COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2020.

Lecture 22

LOGISTICS

were just

- Problem Set 3 grades ~~will be~~ released ~~later today~~.
- Final review sheet will be release imminently.

Last Class: Fast computation of the SVD/eigendecomposition.

$\sim v_1$

- Power method for computing the top singular vector of a matrix.
- Power method is a simple iterative algorithm for solving the *non-convex* optimization problem:

Courant Fischer

$$\max_{\vec{v}:\|\vec{v}\|_2^2=1} |\vec{v}^T \mathbf{A} \vec{v}|.$$

Final Two Weeks of Class:

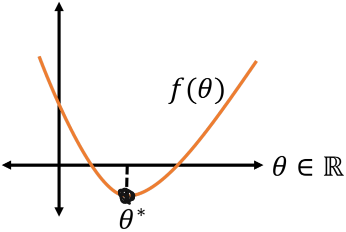
- More general iterative algorithms for optimization, specifically gradient descent and its variants.
- What are these methods, when are they applied, and how do you analyze their performance?
- Small taste of what you can find in COMPSCI 590OP or 690OP.

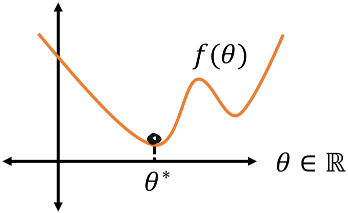
Discrete (Combinatorial) Optimization: (traditional CS algorithms)

- 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

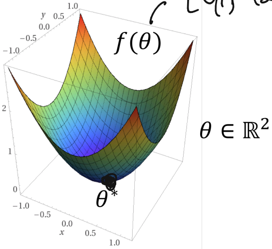


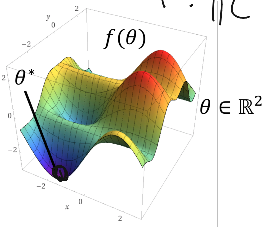


$f: \mathbb{R}^2 \to \mathbb{R}$

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

$[\theta_1, \theta_2]$





$\in \mathbb{R}^d$

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

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

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Typically up to some small approximation factor.

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Typically up to some small approximation factor.

Often under some constraints:

linear programing

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

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) $\theta \in \mathbb{R}^d$
- 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.

Example 1: Linear Regression

house prices from characteristics of house.

Example 1: Linear Regression

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

Example 1: Linear Regression

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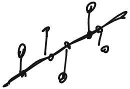
Optimization Problem: Given data points (training points) $\vec{x}_1, \ldots, \vec{x}_n$ (the rows of data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$) and labels $y_1, \ldots, y_n \in \mathbb{R}$, find $\vec{\theta}_*$ minimizing the loss function:

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

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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prediction label

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

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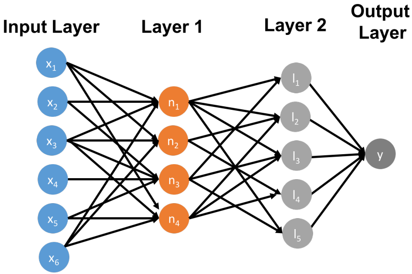
Example 2: Neural Networks



Model: $M_{\vec{\theta}} : \mathbb{R}^d \to \mathbb{R}$. $M_{\vec{\theta}}(\vec{x}) = \langle \vec{w}_{out}, \sigma(\mathbf{W}_2\sigma(\mathbf{W}_1\vec{x}))\rangle$.

Parameter Vector: $\vec{\theta} \in \mathbb{R}^{(\#\ edges)}$ (the weights on every edge)

Optimization Problem: Given data points $\vec{x}_1, \ldots, \vec{x}_n$ and labels $y_1, \ldots, y_n \in \mathbb{R}$, find $\vec{\theta}_*$ minimizing the loss function:

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

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- 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.

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.

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What are some popular optimization algorithms?

