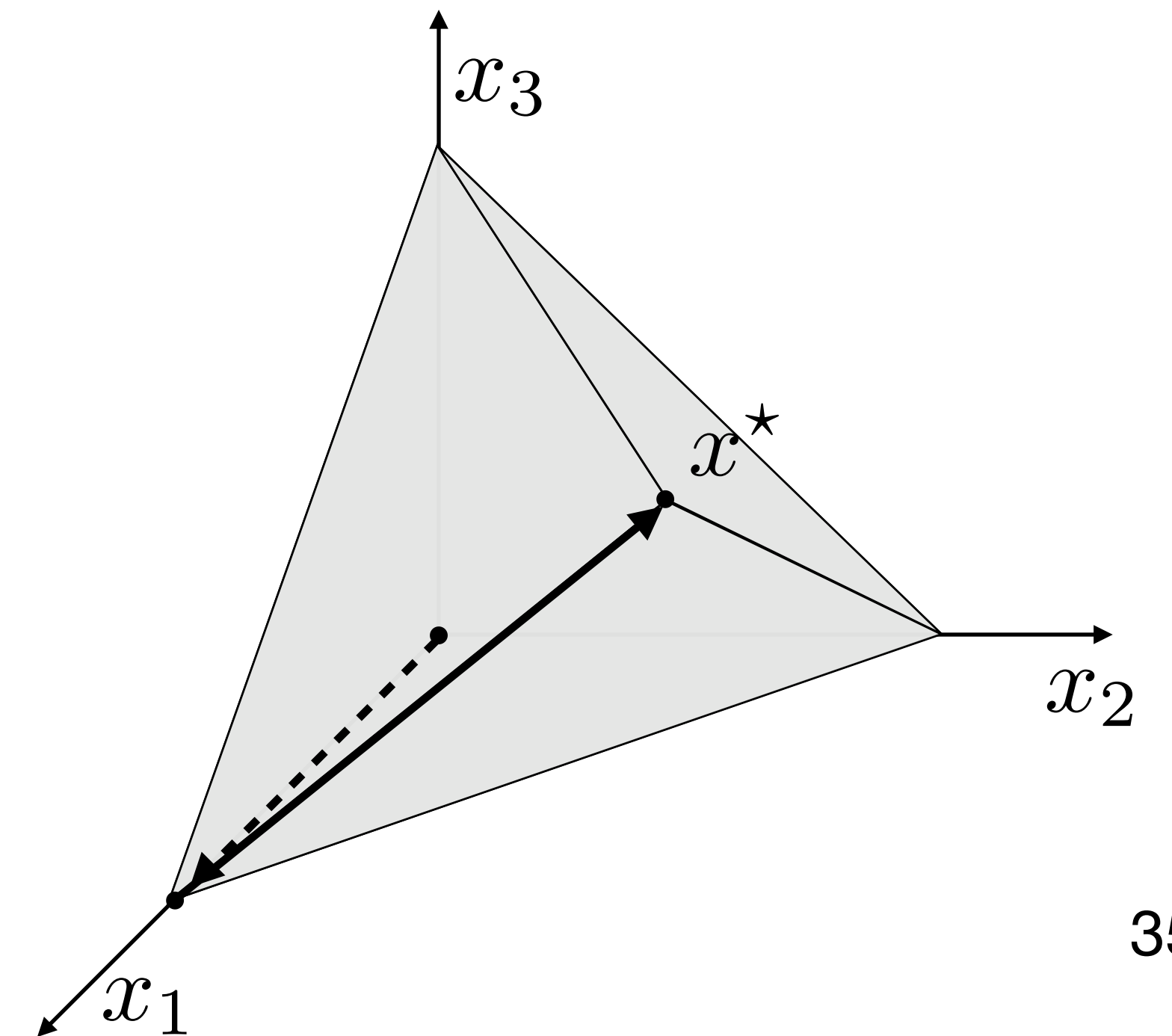
Reduced costs $\bar{c} = (0, 0, 0, 3.6, 1.6, 1.6)$

Solve $A_B^T p = c_B \Rightarrow p = (-3.6, -1.6, -1.6)$

$$\bar{c} = c - A^T p = (0, 0, 0, 3.6, 1.6, 1.6)$$

Optimal

$$\bar{c} \geq 0 \longrightarrow x^* = (4, 4, 4, 0, 0, 0)$$



Simplex tableau implementation

Can we solve LPs by hand?

Minus cost	→	$-c_B^T x_B$		\bar{c}_1	\dots	\bar{c}_n	← Reduced costs
Basic variables	→	$x_B(1)$					
		\vdots		$A_B^{-1} A_1$	\dots	$A_B^{-1} A_n$	
		$x_B(1)$					

People did it **before computers were invented!**

Nobody does it anymore...

