CS-GY 9223 D: Lecture 5
Gradient Descent and Projected Gradient Descent

NYU Tandon School of Engineering, Prof. Christopher Musco

PROJECT

- Choose your partner and email me by **next Wednesday, 10/14**.
- Topic and 1 page proposal due **11/04**.
- See project guidelines on course webpage for details.

What techniques did we learn?

NEW UNIT: CONTINUOUS OPTIMIZATION

Have some function $f : \mathbb{R}^d \to \mathbb{R}$. Want to find $\mathbf{x}^*$ such that:

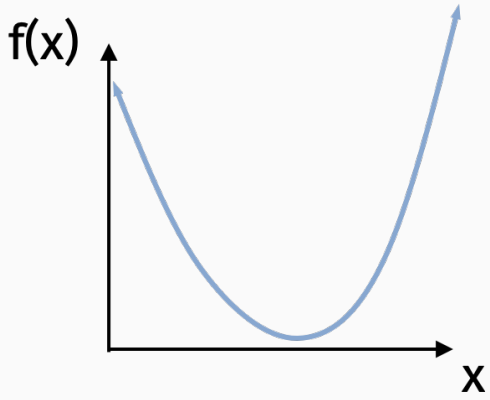
$$f(\mathbf{x}^*) = \min_{\mathbf{x}} f(\mathbf{x}).$$

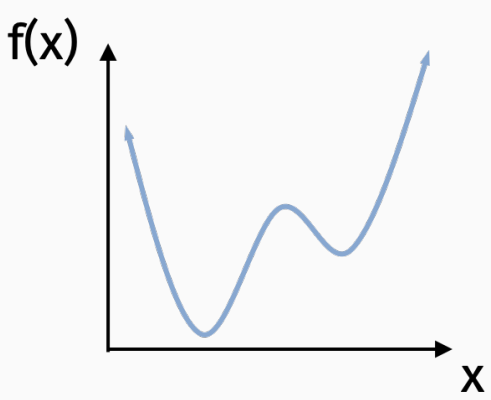
Or at least $\hat{\mathbf{x}}$ which is close to a minimum. E.g.
$f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x}} f(\mathbf{x}) + \epsilon$

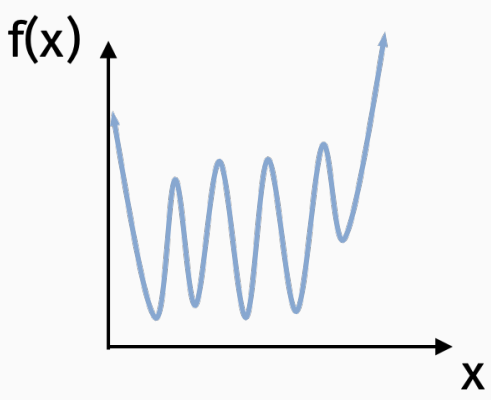
Often we have some additional constraints:

- $\mathbf{x} > 0$.
- $\|\mathbf{x}\|_2 \leq R$, $\|\mathbf{x}\|_1 \leq R$.
- $\mathbf{a}^T\mathbf{x} > c$.

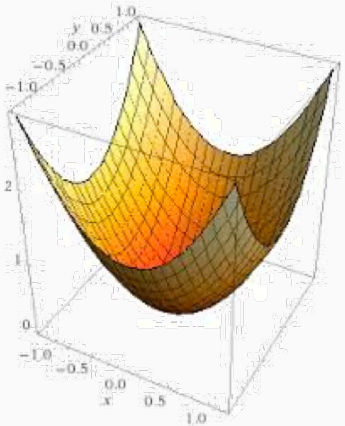
Dimension $d = 1$:

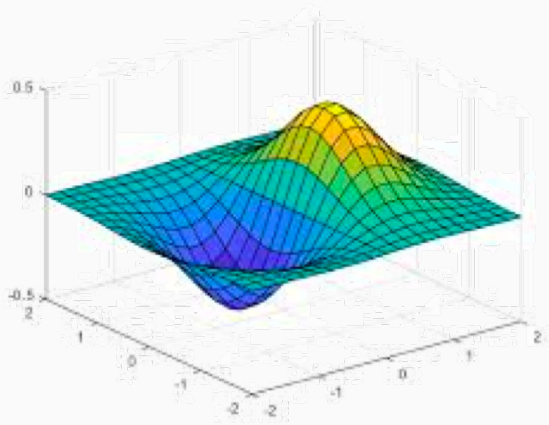


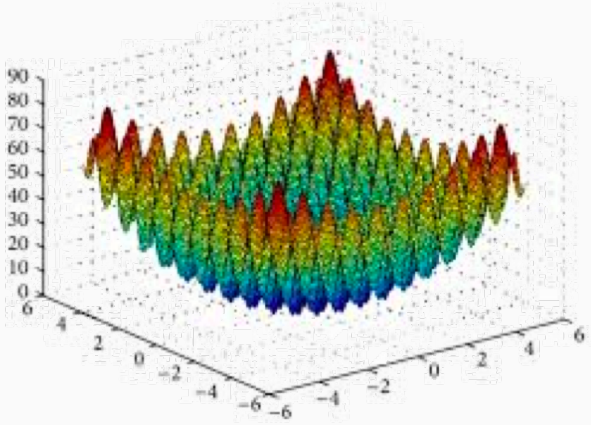




Dimension $d = 2$:







Continuouos optimization is the foundation of modern machine learning.

