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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$$\min_{x} \quad f(x)$$

$$\text{s.t.} \quad x \in \mathcal{C}$$

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

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– Different strategies within each problem
– Different approaches based on computational capabilities
– Different approaches based on constraints

$$\min_{x} \quad f(x)$$
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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

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More complicated models

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Better results ? Provable efficiency Harder problems

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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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- Continuous **optimization** (in general)
  - See syllabus
  - Both theory and practice
- Recent applications that drive research
- When no theory applies, some intuition

Examples

– Least squares / linear regression

(No, we will not re−define it)

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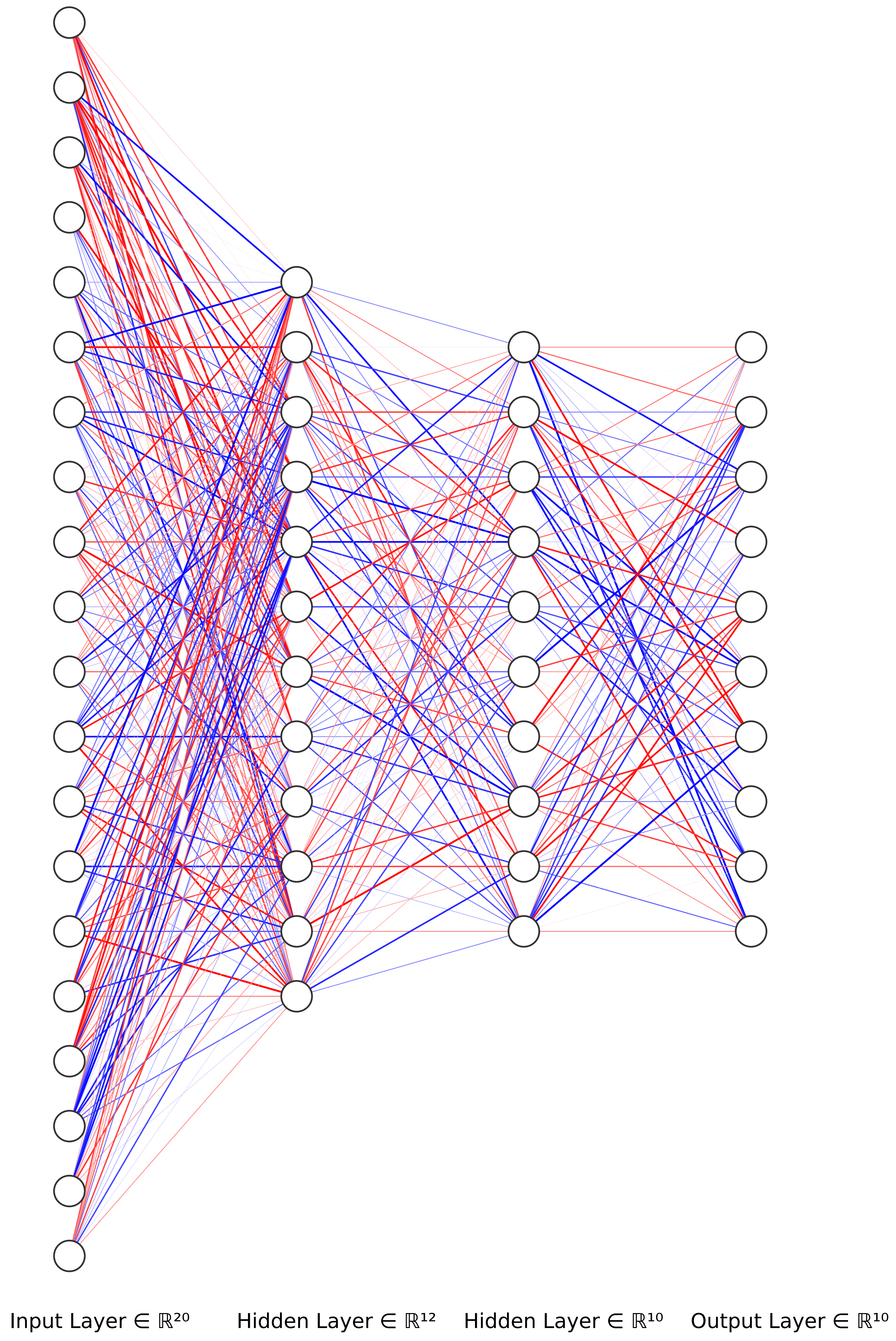
$$\begin{aligned} \min_{X} \quad & f(X) \\ \text{s.t.} \quad & X \in \mathcal{C} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \min_{x\in\{0,1\}^m, y\in\{0,1\}} \quad & f(y) = \sum_{i\in\mathcal{V}} \sum_{k=1}^{p} d_i(1-q)q^{k-1} y_{ik} \\ \text{s.t.} \quad & \sum_{j\in\mathcal{W}_i} x_j \geq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

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

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

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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

– General procedure

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

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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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).

