CS6301: Optimization in Machine Learning

Lecture 1: Introduction and Course Overview

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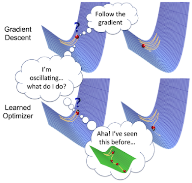
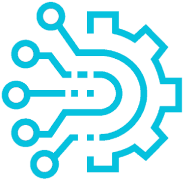
University of Texas, Dallas
https://sites.google.com/view/cs-6301-optml/home

January 13, 2020





Outline

- Why take this course?
- Prerequisites
- Week by Week Course plan
- Course Logistics
- Basics of Linear Algebra
- Applications of Optimization in Machine Learning

Acknowledgements

I would like to acknowledge several sources I have used to create slides

- Martin Jaggi's course at EPFL: https://github.com/epfml/OptML_course
- Mark Schmidt's ML and Advance ML course at UBC: https://www.cs.ubc.ca/~schmidtm/Courses/LecturesOnML
- Several Blogs: geeksforgeeks.org, healthylalgorithms.com
- Prof. Ganesh Ramakrishnan's Convex Optimization course at IIT Bombay: https://www.cse.iitb.ac.in/~cs709/.
- Prof. Ramakrishnan is also the co-creator of this course which he will be teaching at IIT Bombay.

Why take this Course?

Optimization is everywhere: Big Data and Machine Learning, Scheduling and Planning, Operations Research, control theory, data analysis, simulations, almost all technology we use, search engines, computers/laptops, smart-phones, hardware/software of all kinds, ...

- Mathematical Modeling:
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- Computational Optimization:
  - Algorithms to solve these optimization problems optimally or near optimally.

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Machine Learning and AI are embedded in practically every spear of our life: Google/Bing Search & Ads, Amazon product search/recommendation, driverless cars, Google Maps, Uber/Ola matching, Google Photos, Youtube, Facebook, Twitter, Microsoft Office, ...

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- Optimization is one of the important backbones of machine learning.

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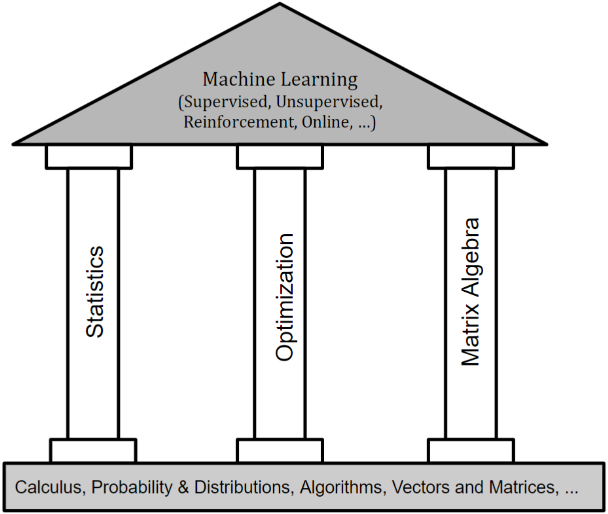

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Optimization one of the pillers of ML!

- Continuous Optimization:
  - Continuous Optimization often appears as *relaxations* of risk/error minimization problem. The *Learning* problem in many parametrized models (whether supervised, semi-supervised, unsupervised, or reinforcement learning) involves **Continuous Optimization**.

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- Mixed Continuous and Discrete Optimization:
  - A growing number of problems including classical problems such as clustering, feature selection, structured sparsity occur as mixed discrete/continuous optimization problems.

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- Even if you don't implement new algorithms, you will have a better idea of which algorithm to use in which sceanrio.

