COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2022.

Lecture 23

Logistics

LGRC A215

- Problem Set 4 is due on Monday at 11:59pm.
- Given the problem set and the exam, there won't be any more quizzes.
- Problem Set 5 is extra credit and will be released over the weekend or on Monday.

4 Pset worth 10%

5th pset worth 5% +

Summary

Last Class Before Break: Fast computation of the SVD/eigendecomposition.

- Power method for approximating the top eigenvector of a matrix.
- Analysis of convergence rate.

Final Three Classes:

- General iterative algorithms for optimization, specifically gradient descent and its variants.
- What are these methods, when are they applied, and how do you analyze their performance?
- Small taste of what you can find in COMPSCI 590OP or 690OP.

Discrete vs. Continuous Optimization

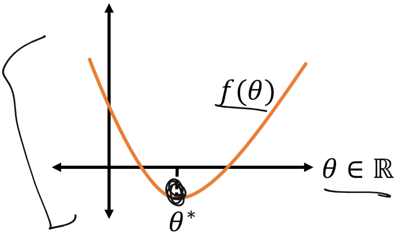
Discrete (Combinatorial) Optimization: (traditional CS algorithms)

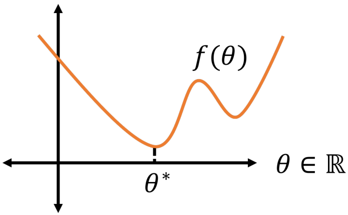
- Graph Problems: min-cut, max flow, shortest path, matchings, maximum independent set, traveling salesman problem
- Problems with discrete constraints or outputs: bin-packing, scheduling, sequence alignment, submodular maximization
- Generally searching over a finite but exponentially large set of possible solutions. Many of these problems are NP-Hard.

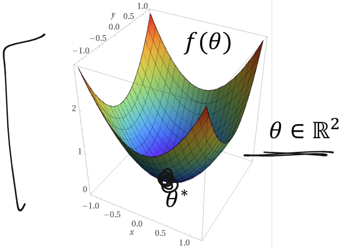
Continuous Optimization: (maybe seen in ML/advanced algorithms)

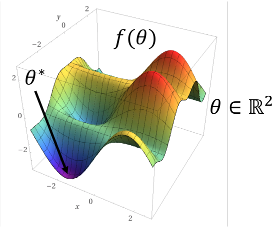
- Unconstrained convex and non-convex optimization.
- Linear programming, quadratic programming, semidefinite programming

Continuous Optimization Examples









θ

Given some function $f : \mathbb{R}^d \to \mathbb{R}$, find $\vec{\theta}_\star$ with:

$$f(\vec{\theta}_\star) = \min_{\vec{\theta} \in R^d} f(\vec{\theta})$$

Mathematical Setup

Given some function $f : \mathbb{R}^d \to \mathbb{R}$, find $\vec{\theta}_\star$ with:

$$f(\vec{\theta}_\star) = \min_{\vec{\theta} \in R^d} f(\vec{\theta}) + \epsilon$$

Typically up to some small approximation factor.

Mathematical Setup

Given some function $f : \mathbb{R}^d \to \mathbb{R}$, find $\vec{\theta}_\star$ with:

$$f(\vec{\theta}_\star) = \min_{\vec{\theta} \in R^d} f(\vec{\theta}) + \epsilon$$

Typically up to some small approximation factor.

Often under some constraints:

- $\|\vec{\theta}\|_2 \leq 1, \quad \|\vec{\theta}\|_1 \leq 1.$
- $\boxed{A\vec{\theta} \leq \vec{b},} \quad \vec{\theta}^T A\vec{\theta} \geq 0.$
- $\sum_{i=1}^{d} \vec{\theta}(i) \leq c.$

entrywise

$A\theta = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \qquad b = \begin{bmatrix} 1.5 \\ 3 \\ 6 \end{bmatrix}$

Why Continuous Optimization?

Modern machine learning centers around continuous optimization.

Typical Set Up: (supervised machine learning)

- Have a model, which is a function mapping inputs to predictions (neural network, linear function, low-degree polynomial etc).
- The model is parameterized by a parameter vector (weights in a neural network, coefficients in a linear function or polynomial)
- Want to train this model on input data, by picking a parameter vector such that the model does a good job mapping inputs to predictions on your training data.

This training step is typically formulated as a continuous optimization problem.

Optimization in ML

Example: Linear Regression

Optimization in ML

Example: Linear Regression house prices

Model: $M_{\vec{\theta}} : \mathbb{R}^d \to \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \stackrel{\text{def}}{=} \langle \vec{\theta}, \vec{x} \rangle$.

predicted price

Optimization in ML

Example: Linear Regression

#bathrooms

sq ft.

Model: $M_{\vec{\theta}} : \mathbb{R}^d \to \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \stackrel{\text{def}}{=} \langle \vec{\theta}, \vec{x} \rangle = \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d)$.

