COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2019.
Lecture 18

LOGISTICS

- Problem Set 3 on Spectral Methods due **this Friday at 8pm**.
- Can turn in without penalty until Sunday at 11:59pm.

SUMMARY

Last Class:

- Power method for computing the top singular vector of a matrix.
- High level discussion of Krylov methods, block versions for computing more singular vectors.

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- Power method for computing the top singular vector of a matrix.
- High level discussion of Krylov methods, block versions for computing more singular vectors.
- Power method is an iterative algorithm for solving the *non-convex* optimization problem:

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

This Class (and until Thanksgiving):

- More general iterative algorithms for optimization, specifically gradient descent and its variants.
- What are they 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
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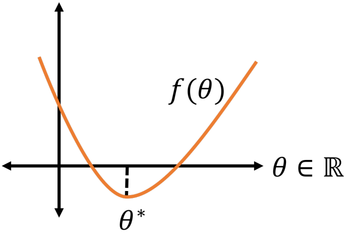
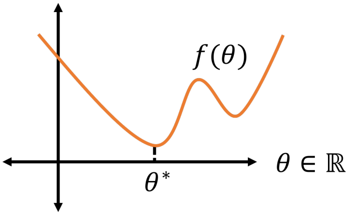
Continuous Optimization: (not covered in core CS curriculum. Touched on in ML/advanced algorithms, maybe.)

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

CONTINUOUS OPTIMIZATION EXAMPLES





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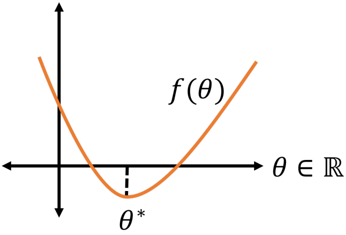

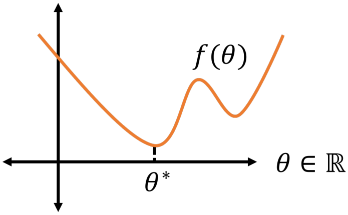

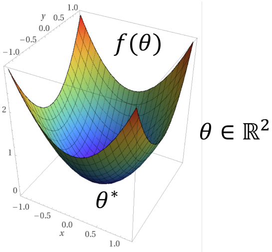

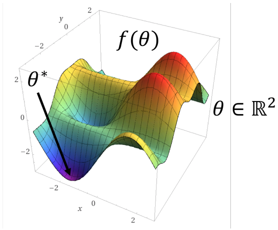

MATHEMATICAL SETUP

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

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Often under some constraints:

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

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

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:

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

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

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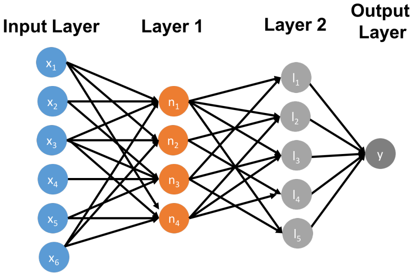

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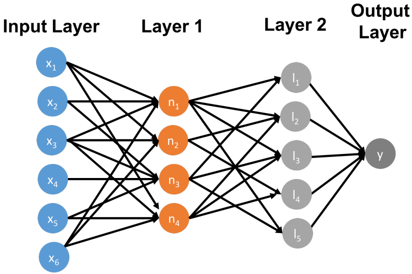

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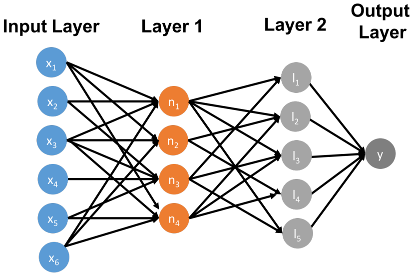

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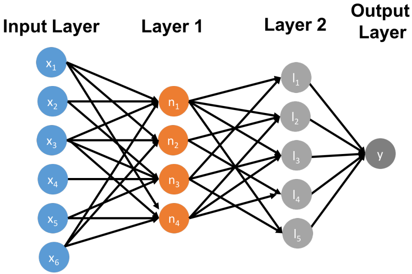

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- Generalization tries to explain why minimizing the loss $L(\vec{\theta}, \mathrm{X})$ on the *training points* minimizes the loss on future *test points*. I.e., makes us have good predictions on future inputs.