About Me

- Undergrad (2007 - 2011) from IIT Bombay $\rightarrow$ Masters + Ph.D at UW Seattle (2011 - 2015) $\rightarrow$ PostDoc at UW Seattle (2015-2016) $\rightarrow$ ML Scientist & Researcher at Microsoft (2016 - 2019) $\rightarrow$ Assistant Professor at UT Dallas (2020 -)

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- Spent good amount of time both in Academia (writing/publishing papers, conferences, giving talks, ...) and Industry (products, impact, solving real world problems)
- Early portion of my Ph.D (proving theorems, theoretical results) $\rightarrow$ later part of Ph.D + Industry (practical aspects of ML, solving problems, getting algorithms to work on real data)

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- Give a flavor of the proofs and proof techniques but will try to not make this course heavily theoretical.
- Focus extensively on implementation aspects and as a part of assignments, we will implement many ML loss functions and algorithms.

Why did you enroll for this Course?

Lets hear from a few of you why you took this course...

Logistics

- Class is Every Mon/Wed 4 PM - 5:15 PM
- Venue: **AD 2.232**
- Office Hours: Wednesdays between 3 to 3:50 PM. Additional Office Hours (by appointment): Mondays 3 to 3:50 PM.
- TA: TBD

Prerequisites

- Calculus Courses
- Basic Linear Algebra: Matrices, Vectors & Matrix Algebra
- Machine Learning (either an undergraduate or graduate ML course)
- Algorithms course (either in undergraduate or graduate version)
- Bonus: Linear Programming or Numerical Optimization
- It is fine if you are concurrently taking the ML course (for e.g. first year students). However you will need to put in extra effort.

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  - A flavor of the proof techniques without going too mathematical
- One of the first courses to provide an overview of the entire spectrum of optimization (discrete & continuous) for ML.

First Half of this Course: Continuous optimization

- Basics of Continuous Optimization
- Convexity
- Gradient Descent
- Projected GD
- Subgradient Descent
- Accelerated Gradient Descent
- Newton & Quasi Newton
- Duality: Legrange, Fenchel
- Coordinate Descent
- Frank Wolfe
- Optimization in Practice

Second Half of this Course: Discrete optimization

- Linear Cost Problems
- Matroids, Spanning Trees
- s-t paths, s-t cuts
- Matchings
- Covers (Set Covers, Vertex Covers, Edge Covers)
- Optimal Transport (if time permits)

- Non-Linear Discrete Optimization
- Submodular Functions
- Submodularity and Convexity
- Submodular Minimization
- Submodular Maximization
- Optimization in Practice

Relevant Books for this Course

- Convex Optimization: Algorithms and Complexity, by Sébastien Bubeck
- Convex Optimization, Stephen Boyd and Lieven Vandenberghe
- Introductory Lectures on Convex Optimization, Yurii Nesterov
- A Course in Combinatorial Optimization, Alexander Schrijver
- Learning with Submodular Functions: A Convex Optimization Perspective, Francis Bach
- Zhang, Lipton, Li and Smola, Dive into Deep Learning (`http://d2l.ai/`)
- Schrijver, Alexander, Combinatorial optimization: polyhedra and efficiency, Vol. 24. Springer Science & Business Media, 2003.
- Fujishige, Satoru. Submodular functions and optimization. Vol. 58. Elsevier, 2005.

Evaluation

- Assignments (50%):
  - Mix of theory and practice.
  - Simple Theory questions, e.g. proving certain loss functions are convex/non-convex, computing gradients etc.
  - Practical implementation in python
  - One assignment every two to three weeks. Around 10 assignments in total.

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- Project: (50%):
  - Examples: Picking a certain real world problem, modeling the problem and optimizing the loss function with different algorithms and drawing insights on its performance.
  - Alternatively,also be a survey on a particular class of optimization algorithms and theoretical results
  - Could also be creating a toolkit (python/c++) of the various optimization/learning algorithms.
  - More on Project Later...

Attendance Policy

- Attendance is compulsory. Since this is a new course, there is not really an official textbook and the classes will be the best source of information!
- Absences due to legitimate reasons/medical etc. are fine
- Attendance policy: Two consecutive classes missed then no penalty, three consecutive classes missed then one letter downgrade, Four consecutive classes missed then an outright Fail.

