CS6301: Optimization in Machine Learning

Lecture 2: Basics of Continuous Optimization

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https://sites.google.com/view/cs-6301-optml/home

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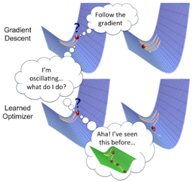
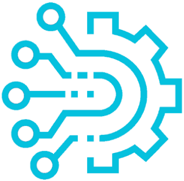
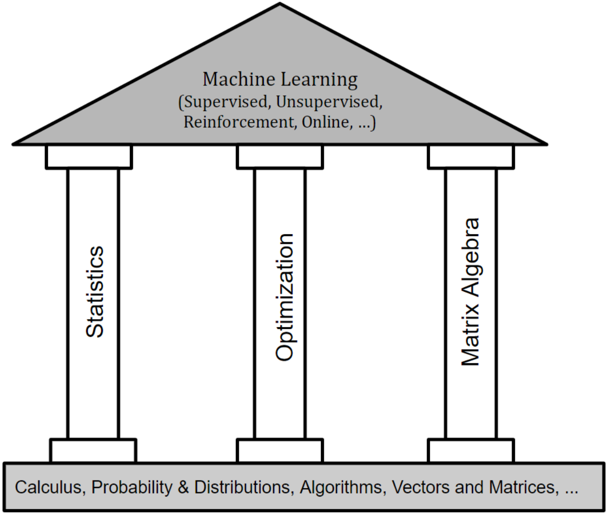




Outline

- Recap from Previous Lecture
- Brief Project Discussion
- Notation and Basics of Continuous optimization: Vectors, Matrices, Gradients, Hessians, ...
- Deriving Gradients and Hessian for various Loss Functions
- Practical Aspects: Implementing Loss Functions and Gradients in Python.

Why take this Course?



Why take this Course?

- Optimization everywhere in Machine Learning.
- Countless number of ML libraries available which implement all kinds of optimization algorithms (Tensorflow, pytorch, scipy, sklearn, Vowpal Wabbit, ...)
- This course will give you the expertise to look inside these algorithms, understand how they work, why they work and how fast they work.
- Invariably in Research, you will come up with new optimization problems which you might need to implement custom algorithms or atleast the loss functions.
- Over 70% of the projects I worked at Microsoft involved new optimization problems (and sometimes new algorithms)
- Even if you don't implement new algorithms, you will have a better idea of which algorithm to use in which sceario.

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: 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

Evaluation

- Assignments (50%):
  - Assignments will comprise of a mix of practical and theoretical.
  - Simple Theory questions, e.g. proving certain loss functions are convex/non-convex, computing gradients etc.
  - Practical $\Rightarrow$ implementing optimization algorithms and loss functions in python.
  - One assignment every week (or maybe every 2 weeks)

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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.

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- 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...

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- We can discuss ideas on this as the class progresses.

Continuous Optimization in Machine Learning

- 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

Supervised Learning: Optimization Problem

- "Loss plus Regularizer" Framework:

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

- L: *Loss function*, Ω: *Regularizer*. Example $F_\theta(x) = \theta^T x$

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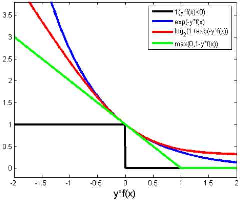
- Examples of L:
  - Logistic Loss: $\log(1 + \exp(-y_i F_\theta(x_i)))$
  - Hinge Loss: $\max\{0, 1 - y_i F_\theta(x_i)\}$
  - Softmax Loss: $-F_{\theta_{y_i}}(x_i) + \log(\sum_{c=1}^{k} \exp(F_{\theta_c}(x_i)))$
  - Absolute Error: $|F_\theta(x_i) - y_i|$
  - Least Squares: $(F_\theta(x_i) - y_i)^2$



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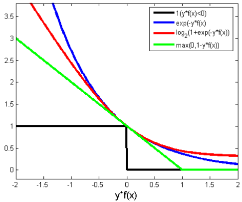

- Examples of Ω:
  - L1 Regularizer: $||\theta||_1 = \sum_{i=1}^{m} |\theta[i]|$
  - L2 Regularizer: $||\theta||_2^2 = \sum_{i=1}^{m} \theta[i]^2$

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- If $y = \frac{f(x)}{g(x)}$, can you compute $\frac{dy}{dx}$?

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- Derivatives for most loss functions can be obtained with the basic derivatives above and with the right choices of product/division/addition and chain rules (basic principal of autograd).

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- Compute the gradient with $L(w_1, w_2) = w_1^2/w_2$:

$$\nabla L(w_1, w_2) = [2w_1/w_2 \quad -w_1^2/w_2^2]$$

Hessian

- We can similarly compute the Hessian of a Function:

$$\nabla^2 f(w) = \begin{pmatrix} \frac{\partial^2 f}{\partial w_1^2} & \frac{\partial^2 f}{\partial w_1 \partial w_2} & \cdots & \frac{\partial^2 f}{\partial w_1 \partial w_n} \\ \frac{\partial^2 f}{\partial w_2 \partial w_1} & \frac{\partial^2 f}{\partial w_2^2} & \cdots & \frac{\partial^2 f}{\partial w_2 \partial w_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial w_n \partial w_1} & \frac{\partial^2 f}{\partial w_n \partial w_2} & \cdots & \frac{\partial^2 f}{\partial w_n^2} \end{pmatrix}$$

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- Notice that the Hessian is:

$$\nabla^2 f(w) = \begin{bmatrix} \nabla \frac{\partial f}{\partial w_1} & \nabla \frac{\partial f}{\partial w_2} & \cdots & \nabla \frac{\partial f}{\partial w_n} \end{bmatrix}$$

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$$\nabla^2 L(w) = \begin{bmatrix} \frac{2}{w_2} & -\frac{2w_1}{w_2^2} \\ -\frac{2w_1}{w_2^2} & \frac{2w_1^2}{w_2^3} \end{bmatrix}$$

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$$\begin{aligned}\nabla L(w) =& \lambda w + \sum_{i=1}^{n} \frac{-y_i \exp(-y_i(w^T x_i))}{1 + \exp(-y_i w^T x_i)} x_i \\ =& \lambda w + \sum_{i=1}^{n} \frac{-y_i}{1 + \exp(y_i w^T x_i)} x_i\end{aligned}$$

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- Define $\sigma(z) = 1/(1 + \exp(-z))$. Then its easy to see that:

$$\nabla^2 L(w) = \sigma(y_i w^T x_i)(1 - \sigma(y_i w^T x_i)) x_i x_i^T + \lambda I$$

Numerical Issues

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import numpy as np
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- Is there any problem with this? Can there be numerical issues?
- Consider the following simpler code:

```
import numpy as np
x = -1000
L = np.log(1 + np.exp(-x))
print(L)
```