COMP 414/514: Optimization – Algorithms, Complexity and Approximations

Lecture 1

Overview

$$
\begin{aligned}
\min_{x} \quad & f(x) \\
\text{s.t.} \quad & x \in \mathcal{C}
\end{aligned}
$$

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- Different objective classes
- Different strategies within each problem
- Different approaches based on computational capabilities
- Different approaches based on constraints

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— Different objective classes
— Different strategies within each problem
— Different approaches based on computational capabilities
— Different approaches based on constraints

And, always having in mind applications in machine learning, AI and signal processing

Motivation (no fancy images included)

Provable efficiency

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Lots of data

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Provable efficiency

Harder problems

Lots of data

Motivation (no fancy images included)

More complicated models

Provable efficiency

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Motivation

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More complicated models

Better results

Provable efficiency

Harder problems

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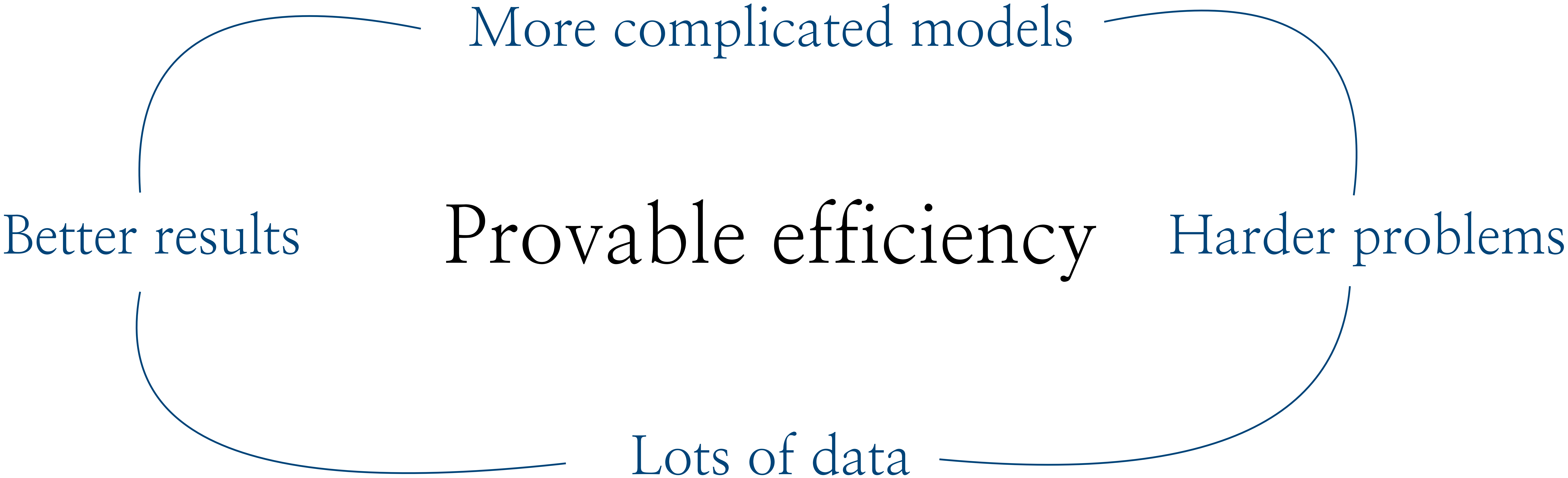