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  (See Anshu's course)

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

Any questions?

Who is this class for?

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(but get in touch with me soon to assess your background)

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- Just auditing is fine by me

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– For starters, this will always be an evolving course

(Any feedback is more than welcome)

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

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: scribing)

Regarding assignments

- Weakly assignments

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- 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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- Consider possible extensions of these works (project)
- Comprehend how optimization is key in ML/AI/SP
- Read and review recent papers

My goals

- Not to judge you on small details in HWs

(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

Prerequisites

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

Grading policy

- 45% HWs
- 50% project/final exam
- 5%: participation, attendance
- 5%: scribing notes (**bonus**)

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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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- Deliverable in LaTEX (template available online)

HWs

– Deliverable in LaTEX

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
  - Main comments + your overall score

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- Grading: slides quality, clarity of main ideas

Presentations (for final projects)

(not certain yet)

Example 1

Example 2

Example 3

Presentation example

Final Project

(Course website)

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(Course website)

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

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

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- **Every week I will try to upload an updated chapter;** however I would appreciate any help with scribing throughout the semester

Length of each session

- There will be longer or shorter sessions

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Setting up the background

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

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$$0 + x = x, \quad x \in \mathbb{R}^p$$

$$\alpha(x + y) = \alpha x + \alpha y, \quad x, y \in \mathbb{R}^p$$ (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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- How does k compare to p, the vector dimension?

- Inner product:

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

Vectors

- Inner production interpretation:

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

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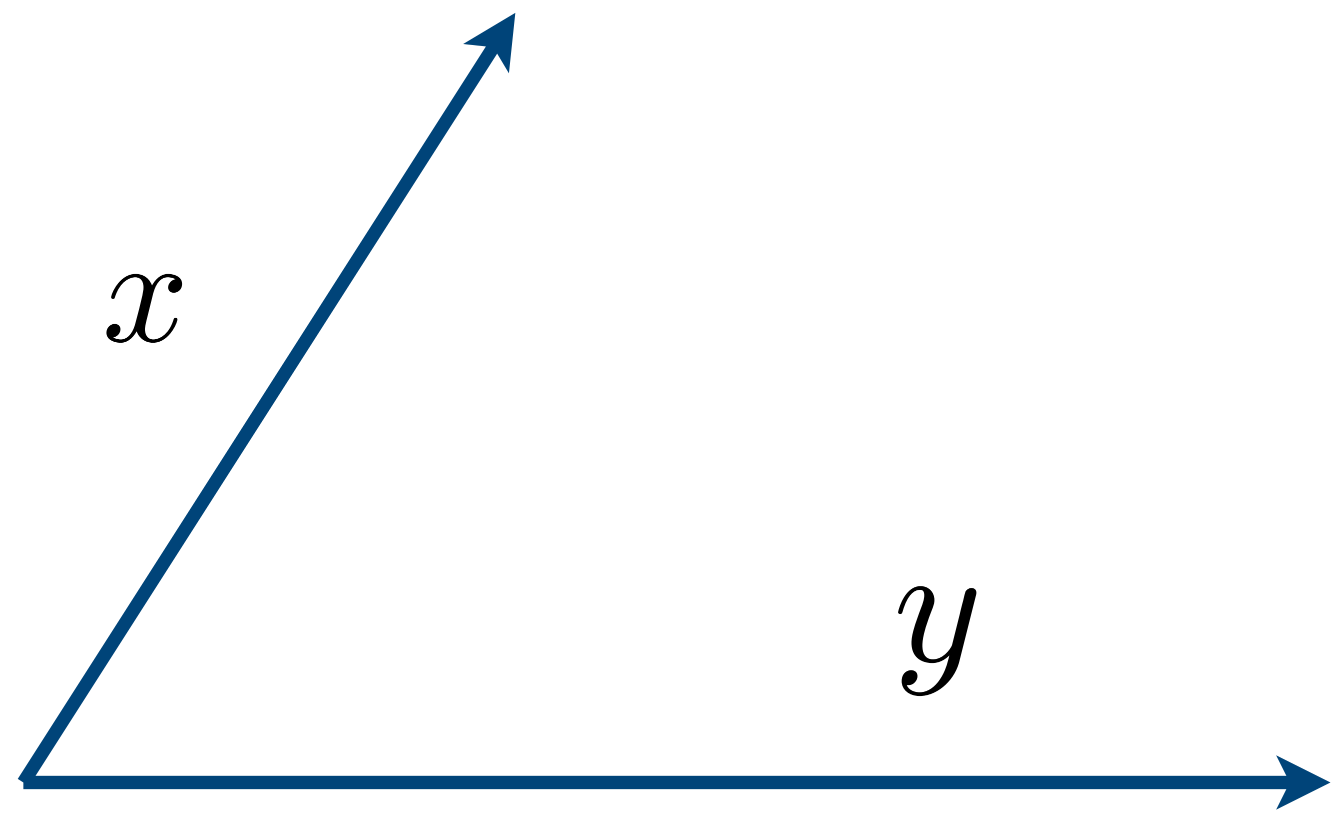