Optimization in ML

Example: Linear Regression

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Parameter Vector: $\vec{\theta} \in \mathbb{R}^d$ (the regression coefficients)

Optimization in ML

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Optimization Problem: Given data points (training points) $\vec{x}_1, \ldots, \vec{x}_n$ (the rows of data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$) and labels $y_1, \ldots, y_n \in \mathbb{R}$, find $\vec{\theta}_*$ minimizing the loss function:

$$L(\vec{\theta}, \mathbf{X}, \vec{y}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

where ℓ is some measurement of how far $M_{\vec{\theta}}(\vec{x}_i)$ is from y_i.

Optimization in ML

Example: Linear Regression

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- $\ell(M_{\vec{\theta}}(\vec{x}_i), y_i) = \left(M_{\vec{\theta}}(\vec{x}_i) - y_i\right)^2$ (least squares regression)
- $y_i \in \{-1, 1\}$ and $\ell(M_{\vec{\theta}}(\vec{x}_i), y_i) = \ln\left(1 + \exp(-y_i M_{\vec{\theta}}(\vec{x}_i))\right)$ (logistic regression)

Optimization in ML

Example: Linear Regression

Model: $M_{\vec{\theta}} : \mathbb{R}^d \to \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \stackrel{\text{def}}{=} \langle \vec{\theta}, \vec{x} \rangle = \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d)$.

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$$\underline{L_{\mathbf{X},y}(\vec{\theta})} = L(\vec{\theta}, \mathbf{X}, \vec{y}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

where ℓ is some measurement of how far $M_{\vec{\theta}}(\vec{x}_i)$ is from y_i.

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Optimization in ML

$$\boxed{L_{\mathbf{X},\vec{y}}(\vec{\theta})} = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

- Supervised means we have labels $y_1, \ldots, y_n$ for the training points.
- Solving the final optimization problem has many different names: likelihood maximization, empirical risk minimization, minimizing training loss, etc.
- Continuous optimization is also very common in unsupervised learning. (PCA, spectral clustering, etc.)
- Generalization tries to explain why minimizing the loss $L_{\mathbf{X},\vec{y}}(\vec{\theta})$ on the *training points* minimizes the loss on future *test points*. I.e., makes us have good predictions on future inputs.

Optimization Algorithms

Choice of optimization algorithm for minimizing $f(\vec{\theta})$ will depend on many things: $L_{x,y}(\vec{\theta})$

- The form of f (in ML, depends on the model & loss function).
- Any constraints on $\vec{\theta}$ (e.g., $\|\vec{\theta}\| < c$).
- Computational constraints, such as memory constraints.

$$L_{\mathbf{X},\vec{y}}(\vec{\theta}) = \sum_{i=1}^{n \sim \text{millions}} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

Optimization Algorithms

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What are some popular optimization algorithms?

"second order"

Stochastic gradient descent

online gradient descent

BFGS, L-BFGS

newton's methods

adaptive gradient descent (Adam, adagrad)

Gradient Descent

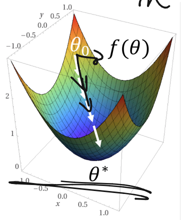
Next few classes: Gradient descent (and some important variants)

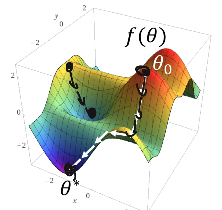
- An extremely simple greedy iterative method, that can be applied to almost any continuous function we care about optimizing.
- Often not the 'best' choice for any given function, but it is the approach of choice in ML since it is simple, general, and often works very well.
- At each step, tries to move towards the lowest nearby point in the function that is can – in the opposite direction of the gradient.

$\eta \cdot \nabla(\theta^{i-1})$

$\mathbb{R}^2 \to \mathbb{R}$

$\theta \begin{bmatrix} \theta(1) \\ \theta(2) \end{bmatrix}$





Multivariate Calculus Review

Let $\vec{e}_i \in \mathbb{R}^d$ denote the i^{th} standard basis vector,
$\vec{e}_i = \underbrace{[0, 0, 1, 0, 0, \ldots, 0]}_{\text{1 at position } i}$.

$f: \mathbb{R}^2 \to \mathbb{R}$

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[θ(1), θ(2), ..θ(i)+ε, θ(i+1)...]

Partial Derivative:

$$\frac{\partial f}{\partial \vec{\theta}(i)} = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \cdot \vec{e}_i) - f(\vec{\theta})}{\epsilon}.$$

$f(x)$

$$\frac{\partial f}{\partial x} = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$$

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$$\frac{\partial f}{\partial \vec{\theta}(i)} = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \cdot \vec{e}_i) - f(\vec{\theta})}{\epsilon}.$$

Directional Derivative: $\|V\|_2 = 1$

$$D_{\vec{v}} f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \vec{v}) - f(\vec{\theta})}{\epsilon}.$$

direction of step

Multivariate Calculus Review

$$f : \mathbb{R}^d \to \mathbb{R} \qquad \nabla f(\vec{\theta}) \in \mathbb{R}^d$$

Gradient: Just a 'list' of the partial derivatives.