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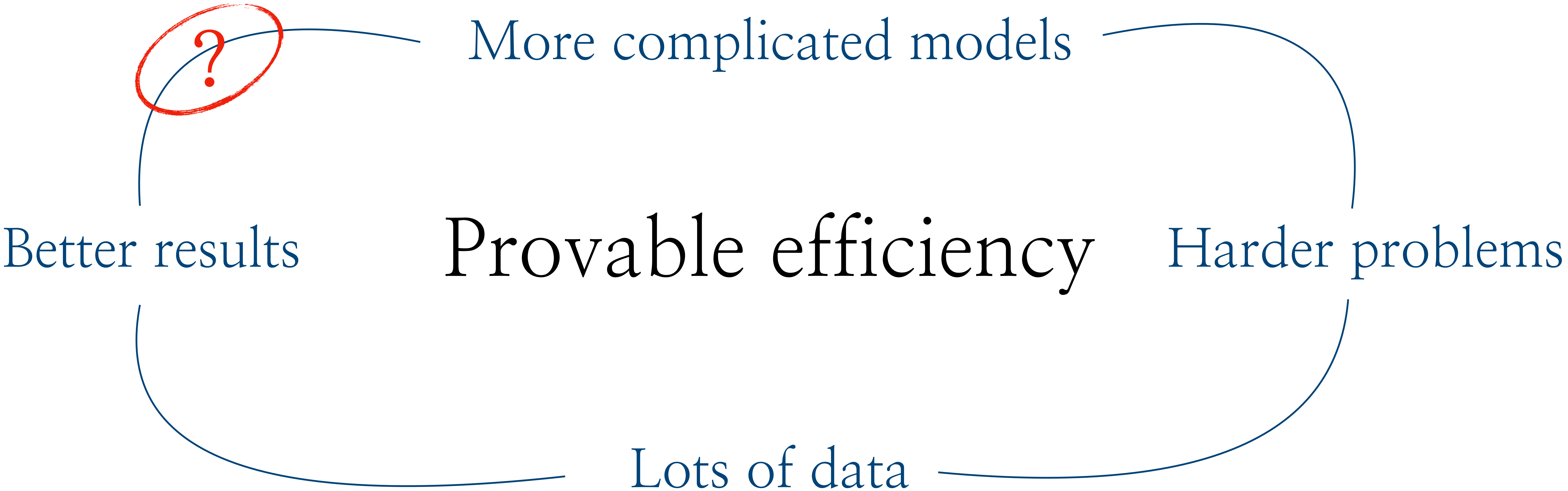

Motivation (no fancy images included)

Provable efficiency

"What shall we do?"

Motivation (no fancy images included)

Provable efficiency

"What shall we do?"

Set up algo nicely

Use prior knowledge

Converge faster

Exploit resources

Topics

- Continuous **optimization** (in general)
  - See syllabus
  - Both theory and practice

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- Recent applications that drive research

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  - Both theory and practice
- Recent applications that drive research
- When no theory applies, some intuition

Topics NOT covered in this course

- (Mixed) integer programming

(See CMOR)

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  (See Anshu's course, Maryam's course)

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- Online algorithms, bandits (See Maryam's course)
- Bayesian algorithms
- Deep learning architectures (See Ankit's course)

Examples

- Least squares / linear regression

(No, we will not re-define it)

$$\min_{x} \quad f(x)$$
$$\text{s.t.} \quad x \in \mathcal{C}$$

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$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & x \in \mathcal{C} \end{aligned} \quad \Rightarrow \quad \min_x \frac{1}{n} \sum_{i=1}^{n} \left(y_i - a_i^\top x \right)^2$$

Examples

- Quantum state tomography from limited samples

$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned}$$

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$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \min_{X} \quad & \sum_{i=1}^{n} \big(y_i - \mathrm{Tr}(A_i^\top X)\big)^2 \\ \text{s.t.} \quad & \mathrm{Tr}(X) \leq 1 \\ & X \succeq 0 \end{aligned}$$

