ECE 8101: Nonconvex Optimization for Machine Learning

Lecture Note 1: Course Info & Introduction

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Course Info (1)

- Instructor: Jia (Kevin) Liu, Assistant Professor
- Office: 420 Dreese Labs
- Email: `liu@ece.osu.edu`
- Time: TTh 11:10AM – 12:30PM
- Location: ~~Journalism Bldg 375~~ Knowlton Hall 190
- Office Hour: Wed 5–6pm or by appointment
- Online Synchronous Zoom Session: `https://osu.zoom.us/j/95738261623?pwd=cWozUmhVbW9pTVpkVHB5OGc4dGJldz09`
- Websites: Carmen: announcements, grade management, course materials)
  Schedule: `https://kevinliu-osu.github.io/teaching/ECE8101_S22/`
- Prerequisite:
  - Working knowledge of Linear Algebra and Probability
  - Exposure to optimization and machine learning is a plus but not required

Course Info (2)

Grading Policy:

- Class Participation (10%): Top Hat (please install on your phone/tablet)
- Paper Reading Assignment (60%)
  - Assigned after each major topic set (approximately)
  - May involve open-ended questions
  - Must be typeset using LaTeX in NeurIPS format
- Final Project (30%)
  - Finished by a team of 2. Project proposal due soon after spring break
  - Project report due in the final exam week. Follow NeurIPS format (Could become a publication of yours! "Automatic A" if determined publishable by instructor ☺)
  - 10-minute in-class presentation at the end of the semester. Final report due by the *beginning* of final exam week ~~(Dec. 9)~~ Apr. 27.
  - Potential ideas of project topics (should contain something new & useful):
    - Nontrivial extension of the results introduced in class
    - Novel applications in your own research area
    - New theoretical analysis/insights of an existing/new algorithm
    - It is important that you justify its novelty!

Course Info (3)

Course Materials:

- No required textbook
- Lecture notes are developed based on:
    - Important & trending papers in the field
    - [BV] S. Boyd and L. Vandenberghe, "*Convex Optimization*," Cambridge University Press, 2004 (available online)
    - [NW] J. Nocedal and S. Wright, "*Numerical Optimization*," Ed. 2, Springer,
    - [BSS] M. Bazarra, H.D. Sherali, and C.M. Shetty, "*Nonlinear Programming: Theory and Algorithms*," John Wiley & Sons, 2006
    - [Nesterov] Y. Nesterov, "*Introductory Lectures on Convex Optimization: A Basic Course*," Springer, 2004 2006

Tentative Topics

- Stochastic Nonconvex Optimization
  - Fundamental of SGD; variance-reduced algorithms (SVRG, SAGA, SPIDER); accelerated algorithms (STORM, Hybrid)
- Federated and Decentralized Optimization
  - Decentralized (stochastic) gradient descent, FedAvg, and variants
- Zeroth-order Optimization
  - One-point and two-point gradient estimator; zeroth-order SGD; zeroth-order variance-reduced optimization methods ...
- Stationary and Saddle Points
  - Saddle points; convergence to saddle points ...
- Geometry of Nonconvex Optimization
  - Landscape of learning models, PL conditions, NTK ...
- Other Emerging Nonconvex Optimization Problems
  - Minimax problems, bilevel problems, meta learning ...

Special Notes

- Advanced, research-oriented
  - There will be paper reading assignments and a term project
- Goal: Prepare & train students for theoretical research
- But will (briefly) mention relevant applications in ML:
  - Deep Learning
  - Big data analytics
  - ...
- Caveat: Focus on theory & proofs, rather than "coding/programming"
  - No "one book fits all" $\Rightarrow$ Many readings required
  - Will try to cover a wide range of major topics
  - Background materials will be introduced but at very fast pace
  - So, mathematical maturity is essential!

How to Best Prepare for the Lectures?

Read, read, read!

