COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2023.

Lecture 22

Logistics

- Problem Set 4 core problems are due Friday. Challenge problems are due Monday.
- Quiz due Monday (last of the semester).
- Problem Set 5 will be released Friday or Saturday, and is optional. The core problems can be used to replace the lowest core problem grade on a previous problem set. It will contain three challenge problems as well.
- Final exam study material has been released on the course webpage/Moodle. I will announce additional office hours for final review shortly.
- Next Monday 12/4 at 3pm in CS 140 I will hold another linear algebra review session.
- Please fill out SRTIs (course reviews)!

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 – we didn't quite finish but we covered the most important ideas.
- Convergence rate depends on the gap between the largest and second largest eigenvalue.

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)

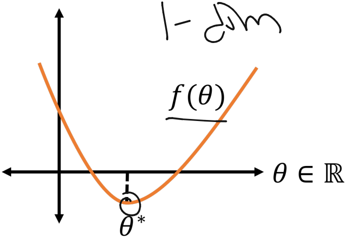
- Graph Problems: min-cut, max flow, shortest path, matchings, maximum independent set, traveling salesman problem
- Problems with discrete constraints or outputs: bin-packing, scheduling, sequence alignment, submodular maximization
- Generally searching over a finite but exponentially large set of possible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

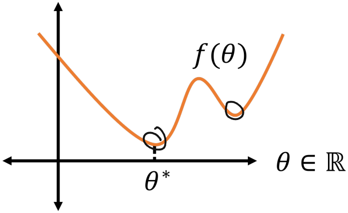
Continuous Optimization: (maybe seen in ML/advanced algorithms)

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

Continuous Optimization Examples

1-dim

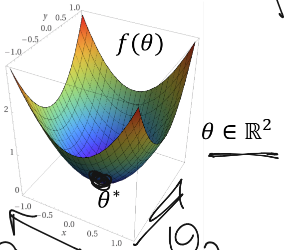




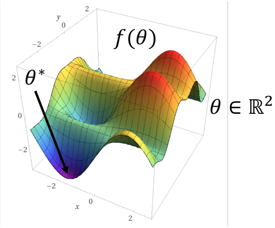
2-dim

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

$f(\theta)$



θ_1 θ_2



Mathematical Setup

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

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

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

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

Typically up to some small approximation factor.

Mathematical Setup

$$\lambda_1 = \max_{x:\|x\|_2=1} \underbrace{x^T A x}_{f(x)}$$

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

$$f(\vec{\theta}_\star) = \min_{\substack{\vec{\theta} \in R^d \\ \|\theta\|_2 \leq 1}} f(\vec{\theta}) + \epsilon$$

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

Optimization in ML

Example: Linear Regression

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

$$\begin{bmatrix} 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Optimization in ML

Example: Linear Regression

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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:

loss $\quad (m_\theta(x_i) - y_i)^2$

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

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

Optimization in ML

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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)

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

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

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

- 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.

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

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$f(x) = x^2$

$\frac{df}{dx} = 2x = 0$ when $x = 0$

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

$x = 0$

What are some popular optimization algorithms?

grid search

randomize search

gradient descent

ADAM

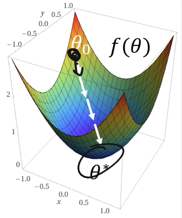
ADAGRAD

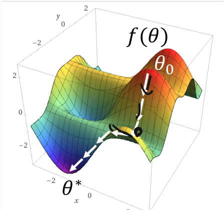
LBFGS

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,
$\vec{e}_i = \underbrace{[0, 0, 1, 0, 0, \ldots, 0]}_{\text{1 at position } i}$.

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

Partial Derivative:

$\frac{\partial f}{\partial \theta(i)}$

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

$$\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \to \begin{bmatrix} 2+\varepsilon \\ 1 \\ 3 \end{bmatrix}$$

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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:

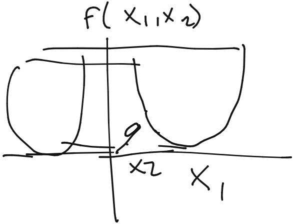
$$D_{\vec{v}} f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \vec{v}) - f(\vec{\theta})}{\epsilon}.$$

V

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} + \varepsilon \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

$$f : \mathbb{R}^d \to \mathbb{R} \qquad \nabla f \in \mathbb{R}^d$$

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



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

$$\nabla f = \begin{bmatrix} 0 \\ x_2 \end{bmatrix}$$

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Directional Derivative in Terms of the Gradient:

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

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

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 $\vec{\theta}$.