Examples

- Fleet management

$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned}$$

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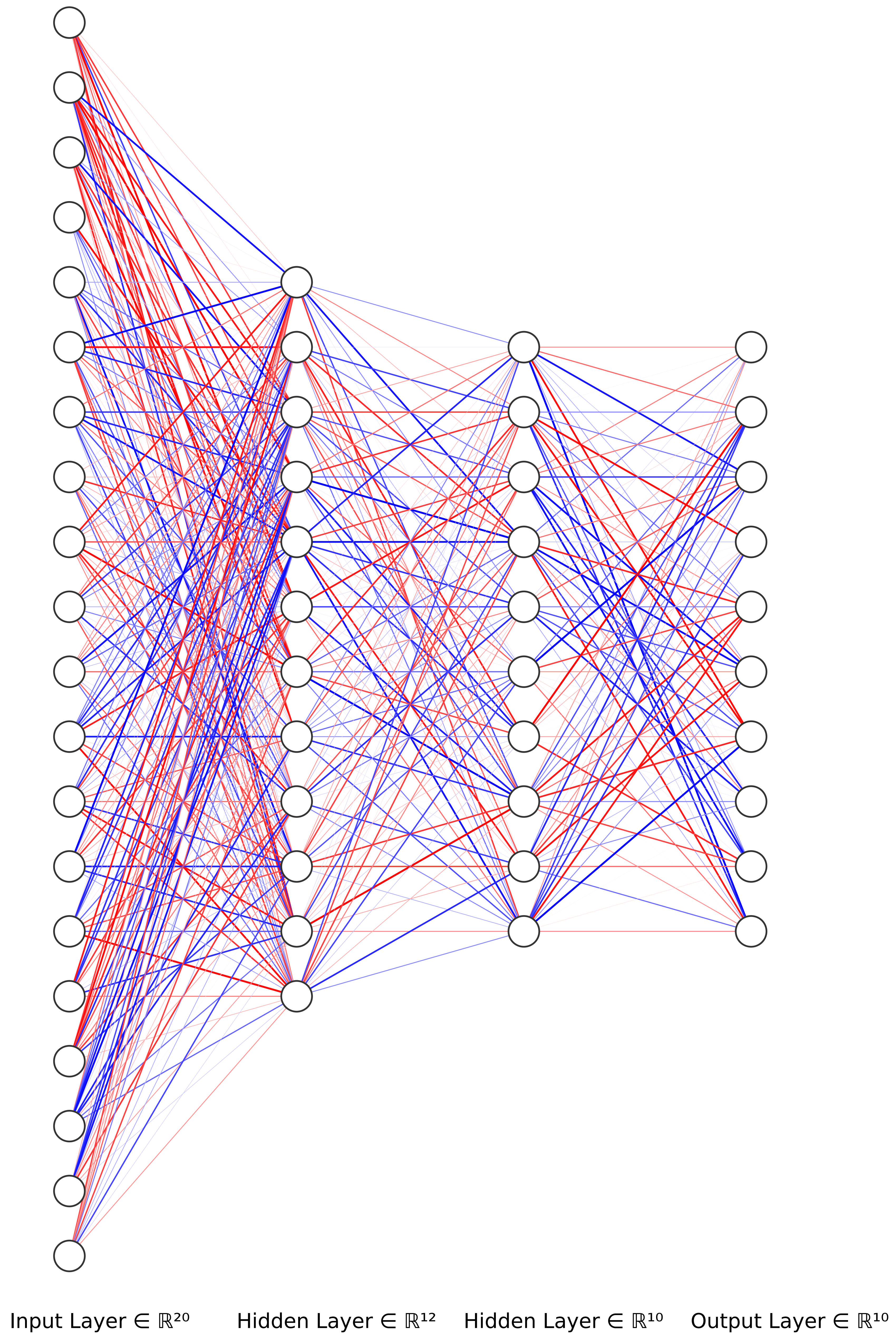
$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \min_{x \in \{0,1\}^m, y \in \{0,1\}} \quad & f(y) = \sum_{i \in \mathcal{V}} \sum_{k=1}^{p} d_i (1-q) q^{k-1} y_{ik} \\ \text{s.t.} \quad & \sum_{j \in \mathcal{W}_i} x_j \geq \sum_{k=1}^{p} y_{ik}, i \in \mathcal{V} \\ & \sum_{j \in \mathcal{W}} x_j = p \\ & x_j \leq p_j \end{aligned}$$

Examples

– Neural networks



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$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned} \quad \Rightarrow$$

$$\min_{W_i} \quad f(W_1, W_2) := \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}\left(\widehat{y}_i, y_i\right).$$

where

$$\widehat{y}_i = \texttt{softmax}\left(\sigma\left(W_2 \cdot \sigma\left(W_1 \cdot x_i\right)\right)\right)$$

Any questions?

