Optimization in Machine Learning

Lecture 1: Introduction and Course Overview

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Outline

- Why take this course?
- Prerequisites
- Week by Week Course plan
- Course Logistics
- Continuous Optimization in Machine Learning
- Discrete Optimization in Machine Learning

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, ...

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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 ackbones of machine learning.

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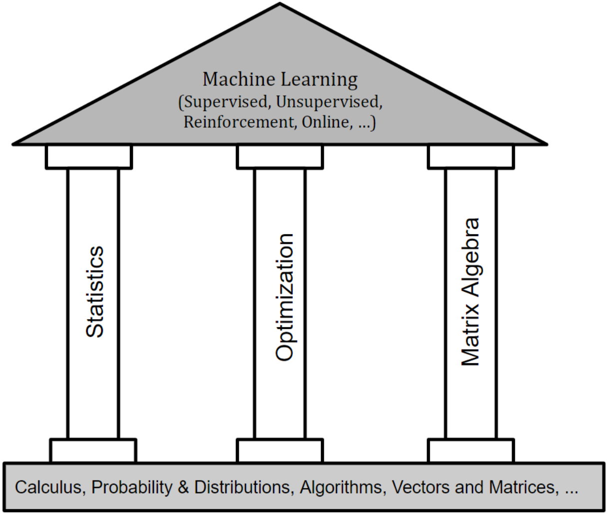

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Optimization one of the pillers of ML!

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  - 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 sceario.

Philosophy of this Course

- The spirit of this course is best summarized by the quote of Thomas Cover: *Theory is only the first term of the Taylor's series of Practice*
- This course will focus on mainly the algorithmic aspects of optimization (both continuous and discrete optimization) and not so much on the modeling.
- Give a flavor of the proofs and proof techniques but will try to not make this course heavily theoretical.
- Focus extensively on implementational 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...

Prerequisites

- Basic Linear Algebra: Matrices, Vectors
- Basics of Machine Learning (Ideally you should have taken either an undergraduate or graduate ML course)
- Algorithms course (either in undergraduate or graduate version)

First Half of this Course: Continuous optimization

- Basics of Continuous Optimization
- Convexity
- Gradient Descent
- Projected/Proximal GD
- Subgradient Descent
- Accelerated Gradient Descent
- Newton & Quasi Newton
- Duality: Lagrange, 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

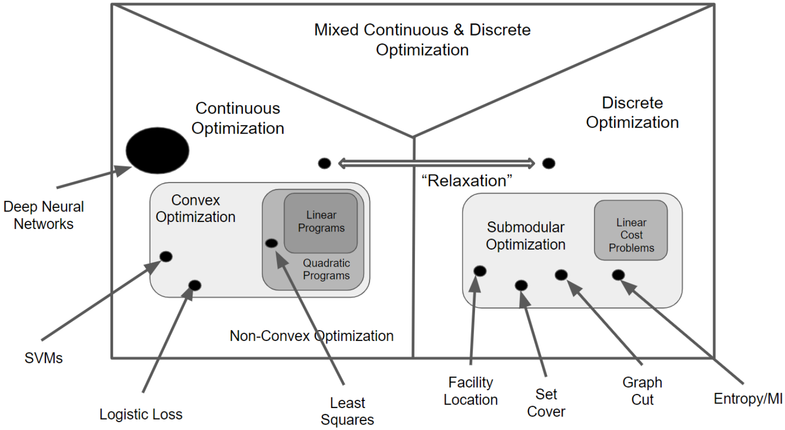
Relevant Books for this Course

- 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.

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

Big Picture: Types of Optimization Problems



Logistics, Grading etc: https://www.cse.iitb.ac.in/~ganesh/cs769/

- Credit/Audit Requirements Anyone who does an exceptional course project that has the potential to be a publishable paper is eligible for a straight AA grade. Otherwise the grading breakup would be:
  - 20% Mid-semester exam
  - 30% End semester exam
  - 20% Project: A basic project will take any of the algorithms we study or any related papers, implement the algorithms in the paper, do a basic performance study and diagnose the performance. However, I would expect most projects to suggest ideas for improvement (atleast in specific settings such as multi core or multiple nodes or reasonable assumptions on matrices etc in the problem for which greater speedup is possible). A more advanced project would take a problem specification for which no solution is publicly available, figure out how to solve it, and implement the solution.
  - 10% Reading and paper presentation.
  - 20% 2 Programming Assignments
- Lectures: In Slot 2, Lectures on MS Teams (Code: 6yxnonu) and will be recorded. All lecture recordings and slides will be organized on moodle.