Supervised learning: Want to learn a model that maps inputs

- numerical data vectors
- images, video
- text documents

to predictions

- numerical value (probability stock price increases)
- label (is the image a cat? does the image contain a car?)
- decision (turn car left, rotate robotic arm)

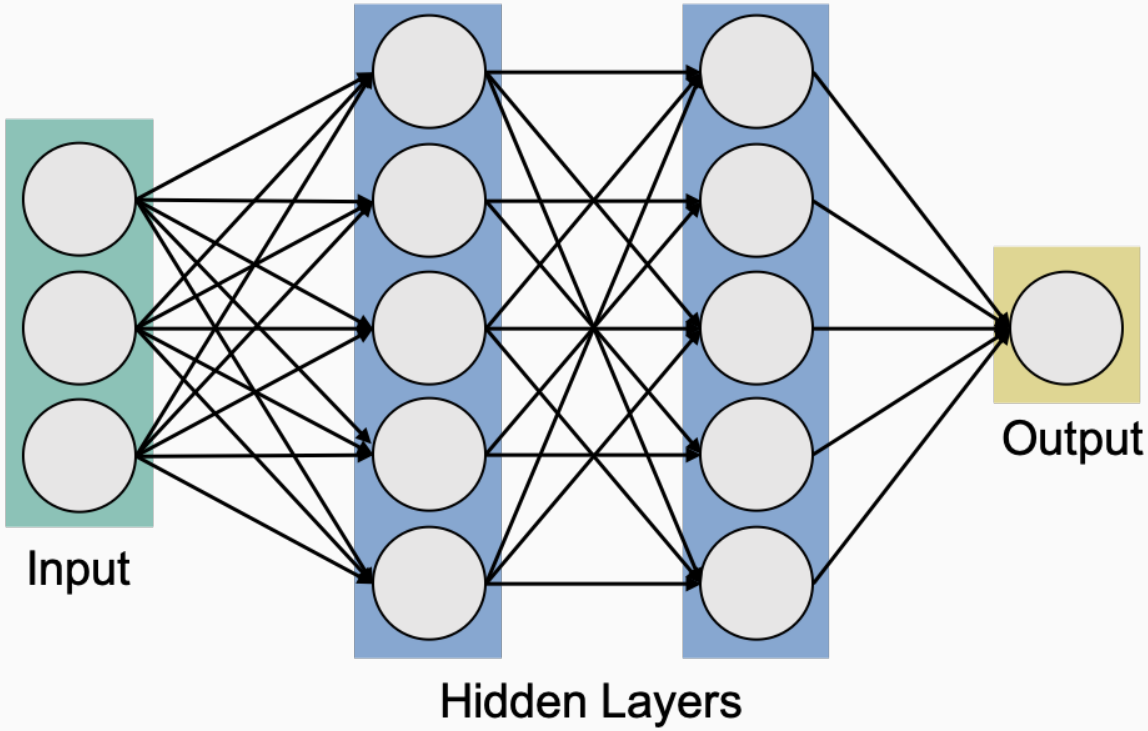
MACHINE LEARNING MODEL

Let $M_{\mathbf{x}}$ be a model with parameters $\mathbf{x} = \{x_1, \ldots, x_k\}$, which takes as input a data vector $\mathbf{a}$ and outputs a prediction.

Example:

$$M_{\mathbf{x}}(\mathbf{a}) = \text{sign}(\mathbf{a}^T\mathbf{x})$$

Example:



$\mathbf{x} \in \mathbb{R}^{(\#\text{ of connections})}$ is the parameter vector containing all the network weights.

Classic approach in supervised learning: Find a model that works well on data that you already have the answer for (labels, values, classes, etc.).

- Model $M_{\mathbf{x}}$ parameterized by a vector of numbers $\mathbf{x}$.
- Dataset $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(n)}$ with outputs $y^{(1)}, \ldots, y^{(n)}$.

Want to find $\hat{\mathbf{x}}$ so that $M_{\hat{\mathbf{x}}}(\mathbf{a}^{(i)}) \approx y^{(i)}$ for $i \in 1, \ldots, n$.

How do we turn this into a function minimization problem?

LOSS FUNCTION

Loss function $L\left(M_{\mathbf{x}}(\mathbf{a}), y\right)$**:** Some measure of distance between prediction $M_{\mathbf{x}}(\mathbf{a})$ and target output y. Increases if they are further apart.

- Squared (ℓ_2) loss: $|M_{\mathbf{x}}(\mathbf{a}) - y|^2$
- Absolute deviation (ℓ_1) loss: $|M_{\mathbf{x}}(\mathbf{a}) - y|$
- Hinge loss: 1 - $y \cdot M_{\mathbf{x}}(\mathbf{a})$
- Cross-entropy loss (log loss).
- Etc.

EMPIRICAL RISK MINIMIZATION

Empirical risk minimization:

$$f(\mathbf{x}) = \sum_{i=1}^{n} L\left(M_{\mathbf{x}}(\mathbf{a}^{(i)}), y^{(i)}\right)$$

Solve the optimization problem $\min_{\mathbf{x}} f(\mathbf{x})$.

