10-701: Introduction to Machine Learning

Lecture 5 – MLE & MAP

Hoda Heidari

* Slides adopted from F24 offering of 10701 by Henry Chai.

Recipe for Linear Regression

1. Define a model and model parameters
   1. Assume $y = \boldsymbol{w}^T \boldsymbol{x}$
   2. Parameters: $\boldsymbol{w} = [w_0, w_1, \dots, w_D]$

2. Write down an objective function
   1. Minimize the mean squared error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2$$

3. Optimize the objective w.r.t. the model parameters
   1. Solve in *closed form*: take partial derivatives, set to 0 and solve

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \frac{1}{N}\sum_{n=1}^{N}\left({\boldsymbol{x}^{(n)}}^T\boldsymbol{w} - y^{(n)}\right)^2$$

$$= \frac{1}{N}\|X\boldsymbol{w} - \boldsymbol{y}\|_2^2 \text{ where } \|\boldsymbol{z}\|_2 = \sqrt{\sum_{d=1}^{D} z_d^2} = \sqrt{\boldsymbol{z}^T\boldsymbol{z}}$$

$$= \frac{1}{N}(X\boldsymbol{w} - \boldsymbol{y})^T(X\boldsymbol{w} - \boldsymbol{y})$$

$$= \frac{1}{N}(\boldsymbol{w}^T X^T X\boldsymbol{w} - 2\boldsymbol{w}^T X^T\boldsymbol{y} + \boldsymbol{y}^T\boldsymbol{y})$$

$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}(\widehat{\boldsymbol{w}}) = \frac{1}{N}(2X^T X\widehat{\boldsymbol{w}} - 2X^T\boldsymbol{y}) = 0$$

$$\rightarrow X^T X\widehat{\boldsymbol{w}} = X^T\boldsymbol{y}$$

$$\rightarrow \widehat{\boldsymbol{w}} = (X^T X)^{-1}X^T\boldsymbol{y}$$

$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

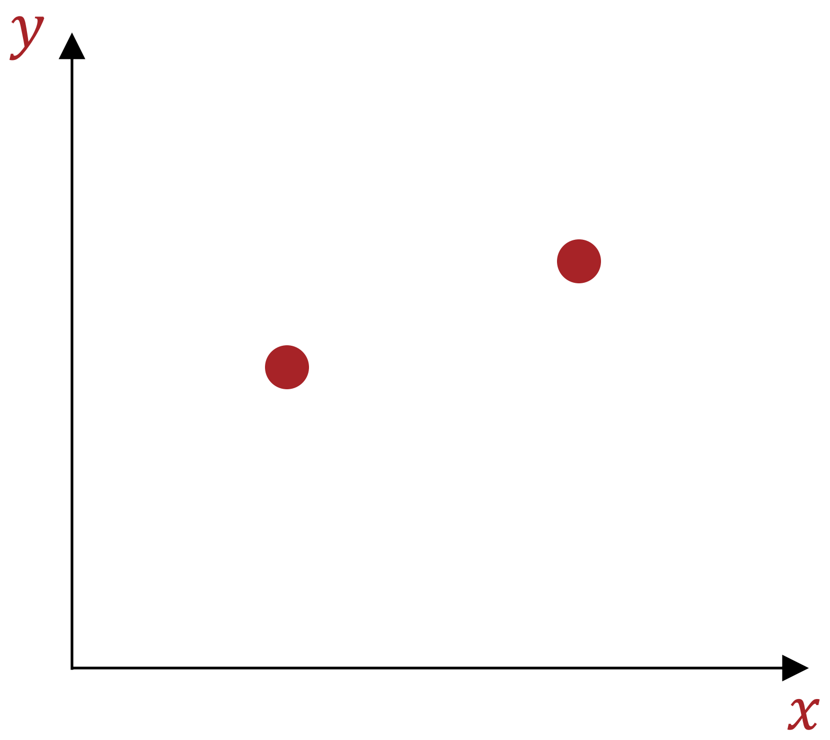
Closed Form Solution

1. Is $X^T X$ invertible?

2. If so, how computationally expensive is inverting $X^T X$?

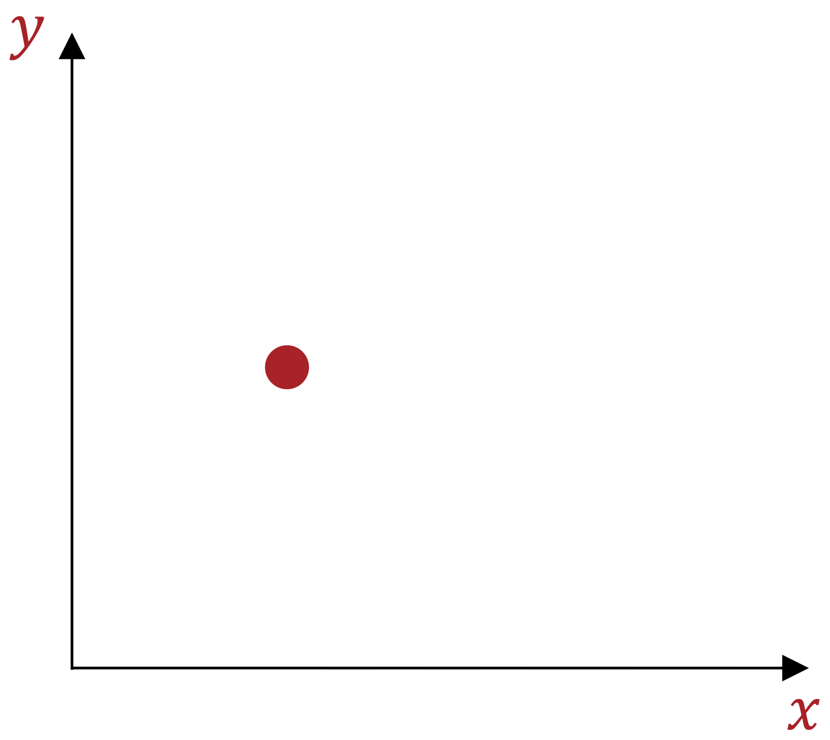
Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



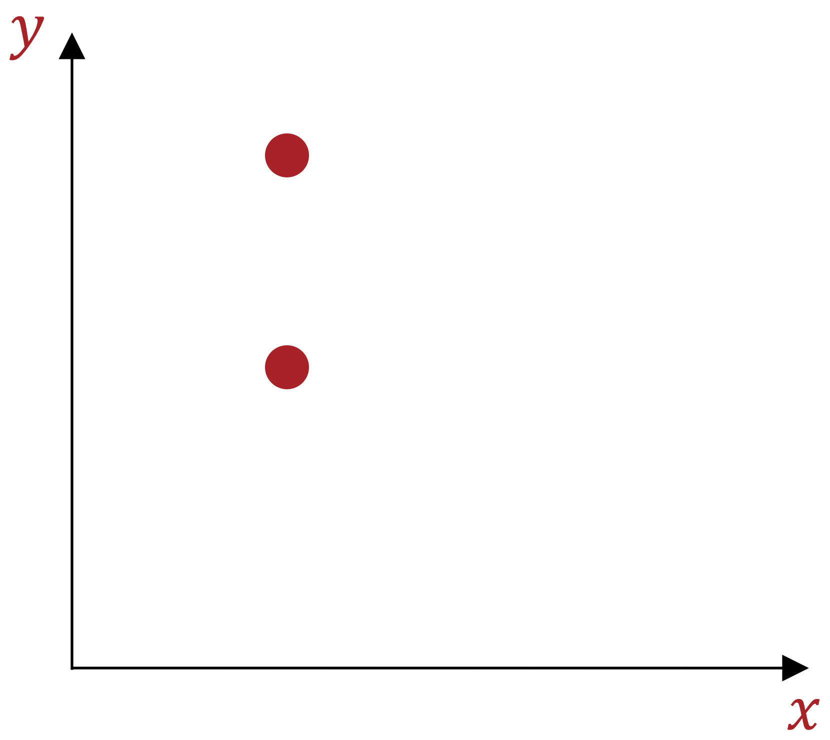
Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



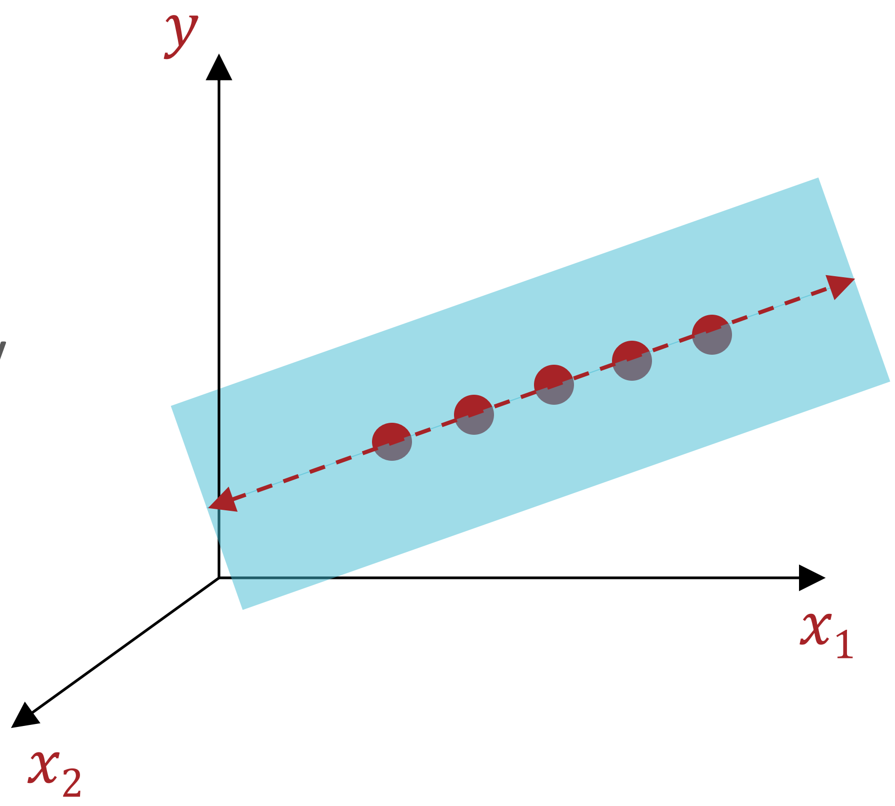
Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