Continuous Optimization in Machine Learning

- Continuous Optimization often appears as *relaxations* of empirical risk minimization problems.
- Supervised Learning: Logistic Regression, Least Squares, Support Vector Machines, Deep Models
- Unsupervised Learning: k-Means Clustering, Principal Component Analysis
- Contextual Bandits and Reinforcement Learning: Soft-Max Estimators, Policy Exponential Models
- Recommender Systems: Matrix Completion, Non-Negative Matrix Factorization, Collaborative Filtering

Reading Material for Linear Algebra

Good Reading Material on the basics of Linear Algebra from my Colleague Prof. Ganesh Ramakrishnan:

`https://www.cse.iitb.ac.in/~cs709/notes/LinearAlgebra.pdf`

Notation: Vectors and Matrices

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- Sometimes we shall refer to L2 as the default norm: $\|w\| = \|w\|_2$.

What is a Norm

A function $f : \mathbb{R}^n \Rightarrow \mathbb{R}_+$ is a norm if:

- $f(x) \geq 0, \forall x$
- $f(x + y) \leq f(x) + f(y)$ [Triangle Inequality]
- $f(\alpha x) = \alpha f(x)$
- $f(x) = 0 \Rightarrow x = 0$

Can you make sure the L1 and L2 norms defined above satisfy all four conditions?

Matrix-Vector Product

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- Matrix vector product is defined as below:

$$\mathbf{Ax} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n \end{bmatrix}$$

Matrix-Vector Product Example

For example, if

$$A = \begin{bmatrix} 1 & -1 & 2 \\ 0 & -3 & 1 \end{bmatrix}$$

and $\mathbf{x} = (2, 1, 0)$, then

$$\begin{aligned} A\mathbf{x} &= \begin{bmatrix} 1 & -1 & 2 \\ 0 & -3 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} 2 \cdot 1 - 1 \cdot 1 + 0 \cdot 2 \\ 2 \cdot 0 - 1 \cdot 3 + 0 \cdot 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 \\ -3 \end{bmatrix}. \end{aligned}$$

DALLAS

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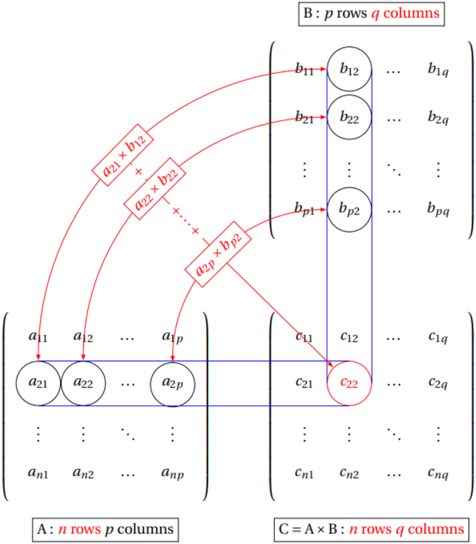
- Hence $AB = [Ab_1 \ Ab_2 \ \cdots \ Ab_p] = [c_1 \ \cdots \ c_p] = C$ is a $m \times p$ Matrix

Matrix-Matrix Product Illustration



Matrix-Matrix Product Example

Compute BC, where

$$B = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}.$$

$$\begin{aligned} BC &= \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \\ &= \begin{bmatrix} 1 \cdot 1 + 2 \cdot 3 + 3 \cdot 5 & 1 \cdot 2 + 2 \cdot 4 + 3 \cdot 6 \\ 4 \cdot 1 + 5 \cdot 3 + 6 \cdot 5 & 4 \cdot 2 + 5 \cdot 4 + 6 \cdot 6 \end{bmatrix} \\ &= \begin{bmatrix} 22 & 28 \\ 49 & 64 \end{bmatrix} \end{aligned}$$

Application 1: Supervised Learning

- Data: Given training examples $\{(x_1, y_1), \cdots, x_n, y_n\}$ where $x_i \in \mathbf{R}^m$ is the feature vectors and y_i is the label.
- Applications: Several different models depending on the applications:
  - Email Spam Filtering: Features are words, phrases, regexps in the email, Label is "+1" for Spam, "0" for Not Spam.
  - Handwritten Digit Recognition: Features are Images of Images, Label is the Digit (say between "0" to "9").
  - Housing price Prediction: Features are House properties (square footage, # Bedrooms/Bathrooms, Location, ...) and Label is the Cost (continuous variable).