- Especially if you're unfamiliar with the background (e.g., linear algebra, probability, ...)
  - Will quickly go over some related background in class
- Appendices in [BV] and [BSS] provide lots of math background
- You are welcome to ask questions in office hours
- But careful self-studies may still be needed

Mathematical Optimization

Mathematical optimization problem:

$$\begin{array}{ll} \text{Minimize} & f_0(\mathbf{x}) \\ \text{subject to} & f_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \end{array}$$

- $\mathbf{x} = [x_1, \ldots, x_N]^\top \in \mathbb{R}^N$: decision variables
- $f_0 : \mathbb{R}^N \to \mathbb{R}$: objective function
- $f_i : \mathbb{R}^N \to \mathbb{R}, i = 1, \ldots, m$: constraint fucntions

Solution or **optimal point** $\mathbf{x}^*$ has the smallest value of f_0 among all vectors that satisfy the constraints

Brief History of Optimization

Theory:

- Early foundations laid by many all-time great mathematicians (e.g., Newton, Gauss, Lagrange, Euler, Fermat, ...)
- Convex analysis 1900–1970 (Duality by von Neumann, KKT conditions...)

Algorithms

- 1947: simplex algorithm for linear programming (Dantzig)
- 1970s: ellipsoid method [Khachiyan 1979], 1st polynomial-time alg. for LP
- 1980s & 90s: polynomial-time interior-point methods for convex optimization [Karmarkar 1984, Nesterov & Nemirovski 1994]
- since 2000s: many methods for large-scale convex optimization

Applications

- before 1990: mostly in operations research, a few in engineering
- since 1990: many applications in engineering (control, signal processing, networking and communications, circuit design,...)
- since 2000s: machine learning

Solving Optimization Problems

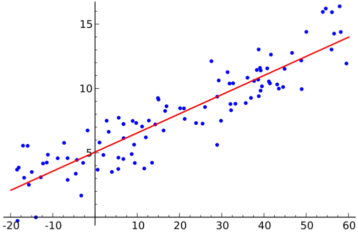
- General optimization problems
  - Very difficult to solve (NP-hard in general)
  - Often involve trade-offs: long computation time, may not find an optimal solution (approximation may be acceptable in practice)
- Exceptions: Problems with special structures
  - Linear programming problems
  - Convex optimization problems
  - Some non-convex optimization problems with strong-duality
- Watershed between Problem Hardness: Convexity
  - This course focuses on nonconvex problems arising from ML context

Applying Optimization Tools in Machine Learning

- Linear Regression
- Variable Selection & Compressed Sensing
- Support Vector Machine
- Logistic Regression (+ Regularization)
- Matrix Completion
- Deep Neural Network Training
- Reinforcement Learning
- Distributed/Federated/Decentralized Learning
- ...

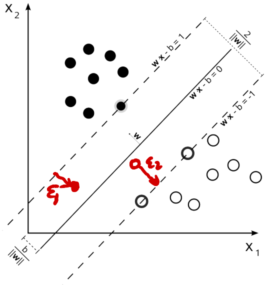
Example 1: Linear Regression (Convex)

$$\text{Minimize}_{\beta} \quad \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$



- Given data samples: $\{(\mathbf{x}_i, y_i), i = 1, \ldots, m\}$, where $\mathbf{x}_i \in \mathbb{R}^n$, $\forall i$
- Find a linear estimator: $y = \boldsymbol{\beta}^\top \mathbf{x}$, so that "error" is small in some sense
- Let $\mathbf{X} \triangleq [\mathbf{x}_1, \ldots, \mathbf{x}_m]^\top \in \mathbb{R}^{m \times n}$, $\mathbf{y} \triangleq [y_1, \ldots, y_m]^\top \in \mathbb{R}^m$
- Linear algebra for $\|\cdot\|_2$: $\boldsymbol{\beta}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ (analytical solution)
- Computation time proportional to $n^2 m$ (less if structured)
- Stochastic gradient if m, n are large

Example 2: Support Vector Machine (Convex)



- Given data samples: $\{(\mathbf{x}_i, y_i), i = 1, \ldots, m\}$
  - $\mathbf{x}_i \in \mathbb{R}^n$ called "feature vectors", $\forall i$
  - $y_i \in \{-1, +1\}$ are "labels"
- Linear classifier: $f(\mathbf{x}) = \mathrm{sgn}(\mathbf{w}^\top \mathbf{x} + b)$:
  - $\mathbf{w} \in \mathbb{R}^n$: weight vector for features
  - $b \in \mathbb{R}$: Some "bias"

If $y_i = 1$, $\underline{w}^T \underline{x}_i + b \geq 1$
$y_i = -1$, $\underline{w}^T \underline{x}_i + b \leq -1$.