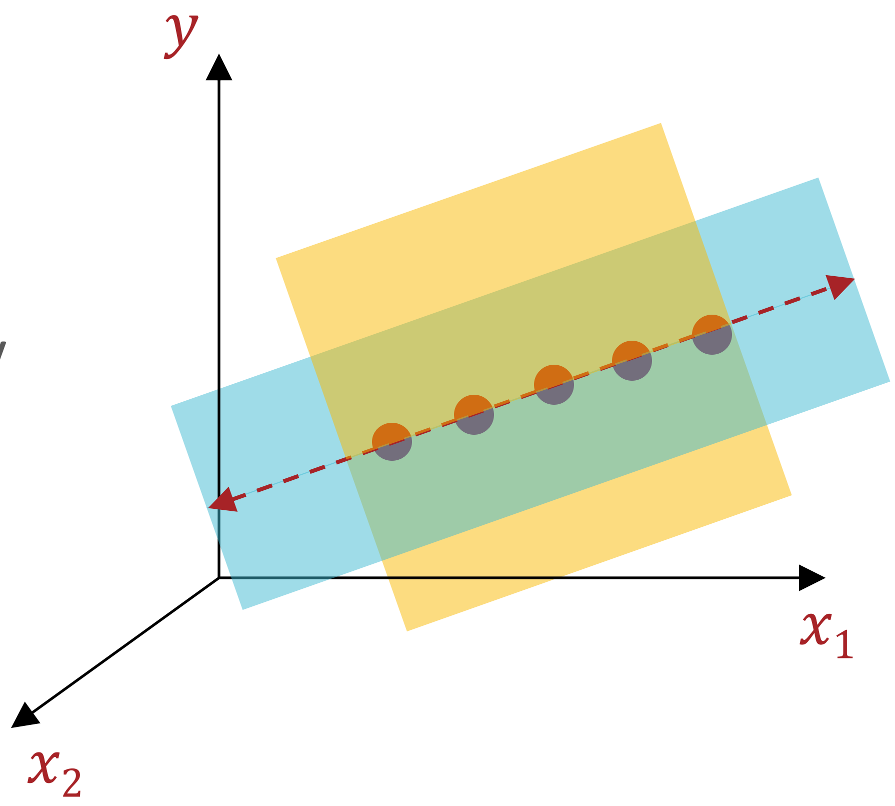
Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



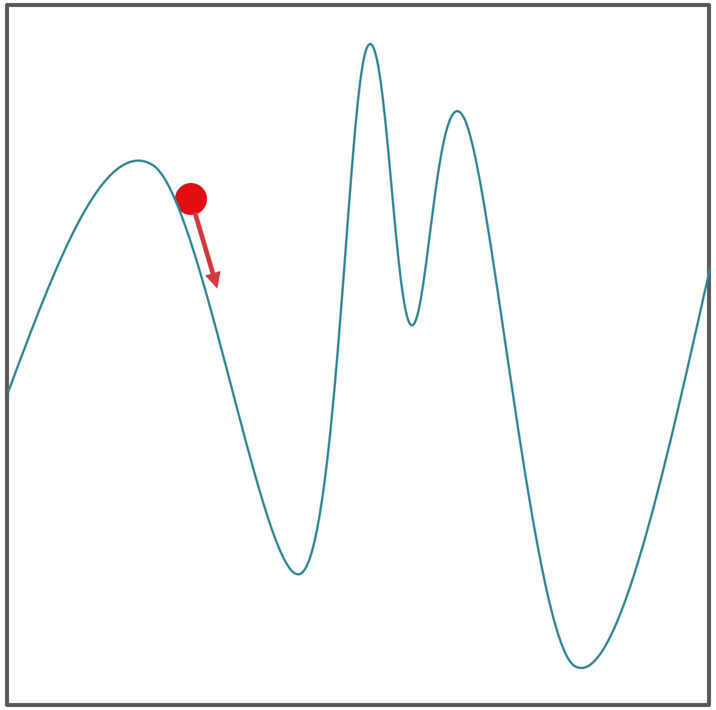
$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Closed Form Solution

1. Is $X^T X$ invertible?
   - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible
   - If $X^T X$ is not invertible (occurs when one of the features is a linear combination of the others) then there are infinitely many solutions.
2. If so, how computationally expensive is inverting $X^T X$?
   - $X^T X \in \mathbb{R}^{D+1 \times D+1}$ so inverting $X^T X$ takes $O(D^3)$ time…
     - Computing $X^T X$ takes $O(ND^2)$ time
   - What alternative optimization method can we use to minimize the mean squared error?

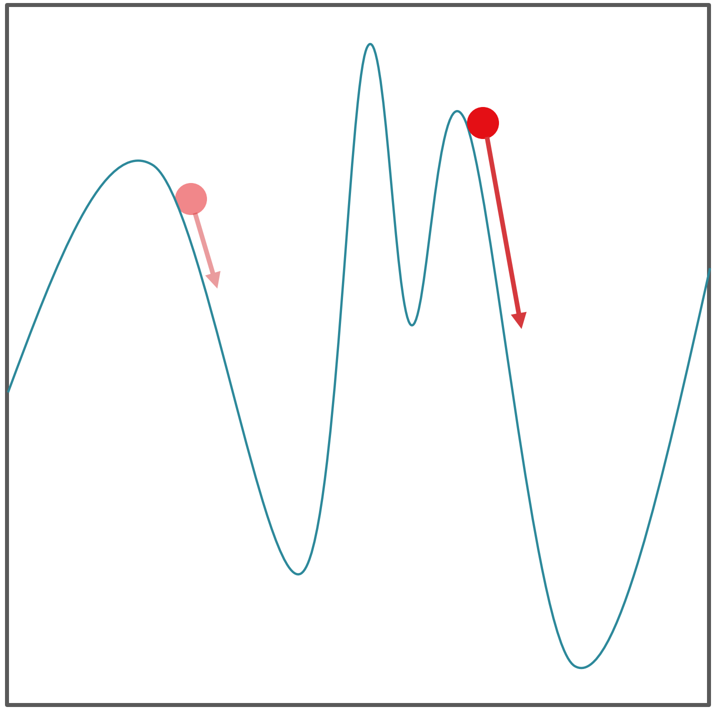
Gradient Descent: Intuition

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



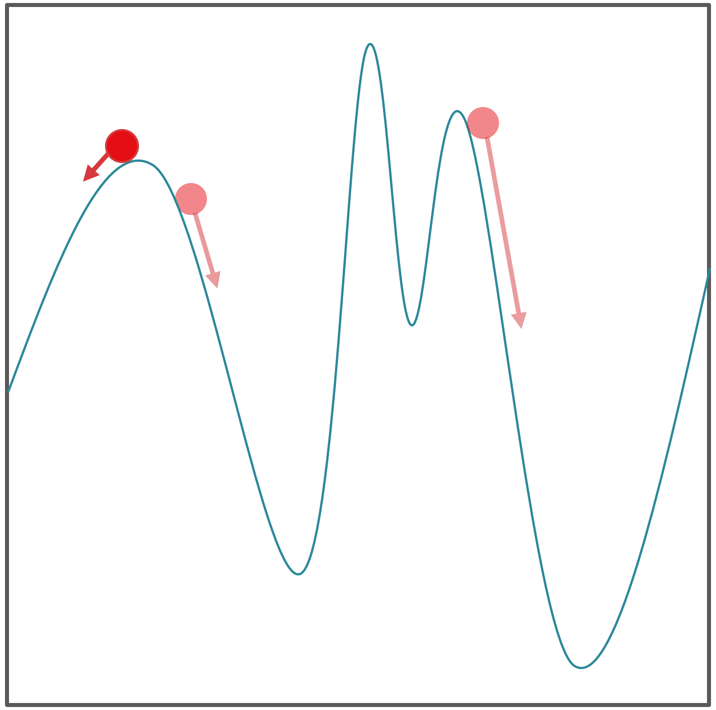
Gradient Descent: Intuition

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



Gradient Descent: Intuition

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



Gradient Descent

- Suppose the current weight vector is $\boldsymbol{w}^{(t)}$
- Move some distance, η, in the "most downhill" direction, $\widehat{\boldsymbol{v}}$:

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta \widehat{\boldsymbol{v}}$$

Gradient Descent: Step Direction

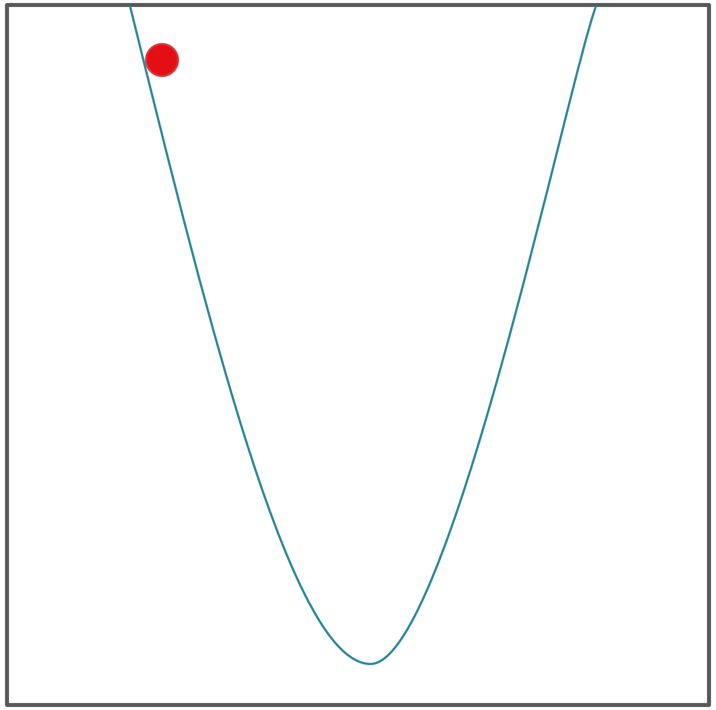
- Suppose the current weight vector is $\boldsymbol{w}^{(t)}$
- Move some distance, η, in the "most downhill" direction, $\hat{\boldsymbol{v}}$:

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta \hat{\boldsymbol{v}}$$

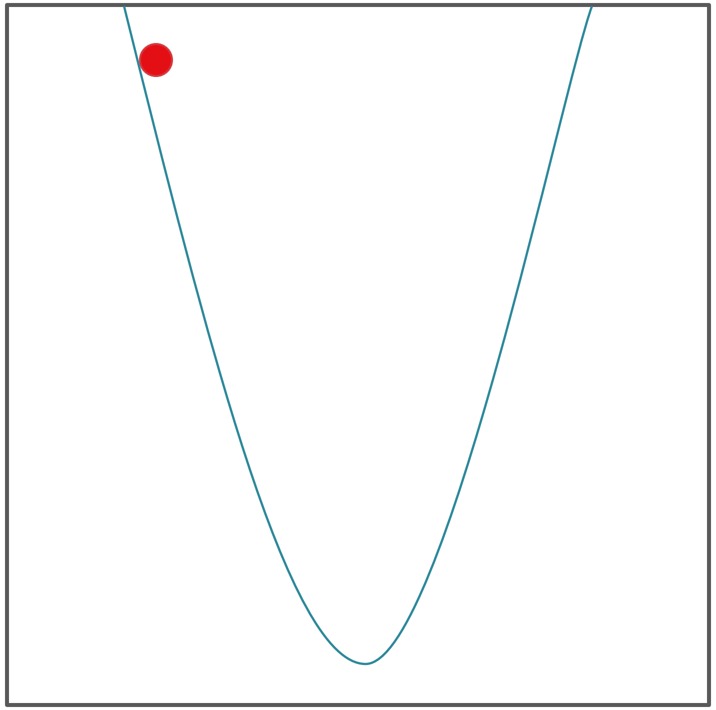
- The gradient points in the direction of steepest *increase* …
- … so $\hat{\boldsymbol{v}}$ should point in the opposite direction:

$$\hat{\boldsymbol{v}}^{(t)} = -\frac{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)}{\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|}$$

Gradient Descent: Step Size

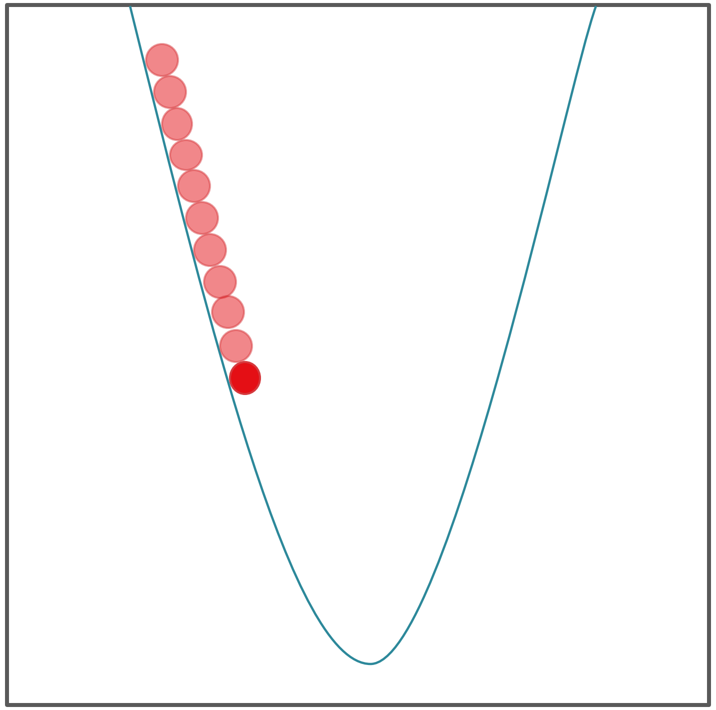


Small η

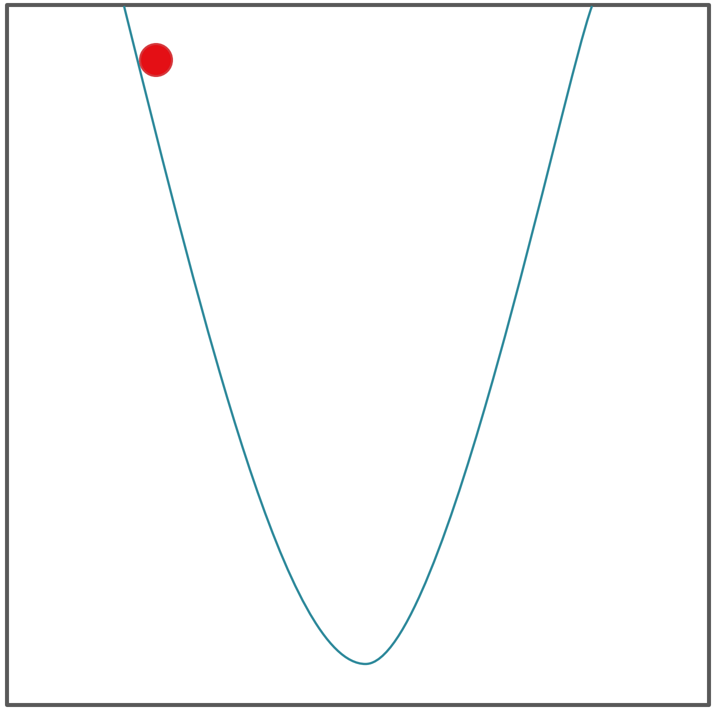


Large η

Gradient Descent: Step Size

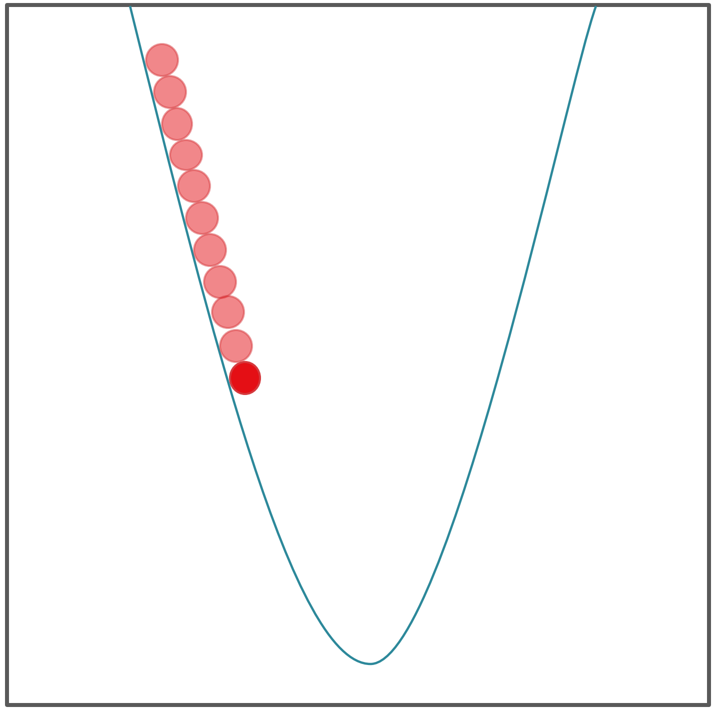


Small η

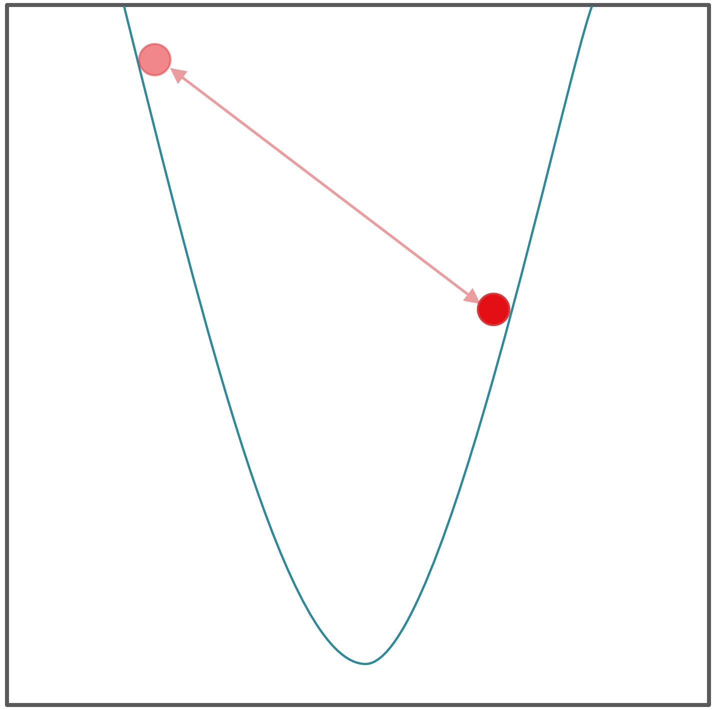


Large η

Gradient Descent: Step Size



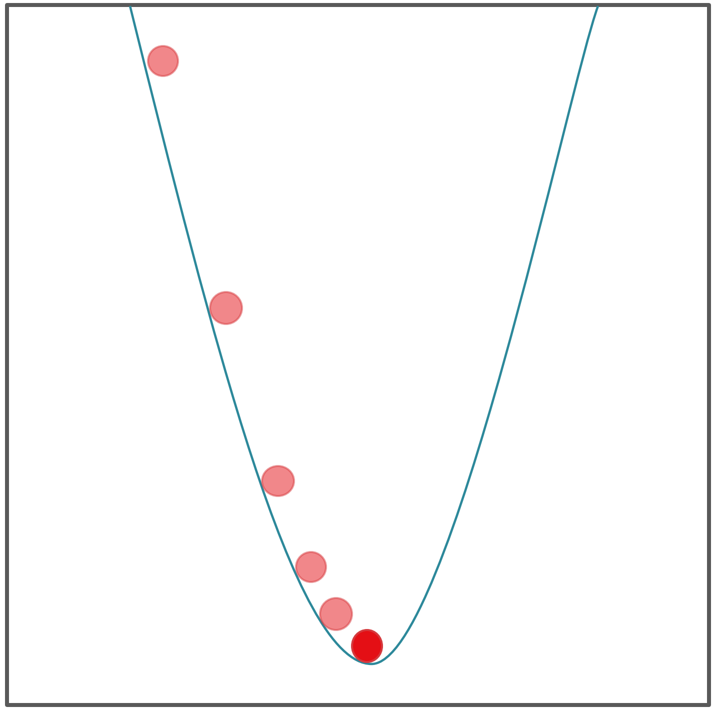
Small η



Large η

Gradient Descent: Step Size

- Use a variable $\eta^{(t)}$ instead of a fixed η!



