COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco

University of Massachusetts Amherst. Fall 2019.
Lecture 18

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

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.

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.
- Power method is an iterative algorithm for solving the *non-convex* optimization problem:

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

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 (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.

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DISCRETE VS. CONTINUOUS OPTIMIZATION

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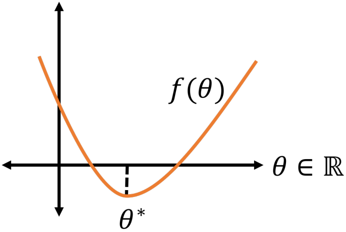
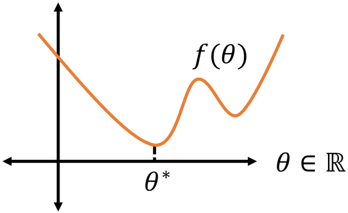
Continuous Optimization: (not covered in core CS curriculum. Touched on in ML/advanced algorithms, maybe.)

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


$f(\theta)$
$\theta \in \mathbb{R}$
θ^*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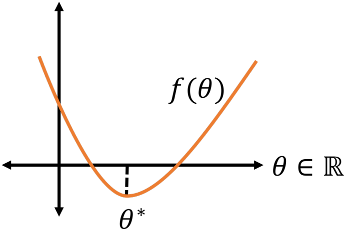
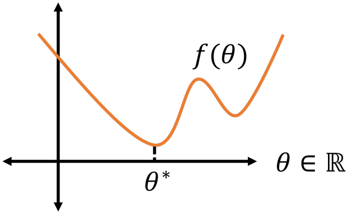
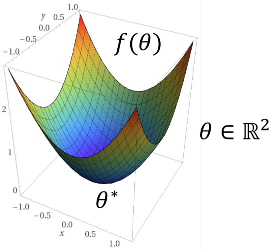
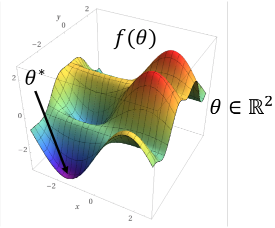
CONTINUOUS OPTIMIZATION EXAMPLES









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Typically up to some small approximation factor.

MATHEMATICAL SETUP

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Typically up to some small approximation factor.

Often under some constraints:

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

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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.

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

Example 1: Linear Regression

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

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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:

param input data

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

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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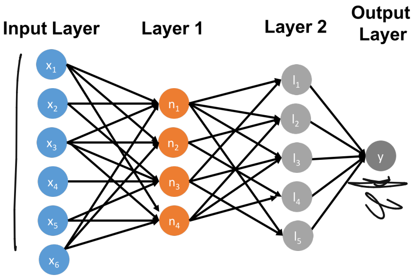

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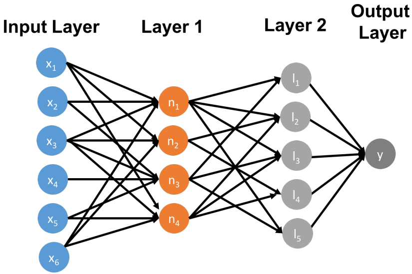

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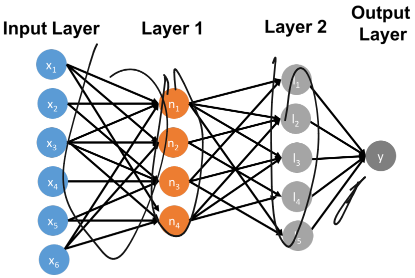

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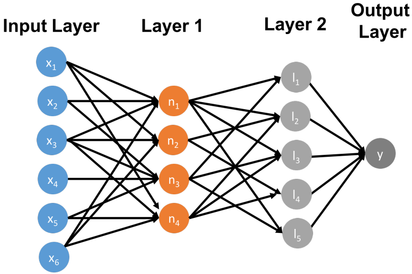

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- Generalization tries to explain why minimizing the loss $L(\vec{\theta}, \mathbf{X})$ on the *training points* minimizes the loss on future *test points*. I.e., makes us have good predictions on future inputs.

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

- The form of f (in ML, depends on the model & loss function).
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What are some popular optimization algorithms?

gradient descent
Adam Adagrad.
power method.

