COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Spring 2020.

Lecture 22

LOGISTICS

- Problem Set 4 on Spectral Methods/Optimization due Wednesday 4/29. Can submit until Sunday 5/3 at 8pm.
- Shorter than the first 3. I may assign some additional extra credit, depending on what we cover in the next few classes.

SUMMARY

Last Class:

- Finish up power method – Krylov methods and connection to random walks.
- Start on continuous optimization.

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- Start on continuous optimization.

This Class:

- Gradient descent.
- Motivation as a greedy method
- Start on analysis for convex functions.

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

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

- Typically up to some small approximation factor: i.e., find $\hat{\theta}$ $\in \mathbb{R}^d$ with $f(\hat{\theta}) = \min_{\vec{\theta} \in \mathbb{R}^d} f(\vec{\theta}) + \epsilon$
- Often under some constraints:
  - $\|\vec{\theta}\|_2 \leq 1, \quad \|\vec{\theta}\|_1 \leq 1.$
  - $A\vec{\theta} \leq \vec{b}, \quad \vec{\theta}^T A \vec{\theta} \geq 0.$
  - $\vec{1}^T \vec{\theta} = \sum_{i=1}^d \vec{\theta}(i) \leq c.$

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

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:

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

MULTIVARIATE CALCULUS REVIEW

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

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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Directional Derivative in Terms of the Gradient:

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

$$D_{\vec{v}} f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon(\vec{e}_1 \cdot \vec{v}(1) + \vec{e}_2 \cdot \vec{v}(2) + \ldots + \vec{e}_d \cdot \vec{v}(d)) - f(\vec{\theta})}{\epsilon}$$

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$$\approx \vec{v}(1) \cdot \frac{\partial f}{\partial \vec{\theta}(1)}$$

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

v = update direction

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

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).

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:

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

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$z^2 \quad 2z$

By Chain rule:

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

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Partial derivative for least squares regression:

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

$$\vec{\nabla} L(\vec{\theta}) = \begin{bmatrix} \frac{\partial L(\vec{\theta})}{\partial \theta(1)} \\ \vdots \\ \frac{\partial L(\vec{\theta})}{\partial \theta(d)} \end{bmatrix} = \begin{bmatrix} \sum 2(\theta^T x_i - y_i) x_i(1) \\ \vdots \\ \sum 2(\theta^T x_i - y_i) x_i(d) \end{bmatrix}$$

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

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

$$\mathbb{R}^{d \times d}$$

$$\theta \in \mathbb{R}^d$$

$$X \in \mathbb{R}^{n \times d} \qquad \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$$

GRADIENT EXAMPLE

Gradient for least squares regression via linear algebraic approach:

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

$x^2 \rightarrow 2x$

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

$$\nabla[(X\theta - y)^T (X\theta - y)] = \nabla[\theta^T X^T X \theta - 2\theta^T X^T y + y^T y]$$

$\theta^T X^T X \theta \rightarrow 2X^T X\theta$, $\quad -2\theta^T X^T y \rightarrow -2X^T y$, $\quad y^T y \rightarrow 0$

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

$f(\theta,)$ $\|v\|=1$

Gradient descent is a greedy iterative optimization algorithm: Starting at $\vec{\theta}_1$, in each iteration let $\vec{\theta}_{i+1} = \vec{\theta}_i + \eta\vec{v}$, where η is a (small) 'step size' and $\vec{v}$ is a direction chosen to minimize $f(\vec{\theta}_i + \eta\vec{v})$.

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So for small η:

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

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So for small η:

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

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$\|v\|_2 = 1$

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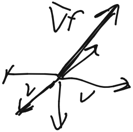

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$$= \eta \cdot \langle \vec{v}, \vec{\nabla} f(\vec{\theta}_i) \rangle.$$

$\langle \vec{v}, \vec{\nabla} f(\vec{\theta}_i) \rangle = 0$

$f(\theta_{i+1}) - f(\theta_i) = 0$

$\theta_1 \quad \theta_2 \quad \theta_3 \ldots \quad \theta_t$ $f(\theta_t)$ be as small as possible

Gradient descent is a greedy iterative optimization algorithm: Starting at $\vec{\theta}_1$, in each iteration let $\vec{\theta}_{i+1} = \vec{\theta}_i + \eta\vec{v}$, where η is a (small) 'step size' and $\vec{v}$ is a direction chosen to minimize $f(\vec{\theta}_i + \eta\vec{v})$.