- Set $\eta^{(t)} = \eta^{(0)} \left\| \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}} \left(\boldsymbol{w}^{(t)} \right) \right\|$
- $\left\| \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}} \left(\boldsymbol{w}^{(t)} \right) \right\|$ decreases as $\ell_{\mathcal{D}}$ approaches its minimum $\rightarrow \eta^{(t)}$ (hopefully) decreases over time

Gradient Descent

- $\hat{\boldsymbol{v}}^{(t)} = -\frac{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)}{\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|}$

- $\eta^{(t)} = \eta^{(0)}\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|$

- $\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta^{(t)}\hat{\boldsymbol{v}}^{(t)}$
  $=$

Gradient Descent

- $\hat{\boldsymbol{v}}^{(t)} = -\frac{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)}{\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|}$

- $\eta^{(t)} = \eta^{(0)} \left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|$

- $$\begin{aligned}\boldsymbol{w}^{(t+1)} &= \boldsymbol{w}^{(t)} + \eta^{(t)} \hat{\boldsymbol{v}}^{(t)} \\ &= \boldsymbol{w}^{(t)} + \left(\eta^{(0)} \left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|\right)\left(-\frac{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)}{\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\|}\right) \\ &= \boldsymbol{w}^{(t)} - \eta^{(0)} \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\end{aligned}$$

Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}, \eta$

1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Compute the gradient:
      $\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   b. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}, \eta, \epsilon$

1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While $\left\|\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)\right\| > \epsilon$
   a. Compute the gradient:
      $\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   b. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Gradient Descent

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}, \eta, T$

1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While $t < T$
   a. Compute the gradient:
      $\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   b. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Why Gradient Descent for linear regression?

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}, \eta, T$

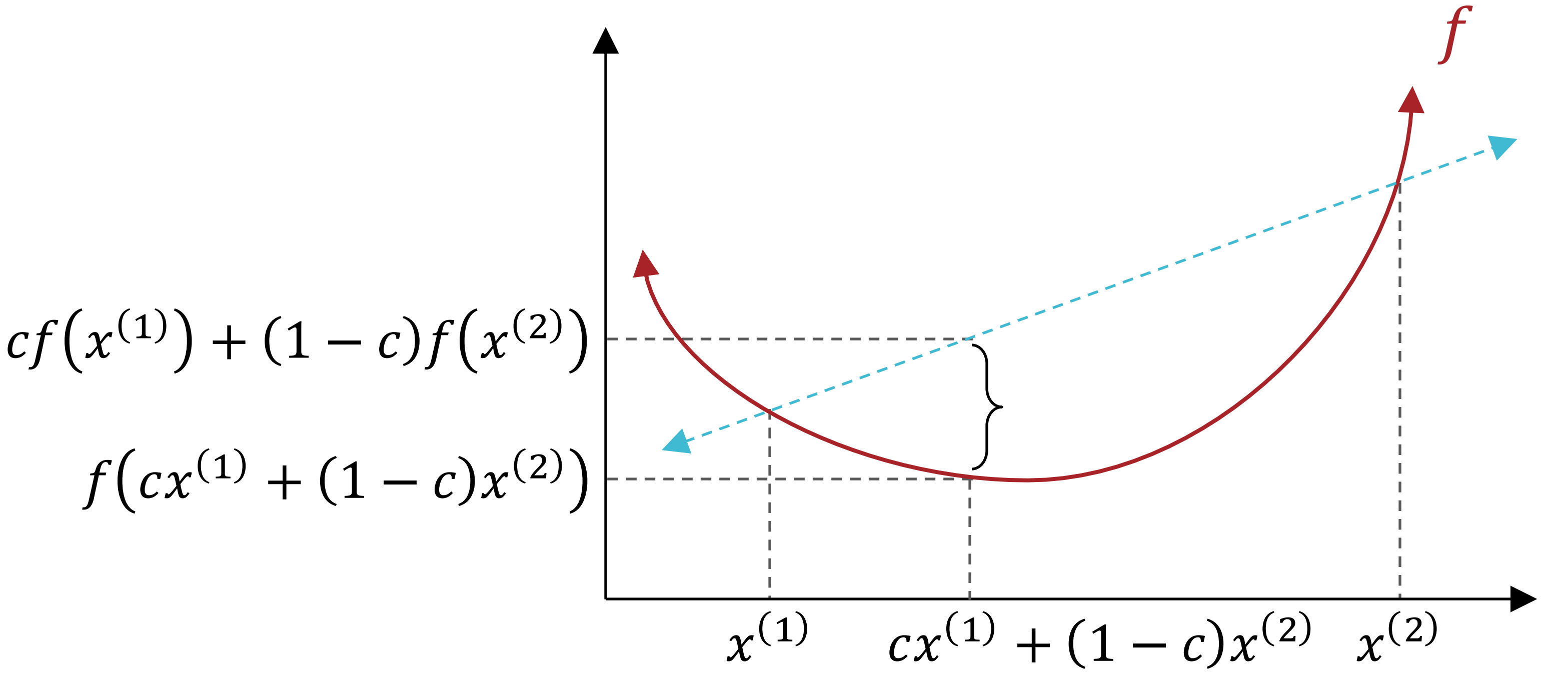
1. Initialize $\boldsymbol{w}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Compute the gradient:
      $\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   b. Update $\boldsymbol{w}$: $\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$
   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{w}^{(t)}$

Convexity

- A function $f: \mathbb{R}^D \rightarrow \mathbb{R}$ is convex if $\forall\, \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

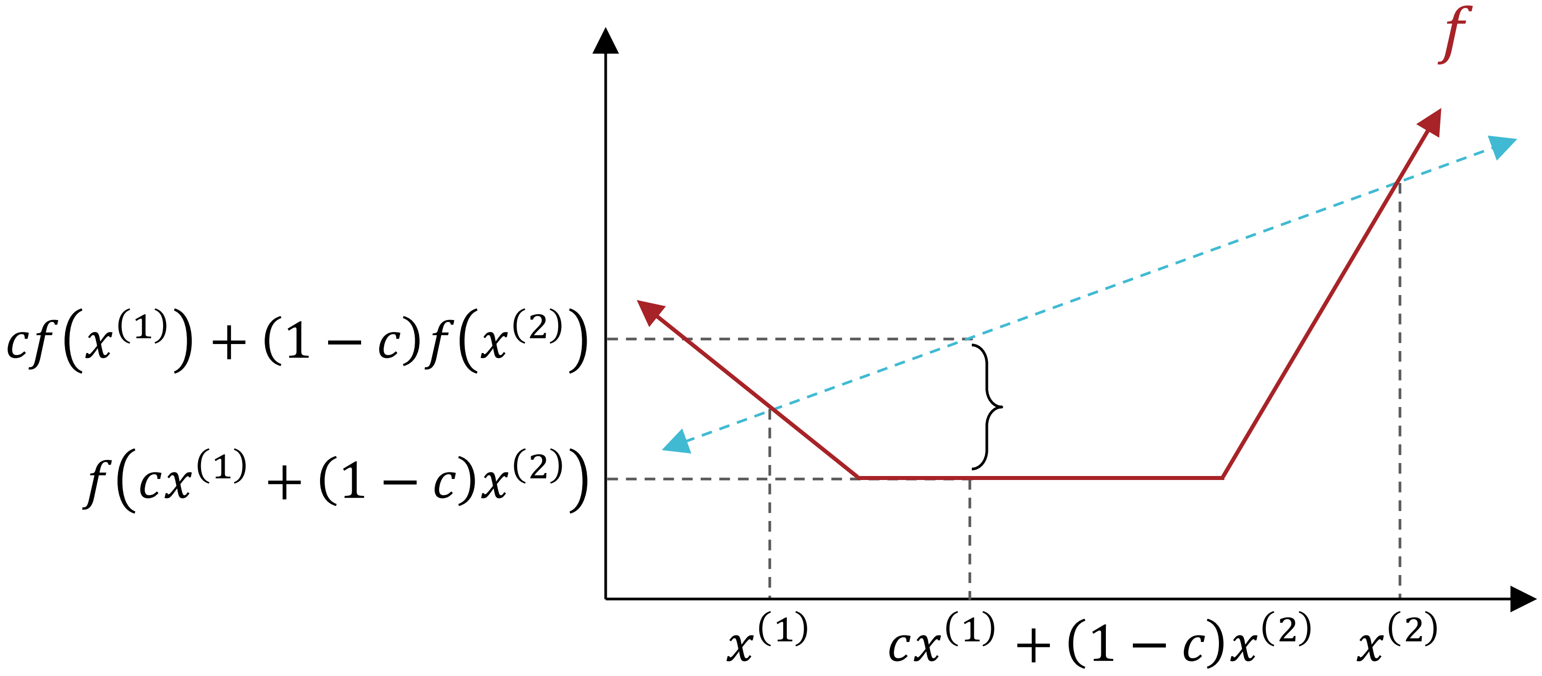
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f: \mathbb{R}^D \to \mathbb{R}$ is convex if $\forall\, \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