ADAM, Adaboost

[Stochastic gradient descent

interior point methods,

simplex method

lbfgs

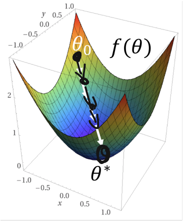
(Newton methods

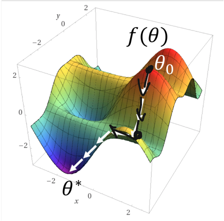
quasi newton

methods)

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 isthe 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.





Let $\vec{e}_i \in \mathbb{R}^d$ denote the i^{th} standard basis vector,
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$f: \mathbb{R}^d \to \mathbb{R}$

Partial Derivative:

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

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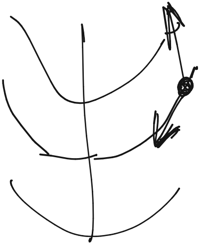

Directional Derivative:

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

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

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

$f'(\vec{\theta})$

$\vec{\nabla} f(\theta) = [f'(\theta)]$

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Directional Derivative in Terms of the Gradient:

$V = [1, 2, 3]$

$$\underbrace{D_{\vec{v}} f(\vec{\theta})}_{\text{change when moving in the direction of } V} = \underbrace{\langle \vec{v}, \vec{\nabla} f(\vec{\theta}) \rangle}_{\text{dot product}} = \sum v(i) \frac{\partial f}{\partial \theta(i)}$$

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

$\parallel$

$f(\theta^i)$

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

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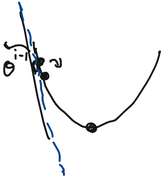

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$$\begin{aligned}\underbrace{f(\vec{\theta}^{(i)}) - f(\vec{\theta}^{(i-1)})}_{\text{minimize}} = f(\vec{\theta}^{(i-1)} + \eta\vec{v}) - f(\vec{\theta}^{(i-1)}) &\approx \eta \cdot D_{\vec{v}} f(\vec{\theta}^{(i-1)}) \\ &= \eta \cdot \langle \underbrace{\vec{v}}_{-\nabla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

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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.

$f(\vec{\theta}^{(t)}) \leq \min_{\theta} f(\vec{\theta}) + \epsilon$

Gradient Descent

- Choose some initialization $\vec{\theta}^{(0)}$.
- For $i = 1, \ldots, t$ $\quad v = -\nabla f(\theta^{i-1})$
  - $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
- 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.)

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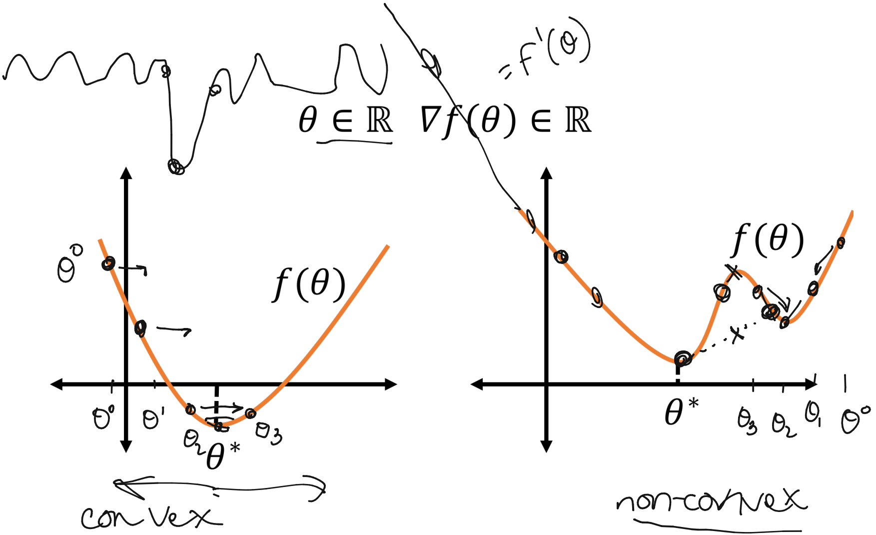
- For now assume η stays the same in each iteration.