EXAMPLE: LINEAR REGRESSION

- $M_{\mathbf{x}}(\mathbf{a}) = \mathbf{x}^T\mathbf{a}$. $\mathbf{x}$ contains the regression coefficients.
- $L(z, y) = |z - y|^2$.
- $f(\mathbf{x}) = \sum_{i=1}^{n} |\mathbf{x}^T\mathbf{a}^{(i)} - y^{(i)}|^2$

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2$$

where $\mathbf{A}$ is a matrix with $\mathbf{a}^{(i)}$ as its i^{th} row and $\mathbf{y}$ is a vector with $y^{(i)}$ as its i^{th} entry.

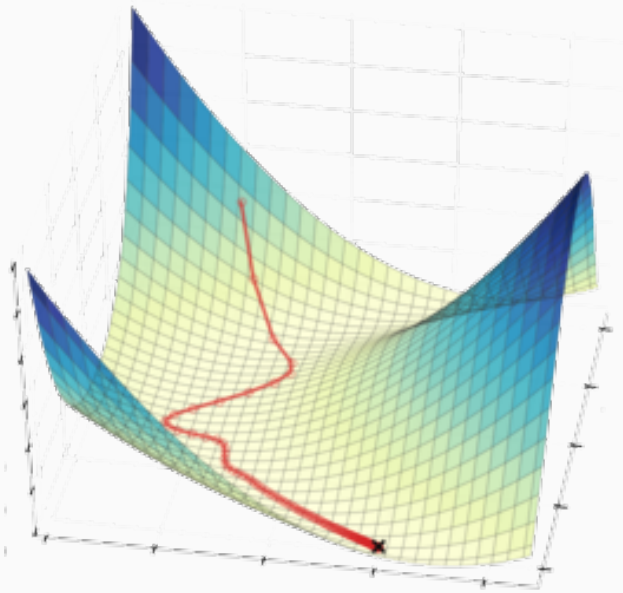
The choice of algorithm to minimize $f(\mathbf{x})$ will depend on:

- The form of $f(\mathbf{x})$ (is it linear, is it quadratic, does it have finite sum structure, etc.)
- If there are any additional constraints imposed on $\mathbf{x}$. E.g. $\|\mathbf{x}\|_2 \leq c$.

What are some example algorithms for continuous optimization?

GRADIENT DESCENT

Gradient descent: A greedy algorithm for minimizing functions of multiple variables that often works amazingly well.



For $i = 1, \ldots, d$, let x_i be the i^{th} entry of $\mathbf{x}$. Let $\mathbf{e}^{(i)}$ be the i^{th} standard basis vector.

Partial derivative:

$$\frac{\partial f}{\partial x_i}(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{e}^{(i)}) - f(\mathbf{x})}{t}$$

Directional derivative:

$$D_{\mathbf{v}} f(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{v}) - f(\mathbf{x})}{t}$$

Gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \frac{\partial f}{\partial x_2}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix}$$

Directional derivative:

$$D_{\mathbf{v}} f(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{v}) - f(\mathbf{x})}{t} = \nabla f(\mathbf{x})^T \mathbf{v}.$$

Given a function f to minimize, assume we have:

- **Function oracle**: Evaluate $f(\mathbf{x})$ for any $\mathbf{x}$.
- **Gradient oracle**: Evaluate $\nabla f(\mathbf{x})$ for any $\mathbf{x}$.

We view the implementation of these oracles as black-boxes, but they can often require a fair bit of computation.

EXAMPLE GRADIENT EVALUATION

Linear least-squares regression:

- Given $\mathbf{a}^{(1)}, \ldots \mathbf{a}^{(n)} \in \mathbb{R}^d$, $y^{(1)}, \ldots y^{(n)} \in \mathbb{R}$.
- Want to minimize:

$$f(\mathbf{x}) = \sum_{i=1}^{n} \left(\mathbf{x}^T \mathbf{a}^{(i)} - y^{(i)} \right)^2 = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2.$$

$$\frac{\partial f}{\partial x_j} = \sum_{i=1}^{n} 2 \left(\mathbf{x}^T \mathbf{a}^{(i)} - y^{(i)} \right) \cdot a_j^{(i)} = (2\mathbf{A}\mathbf{x} - \mathbf{y})^T \boldsymbol{\alpha}^{(j)}$$

where $\boldsymbol{\alpha}^{(j)}$ is the i^{th} column of $\mathbf{A}$.

$$\nabla f(\mathbf{x}) = 2\mathbf{A}^T (\mathbf{A}\mathbf{x} - \mathbf{y})$$

What is the time complexity of a gradient oracle for $\nabla f(\mathbf{x})$?

Greedy approach: Given a starting point $\mathbf{x}$, make a small adjustment that decreases $f(\mathbf{x})$. In particular, $\mathbf{x} \leftarrow \mathbf{x} + \eta\mathbf{v}$ and $f(\mathbf{x}) \leftarrow f(\mathbf{x} + \eta\mathbf{v})$.

What property do I want in $\mathbf{v}$?

