COMPSCI 514: Algorithms for Data Science

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Lecture 23

Logistics

- 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.

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

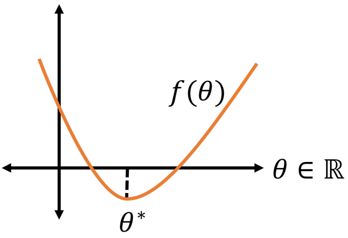
Discrete (Combinatorial) Optimization: (traditional CS algorithms)

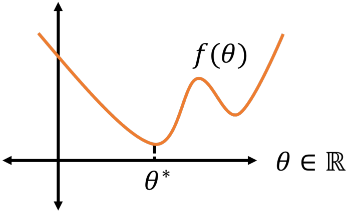
- Graph Problems: min-cut, max flow, shortest path, matchings, maximum independent set, traveling salesman problem
- Problems with discrete constraints or outputs: bin-packing, scheduling, sequence alignment, submodular maximization
- Generally searching over a finite but exponentially large set of possible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

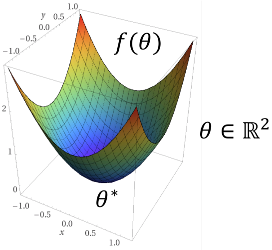
Continuous Optimization: (maybe seen in ML/advanced algorithms)

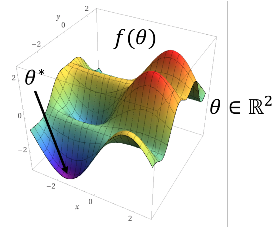
- Unconstrained convex and non-convex optimization.
- Linear programming, quadratic programming, semidefinite programming

Continuous Optimization Examples









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:

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

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

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

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

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:

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

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

- $\ell(M_{\vec{\theta}}(\vec{x}_i), y_i) = \left(M_{\vec{\theta}}(\vec{x}_i) - y_i\right)^2$ (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

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

- 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:

- 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.

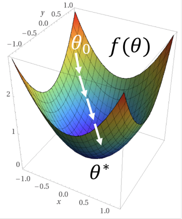
$$L_{\mathbf{X},\vec{y}}(\vec{\theta}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

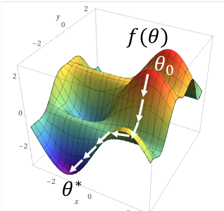
What are some popular optimization algorithms?

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.





Multivariate Calculus Review

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

Partial Derivative:

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

Directional Derivative:

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

Multivariate Calculus Review

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

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

Directional Derivative in Terms of the Gradient:

$$D_{\vec{v}}\, f(\vec{\theta}) = \langle \vec{v}, \vec{\nabla} f(\vec{\theta}) \rangle.$$

Function Access

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 $\vec{\theta}$.

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 $f(\vec{\theta}^{(i-1)} + \eta\vec{v})$.

$$D_{\vec{v}}\, f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon\vec{v}) - f(\vec{\theta})}{\epsilon}. D_{\vec{v}}\, f(\vec{\theta}^{(i-1)}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta}^{(i-1)} + \epsilon\vec{v}) - f(\vec{\theta}^{(i-1)})}{\epsilon}.$$

So for small η:

$$\begin{aligned} f(\vec{\theta}^{(i)}) - f(\vec{\theta}^{(i-1)}) = f(\vec{\theta}^{(i-1)} + \eta\vec{v}) - f(\vec{\theta}^{(i-1)}) &\approx \eta \cdot D_{\vec{v}} f(\vec{\theta}^{(i-1)}) \\ &= \eta \cdot \langle \vec{v}, \vec{\nabla} f(\vec{\theta}^{(i-1)}) \rangle. \end{aligned}$$