- Goal: To find a pair $(\mathbf{w}, b)$ to minimize a weighted sum such that
  - Minimize classification error on training samples
  - Robust to random noise in the training samples

$y_i(\underline{w}^T \underline{x}_i + b) \geq 1$.

$$\underset{\mathbf{w}, b, \boldsymbol{\epsilon}}{\text{Minimize}} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m} \epsilon_i$$

$$\text{subject to} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0, \quad i = 1, \ldots, m$$

Optimization Algorithms for SVM

- Coordinate Descent [Platt, 1999; Chang and Lin, 2011]
- Stochastic gradient [Bottou and LeCun, 2004; Shalev-Shwartz et al., 2007]
- Higher-order methods (interior-point) [Ferris and Munson, 2002; Fine and Scheinberg, 2001]; (on reduced space) [Joachims, 1999]
- Shrink Algorithms [Duchi and Singer, 2009; Xiao, 2010]
- Stochastic gradient + shrink + higher-order [Lee and Wright, 2012]

Nonconvex Optimization Problems in ML

- Lower complexity bound for solving general nonconvex problems
  - Consider, w.l.o.g., $\min_{\mathbf{x}\in[0,1]^d} f(\mathbf{x})$
  - f is nonconvex and L-Lipschitz-continuous, with global optimal $f^* > -\infty$
  - To find an ϵ-approximate solution $\hat{\mathbf{x}}$ (i.e., $f(\hat{\mathbf{x}}) - f^* \leq \epsilon$), number of iterations required: $\Omega(L^d \epsilon^{-d})$ (exponential)

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- Several ways to relax this challenging goal:
  - Finding hidden convexity or reformulate into an equivalent convex problem
    - ⋆ Need to exploit special problem structure as much as possible
    - ⋆ However, solution approaches cannot be generalized
  - Change the goal to finding a stationary point or a local extremum
    - ⋆ Often possible to obtain FO methods with polynomial dependence of the complexity on the dimension of the problem and desired accuracy
  - Identify a class of problems:
    - ⋆ General enough to characterize a wide range of applications (in ML)
    - ⋆ Allow one to obtain global performance guarantees of an algorithm
    - ⋆ E.g., Polyak-Lojasiewicz condition (linear convergence), α-weakly-quasi-convexity (sublinear convergence), etc.

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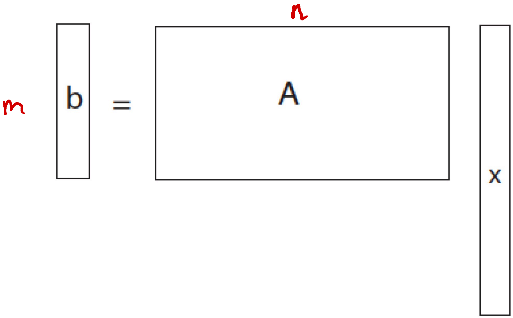
    - ⋆ E.g., Polyak-Lojasiewicz condition (linear convergence), α-weakly-quasi-convexity (sublinear convergence), etc.
  - But what if gradients are hard to obtain?
    - ⋆ E.g., reinforcement learning, blackbox adversarial attacks on DNN?
    - ⋆ Zeroth-order or derivative-free methods

Tractable Nonconvex Optimization Problems in ML

- Problems with hidden convexity or analytic solutions
  - Eigen-problems (e.g., PCA, multi-dimensional scaling, ...)
  - Non-convex proximal operators (e.g., Hard-thresholding, Potts minimization)
  - Some discrete problems (binary graph segmentation, discrete Potts minimization, nearly optimal K-means)
  - Infinite-dimensional problems (smoothing splines, locally adaptive regression splines, reproducing kernel Hilbert spaces)
  - Non-negative matrix factorization (NMF)
  - Compressive sensing with ℓ_1 regularization
- Problems with (global) convergence results
  - Phase retrieval problem
  - Low-rank matrix completion
  - Deep learning
- Problems with certain properties of symmetry
  - Rotational symmetry, discrete symmetry, etc.