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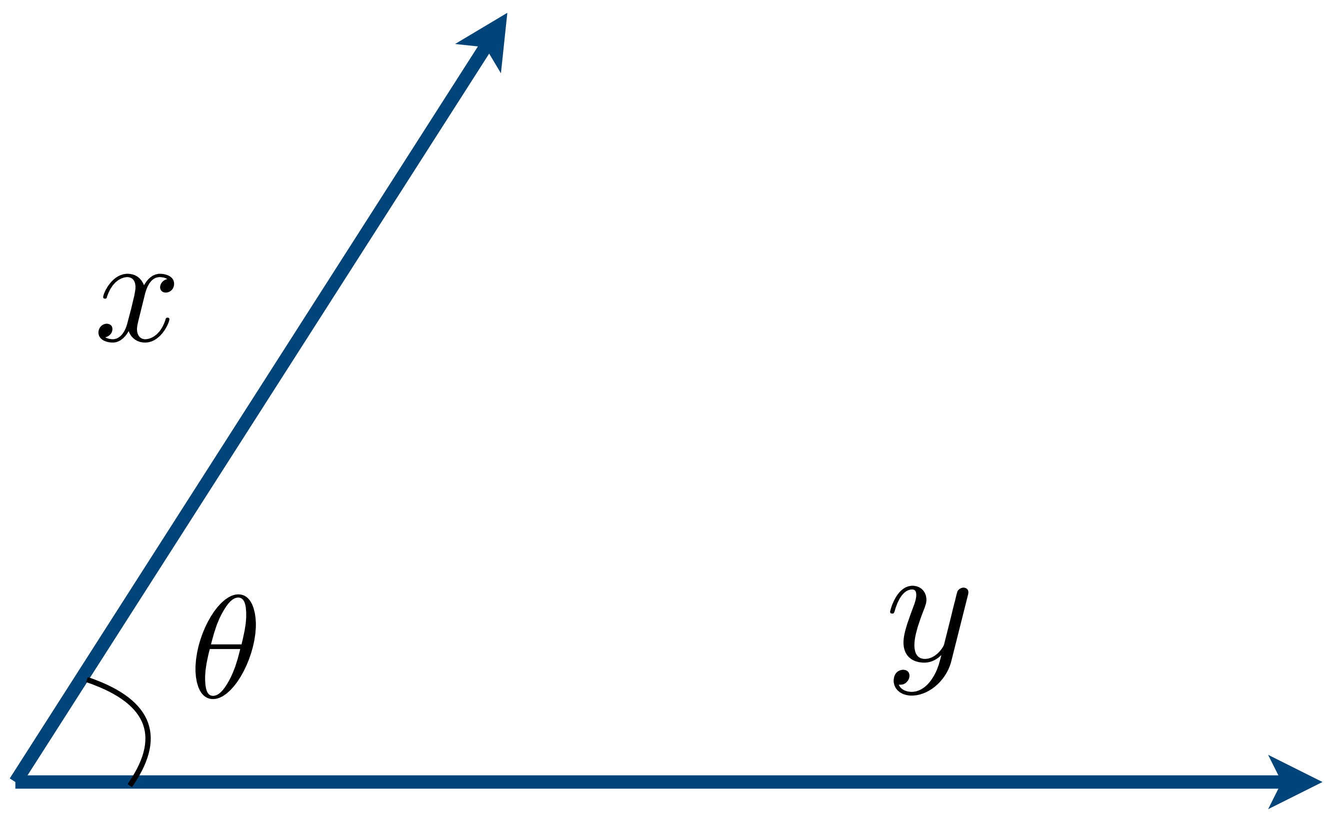