Supervised Learning: Modeling

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- Model: Denote the Model by $F_\theta(x)$ with θ being the parameters of the model. Model examples: $F_\theta(x) = \theta^T x$ as a simple linear model. Deep Models are recursive functions:

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- Loss Functions: The Loss Function L tries to measure the *distance* between $F_\theta(x_i)$ and y_i.

Supervised Learning: Optimization Problem

- "Loss plus Regularizer" Framework:

$$\min_{\theta} G(\theta) = \sum_{i=1}^{n} L(F_\theta(x_i), y_i) + \lambda \Omega(\theta)$$

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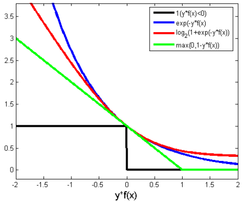
  - Hinge Loss: $\max\{0, 1 - y_i F_\theta(x_i)\}$
  - Softmax Loss: $-F_{\theta_{y_i}}(x_i) + \log(\sum_{c=1}^{k} \exp(F_{\theta_c}(x_i)))$
  - Absolute Error: $|F_\theta(x_i) - y_i|$
  - Least Squares: $(F_\theta(x_i) - y_i)^2$



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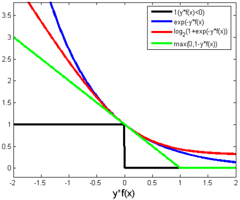

- Examples of Ω:
    - L1 Regularizer: $||\theta||_1 = \sum_{i=1}^{m} |\theta[i]|$
    - L2 Regularizer: $||\theta||_2^2 = \sum_{i=1}^{m} \theta[i]^2$

Some Concrete Supervised Learning Instances

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- This problem can actually be viewed as a joint discrete and continuous problem.

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$$\min_{U:U^T U = I} \sum_{i=1}^{n} ||x_i - UU^T x_i||_2^2$$

Application 4: Matrix Completion

- Data: Given observations $y_1, \cdots, y_n$, such that each $y_j = A_j(X)$ where A_j could be a single element or a combination of elements in $X \in \mathbb{R}^{m \times n}$. Consider for example X being product recommendation matrix.

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- Another way is to explicitly model this is by assuming $X = LR$ where $L \in \mathbb{R}^{m \times k}$ and $R \in \mathbb{R}^{k \times n}$ (and hence X is rank r), and optimize for L and R.

Application 5: Low Rank and Non Negative Matrix Factorization

- Goal: Find low rank matrices L, R with $L \in \mathbb{R}^{m \times k}$ and $R \in \mathbb{R}^{k \times n}$ s.t $A_j(LR) \approx y_j, \forall j \in 1, \cdots, n$

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No need of matrix regularization.

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- Sometimes Y is fully observed and we want a non-negative low rank factorization of $Y \approx LR$. The optimization problem is: $\min_{L,R:L \geq 0, R \geq 0} \sum_{i=1}^{n} ||Y - LR||_2^2$.

Application 6: Contextual Bandits and Learning from Logged Data

- Scenario: Learn from logged contextual bandit data. Example: We need to show k ads to users with each ad comprising of features (title, ad text, query etc.), and given an online policy which (with certain randomization) picks ads to show to users and the system logs feedback (whether the user clicks on the ad or not).

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  - Define our policy as $\pi_\theta(x) = \text{argmax}_{i=1:k} F_\theta(x^i)$. Again the simplest example of $F_\theta(x) = \theta^T x$.