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- Just auditing is fine by me

What is the vision for this course?

- For starters, this will always be an evolving course

(Any feedback is more than welcome)

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- My purpose and vision is to introduce a series of optimization courses in the CS (and Duncan Hall's in general) curriculum

- The vision is for this course to be part of a sequence of courses that will focus on the theory+practice of methods

(I'm also teaching COMP182)

Course format

- Lectures (slides) + whiteboard + in-class code running

(Some lectures have presentations, others will be handwritten)

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- Your workload:

  Graduate – HWs, final project
  Undergraduate – HWs, final exam
  (Additional workload: possible midterm, scribing)

Regarding assignments

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- Some questions might not feel intuitive

  ("I'm a computer scientist! Why should I care about optimization?")
- Try to do the best you can

  (There will be a reweighing at the end of the course, only if necessary)

Goals + outcomes

- Learn about research in related fields

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- Read and review recent papers

My goals

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(But judge whether you have thought about solving the questions)

My goals

- Not to judge you on small details in HWs

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- Spark your interest in research
  where math and practice are combined together

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- A quiz was usually provided for self-assessment, but I decided to make it an additional HW

Grading policy

- 50% HWs
- 50% project/final exam
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Usually there is scaling in final grades. For me, a good grade is given based on the overall performance of the students: I value self-motivation, being proactive and enthusiasm.

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(Moderation is key)

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  (it will depend on the attendance)
- Deliverable in LaTEX
  (template available online)

HWs

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Reviews (when applicable)

- Select papers from a pile of .pdfs that will be provided

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- Single page reviews, similar to NIPS/ICML standards:

  (but not random as it usually is now)

  - Comment on novelty, clarity, importance
  - Strengths and weaknesses
  - Main comments + your overall score

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- Grading: slides quality, clarity of main ideas

Presentations (for final projects)

(not certain yet)

(Course website)

Final Project

(Course website)

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Please come find me the earliest to discuss projects

Final Project

(Course website)

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You should start reading papers soon, so that around mid-way you have a good project proposal

Communication

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- **HWs**: will be sent to you via Canvas every week.
  (please do not distribute)

Notes

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- Every week I will try to update every chapter; however I would appreciate any help with scribing throughout the semester

(Course website)

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- In case I don't have the time to cover fully a session, I will decide whether you will read it yourself, or I will teach it the next time.

Any questions?

Setting up the background

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- Notation convention: vectors = lowercase, matrices = uppercase

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$$x + y = y + x, \quad x, y \in \mathbb{R}^p$$

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$$x + y = y + x, \quad x, y \in \mathbb{R}^p$$ (Commutative)

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$$\alpha(x + y) = \alpha x + \alpha y, \quad x, y \in \mathbb{R}^p$$ (Distributive)

Vectors

- Span of a set of vectors:

$$\text{span}\{x_1, x_2, \ldots, x_k\} = \{\alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_k x_k \mid \alpha_i \in \mathbb{R}, i = [1, k]\}$$

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- Inner product:

$$x^\top y = \langle x, y \rangle = \sum_{i=1}^{p} x_i \cdot y_i$$

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– Inner production interpretation:

$$\langle x, y \rangle = \|x\| \cdot \|y\| \cdot \cos\theta$$

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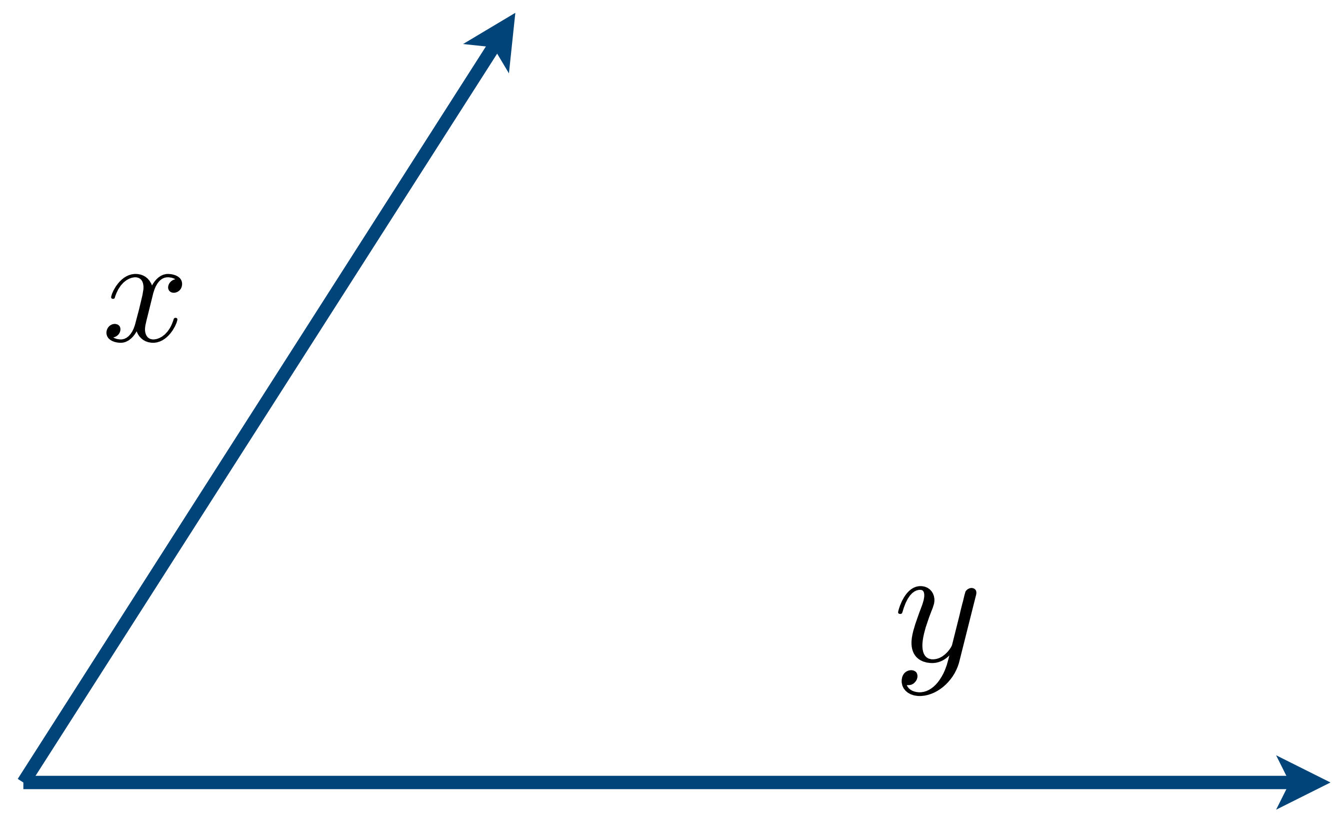