Leading question: When η is small, what's an approximation for $f(\mathbf{x} + \eta\mathbf{v}) - f(\mathbf{x})$?

$$f(\mathbf{x} + \eta\mathbf{v}) - f(\mathbf{x}) \approx$$

DIRECTIONAL DERIVATIVES

$$D_{\mathbf{v}} f(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{v}) - f(\mathbf{x})}{t} = \nabla f(\mathbf{x})^T \mathbf{v}.$$

So:

$$f(\mathbf{x} + \eta\mathbf{v}) - f(\mathbf{x}) \approx$$

How should we choose $\mathbf{v}$ so that $f(\mathbf{x} + \eta\mathbf{v}) < f(\mathbf{x})$?

Prototype algorithm:

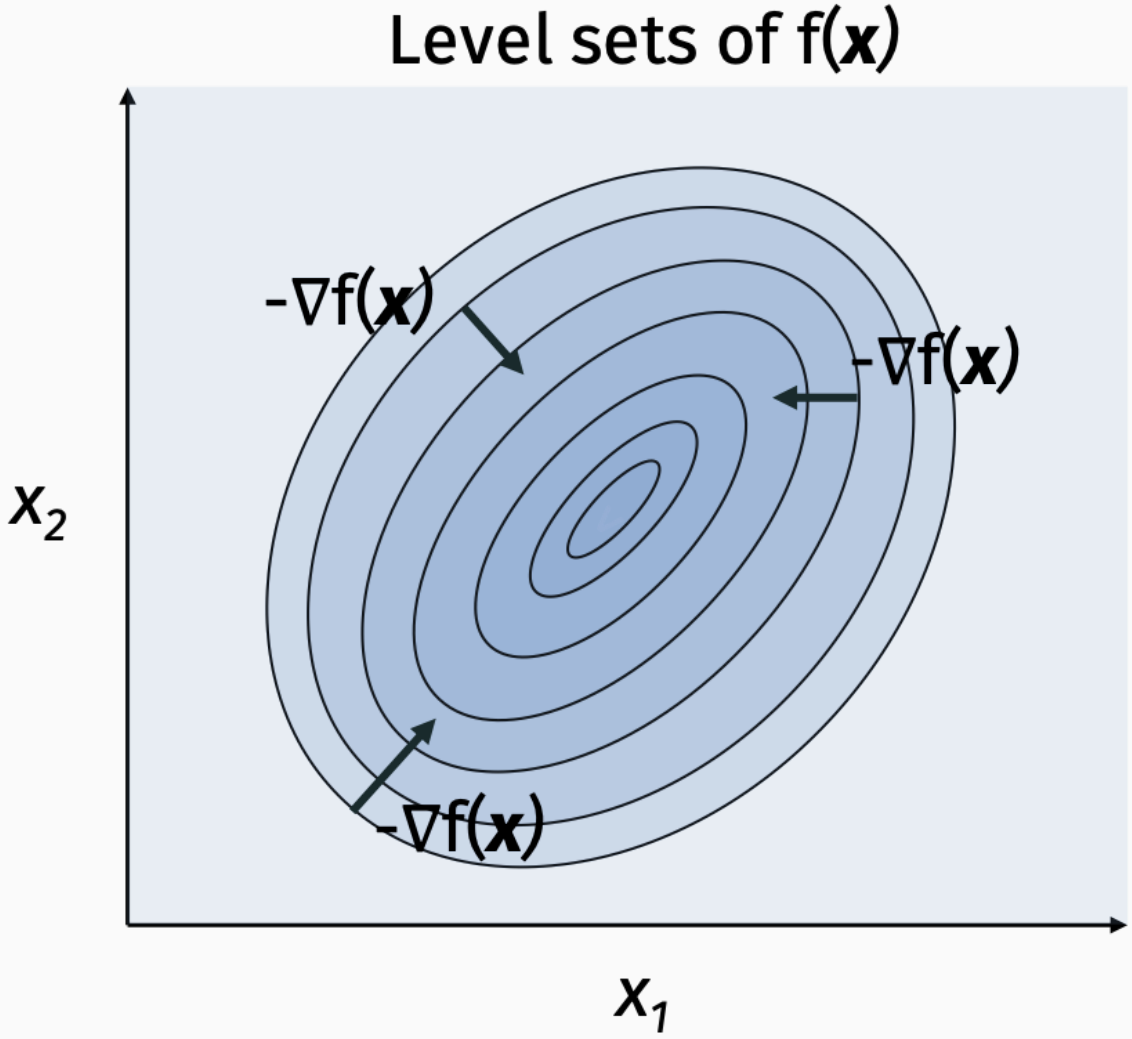
- For $i = 0, \ldots, T$:
  - $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$
- Return $\mathbf{x}^{(T)}$.

η is a step-size parameter, which is often adapted on the go. For now, assume it is fixed ahead of time.