Application 6: Contextual Bandits and Learning from Logged Data

- Optimization Problem: The Inverse Propensity Estimate of the Reward (which is an unbiased estimate of the Reward function is):

$$\max_{\theta} \text{IPS}(\theta) = \max_{\theta} \sum_{i=1}^{n} r_i / p_i I(\pi_\theta(x_i) == a_i)$$

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- SoftMax Relaxation: The IPS objective above is not continuous and non differentiable. We can define a softmax relaxation as:

$$\max_{\theta} \text{SM}(\theta) = \max_{\theta} \sum_{i=1}^{n} r_i / p_i \frac{\exp(F_\theta(x_i^{a_i}))}{\sum_{j=1}^{k} \exp(F_\theta(x_i^j))}$$

Discrete Optimization in Machine Learning

- MAP inference in Probabilistic Models: Ising Models, DPPs
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- Data Partitioning
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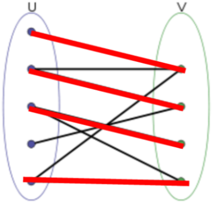
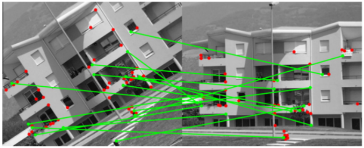
- Natural Language Processing: words, phrases, n-grams, syntax trees, semantic structures
- Computer Vision: Image Segmentation, Image Correspondence
- Genomics and Computational Biology: cell types or assay selection, selecting peptides and proteins

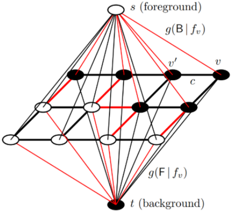
Application 1: Image Segmentation and Correspondence

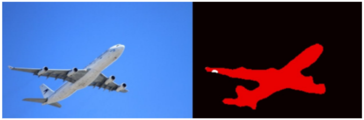
Bipartite Matchings





Minimum Cuts





Application 2: Feature Selection

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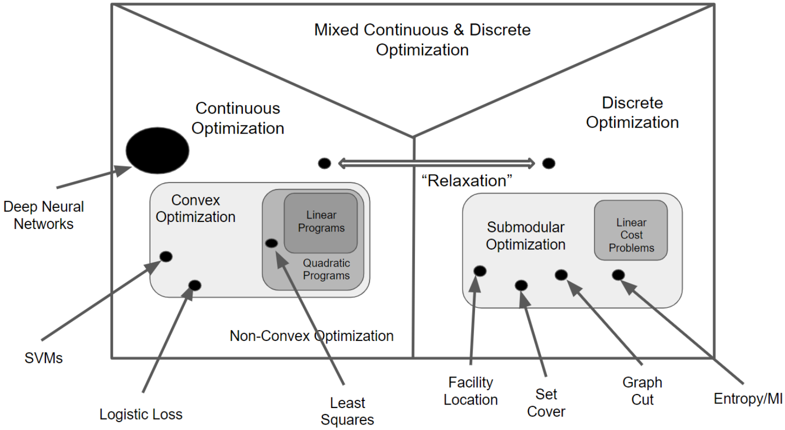
- We will see in the second part of this course that this problem is called *Facility Location* also related to the concept of *submodularity*.

Big Picture: Types of Optimization Problems



Course Project Ideas

- Let's spend a few minutes discussing some ideas for course project(s)
- Why not we all jointly create a *OptML* python toolkit which implements several (discrete and continuous) loss functions, optimization algorithms along with wrappers to machine learning models (e.g. classification, recommender systems, regression etc.)
- Why another toolkit when there are already so many out there?
- A lot of the base for this toolkit will already be covered in this course
- Each group can take on a particular component of the toolkit: with components as a) linear classification/regression, b) non-linear classification/regression, c) recommendation and matrix factorization, d) contextual bandits, e) submodular minimization, f) submodular maximization g) graph algorithms and so on...
- We can discuss ideas on this as the class progresses.