BFGS.

Newtons

interior point methods
ellipsoid.

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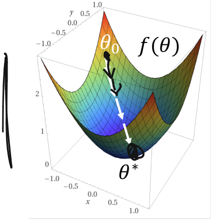
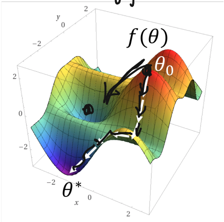
"opposite





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Partial Derivative:

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

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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.

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

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Directional Derivative in Terms of the Gradient: √

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$$\approx \vec{v}(1) \cdot \frac{\partial f}{\partial \vec{\theta}(1)} + \vec{v}(2) \cdot \frac{\partial f}{\partial \vec{\theta}(2)} + \ldots + \vec{v}(d) \cdot \frac{\partial f}{\partial \vec{\theta}(d)}$$

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$\theta(1) : \theta(2)$

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Directional Derivative in Terms of the Gradient:

$$\begin{aligned} D_{\vec{v}}\, f(\vec{\theta}) &= \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon(\vec{e}_1 \cdot \vec{v}(1) + \vec{e}_2 \cdot \vec{v}(2) + \ldots + \vec{e}_d \cdot \vec{v}(d)) - f(\vec{\theta})}{\epsilon} \\ &\approx \vec{v}(1) \cdot \frac{\partial f}{\partial \vec{\theta}(1)} + \vec{v}(2) \cdot \frac{\partial f}{\partial \vec{\theta}(2)} + \ldots + \vec{v}(d) \cdot \frac{\partial f}{\partial \vec{\theta}(d)} \\ &= \langle \vec{v}, \vec{\nabla} f(\vec{\theta}) \rangle. \end{aligned}$$

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

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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).

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:

$\nabla L(\vec{\theta}, X)$

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

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:

$$L(\vec{\theta}, \mathbf{X}) = \sum_{i=1}^{n} \left(\vec{\theta}^T \vec{x}_i - y_i\right)^2 = \|\mathbf{X}\vec{\theta} - \vec{y}\|_2^2.$$

By Chain rule:

$f(x) = x^2$

$f'(x) = 2x$

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

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$\cancel{\theta^T x_i - \theta^T x_i}^{\,0} - \epsilon e_j^T x_i$

$-\epsilon x_i(j)$

$-x_i(j)$

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GRADIENT EXAMPLE

Partial derivative for least squares regression:

$X_1 \ldots X_n$

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

Partial derivative for least squares regression:

$$\begin{bmatrix} \frac{\partial L}{\partial \theta(1)} \\ \vdots \\ \frac{\partial L}{\partial \theta(d)} \end{bmatrix}$$

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$$\begin{bmatrix} x_i(1) \\ \vdots \\ x_i(d) \end{bmatrix}$$

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$$= 2\mathbf{X}^T(\mathbf{X}\vec{\theta} - \vec{y}).$$

$$\begin{bmatrix} \vec{\theta}^T \vec{x}_1 \\ \theta^T x_2 \\ \vdots \\ \theta^T x_n \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

GRADIENT EXAMPLE

Gradient for least squares regression via linear algebraic approach:

$$\sum_{i=1}^{n}(\theta^T x_i - y_i)^2$$

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

$$(X\theta - y)^T(X\theta - y)$$

$$\theta^T X^T X\theta - 2\theta^T X^T y + \cancel{y^T y}^{\,0}$$

$$2X^T X\theta \qquad -2X^T y \qquad \langle \theta, X^T y\rangle$$

$$= \sum \theta(i)[X^T y](i)$$

$$y^T X^T \theta$$

$$2(X^T X\theta - 2X^T y)$$

$$2X^T(X\theta - y)$$

$\theta^{i-1} \rightarrow \theta^{i}$

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

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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

- 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.)