GRADIENT DESCENT INTUITION

1 dimensional example:

2 dimensional example:



For a convex function $f(\mathbf{x})$: For sufficiently small η and a sufficiently large number of iterations T, gradient descent will converge to a near global minimum:

$$f(\mathbf{x}^{(T)}) \leq f(\mathbf{x}^*) + \epsilon.$$

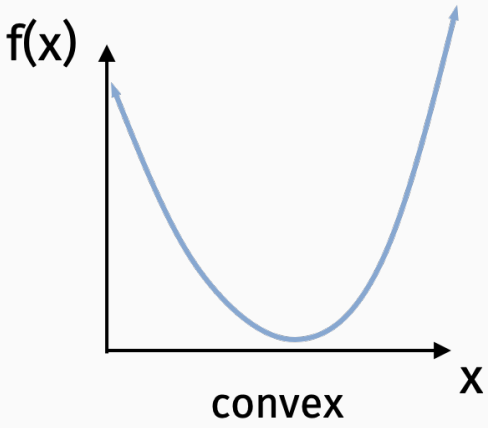
Examples: least squares regression, logistic regression, kernel regression, SVMs.

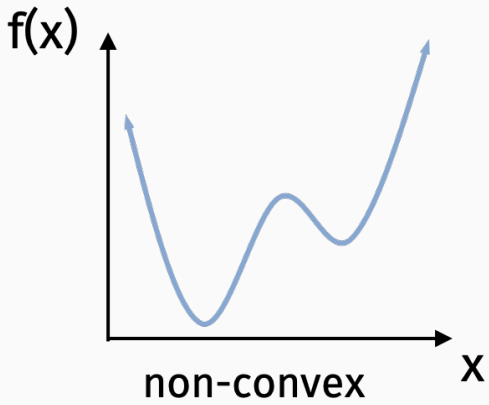
For a non-convex function $f(\mathbf{x})$: For sufficiently small η and a sufficiently large number of iterations T, gradient descent will converge to a near stationary point:

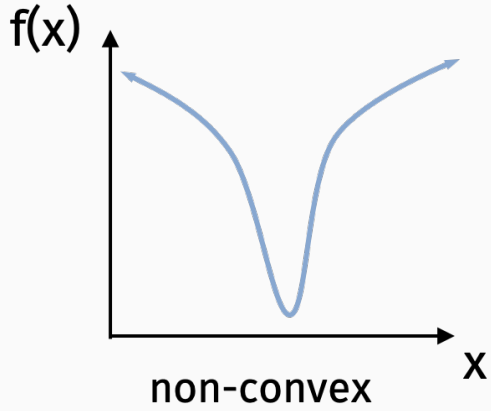
$$\|\nabla f(\mathbf{x}^{(T)})\|_2 \leq \epsilon.$$

Examples: neural networks, matrix completion problems, mixture models.

CONVEX VS. NON-CONVEX







One issue with non-convex functions is that they can have local minima. Even when they don't, convergence analysis requires different assumptions than convex functions.

APPROACH FOR THIS UNIT

We care about how fast gradient descent and related methods converge, not just that they do converge.

- Bounding iteration complexity requires placing some assumptions on $f(\mathbf{x})$.
- Stronger assumptions lead to better bounds on the convergence.

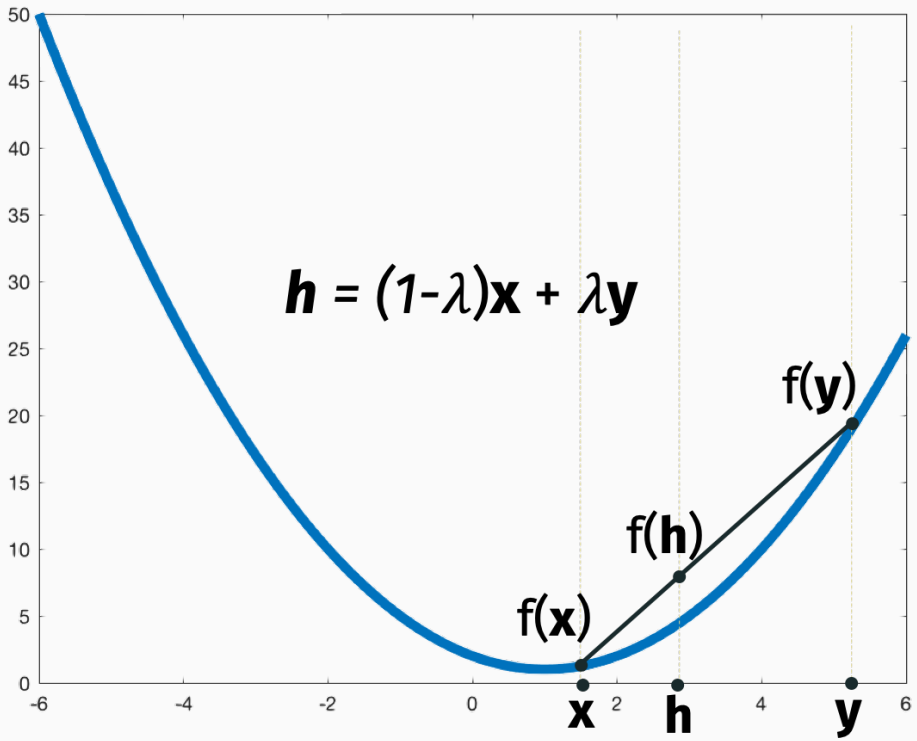
Understanding these assumptions can help us design faster variants of gradient descent (there are many!).

Today, we will start with **convex functions** only.