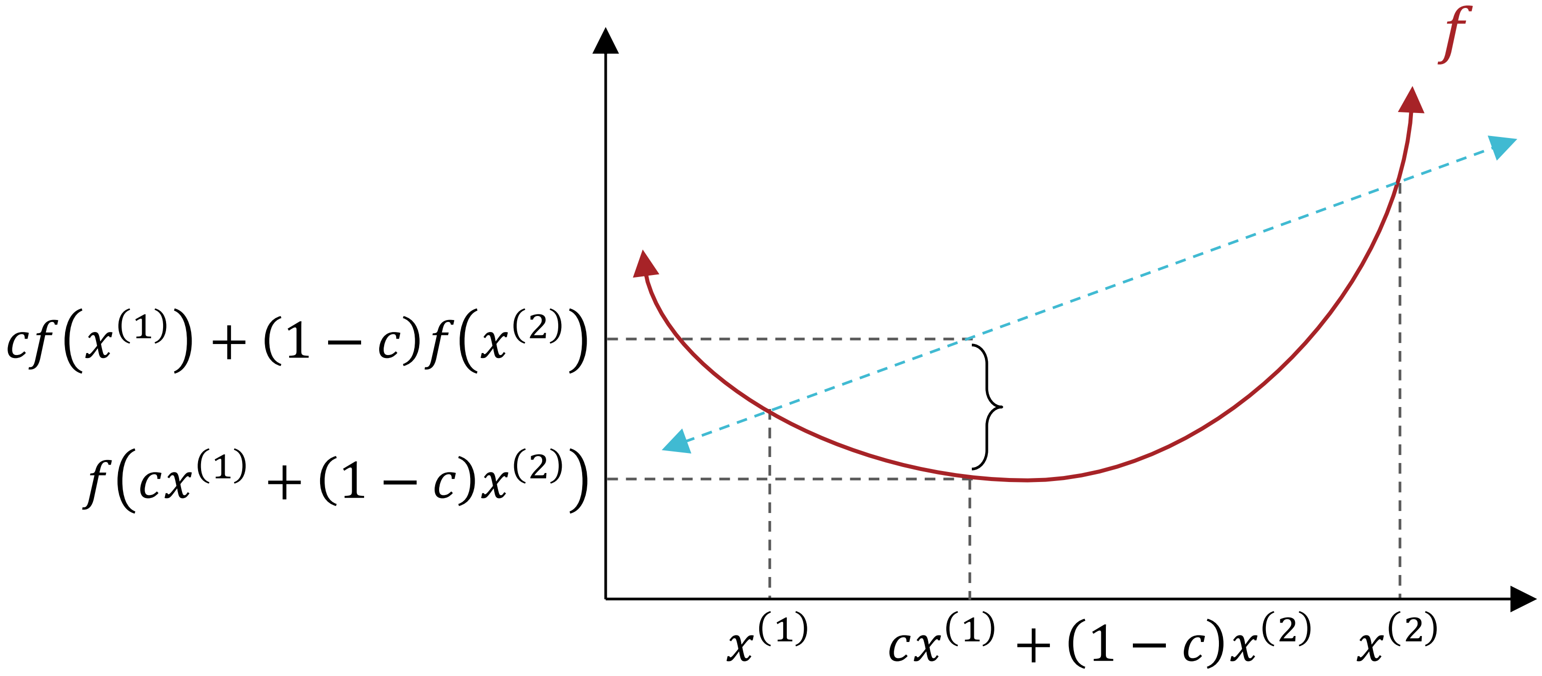
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



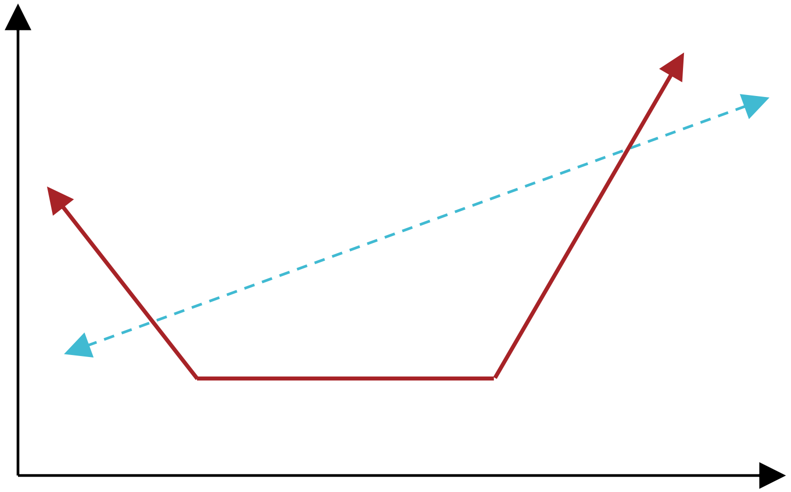
Strict Convexity

- A function $f: \mathbb{R}^D \to \mathbb{R}$ is *strictly* convex if $\forall\, \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 < c < 1$

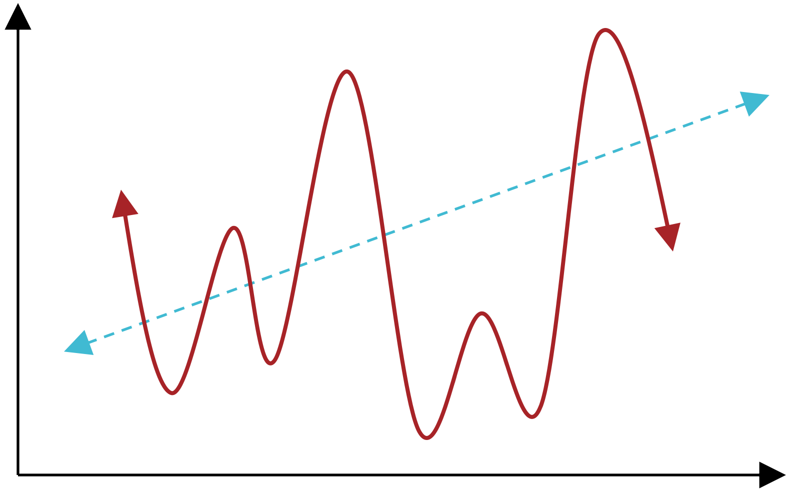
  $f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) < cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$



Examples

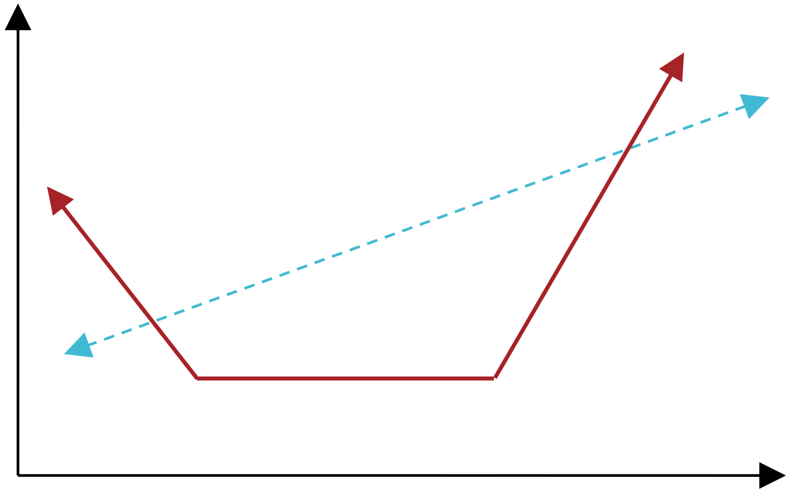


Convex functions



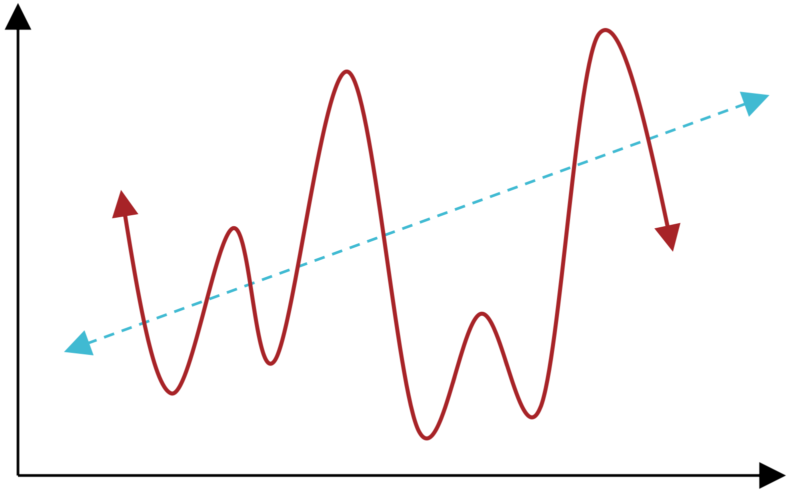
Non-convex functions

Local vs. Global Minimum



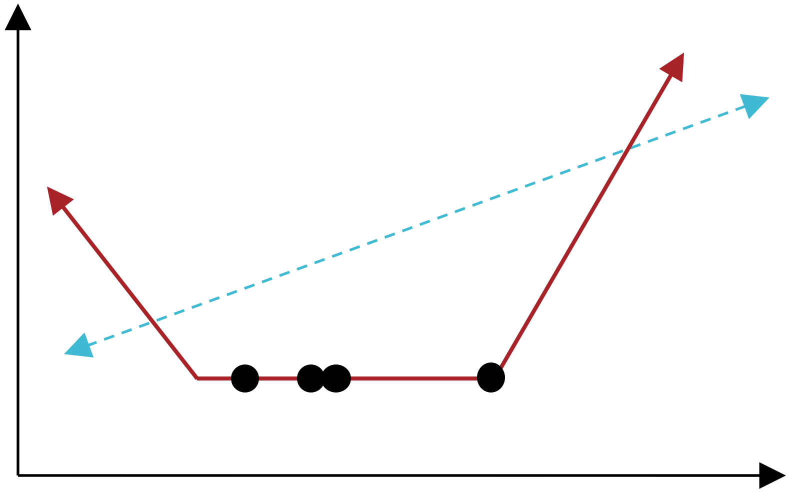
Given a function $f: \mathbb{R}^D \to \mathbb{R}$