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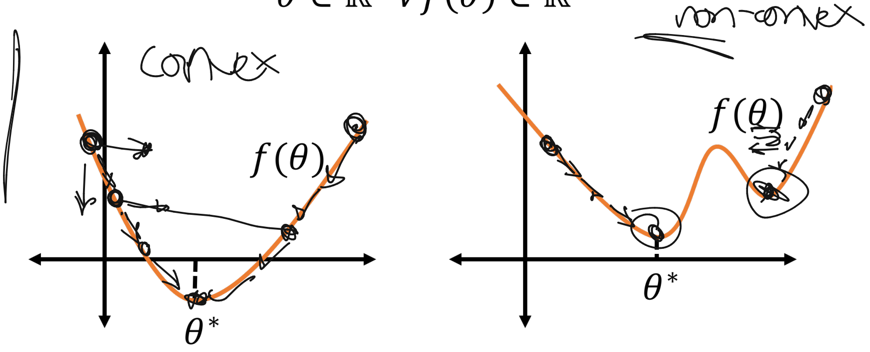
When will this algorithm work well?

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



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

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.

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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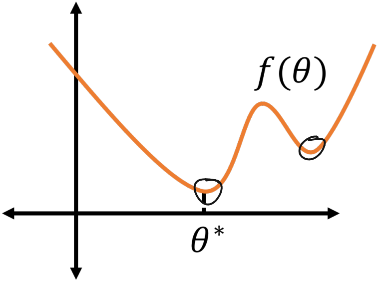

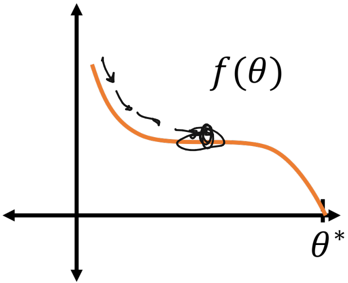

Adam Adagrad.

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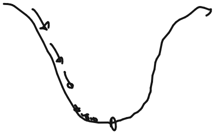

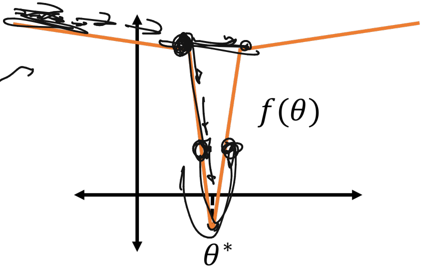

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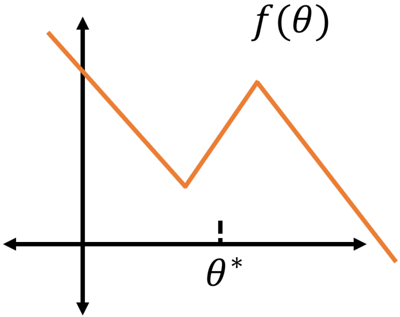

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- Lipschitz (size of gradient is bounded): For all $\vec{\theta}$ and some G,

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

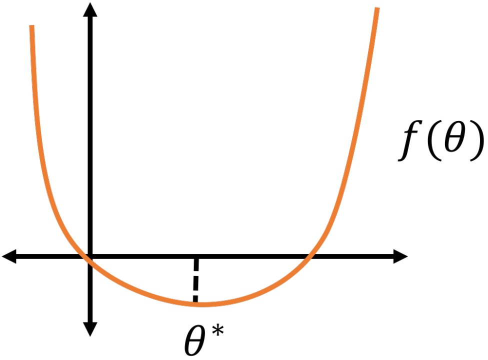
- Smooth (direction/size of gradient is not changing too quickly): For all $\vec{\theta}_1, \vec{\theta}_2$ and some β,

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

Gradient Descent analysis for convex functions.

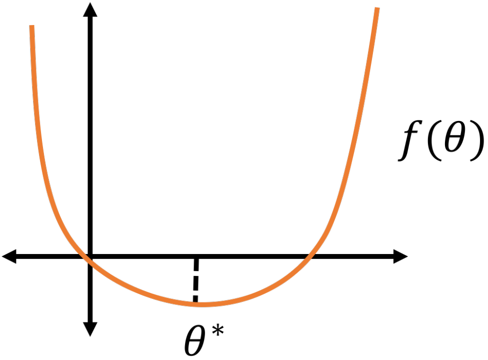
Definition – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0,1]$:

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



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

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



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 $\hat{\theta} = \arg\min_{\vec{\theta}_0, \ldots \vec{\theta}_t} f(\vec{\theta}_i)$.

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

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Questions on Gradient Descent?