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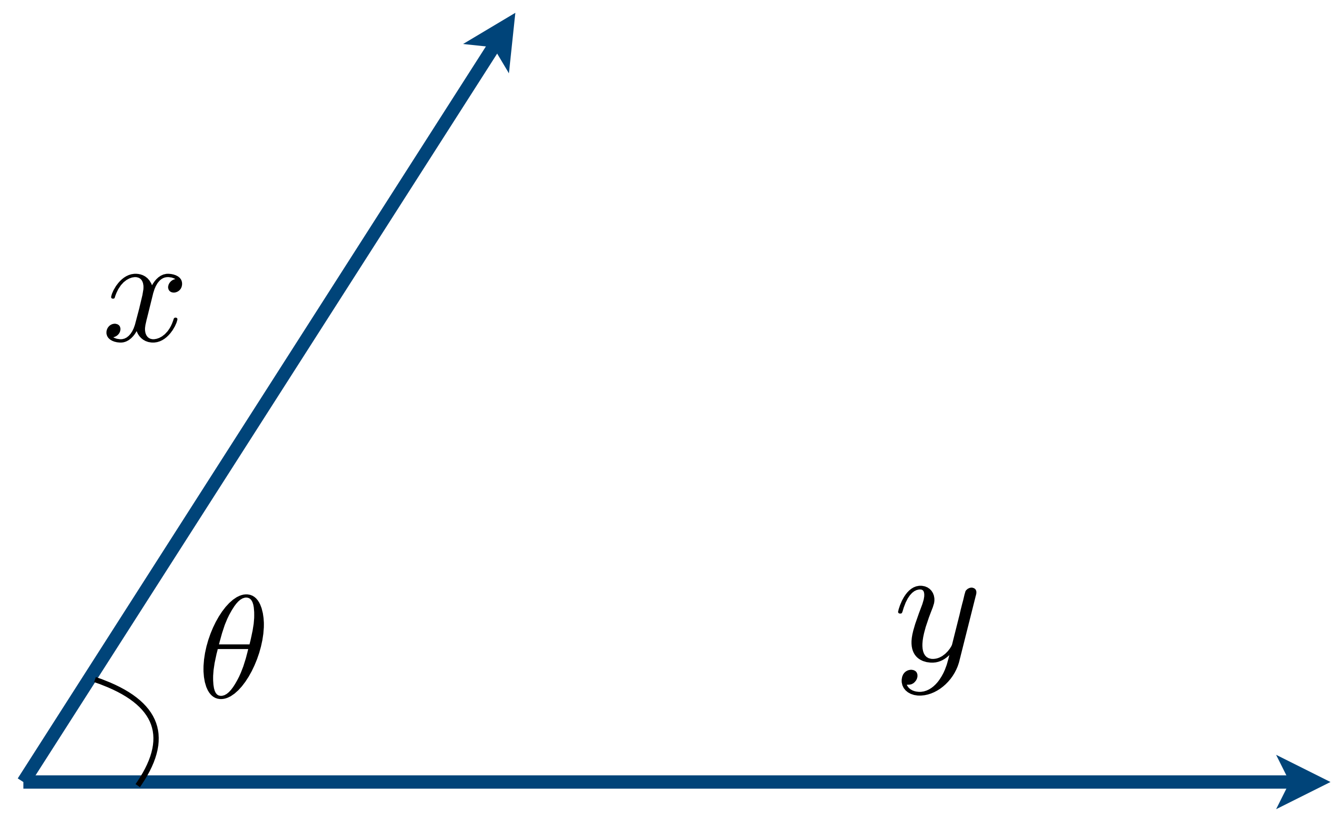