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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 $\vec{\theta}^{(0)}$ $=0$, 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 $f(\vec{\theta}^{(i-1)} + \eta\vec{v})$.

$$\theta^{i-1} \xrightarrow{\eta \vec{v}} \theta^{i}$$

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So for small η:

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

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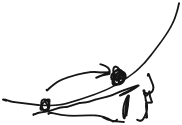

So for small η:

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

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θ^0

θ^1

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θ^*

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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.

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

v

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

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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?

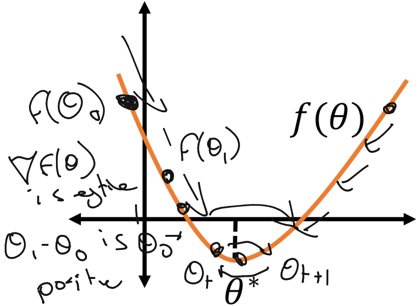
$\frac{\theta_0 - \theta_*}{\nabla f \theta_0} = \eta^*$

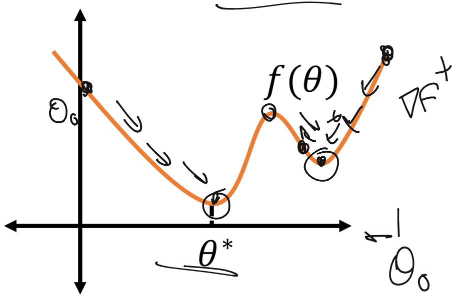
convex

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

$\frac{df}{d\theta} = f'(\theta)$

non-convex





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

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

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 $\lambda \in [0, 1]$:

.5 .5

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

$f''(\theta) \geq 0$ for all θ

$f(x) = 3x$

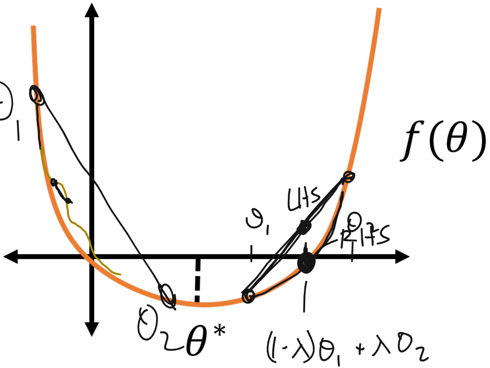
$(1-\lambda)3\theta_1 + \lambda 3\theta_2$

$\shortparallel$

$3((1-\lambda)\theta_1 + \lambda\theta_2)$

$= (1-\lambda)3\theta_1 + \lambda 3\theta_2$

$\lambda = .5$



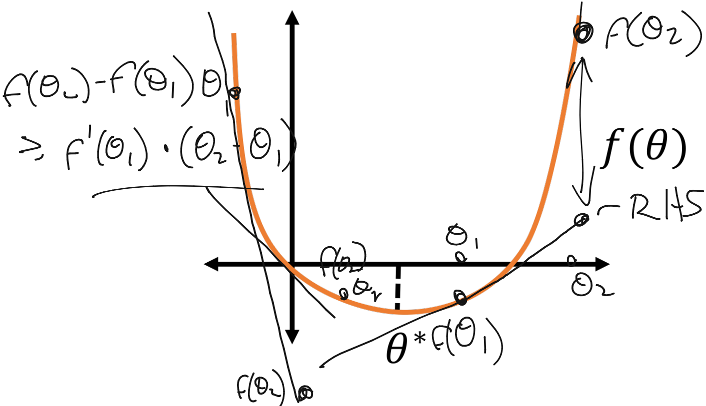
Convexity

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

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

$f(x) = x^2$

$\langle \nabla f(\theta_1), \theta_2 - \theta_1 \rangle$



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,...

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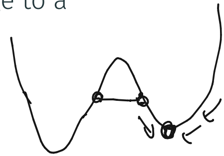
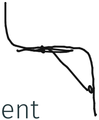


Examples: least squares regression, logistic regression, sparse regression (lasso), regularized regression, SVMS,...



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

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

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.