Example 3: Compressive Sensing (Nonconvex)

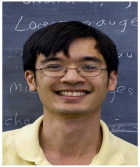
Interested in solving undetermined systems of linear equations:



- Estimate $\mathbf{x} \in \mathbb{R}^n$ from linear measurements $\mathbf{b} = \mathbf{A}\mathbf{x} \in \mathbb{R}^m$, where $m \ll n$.
- Seems to be hopelessly ill-posed, since more unknowns than equations...
- Or does it?

A Little History of Compressive Sensing (CS)

- Name coined by David Donoho
- Pioneered by Donoho and Candès, Tao and Romberg in 2004

Compressed sensing
DL Donoho - Information Theory, IEEE Transactions on, 2006 - ieeexplore.ieee.org
Abstract—Suppose is an unknown vector in(a digital image or signal); we plan to measure general linear functionals of and then reconstruct. If is known to be compressible by transform coding with a known transform, and we reconstruct via the nonlinear procedure ...
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30,039

Robust uncertainty principles: Exact signal reconstruction from highly incomplete frequency information
EJ Candès, J Romberg, T Tao - Information Theory, IEEE ..., 2006 - ieeexplore.ieee.org
Abstract—This paper considers the model problem of recon-structing an object from incomplete frequency samples. Consider a discrete-time signal and a randomly chosen set of frequencies. Is it possible to reconstruct from the partial knowledge of its Fourier ...
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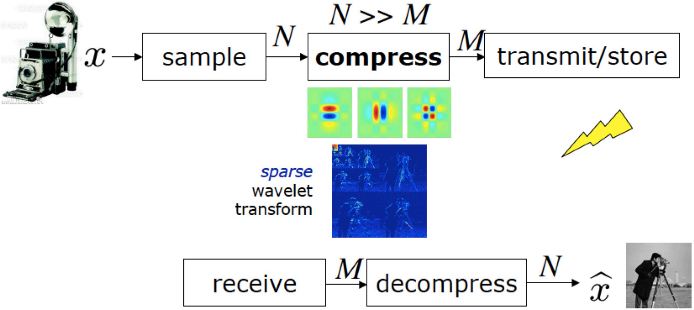
17,652.

Sensing and Signal Recovery

Conventional paradigm of data acquisition: Acquire then compress



Q: Why compression works?

A: Quite often, there's only marginal loss in "quality" between the raw data and its compression form.

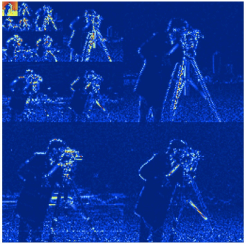
Q: But still, why marginal loss?

Sparse Representation

- **Sparsity:** Many real world data admit sparse representation. The signal $\mathbf{s} \in \mathbb{C}^n$ is sparse in a basis $\mathbf{\Phi} \in \mathbb{C}^{n \times n}$ if

$$\mathbf{s} = \mathbf{\Phi}\mathbf{x} \quad \text{and} \quad \mathbf{x} \in \mathbb{R}^n \text{ only has very few non-zero elements}$$

- For example, images are sparse in the wavelet domain



- The # of large coefficients in the wavelet domain is small ⇒ compression

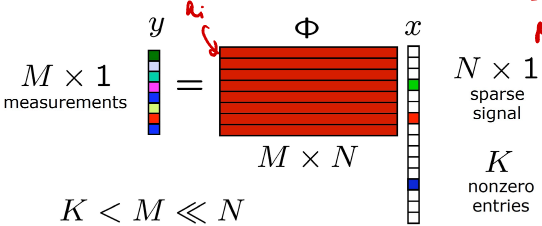
Compressed Sensing: Compression on the Fly!

Q: Could we directly compress data and then reconstruct?