Empirical complexity

Example with real solver

GLPK (open-source)

Code

```
import numpy as np
import cvxpy as cp

c = np.array([-10, -12, -12])
A = np.array([[1, 2, 2],
              [2, 1, 2],
              [2, 2, 1]])
b = np.array([20, 20, 20])
n = len(c)

x = cp.Variable(n)
problem = cp.Problem(cp.Minimize(c @ x),
                     [A @ x <= b, x >= 0])
problem.solve(solver=cp.GLPK, verbose=True)
```

Output

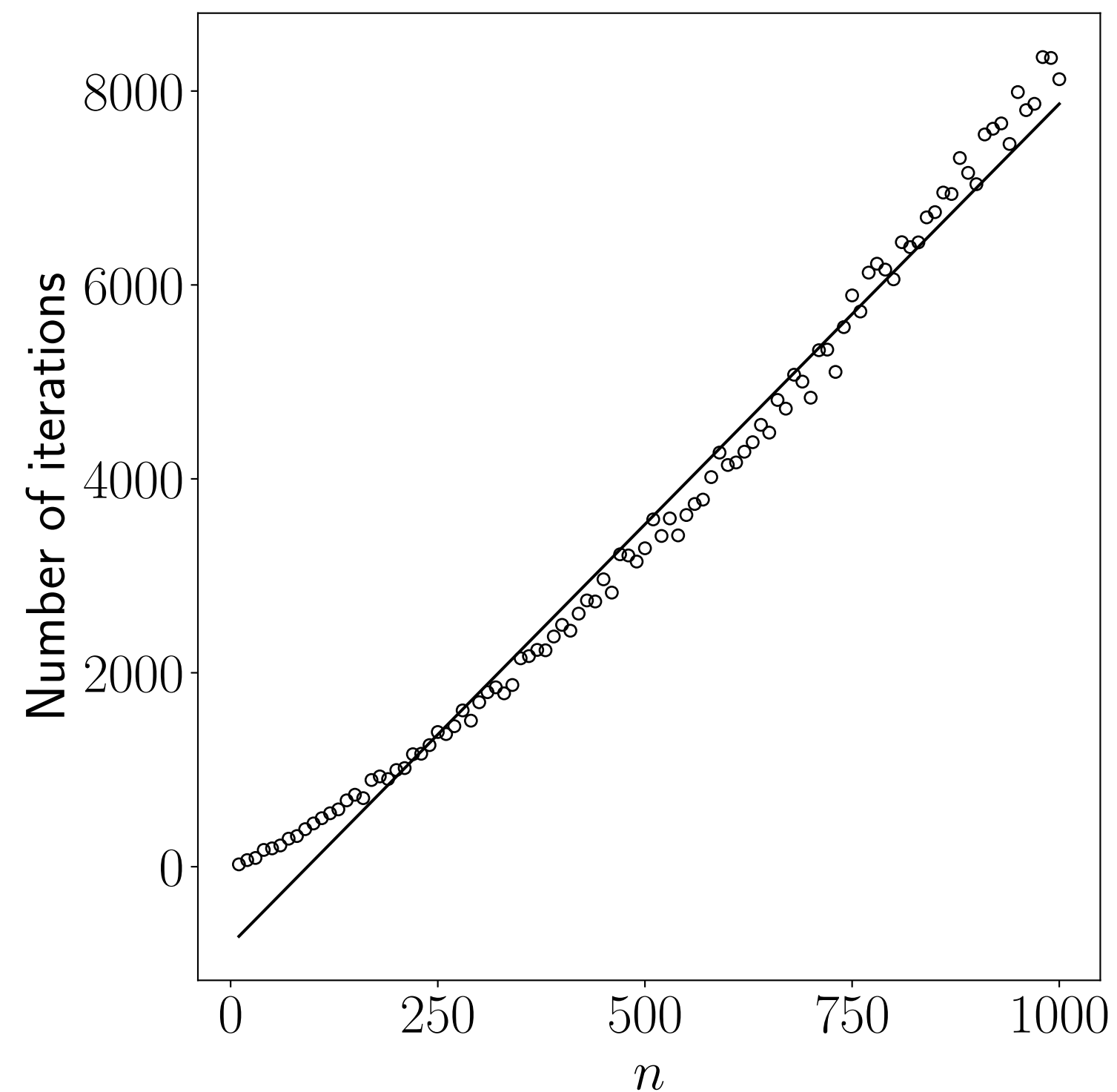
```
GLPK Simplex Optimizer, v4.65
6 rows, 3 columns, 12 non-zeros
*      0: obj =  0.000000000e+00  inf =  0.000e+00 (3)
*      3: obj = -1.360000000e+02  inf =  0.000e+00 (0)
OPTIMAL LP SOLUTION FOUND
```