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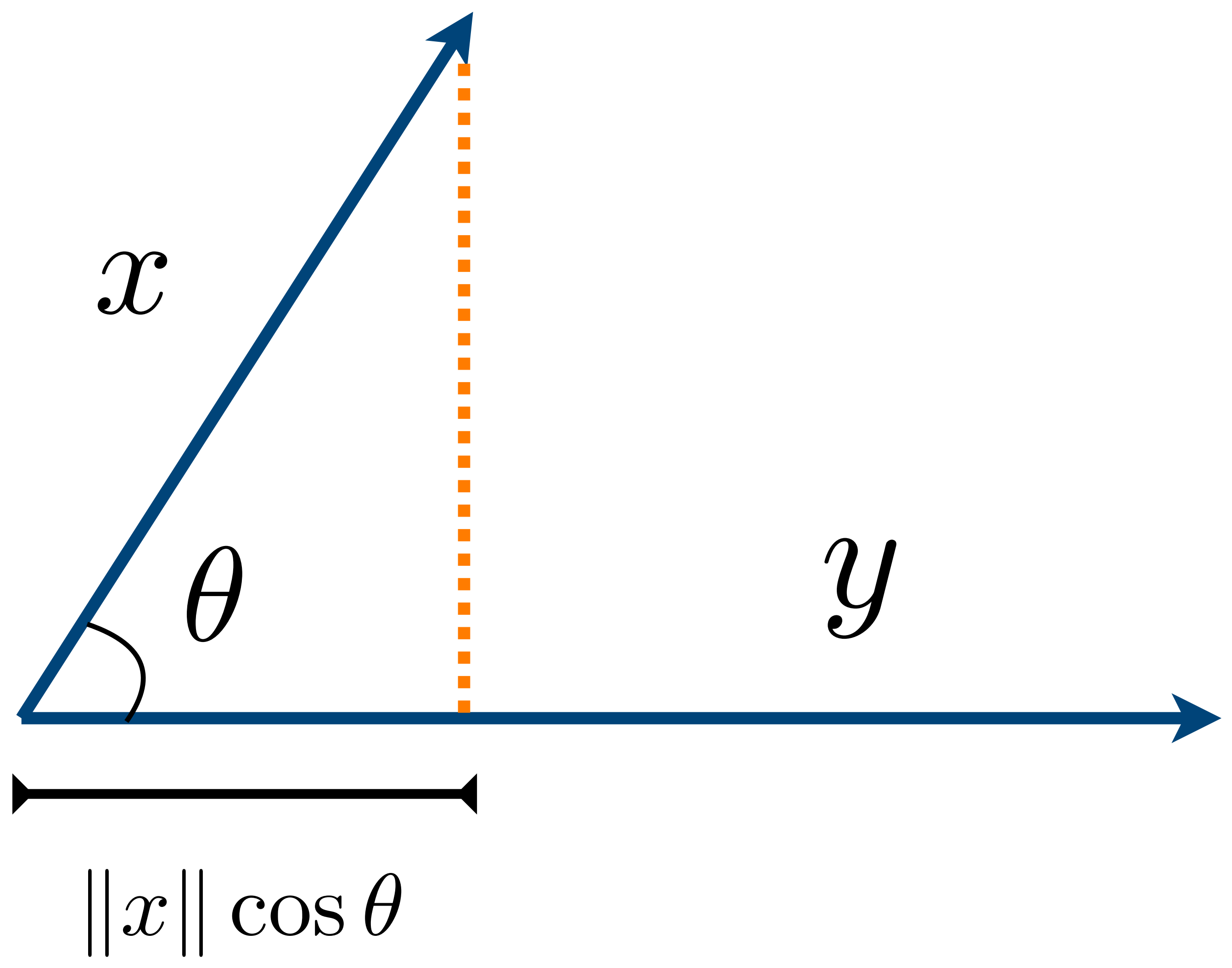

$$\langle x, y \rangle = \|x\| \cdot \|y\| \cdot \cos\theta$$

Vectors

- Norms = notion of distance in multiple dimensions

Properties:

$$\|x\| \geq 0, \forall x \in \mathbb{R}^p$$

$$\|x\| = 0, \text{ iff } x = 0$$

$$\|\alpha x\| = |\alpha| \|x\|, \forall \alpha \in \mathbb{R}$$

$$\|x + y\| \leq \|x\| + \|y\|$$ (Triangle inequality)

$$|x^\top y| \leq \|x\| \|y\|$$ (Cauchy–Schwarz)

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- Famous wanna-be norms: $\|x\|_0 = \text{card}(x)$

Matrices

- Matrix in m, n dimensions: $A \in \mathbb{R}^{m \times n}$

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

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- Names: Square, tall, fat, zero, identity, diagonal
- Properties:

$$A + B = B + A,\ \forall A, B \in \mathbb{R}^{m \times n}$$
$$(A + B) + C = A + (B + C),\ \forall A, B, C \in \mathbb{R}^{m \times n}$$
$$A + 0 = 0 + A,\ \forall A \in \mathbb{R}^{m \times n}$$
$$(A + B)^\top = A^\top + B^\top,\ \forall A, B \in \mathbb{R}^{m \times n}$$

Matrices

– Matrix multiplication： $C = AB$ where $C \in \mathbb{R}^{m\times p}$, $A \in \mathbb{R}^{m\times n}$, and $B \in \mathbb{R}^{n\times p}$