$\min \cancel{\|\mathbf{x}\|_0}$ $\|\mathbf{x}\|_1$

s.t. $\|\Phi \mathbf{x} - \mathbf{y}\| \le \delta$

$$y_i = \langle \mathbf{a}_i, \mathbf{x} \rangle, \quad i = 1, \ldots, m$$



RIP: restricted isometry property

- Goal: To learn (recover) $\mathbf{x}$'s value through some given (noisy) samples y_i?
- Mathematically, this gives rise to an underdetermined system of equations, where the signal of interests is *sparse*

Sparse Recovery

In optimization, CS can be written in the form of:

$$\underset{\mathbf{x}\in\mathbb{R}^n}{\text{Minimize}}\ \phi_\gamma(\mathbf{x}) \triangleq \underbrace{f(\mathbf{y},\mathbf{\Phi};\mathbf{x})}_{\text{error}} + \gamma\underbrace{\|\mathbf{x}\|_1}_{\text{reg.}}$$

In machine learning context, questions of interests include:

- How to design the measurement/sampling matrix $\mathbf{\Phi}$?
- What are the efficient algorithms to search for $\mathbf{x}$?
- Are they stable under noisy inputs?
- How many measurements/samples are necessary/sufficient (i.e., size of $\mathbf{y}$)?

Insight: Turns out $m = \Omega(\log(n))$ random samples will suffice

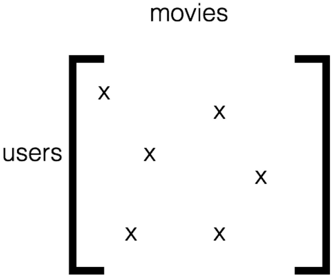
Some Optimization Algorithms for Compressed Sensing

- Shrink algorithms (for l_1 term) [Wright et al., 2009]
- Accelerated gradient [Beck and Teboulle, 2009b]
- ADMM [Zhang et al., 2010]
- Higher-order: Reduced inexact Newton [Wen et al., 2010]; Interior-point [Fountoulakis and Gondzio, 2013]

Example 4: Matrix Completion (Nonconvex)

In 2006, Netflix offered $1 million prize to improve movie rating prediction

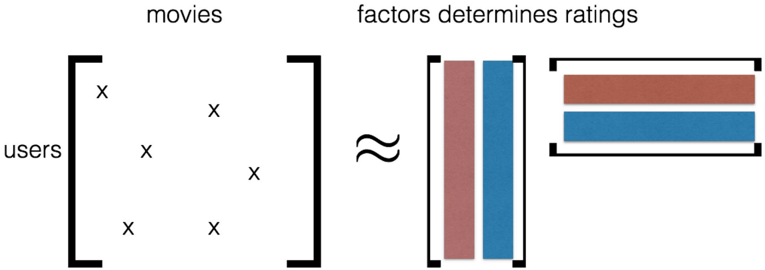
- How to estimate the missing ratings?



- About a million users, and 25,000 movies, with sparsely sampled ratings
- In essence, a low-rank matrix completion problem

Low-Rank Matrix Completion

- Completion Problem: Consider $\mathbf{M} \in \mathbb{R}^{n_1 \times n_2}$ to represent Netflix data, we may model it through factorization:



- In other words, the rank r of $\mathbf{M}$ is much smaller than its dimension $r \ll \min\{n_1, n_2\}$

Low-Rank Matrix Completion

In optimization, the low-rank matrix completion problem can be written as:

$$\begin{array}{ll} \underset{\mathbf{X}}{\text{Minimize}} & \cancel{\mathrm{rank}(\mathbf{X})} \quad \|\underline{X}\|_* \text{ : nuclear norm.} \\ \text{subject to} & (\mathbf{X})_{ij} = (\mathbf{M})_{ij}, \quad \forall i,j \in \text{observed entries} \end{array}$$

In machine learning context, questions of interests include:

- What are the efficient algorithms to search for $\mathbf{X}$?
- Are they stable under noisy inputs and outliers?
- How many samples are necessary/sufficient (i.e., size of $(\mathbf{M})_{i,j}$)?