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

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What are some popular optimization algorithms?

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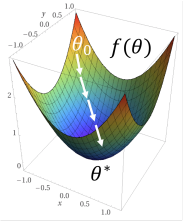

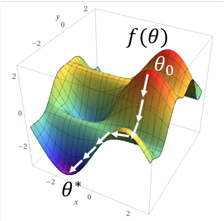

MULTIVARIATE CALCULUS REVIEW

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

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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 $\vec{\theta}$.

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 EXAMPLE

Running Example: Least squares regression.

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

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By Chain rule:

$$\frac{\partial L(\vec{\theta}, \mathbf{X})}{\partial \vec{\theta}(j)} = \sum_{i=1}^{n} 2 \cdot \left(\vec{\theta}^T \vec{x}_i - y_i\right) \cdot \frac{\partial \left(\vec{\theta}^T \vec{x}_i - y_i\right)}{\partial \vec{\theta}(j)}$$

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Partial derivative for least squares regression:

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GRADIENT EXAMPLE

Gradient for least squares regression via linear algebraic approach:

$$\nabla L(\vec{\theta}, \mathsf{X}) = \nabla \|\mathsf{X}\vec{\theta} - \vec{y}\|_2^2$$

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

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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.

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

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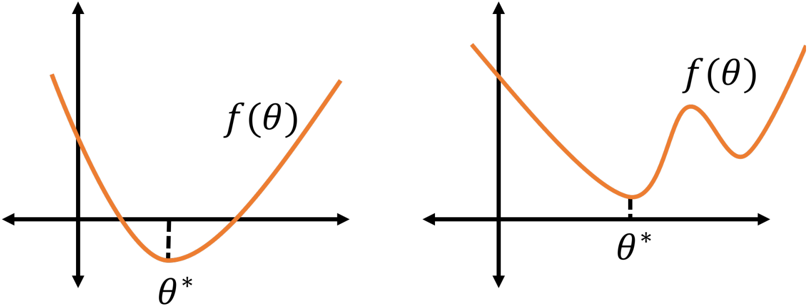
When will this algorithm work well?

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



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

CONDITIONS FOR GRADIENT DESCENT CONVERGENCE

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

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Examples: neural networks, clustering, mixture models.

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Why for non-convex functions do we only guarantee convergence to a approximate stationary point rather than an approximate local minimum?

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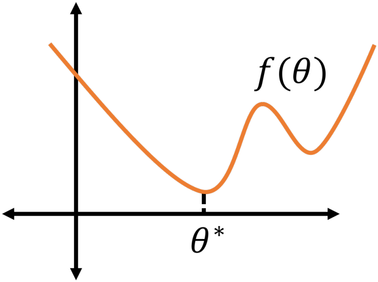
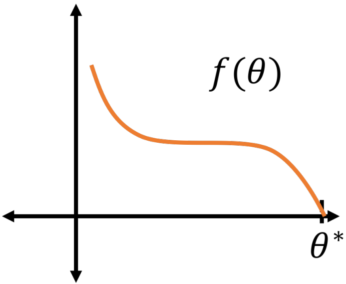
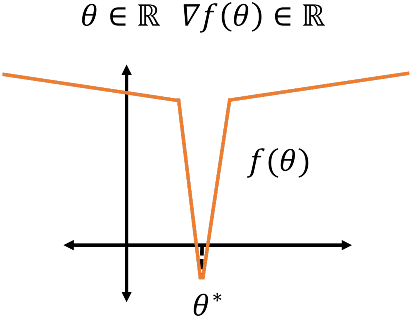