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

$f(\theta_{i+1}) \approx f(\theta_i) + \eta\langle v, \nabla f(\theta_i)\rangle$

So for small η:

$$\min \quad f(\vec{\theta}_{i+1}) - f(\vec{\theta}_i) = f(\vec{\theta}_i + \eta\vec{v}) - f(\vec{\theta}_i) \approx \eta \cdot D_{\vec{v}} f(\vec{\theta}_i)$$

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

$\Updownarrow$

$\min \; f(\theta_{i+1})$

We want to choose $\vec{v}$ minimizing $\langle \vec{v}, \vec{\nabla} f(\vec{\theta}_i)\rangle$ – i.e., pointing in the direction of $\vec{\nabla} f(\vec{\theta}_i)$ but with the opposite sign.

Gradient Descent

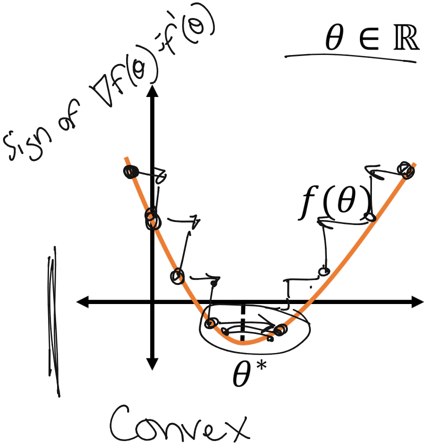
- Choose some initialization $\vec{\theta}_1$.
- For $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_i} f(\vec{\theta}_i)$, as an approximate minimizer.

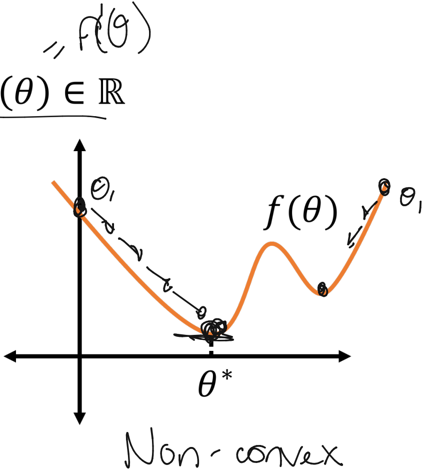
$f(\hat{\theta}) \leq f(\theta^*) + \epsilon$

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.

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





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

CONDITIONS FOR GRADIENT DESCENT CONVERGENCE

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

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

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

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

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

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CONDITIONS FOR GRADIENT DESCENT CONVERGENCE

Convex Functions: After sufficient iterations, 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.

STATIONARY POINT VS. LOCAL MINIMUM

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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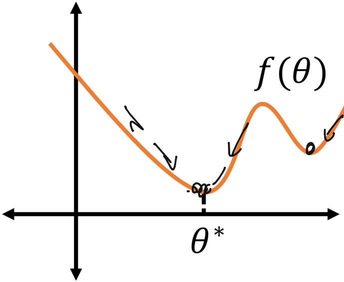

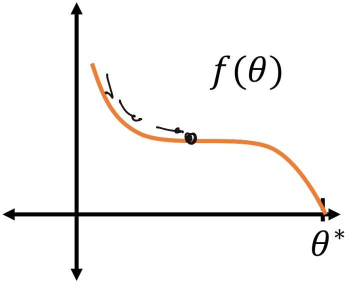

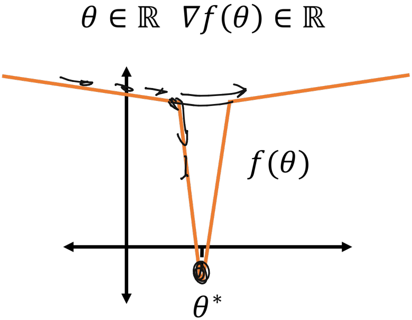

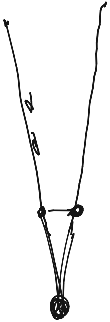

Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

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

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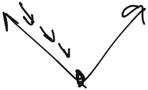
- Lipschitz (size of gradient is bounded): There is some G s.t.:

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

$f(\theta) = |\theta|$

$f'(\theta) = 1$ for $\theta > 0$, -1 for $\theta < 0$



$G = 1$

$||\theta_1| - |\theta_2|| \leq |\theta_1 - \theta_2|$

- Smooth/Lipschitz gradient (direction/size of gradient is not changing too quickly): There is some β s.t.:

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

$\theta_1 = \varepsilon \quad \theta_2 = -\varepsilon$

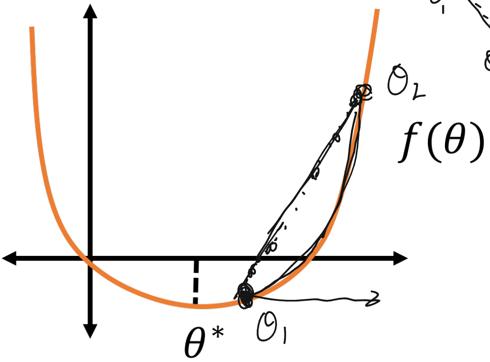
$\|1 - (-1)\| = 2$

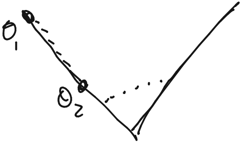
$|\varepsilon - (-\varepsilon)| = 2\varepsilon$