$$\vec{\nabla} f(\vec{\theta}) = \begin{bmatrix} \frac{\partial f}{\partial \vec{\theta}(1)} \\ \frac{\partial f}{\partial \vec{\theta}(2)} \\ \vdots \\ \frac{\partial f}{\partial \vec{\theta}(d)} \end{bmatrix}$$

Multivariate Calculus Review

coordinate descent

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Directional Derivative in Terms of the Gradient:

$$\overset{\mathbb{R}}{D_{\vec{v}} f(\vec{\theta})} = \langle \overset{\mathbb{R}^d}{\vec{v}}, \overset{\mathbb{R}^d}{\vec{\nabla} f(\vec{\theta})} \rangle.$$

$$V = \begin{bmatrix} \vdots \end{bmatrix}$$

$$V(1) \cdot \frac{\partial f}{\partial \theta(1)} + V(2) \cdot \frac{\partial f}{\partial \theta(2)} + \ldots$$

Function Access

$x^2 + 3x + 1$

Often the functions we are trying to optimize are very complex (e.g., a neural network). We will assume access to:

Function Evaluation: Can compute $f(\vec{\theta})$ for any $\vec{\theta}$.

Gradient Evaluation: Can compute $\vec{\nabla} f(\vec{\theta})$ for any $\vec{\theta}$.

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In neural networks:

- Function evaluation is called a forward pass (propogate an input through the network).
- Gradient evaluation is called a backward pass (compute the gradient via chain rule, using backpropagation).

Gradient Descent Greedy Approach

Gradient descent is a greedy iterative optimization algorithm: Starting at $\vec{\theta}^{(0)}$, in each iteration let $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} + \eta\vec{v}$, where η is a (small) 'step size' and $\vec{v}$ is a direction chosen to minimize $f(\vec{\theta}^{(i-1)} + \eta\vec{v})$.

$F(\theta^{(i+1)})$

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So for small η:

$$\underbrace{f(\vec{\theta}^{(i)}) - f(\vec{\theta}^{(i-1)})}_{\text{minimize}} = f(\vec{\theta}^{(i-1)} + \eta\vec{v}) - f(\vec{\theta}^{(i-1)})$$

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$\|v\|_2 = 1$

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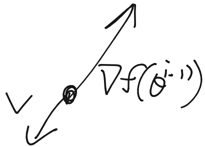
$$\underbrace{f(\vec{\theta}^{(i)}) - f(\vec{\theta}^{(i-1)})}_{\text{minimize}} = f(\vec{\theta}^{(i-1)} + \eta\vec{v}) - f(\vec{\theta}^{(i-1)}) \approx \eta \cdot D_{\vec{v}} f(\vec{\theta}^{(i-1)})$$

$\eta \cdot \langle \vec{v}, \nabla f(\theta^{i-1}) \rangle$



$\boxed{v = -\nabla f(\theta^{i-1})}$

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$= -\nabla f(\theta^{i-1})$

We want to choose $\vec{v}$ minimizing $\langle \vec{v}, \vec{\nabla} f(\vec{\theta}^{(i-1)}) \rangle$ – i.e., pointing in the direction of $\vec{\nabla} f(\vec{\theta}^{(i-1)})$ but with the opposite sign.

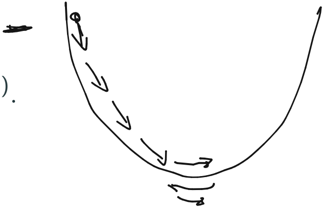
Gradient Descent

- Choose some initialization $\vec{\theta}^{(0)}$.
- For $i = 1, \ldots, t$
  - $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
- Return $\vec{\theta}^{(t)}$, as an approximate minimizer of $f(\vec{\theta})$.

Step size η is chosen ahead of time or adapted during the algorithm (details to come.)

Gradient Descent Psuedocode

Gradient Descent



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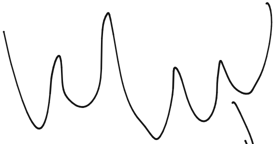
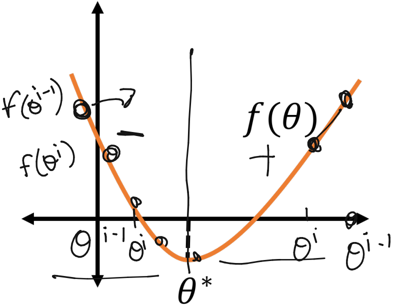
Step size η is chosen ahead of time or adapted during the algorithm (details to come.)

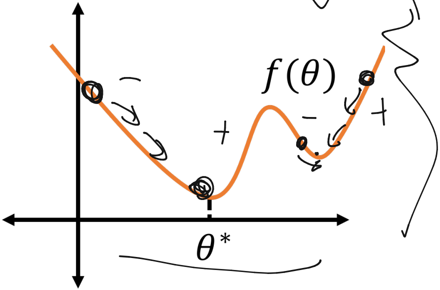
- For now assume η stays the same in each iteration.

When Does Gradient Descent Work?

$\theta \in \mathbb{R} \quad \nabla f(\theta) \in \mathbb{R}$







Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$