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- Special cases: vector inner product, matrix–vector mult., outer product

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– Properties：

$$(AB)C = A(BC),\ \forall A, B, C$$

$$\alpha(AB) = (\alpha A)B,\ \forall A, B$$

$$A(B + C) = AB + AC,\ \forall A, B, C$$

$$(AB)^\top = B^\top A^\top,\ \forall, A, B$$

$$AB \neq BA$$

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$$\mathrm{Tr}(A^\top B) = \sum_{i=1}^m A_{i1}\cdot B_{i1} + \sum_{i=1}^m A_{i2}\cdot B_{i2} + \cdots + \sum_{i=1}^m A_{in}\cdot B_{in}$$

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$$\mathrm{Tr}(A^\top B) = \mathtt{vec}(A)^\top \mathtt{vec}(B) = \langle \mathtt{vec}(A), \mathtt{vec}(B) \rangle$$

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– Positive semi–definite matrices： $A \succeq 0$

1. $A \in \mathbb{R}^{n \times n}$
2. A is symmetric
3. $x^\top Ax \geq 0,\ \forall x \in \mathbb{R}^n,\ x \neq 0$

Matrices

- Matrix singular value decomposition: $A \in \mathbb{R}^{m \times n}$

$$A = U\Sigma V^\top = \sum_{i=1}^{r} \sigma_i u_i v_i^\top,\ U \in \mathbb{R}^{m\times r}, \Sigma \in \mathbb{R}^{r\times r}, V \in \mathbb{R}^{n\times r} \qquad r \leq \{m, n\}$$

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- $\Sigma = \mathtt{diag}(\sigma_1, \ldots, \sigma_r)$ contains singular values where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$
- Left and right singular vectors are orthogonal: $U^\top U = I$ and $V^\top V = I$

Matrices

- Norms:

$$\|A\|_F = \sqrt{\sum_{ij} A_{ij}^2}$$

(Frobenius norm)

$$\|A\|_* = \sum_{i}^{r} \sigma_i$$

(Nuclear norm)

$$\|A\|_2 = \max_i \sigma_i$$

(Spectral norm)

..there are more norms to worry about (e.g., operator norms)
but we will skip them here..

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– Matrix inverses are defined on square matrices

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- Matrix inverse definition as a collection of properties:
  - A is full rank

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  - The linear system $Ax = b$ has a unique solution
  - The columns and rows of A are linearly independent
  - There exists a square matrix, A^{-1}, such that $A^{-1}A = AA^{-1} = I$

Overview

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & x \in \mathcal{C} \end{aligned}$$

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Unconstrained optimization

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Disclaimer

Optimization is generally **unsolvable**..

(Closed form expressions vs. Iterative methods)

(Naive solvers that work well on specific cases)

This course focuses on iterative methods

(..or what is the difference to specific, deterministic algorithms)

- General procedure

$$\min_x \quad f(x)$$
$$\text{s.t.} \quad x \in \mathcal{C}$$

1. Start from an initial point x_0.
2. Given an oracle $\mathcal{O}$, make queries to $\mathcal{O}$.
3. Obtain oracle's answer and exploit such a knowledge to reach to a new point as a putative solution.
4. Repeat steps 2.-3. until we get to a point where we are satisfied, according to a stopping criterion.

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- The notion of the Black−Box model

Common types of oracles. Some common types of oracles are:

- *Zeroth-order oracle*: Given a query point x, the oracle only returns $f(x)$.
- *First-order oracle*: Given a query point x, the oracle returns $f(x)$, and its gradient at x, $\nabla f(x)$ (assuming differentiability).
- *Second-order oracle*: Given a query point x, the oracle returns $f(x)$, its gradient $\nabla f(x)$, and the Hessian at x, $\nabla^2 f(x)$ (assuming twice-differentiability).

Conclusion

- We have set up background and notation w.r.t. linear algebra
- We saw a toy example where non-convex operations happen

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Next lecture

- Brief introduction to convex optimization and related topics

Demo