- $\boldsymbol{x}^*$ is a *global* minimum iff $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \ \forall \ \boldsymbol{x} \in \mathbb{R}^D$



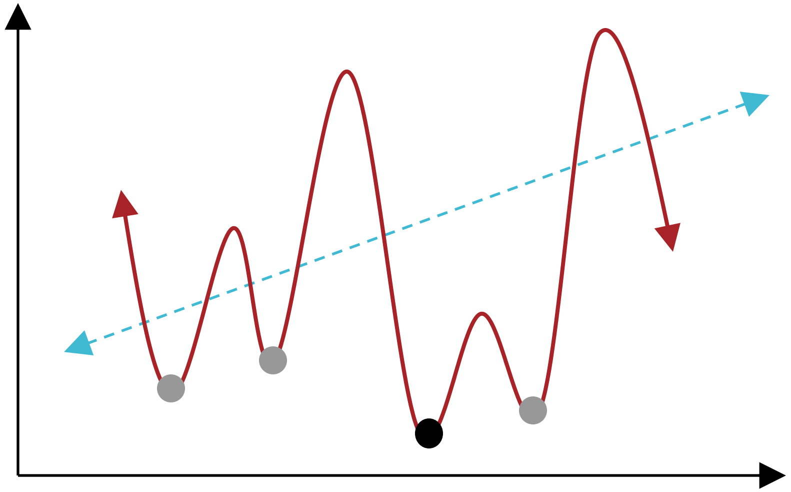
- $\boldsymbol{x}^*$ is a *local* minimum iff $\exists \ \epsilon$ s.t. $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \ \forall \ \boldsymbol{x}$ s.t. $\|\boldsymbol{x} - \boldsymbol{x}^*\|_2 < \epsilon$

Convexity



Convex functions:

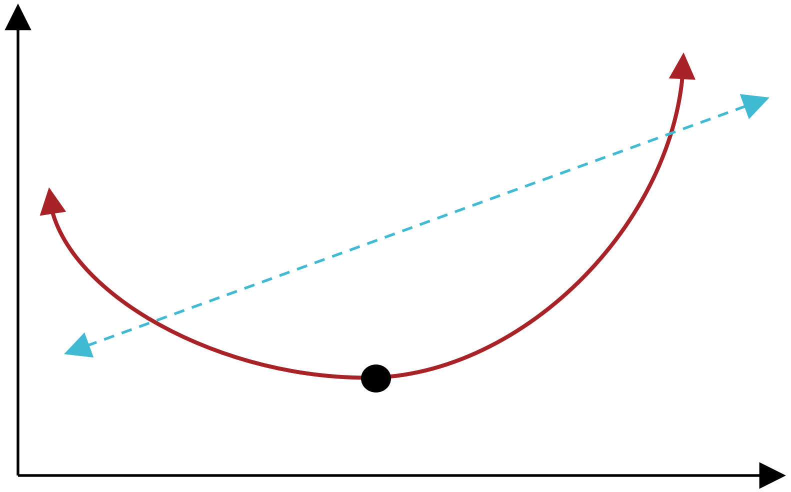
Each local minimum is a global minimum!



Non-convex functions:

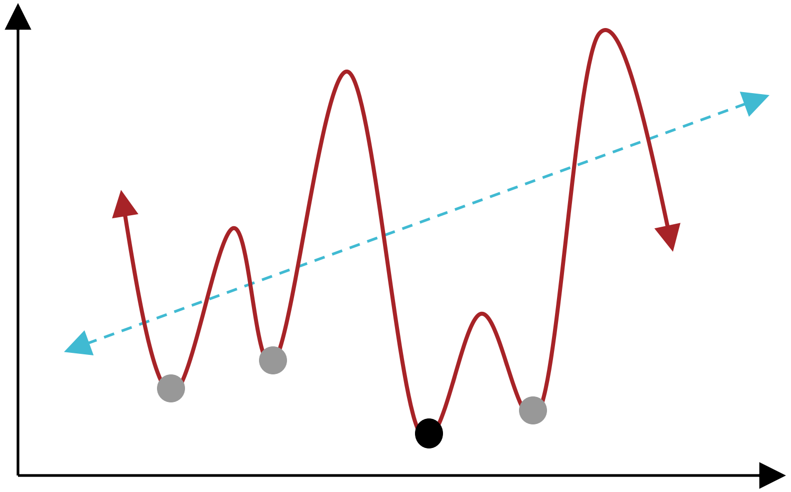
A local minimum may or may not be a global minimum…

Convexity



Strictly convex functions:

There exists a unique global minimum!

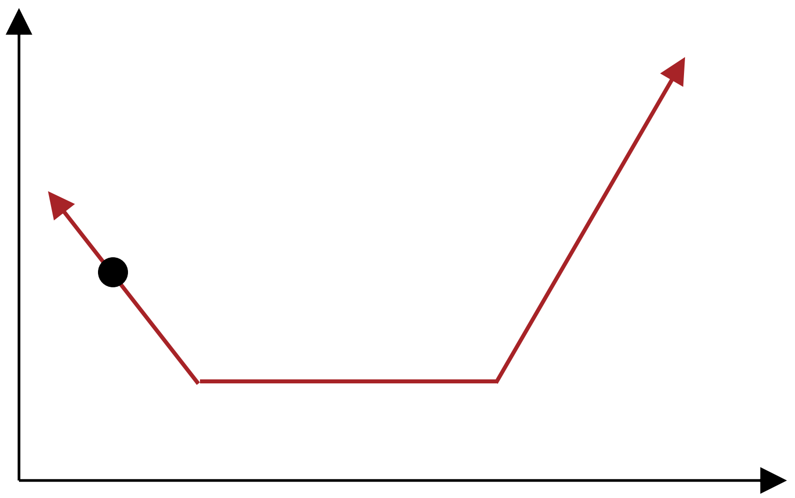


Non-convex functions:

A local minimum may or may not be a global minimum…

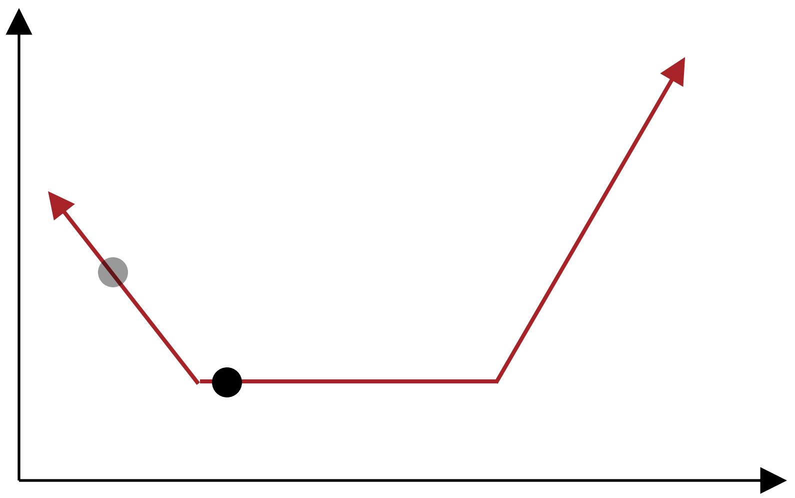
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



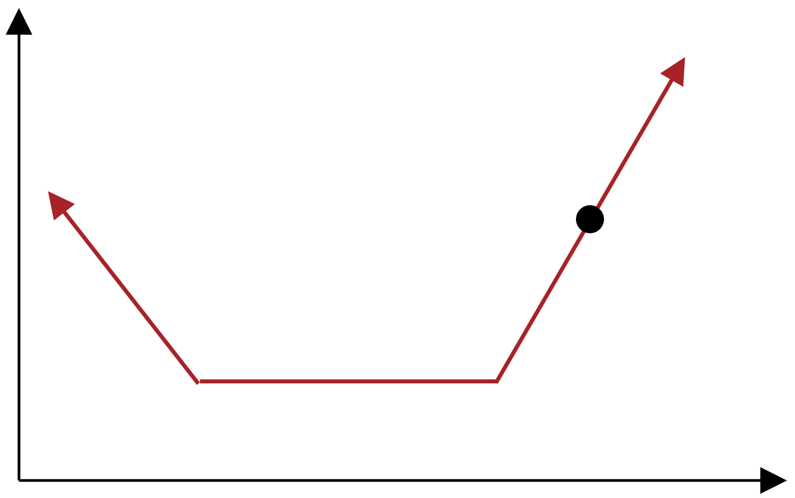
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



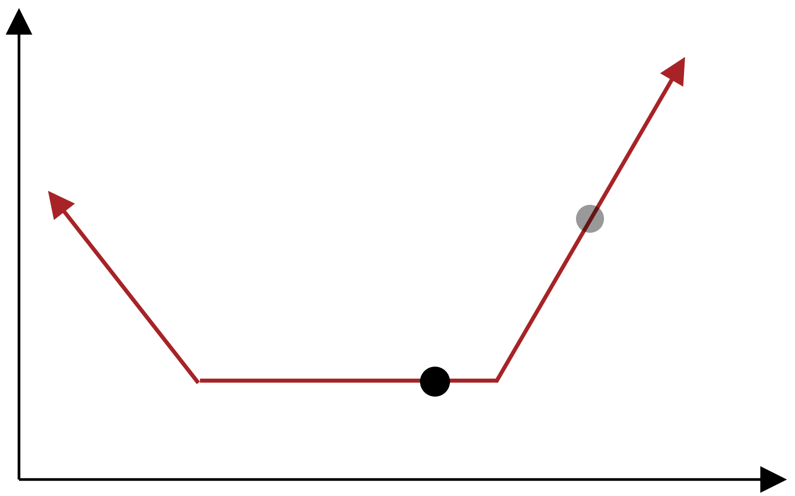
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