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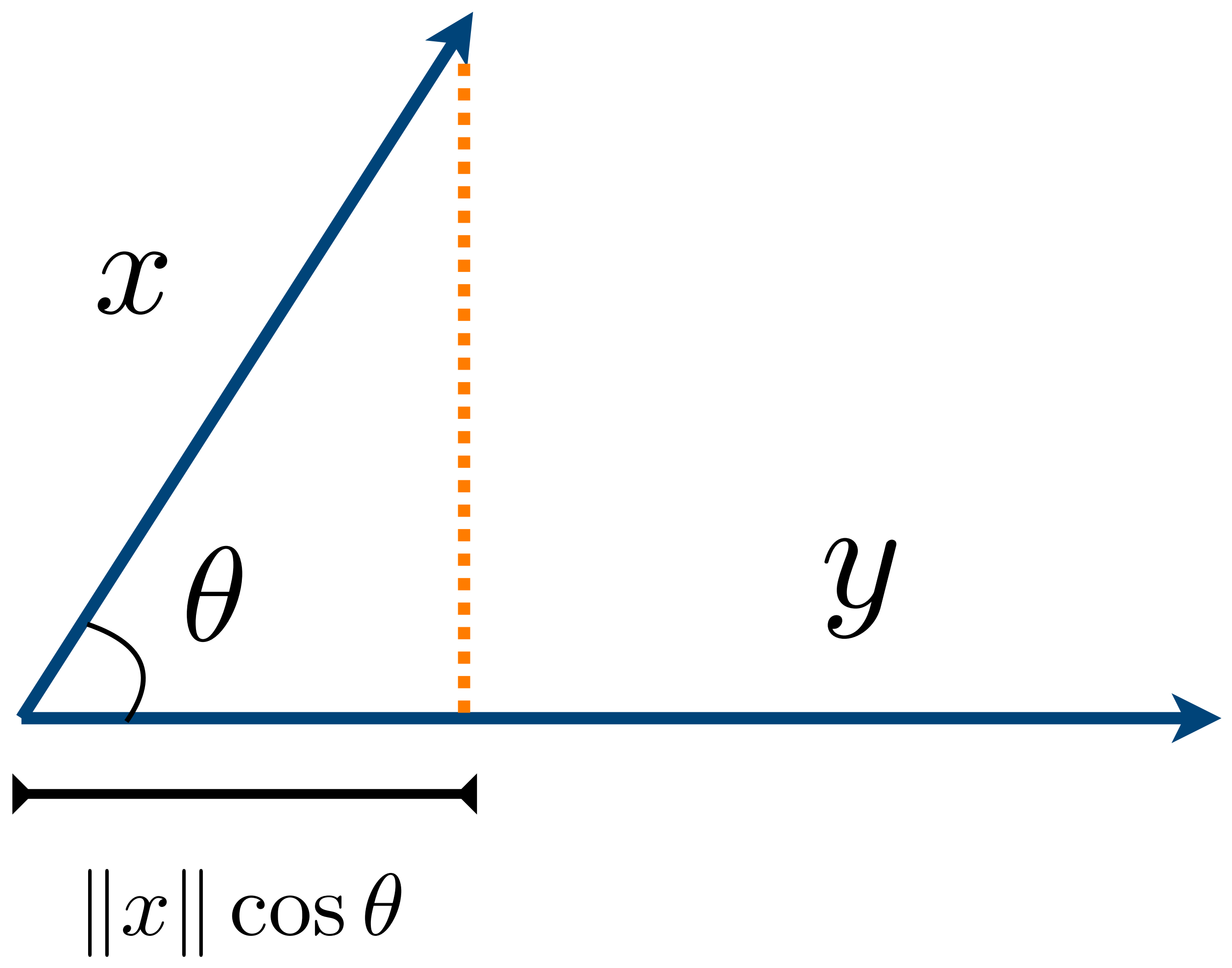

$$\langle x, y \rangle = \|x\| \cdot \|y\| \cdot \cos\theta$$

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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$$\|\alpha x\| = |\alpha|\|x\|, \forall \alpha \in \mathbb{R}$$
$$\|x + y\| \leq \|x\| + \|y\|$$ (Triangle inequality)
$$|x^\top y| \leq \|x\|\|y\|$$ (Cauchy−Schwarz)

- Standard vector norms:

$$\|x\|_2 = \sqrt{\sum_i x_i^2} \qquad \|x\|_1 = \sum_i |x_i| \qquad \|x\|_\infty = \max_i |x_i|$$

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$$\|x\| \geq 0, \forall x \in \mathbb{R}^p$$
$$\|x\| = 0, \text{ iff } x = 0$$
$$\|\alpha x\| = |\alpha|\|x\|, \forall \alpha \in \mathbb{R}$$
$$\|x + y\| \leq \|x\| + \|y\|$$ (Triangle inequality)
$$|x^\top y| \leq \|x\|\|y\|$$ (Cauchy−Schwarz)

- Standard vector norms:

$$\|x\|_2 = \sqrt{\sum_i x_i^2} \qquad \|x\|_1 = \sum_i |x_i| \qquad \|x\|_\infty = \max_i |x_i|$$

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

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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– 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

– Properties：

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

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

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

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

$$AB \neq BA$$

Matrices

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$$\langle A, B\rangle = \mathrm{Tr}(A^\top B) = \mathrm{Tr}(B^\top A), \forall A, B \in \mathbb{R}^{m\times n}$$

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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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- 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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  - 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 $A^{-1}A = AA^{-1} = I$

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