Insight: Turns out $m = \Omega(r \max\{n_1, n_2\} \log^2(\max\{n_1, n_2\}))$ samples will suffice

Some Optimization Algorithms for Matrix Completion

- (Block) Coordinate Descent [Wen et al., 2012]
- Shrink [Cai et al., 2010a; Lee et al., 2010]
- Stochastic Gradient [Lee et al., 2010]

Example 5: Phase Retrieval (Nonconvex)

- A classical topic from at least 1980s:
  - Recovery of a function given magnitude of its Fourier transform
  - Applications: optimal imaging, electron microscopy, crystallography, etc.

- Recover an $\mathbf{x}^* \in \mathbb{C}^d$ from a phase-less measurements:

$$y_k = |\langle \mathbf{a}_k, \mathbf{x} \rangle|^2, \quad k = 1, \ldots, M,$$

where $\mathbf{a}_k$ denotes some measurement vectors. The phase-retrieval problem can be formulated as an empirical risk minimization (ERM): problem

$$\min_{\mathbf{x}} \sum_{k=1}^{M} (y_k - |\langle \mathbf{a}_k, \mathbf{x} \rangle|^2)^2.$$

- Phase retrieval is nonconvex and unclear how to find a global minimum
  - Provable convergence result: [Candes et al. '15], [Yang et al. '19], [Wu and Rebeschini, '20], [Tan and Vershynin, '16], [Chen et al. '19]

Wirtinger Flow. Alg.

Example 6: Deep Learning (Nonconvex)

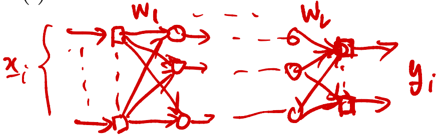
- Example: Train an L-layer fully-connected NN for supervised learning:

$$\min_{\mathbf{W}} \left\{ F(\mathbf{W}) \triangleq \frac{1}{m} \sum_{i=1}^{m} \ell(\mathbf{y}_i, f(\mathbf{x}_i, \mathbf{W})) \right\},$$

  - $\mathbf{W} = \{\mathbf{W}_1, \ldots, \mathbf{W}_L\}$, with $\mathbf{W}_i \in \mathbb{R}^{n_i \times n_{i-1}}$, are weights of NN model
  - $\{(\mathbf{x}_i, \mathbf{y}_i)_{i=1}^{m}\}$, $\mathbf{x}_i \in \mathbb{R}^{n_0}$, are training samples
  - $\ell(\cdot, \cdot)$ is a loss function (e.g., quadratic or logistic loss)
  - NN model can be written as:

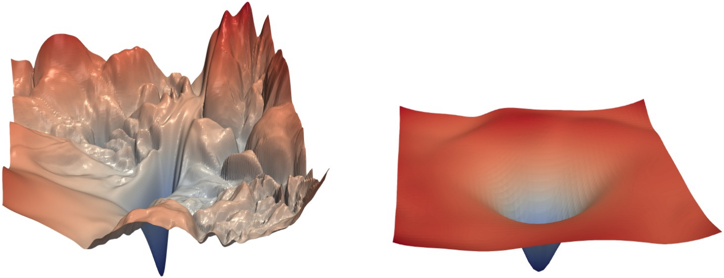
$$f(\mathbf{x}_i, \mathbf{W}) = \mathbf{W}_L \sigma(\mathbf{W}_{L-1} \sigma(\ldots, \sigma(\mathbf{W}_2 \sigma(\mathbf{W}_1 \mathbf{x}_i)) \ldots)),$$

  where $\sigma(\cdot)$ is scalar-valued and called activation function.



Example 6: Deep Learning (Nonconvex)

- Landscape of deep neural networks
  - Loss surfaces of ResNet-56 with/without skip connections [Li et al. '18]



(a) without skip connections (b) with skip connections

- Training NN is NP-complete in general [Blum and Rivest, '89], but:
  - All local minima are global for 1-layer NN: [Soltanolkotabi et al. '18], [Haeffele and Vidal, '17], [Feizi et al. '17]
  - GD/SGD converge to global min for linear networks [Arora et al. '18], [Ji and Telgarsky, '19], [Shin, '19], wide over-parameterized networks [Allen-Zhu et al., '19], and pyramid networks [Nguyen and Mondelli, '19]

Next Class...

We will start from some related math background.