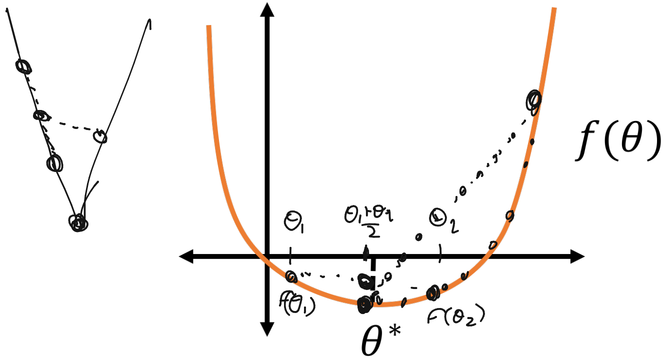


Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

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 $\lambda \in [0, 1]$: $\lambda = 1/2$

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

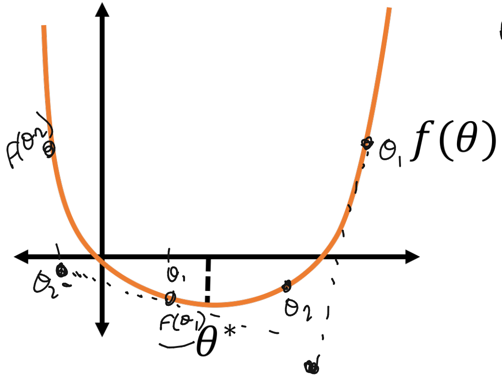
simulated annealing



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

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

F is convex iff
$F''(x) \geq 0 \ \forall x$



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

$(\theta^+$

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

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

CONDITIONS FOR GRADIENT DESCENT CONVERGENCE

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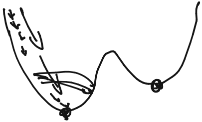
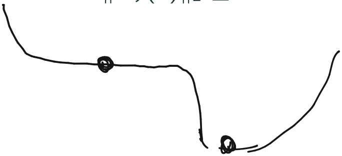
Non-Convex Functions: After sufficient iterations, gradient descent will converge to a approximate stationary point $\hat{\theta}$ with:



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



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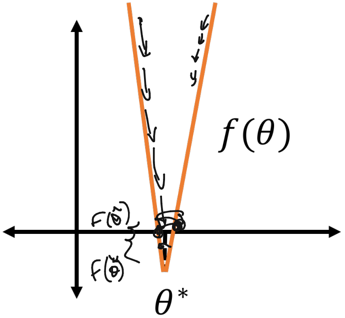
Examples: least squares regression, logistic regression, sparse regression (lasso), regularized regression, SVMS,...

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

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

Examples: neural networks, clustering, mixture models.

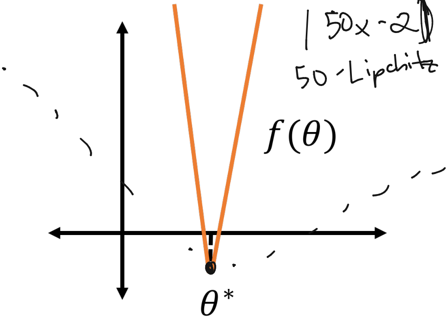
$\theta \in \mathbb{R} \quad \nabla f(\theta) \in \mathbb{R}$



Gradient Descent Update:

$$\vec{\theta}_{i+1} = \vec{\theta}_i - \underbrace{\eta \nabla f(\vec{\theta}_i)}_{\text{Very large}}$$

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



$|50x - 2|$

50-Lipchitz

Gradient Descent Update:

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

For fast convergence, need to assume that the function is

G Lipschitz (size of gradient is bounded): There is some G s.t.:

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

Gradient Descent analysis for convex, Lipschitz functions.