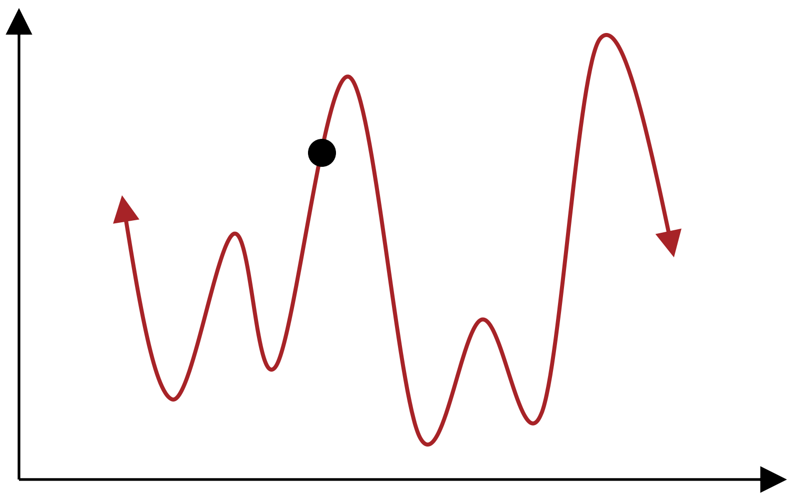
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



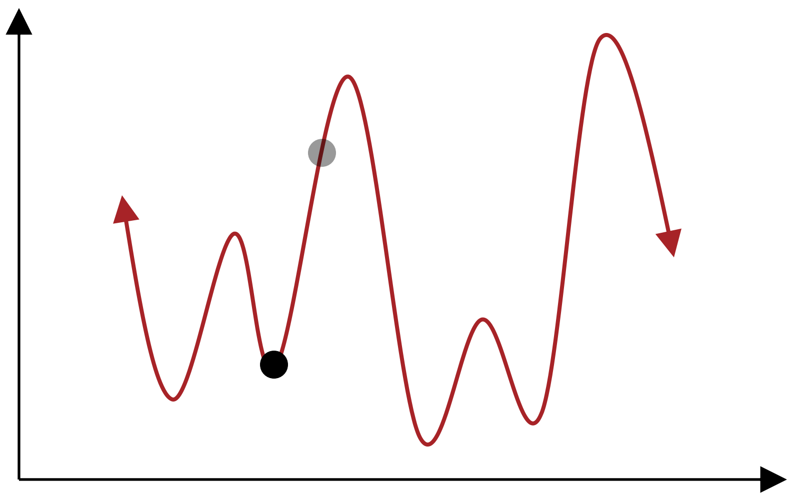
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



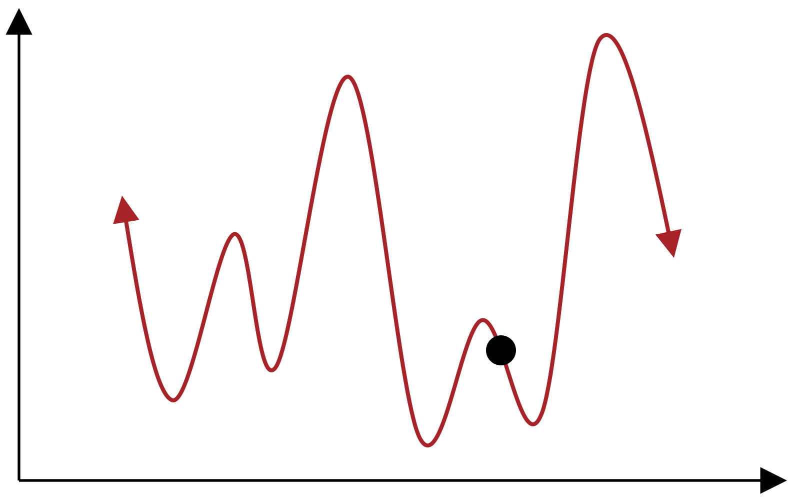
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



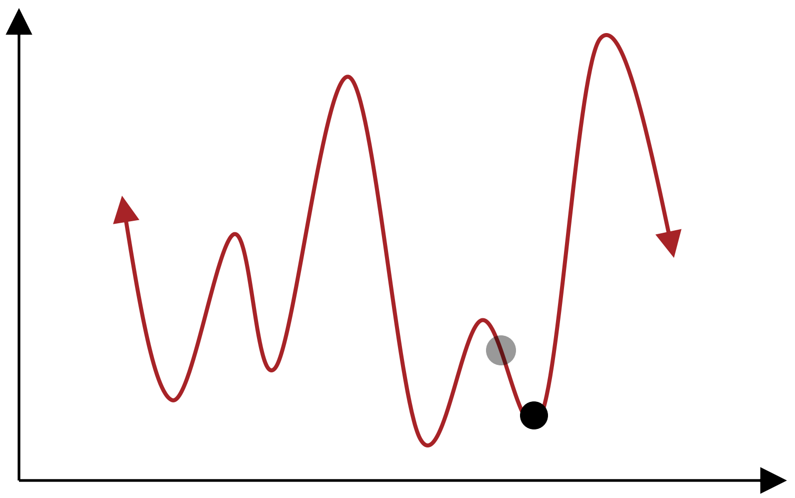
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



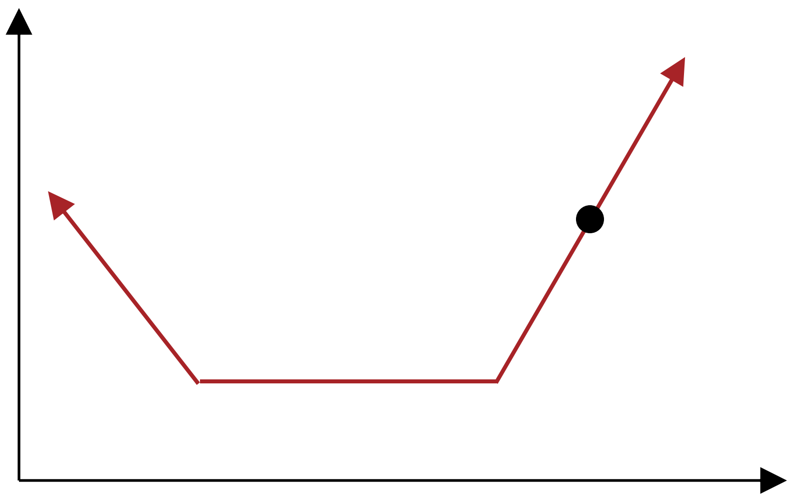
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



The squared error for linear regression is convex (but not strictly convex)!

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



$H_{\boldsymbol{w}} \ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{2}{N} X^T X$ which is positive *semi*-definite

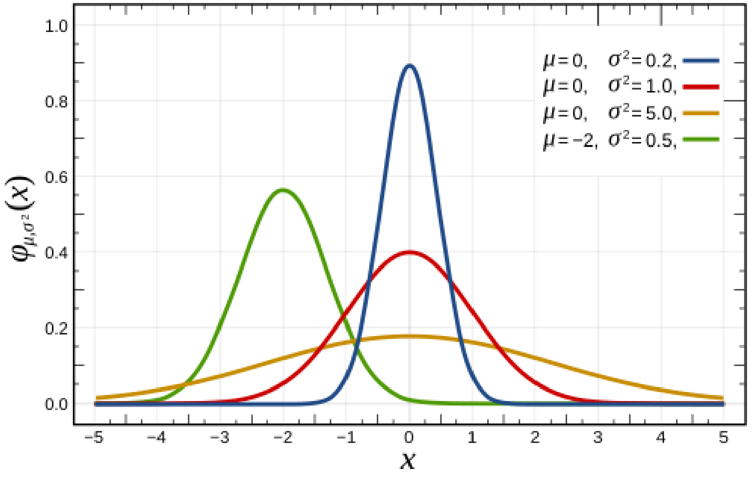
Key Takeaways

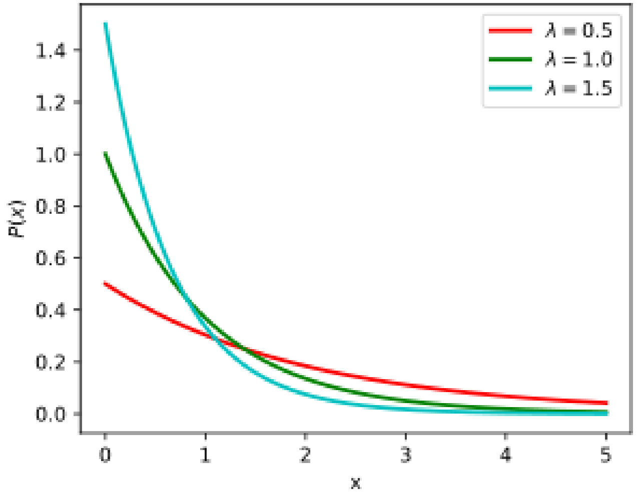
- Closed form solution for linear regression
  - Setting the gradient equal to 0 and solving for critical points
  - Potential issues: invertibility and computational costs
- Gradient descent
  - Effect of step size
  - Termination criteria
- Convexity vs. non-convexity
  - Strong vs. weak convexity
  - Implications for local, global and unique optima

Probabilistic Learning

- Previously:
  - (Unknown) Target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
  - Classifier, $h : \mathcal{X} \rightarrow \mathcal{Y}$
  - Goal: find a classifier, h, that best approximates c^*
- Now:
  - (Unknown) Target *distribution*, $y \sim p^*(Y|\boldsymbol{x})$
  - Distribution, $p(Y|\boldsymbol{x})$
  - Goal: find a distribution, p, that best approximates p^*
  - Suppose p comes from a parametric family of distributions, parameterized by θ

Parametric Distributions





Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \ldots, x^{(N)}\}$ of a random variable X
  - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{n=1}^{N} p\left(x^{(n)}|\theta\right)$$

  - If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{n=1}^{N} f\left(x^{(n)}|\theta\right)$$

Log-Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ of a random variable X
  - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