Definition (Convex)

A function f is convex iff for any $\mathbf{x}, \mathbf{y}, \lambda \in [0, 1]$:

$$(1 - \lambda) \cdot f(\mathbf{x}) + \lambda \cdot f(\mathbf{y}) \geq f((1 - \lambda) \cdot \mathbf{x} + \lambda \cdot \mathbf{y})$$



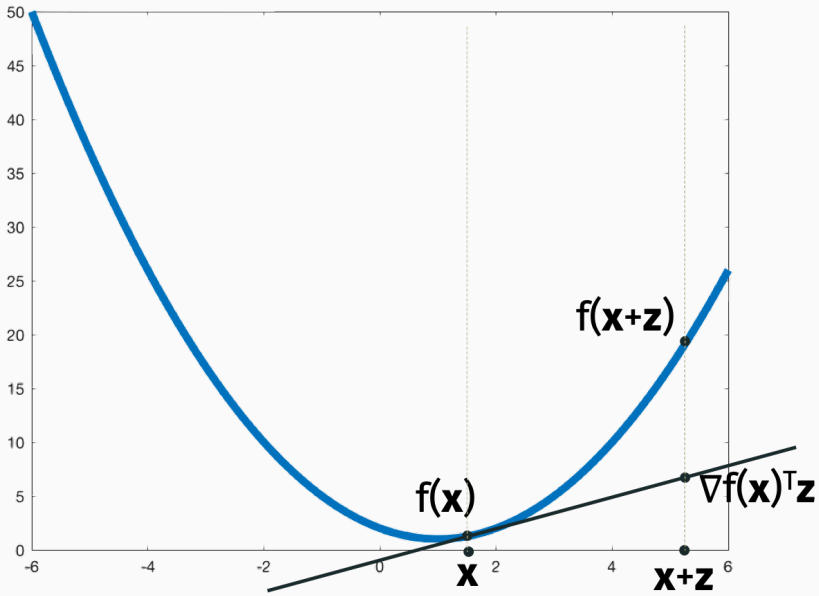
Definition (Convex)

A function f is convex if and only if for any $\mathbf{x}, \mathbf{y}$:

$$f(\mathbf{x}+\mathbf{z}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{z}$$

Equivalently:

$$f(\mathbf{x}) - f(\mathbf{y}) \leq \nabla f(\mathbf{x})^T (\mathbf{x}-\mathbf{y})$$



Assume:

- f is convex.
- Lipschitz function: for all $\mathbf{x}$, $\|\nabla f(\mathbf{x})\|_2 \leq G$.
- Starting radius: $\|\mathbf{x}^* - \mathbf{x}^{(0)}\|_2 \leq R$.

Gradient descent:

- Choose number of steps T.
- $\eta = \frac{R}{G\sqrt{T}}$
- For $i = 0, \ldots, T$:
  - $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$
- Return $\hat{\mathbf{x}} = \arg\min_i f(\mathbf{x}^{(i)})$.

Claim (GD Convergence Bound)

If $T \geq \frac{R^2 G^2}{\epsilon^2}$, *then* $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Proof is made tricky by the fact that $f(\mathbf{x}^{(i)})$ does not improve monotonically. We can "overshoot" the minimum.

Claim (GD Convergence Bound)

If $T \geq \frac{R^2 G^2}{\epsilon^2}$ *and* $\eta = \frac{R}{G\sqrt{T}}$, *then* $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Claim 1: For all $i = 0, \ldots, T$,

$$f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(i+1)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$

Claim (GD Convergence Bound)

If $T \geq \frac{R^2 G^2}{\epsilon^2}$ *and* $\eta = \frac{R}{G\sqrt{T}} = \frac{\epsilon}{G^2}$, *then* $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

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Telescoping sum:

$$\sum_{i=0}^{T-1} \left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right] \leq \frac{\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{T\eta G^2}{2}$$

$$\frac{1}{T} \sum_{i=0}^{T-1} \left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right] \leq \frac{R^2}{2T\eta} + \frac{\eta G^2}{2}$$

Claim (GD Convergence Bound)

If $T \geq \frac{R^2 G^2}{\epsilon^2}$ *and* $\eta = \frac{R}{G\sqrt{T}} = \frac{\epsilon}{G^2}$, *then* $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Final step:

$$\frac{1}{T}\sum_{i=0}^{T-1}\left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*)\right] \leq \epsilon$$

$$\left[\frac{1}{T}\sum_{i=0}^{T-1} f(\mathbf{x}^{(i)})\right] - f(\mathbf{x}^*) \leq \epsilon$$