Average simplex complexity

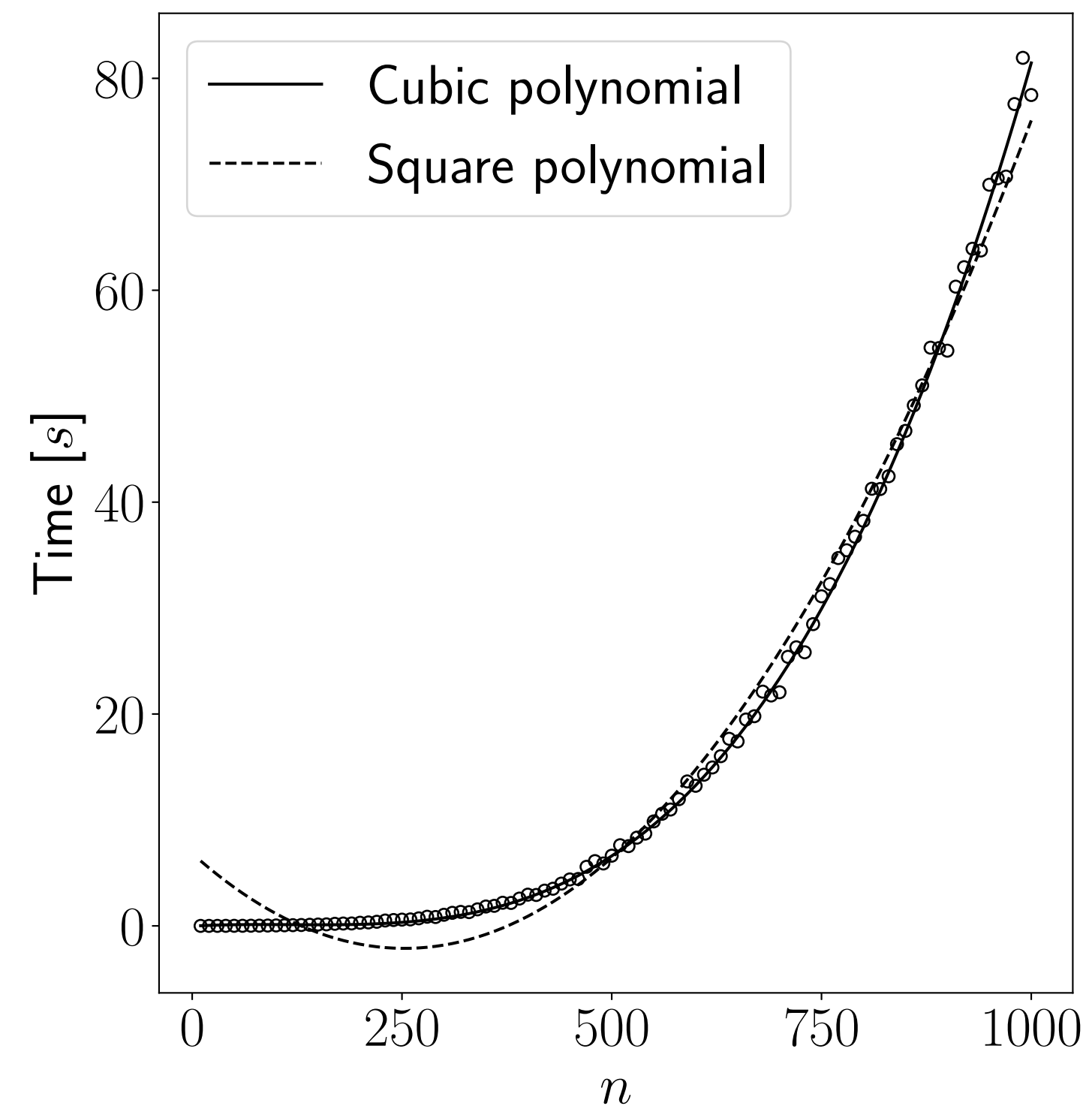
Random LPs

minimize $c^T x$ n variables
subject to $Ax \leq b$ $3n$ constraints

Iterations: $O(n)$



Time: $O(nn^2) = O(n^3)$



Numerical linear algebra and simplex implementation

Today, we learned to:

- **Identify** the pros and cons of different methods to solve a linear system
- **Derive** the computational complexity of the factor-solve method
- **Implement** a “realistic” version of the simplex method
- **Empirically** analyze the average complexity of the simplex method

Next lecture

- Linear optimization duality