Course Project Ideas

- Let's spend a few minutes discussing some ideas for course project(s)
- Why not we all jointly contribute to our **DECILE** `https://decile.org/` python toolkit and add to it a component **OptML** 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.

Adding **OptML** to DECILE

The **DECILE** (`https://decile.org/`) python toolkit is being built toward principled human-machine interaction for machine learning, has 4 important components and we can have **OptML** as the fifth!

1. Submodlib (in C++ with Python wrappers) `https://github.com/vishkaush/submodlib/`: Submodlib is an efficient and scalable library for submodular optimization which finds its application in summarization, data subset selection, hyper parameter tuning etc.
2. DISTIL (`https://github.com/decile-team/distil`): This is a library in python for Deep dIverSified inTeractIve Learning
3. CORDS (`https://github.com/decile-team/cords`): This is a library in python for COResets and Data Subset selection
4. DOMAIN (`https://github.com/oishik75/CAGE`): This is a library (work-in-progress) in python for Data prOgraMming viA rule induction through human INteraction
5. **OptML** can implement several continuous loss functions optimization algorithms along with wrappers to machine learning models (*e.g.*, classification, recommender systems, regression *etc.*).

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).

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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:

$$F_{\theta_1,\theta_2,\cdots,\theta_l}(x) = f_1(\theta_1^T f_2(\cdots \theta_{l-1}^T f_l(\theta_l^T x)))$$

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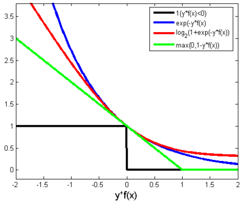
- Examples of L:
  - Logistic Loss: $\log(1 + \exp(-y_i F_\theta(x_i)))$
  - Hinge Loss: $\max\{0, 1 - y_i F_\theta(x_i)\}$
  - Softmax Loss: $-F_{\theta_{y_i}}(x_i) + \log(\sum_{c=1}^{k} \exp(F_{\theta_c}(x_i)))$
  - Absolute Error: $|F_\theta(x_i) - y_i|$
  - Least Squares: $(F_\theta(x_i) - y_i)^2$



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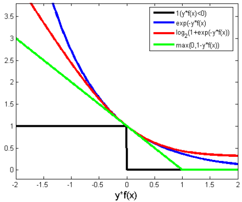

- Examples of Ω:
  - L1 Regularizer: $\sum_{i=1}^{m} |\theta[i]|$
  - L2 Regularizer: $\sum_{i=1}^{m} \theta[i]^2$

Some Concrete Supervised Learning Instances

- L1 Regularized Logistic Regression:
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- Optimization Problem: The k-means optimization problem is:

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

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- Optimization Problem: The PCA optimization problem is:

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

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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- 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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  - Denote r_i as the Reward obtained by choosing action a_i
  - Define our policy as $\pi_\theta(x) = \text{argmax}_{i=1:k} F_\theta(x^i)$. Again the simplest example of $F_\theta(x) = \theta^T x$.

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

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

Discrete Optimization in Machine Learning

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- Feature Subset Selection
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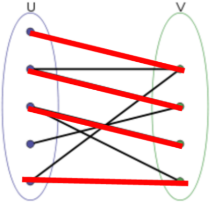
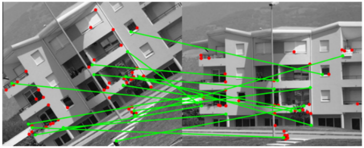
- Computer Vision: Image Segmentation, Image Correspondence
- Genomics and Computational Biology: cell types or assay selection, selecting peptides and proteins

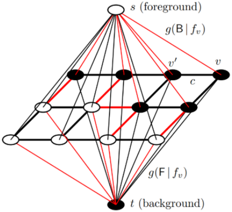
Application 1: Image Segmentation and Correspondence

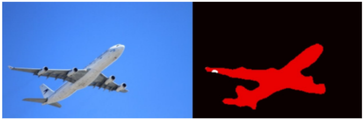
Bipartite Matchings





Minimum Cuts





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Big Picture: Types of Optimization Problems