WELL-BEHAVED FUNCTIONS



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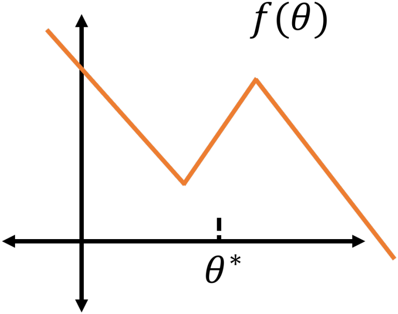

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Both Convex and Non-convex: Need to assume the function is well behaved in some way.

- Lipschitz (size of gradient is bounded): For all $\vec{\theta}$ and some G,

$$\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G.$$

- Smooth (direction/size of gradient is not changing too quickly): For all $\vec{\theta}_1, \vec{\theta}_2$ and some β,

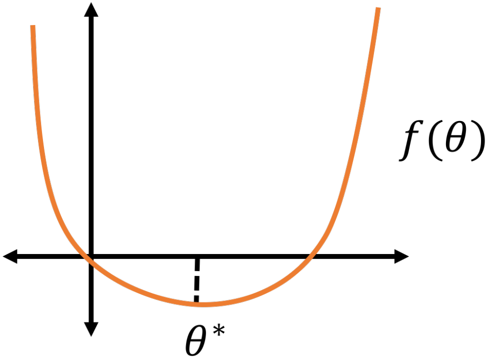
$$\|\vec{\nabla} f(\vec{\theta}_1) - \vec{\nabla} f(\vec{\theta}_2)\|_2 \leq \beta \cdot \|\vec{\theta}_1 - \vec{\theta}_2\|_2.$$

Gradient Descent analysis for convex functions.

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

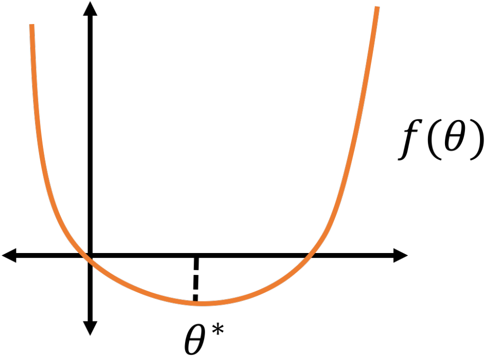
$$(1-\lambda)\cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda)\cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$



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

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



GD ANALYSIS – CONVEX FUNCTIONS

Assume that:

- f is convex.
- f is G Lipschitz (i.e., $\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$.
- $\|\vec{\theta}_0 - \vec{\theta}_*\|_2 \leq R$ where θ_0 is the initialization point.

Gradient Descent

- Choose some initialization $\vec{\theta}_0$ and set $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t$
  - $\vec{\theta}_i = \vec{\theta}_{i-1} - \eta \nabla f(\vec{\theta}_{i-1})$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_0, \ldots \vec{\theta}_t} f(\vec{\theta}_i)$.

GD ANALYSIS PROOF

Theorem – GD on Convex Lipschitz Functions: For convex G Lipschitz function f, GD run with $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of θ_*, outputs $\hat{\theta}$ satisfying:

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Step 1: For all i, $f(\theta_i) - f(\theta_*) \leq \frac{\|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$. Visually:

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GD ANALYSIS PROOF

Theorem – GD on Convex Lipschitz Functions: For convex G Lipschitz function f, GD run with $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of θ_*, outputs $\hat{\theta}$ satisfying:

$$f(\hat{\theta}) \leq f(\theta_*) + \epsilon.$$

Step 1: For all i, $f(\theta_i) - f(\theta_*) \leq \frac{\|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$

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Step 2: $\frac{1}{T}\sum_{i=1}^{T} f(\theta_i) - f(\theta_*) \leq \frac{R^2}{2\eta \cdot T} + \frac{\eta G^2}{2}$.

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Questions on Gradient Descent?