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 Psuedocode

Gradient Descent

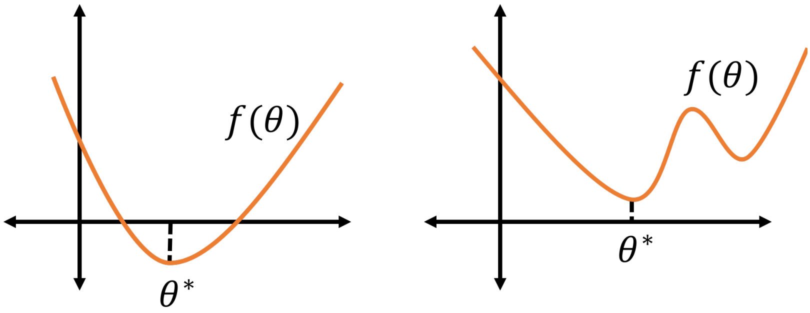
- Choose some initialization $\vec{\theta}^{(0)}$.
- For $i = 1, \ldots, t$
  - $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
- Return $\vec{\theta}^{(t)}$, as an approximate minimizer of $f(\vec{\theta})$.

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

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

When Does Gradient Descent Work?

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

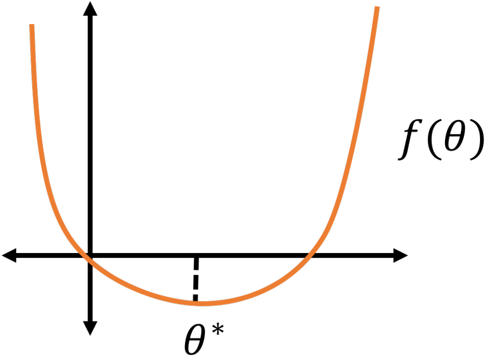


Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

Convexity

Definition – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

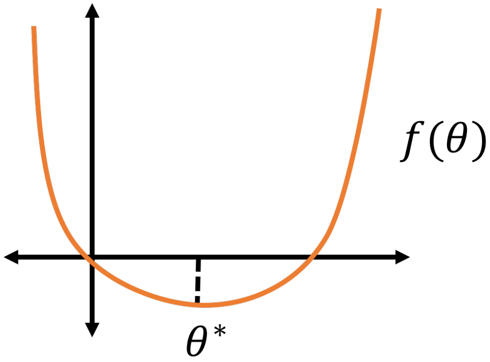
$$(1-\lambda) \cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda) \cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$



Convexity

Corollary – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$f(\vec{\theta}_2) - f(\vec{\theta}_1) \geq \vec{\nabla} f(\vec{\theta}_1)^T \left(\vec{\theta}_2 - \vec{\theta}_1\right)$$



Conditions for Gradient Descent Convergence

Convex Functions: After sufficient iterations, if the step size η is chosen appropriately, gradient descent will converge to a approximate minimizer $\hat{\theta}$ with:

$$f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon = \min_{\vec{\theta}} f(\vec{\theta}) + \epsilon.$$

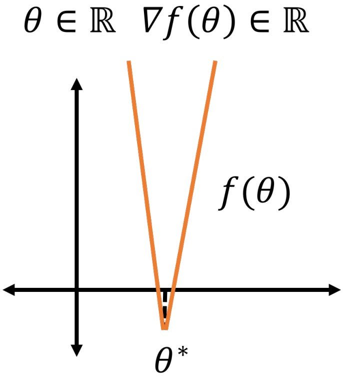
Examples: least squares regression, logistic regression, sparse regression (lasso), regularized regression, SVMS,...

Non-Convex Functions: After sufficient iterations, gradient descent will converge to a approximate stationary point $\hat{\theta}$ with:

$$\|\nabla f(\hat{\theta})\|_2 \leq \epsilon.$$

Examples: neural networks, clustering, mixture models.

Lipschitz Functions



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

Need to assume that the function is Lipschitz (size of gradient is bounded): There is some G s.t.:

$$\forall \vec{\theta}: \quad \|\vec{\nabla} f(\vec{\theta})\|_2 \leq G \Leftrightarrow \forall \vec{\theta}_1, \vec{\theta}_2: \quad |f(\vec{\theta}_1) - f(\vec{\theta}_2)| \leq G \cdot \|\vec{\theta}_1 - \vec{\theta}_2\|_2$$

Definition – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$(1-\lambda) \cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda) \cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$

Corollary – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$f(\vec{\theta}_2) - f(\vec{\theta}_1) \geq \vec{\nabla} f(\vec{\theta}_1)^T \left(\vec{\theta}_2 - \vec{\theta}_1\right)$$

Definition – Lipschitz Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is G-Lipschitz if $\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$.