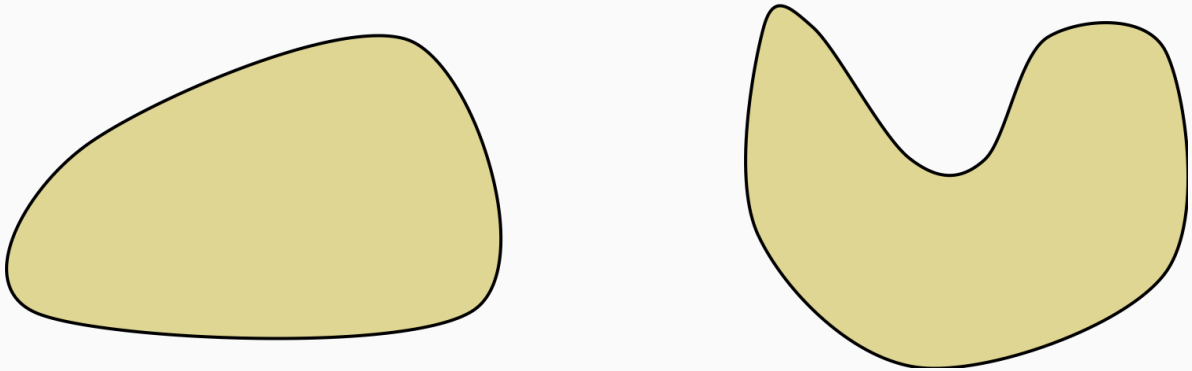
We always have that $\min_i f(\mathbf{x}^{(i)}) \leq \frac{1}{T}\sum_{i=0}^{T-1} f(\mathbf{x}^{(i)})$, so this is what we return:

$$f(\hat{\mathbf{x}}) = \min_{i \in 1,\ldots,T} f(\mathbf{x}^{(i)}) \leq f(\mathbf{x}^*) + \epsilon.$$

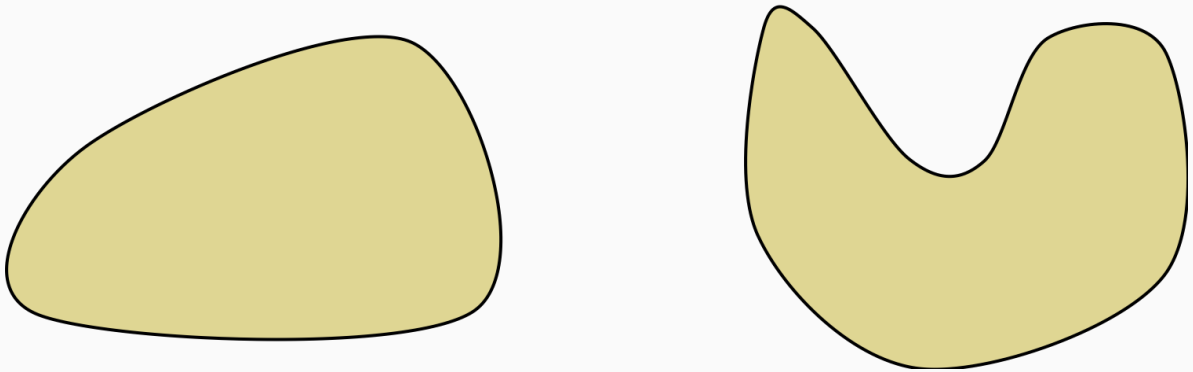
Typical goal: Solve a convex minimization problem with additional convex constraints.

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x})$$

where $\mathcal{S}$ is a convex set.



Which of these is convex?



Definition (Convex set)

A set $\mathcal{S}$ is convex if for any $\mathbf{x}, \mathbf{y} \in \mathcal{S}, \lambda \in [0, 1]$:

$$(1 - \lambda)\mathbf{x} + \lambda\mathbf{y} \in \mathcal{S}.$$

PROBLEM WITH GRADIENT DESCENT

Gradient descent:

- For $i = 0, \ldots, T$:
  - $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$
- Return $\hat{\mathbf{x}} = \arg\min_i f(\mathbf{x}^{(i)})$.

Even if we start with $\mathbf{x}^{(0)} \in \mathcal{S}$, there is no guarantee that $\mathbf{x}^{(0)} - \eta \nabla f(\mathbf{x}^{(0)})$ will remain in our set.

Extremely simple modification: Force $\mathbf{x}^{(i)}$ to be in $\mathcal{S}$ by projecting onto the set.

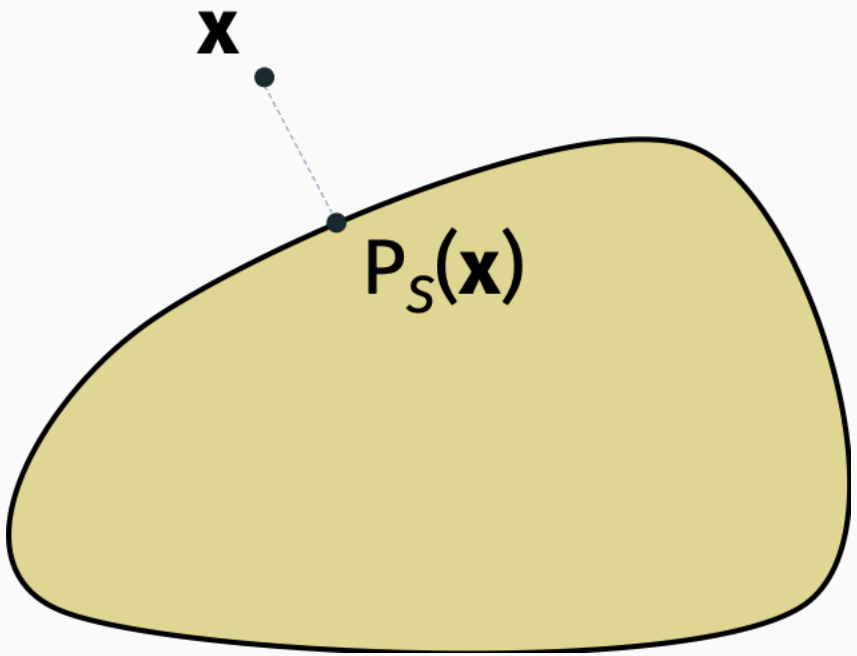
Given a function f to minimize and a convex constraint set $\mathcal{S}$, assume we have:

- **Function oracle**: Evaluate $f(\mathbf{x})$ for any $\mathbf{x}$.
- **Gradient oracle**: Evaluate $\nabla f(\mathbf{x})$ for any $\mathbf{x}$.
- Projection oracle: Evaluate $P_{\mathcal{S}}(\mathbf{x})$ for any $\mathbf{x}$.

$$P_{\mathcal{S}}(\mathbf{x}) = \arg\min_{\mathbf{y} \in \mathcal{S}} \|\mathbf{x} - \mathbf{y}\|_2$$

PROJECTION ORACLES

- How would you implement $P_{\mathcal{S}}$ for $\mathcal{S} = \{\mathbf{y} : \|\mathbf{y}\|_2 \leq 1\}$.
- How would you implement $P_{\mathcal{S}}$ for $\mathcal{S} = \{\mathbf{y} : \mathbf{y} = \mathbf{Q}\mathbf{z}\}$.



Given function $f(\mathbf{x})$ and set $\mathcal{S}$, such that $\|\nabla f(\mathbf{x})\|_2 \leq G$ for all $\mathbf{x} \in \mathcal{S}$ and starting point $\mathbf{x}^{(0)}$ with $\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2 \leq R$.

Projected gradient descent:

- Select starting point $\mathbf{x}^{(0)}$, $\eta = \frac{R}{G\sqrt{T}}$.
- For $i = 0, \ldots, T$:
  - $\mathbf{z} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$
  - $\mathbf{x}^{(i+1)} = P_{\mathcal{S}}(\mathbf{z})$
- Return $\hat{\mathbf{x}} = \arg\min_i f(\mathbf{x}^{(i)})$.

Claim (PGD Convergence Bound)

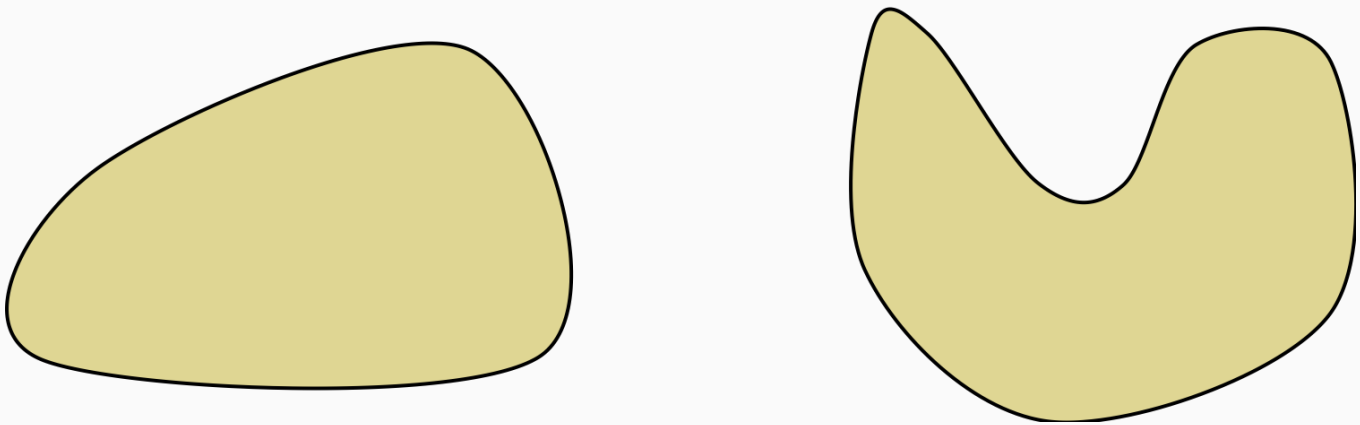
If $f, \mathcal{S}$ are convex and $T \geq \frac{R^2 G^2}{\epsilon^2}$, then $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Analysis is almost identical to standard gradient descent! We just need one additional claim:

Claim (Contraction Property of Convex Projection)

If $\mathcal{S}$ is convex, then for <u>any</u> $\mathbf{y} \in \mathcal{S}$,

$$\|\mathbf{y} - P_{\mathcal{S}}(\mathbf{x})\|_2 \leq \|\mathbf{y} - \mathbf{x}\|_2.$$



Claim (PGD Convergence Bound)

If $f, \mathcal{S}$ are convex and $T \geq \frac{R^2 G^2}{\epsilon^2}$, then $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Claim 1: For all $i = 0, \ldots, T$,

$$f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{z} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$
$$\leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(i+1)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$

Same telescoping sum argument:

$$\left[\frac{1}{T}\sum_{i=0}^{T-1} f(\mathbf{x}^{(i)})\right] - f(\mathbf{x}^*) \leq \frac{R^2}{2T\eta} + \frac{\eta G^2}{2}.$$