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

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





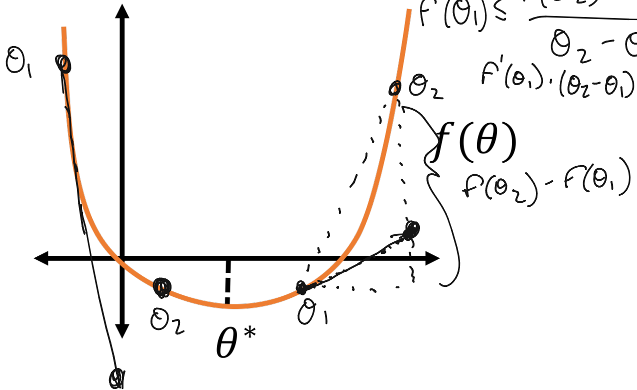
Corollary – Convex Function: A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

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

$\nabla f(\theta)^T$ ✓

$$f'(\theta_1) \leq \frac{f(\theta_2) - f(\theta_1)}{\theta_2 - \theta_1}$$

$$f'(\theta_1) \cdot (\theta_2 - \theta_1) \leq f(\theta_2) - f(\theta_1)$$



Assume that:

- f is convex.
- f is G Lipschitz ($\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$).
- $\|\vec{\theta}_1 - \vec{\theta}_*\|_2 \leq R$ where $\vec{\theta}_1$ is the initialization point.

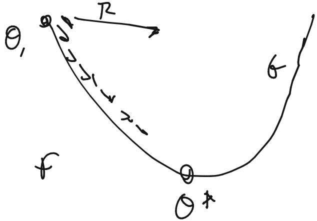
Gradient Descent

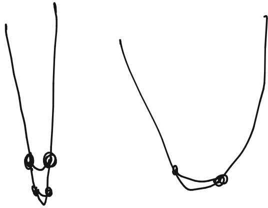
- Choose some initialization $\vec{\theta}_1$ and set $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_1, \ldots \vec{\theta}_t} f(\vec{\theta}_i)$.

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

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

$$t \geq \frac{R^2 G^2}{\epsilon^2} \qquad \eta = \frac{R}{G\sqrt{t}}$$





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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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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?

CONSTRAINED CONVEX OPTIMIZATION

Often want to perform convex optimization with convex constraints.

$$\theta^* = \arg\min_{\theta \in \mathcal{S}} f(\theta),$$

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E.g. $\mathcal{S} = \{\vec{\theta} \in \mathbb{R}^d : \|\vec{\theta}\|_2 \leq 1\}$.

PROJECTED GRADIENT DESCENT

For any convex set let $P_{\mathcal{S}}(\cdot)$ denote the projection function onto $\mathcal{S}$.

- $P_{\mathcal{S}}(\vec{y}) = \arg\min_{\vec{\theta} \in \mathcal{S}} \|\vec{\theta} - \vec{y}\|_2$.

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- For $\mathcal{S} = \{\vec{\theta} \in \mathbb{R}^d : \|\vec{\theta}\|_2 \leq 1\}$ what is $P_{\mathcal{S}}(\vec{y})$?
- For $\mathcal{S}$ being a k dimensional subspace of $\mathbb{R}^d$, what is $P_{\mathcal{S}}(\vec{y})$?

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Projected Gradient Descent

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- For $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1}^{(out)} = \vec{\theta}_i - \eta \cdot \nabla f(\vec{\theta}_i)$
  - $\vec{\theta}_{i+1} = P_{\mathcal{S}}(\vec{\theta}_{i+1}^{(out)})$.
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_i} f(\vec{\theta}_i)$.

Visually:

CONVEX PROJECTIONS

Projected gradient descent can be analyzed identically to gradient descent!

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Theorem – Projection to a convex set: For any convex set $\mathcal{S} \subseteq \mathbb{R}^d$, $\vec{y} \in \mathbb{R}^d$, and $\vec{\theta} \in \mathcal{S}$,

$$\|P_{\mathcal{S}}(\vec{y}) - \vec{\theta}\|_2 \leq \|\vec{y} - \vec{\theta}\|_2.$$

Theorem – Projected GD: For convex G-Lipschitz function f, and convex set $\mathcal{S}$, Projected 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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