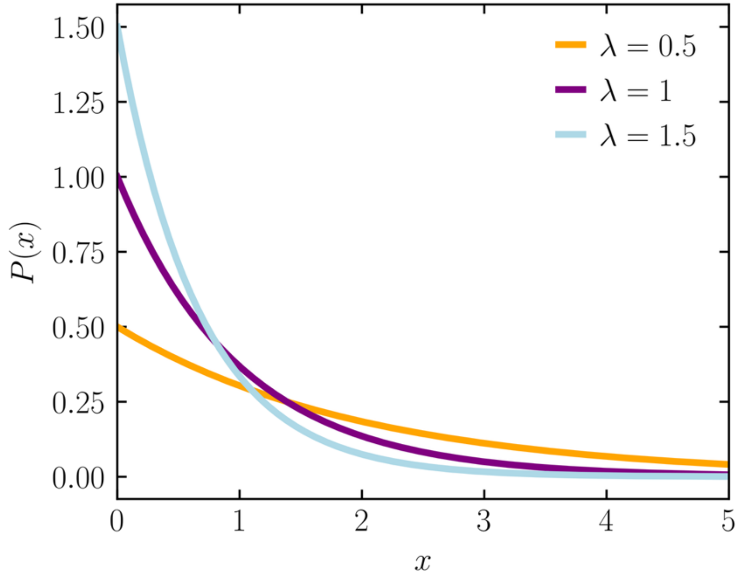
$$\ell(\theta) = \log \prod_{n=1}^{N} p\left(x^{(n)}|\theta\right) = \sum_{n=1}^{N} \log p\left(x^{(n)}|\theta\right)$$

  - If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

$$\ell(\theta) = \log \prod_{n=1}^{N} f\left(x^{(n)}|\theta\right) = \sum_{n=1}^{N} \log f\left(x^{(n)}|\theta\right)$$

Maximum Likelihood Estimation (MLE)

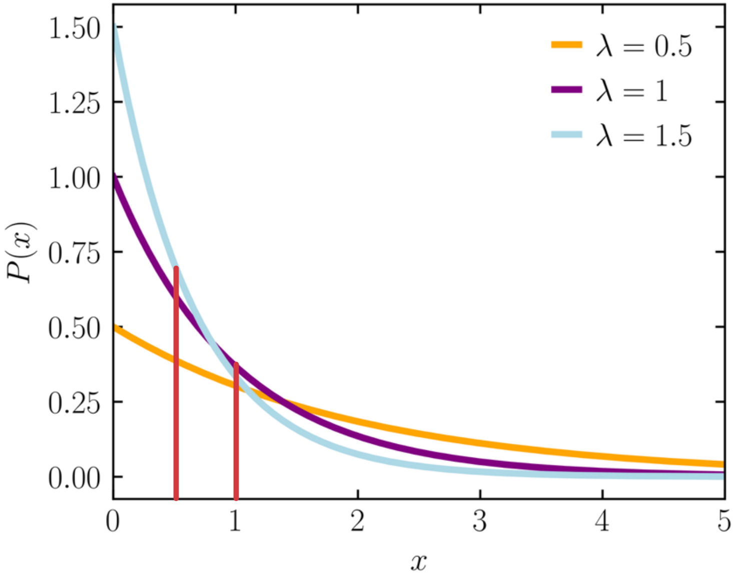
- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution

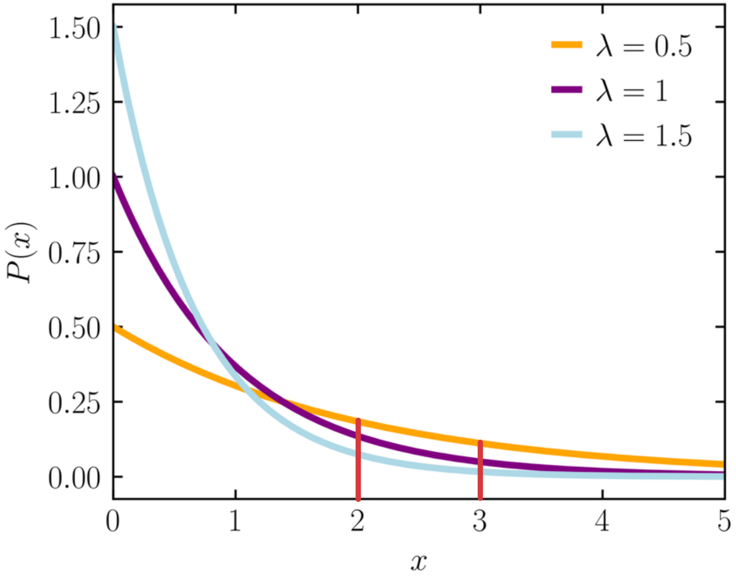


$\{x^{(1)} = 0.5, x^{(2)} = 1\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



$\{x^{(1)} = 2, x^{(2)} = 3\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N **iid** (independent and identically distributed) samples $\{x^{(1)}, \dots, x^{(N)}\}$, the likelihood is

$$L(\lambda) = \prod_{n=1}^{N} f\left(x^{(n)}|\lambda\right) = \prod_{n=1}^{N} \lambda e^{-\lambda x^{(n)}}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is
$$f(x|\lambda) = \lambda e^{-\lambda x}$$
- Given N **iid** (independent and identically distributed) samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is
$$\ell(\lambda) = \sum_{n=1}^{N} \log f\left(x^{(n)}|\lambda\right) = \sum_{n=1}^{N} \log \lambda e^{-\lambda x^{(n)}}$$
$$= \sum_{n=1}^{N} \log \lambda + \log e^{-\lambda x^{(n)}} = N \log \lambda - \lambda \sum_{n=1}^{N} x^{(n)}$$
- Taking the partial derivative and setting it equal to 0 gives
$$\frac{\partial \ell}{\partial \lambda} = \frac{N}{\lambda} - \sum_{n=1}^{N} x^{(n)}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is
$$f(x|\lambda) = \lambda e^{-\lambda x}$$
- Given N **iid** (independent and identically distributed) samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is
$$\ell(\lambda) = \sum_{n=1}^{N} \log f\left(x^{(n)} | \lambda\right) = \sum_{n=1}^{N} \log \lambda e^{-\lambda x^{(n)}}$$
$$= \sum_{n=1}^{N} \log \lambda + \log e^{-\lambda x^{(n)}} = N \log \lambda - \lambda \sum_{n=1}^{N} x^{(n)}$$
- Taking the partial derivative and setting it equal to 0 gives
$$\frac{N}{\hat{\lambda}} - \sum_{n=1}^{N} x^{(n)} = 0 \rightarrow \frac{N}{\hat{\lambda}} = \sum_{n=1}^{N} x^{(n)} \rightarrow \hat{\lambda} = \frac{N}{\sum_{n=1}^{N} x^{(n)}}$$

M(C)LE for Linear Regression

- If we assume a linear model with additive Gaussian noise

$$y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \ldots$$

then given $X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix}$ and $\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$, the MLE of $\boldsymbol{\omega}$ is

$$\widehat{\boldsymbol{\omega}} = \underset{\boldsymbol{\omega}}{\operatorname{argmax}} \log P(\boldsymbol{y} | X, \boldsymbol{\omega})$$

$$\vdots$$

$$= (X^T X)^{-1} X^T \boldsymbol{y}$$

Bernoulli Distribution MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is
$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$
- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the log-likelihood is

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is
$$p(x|\phi) = \phi^x (1-\phi)^{1-x}$$
- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the log-likelihood is
$$\ell(\phi) = \sum_{n=1}^{N} \log p\left(x^{(n)}|\phi\right) = \sum_{n=1}^{N} \log \phi^{x^{(n)}} (1-\phi)^{1-x^{(n)}}$$
$$= \sum_{n=1}^{N} x \log \phi + (1-x) \log(1-\phi)$$
$$= N_1 \log \phi + N_0 \log(1-\phi)$$
- where N_1 is the number of 1's in $\{x^{(1)}, \ldots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1-\phi$
- The pmf of the Bernoulli distribution is
$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$
- The partial derivative of the log-likelihood is
- where N_1 is the number of 1's in $\{x^{(1)}, \ldots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- The partial derivative of the log-likelihood is

$$\frac{\partial \ell}{\partial \phi} = \frac{N_1}{\phi} - \frac{N_0}{1 - \phi}$$

- where N_1 is the number of 1's in $\{x^{(1)}, \dots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- The partial derivative of the log-likelihood at $\hat{\phi}$ is

- where N_1 is the number of 1's in $\{x^{(1)}, \dots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- The partial derivative of the log-likelihood at $\hat{\phi}$ is

$$\frac{N_1}{\hat{\phi}} - \frac{N_0}{1 - \hat{\phi}} = 0 \rightarrow \frac{N_1}{\hat{\phi}} = \frac{N_0}{1 - \hat{\phi}}$$

$$\rightarrow N_1 \left(1 - \hat{\phi}\right) = N_0 \hat{\phi} \rightarrow N_1 = \hat{\phi}(N_0 + N_1)$$

$$\rightarrow \hat{\phi} = \frac{N_1}{N_0 + N_1}$$

- where N_1 is the number of 1's in $\left\{x^{(1)}, \ldots, x^{(N)}\right\}$ and N_0 is the number of 0's

Maximum a Posteriori (MAP) Estimation

- Insight: sometimes we have *prior* information we want to incorporate into parameter estimation
- Idea: use Bayes rule to reason about the *posterior* distribution over the parameters
  - MLE finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\mathcal{D}|\theta)$
  - MAP finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\theta|\mathcal{D})$

Maximum a Posteriori (MAP) Estimation

- Insight: sometimes we have *prior* information we want to incorporate into parameter estimation
- Idea: use Bayes rule to reason about the *posterior* distribution over the parameters
  - MLE finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\mathcal{D}|\theta)$
  - MAP finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\theta|\mathcal{D})$

$$= \underset{\theta}{\operatorname{argmax}}\ p(\mathcal{D}|\theta)p(\theta)/p(\mathcal{D})$$

$$= \underset{\theta}{\operatorname{argmax}}\ \underbrace{p(\mathcal{D}|\theta)}_{\text{likelihood}}\underbrace{p(\theta)}_{\text{prior}}$$

$$= \underset{\theta}{\operatorname{argmax}}\ \underbrace{\log p(\mathcal{D}|\theta) + \log p(\theta)}_{\text{log-posterior}}$$

Coin Flipping MAP

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

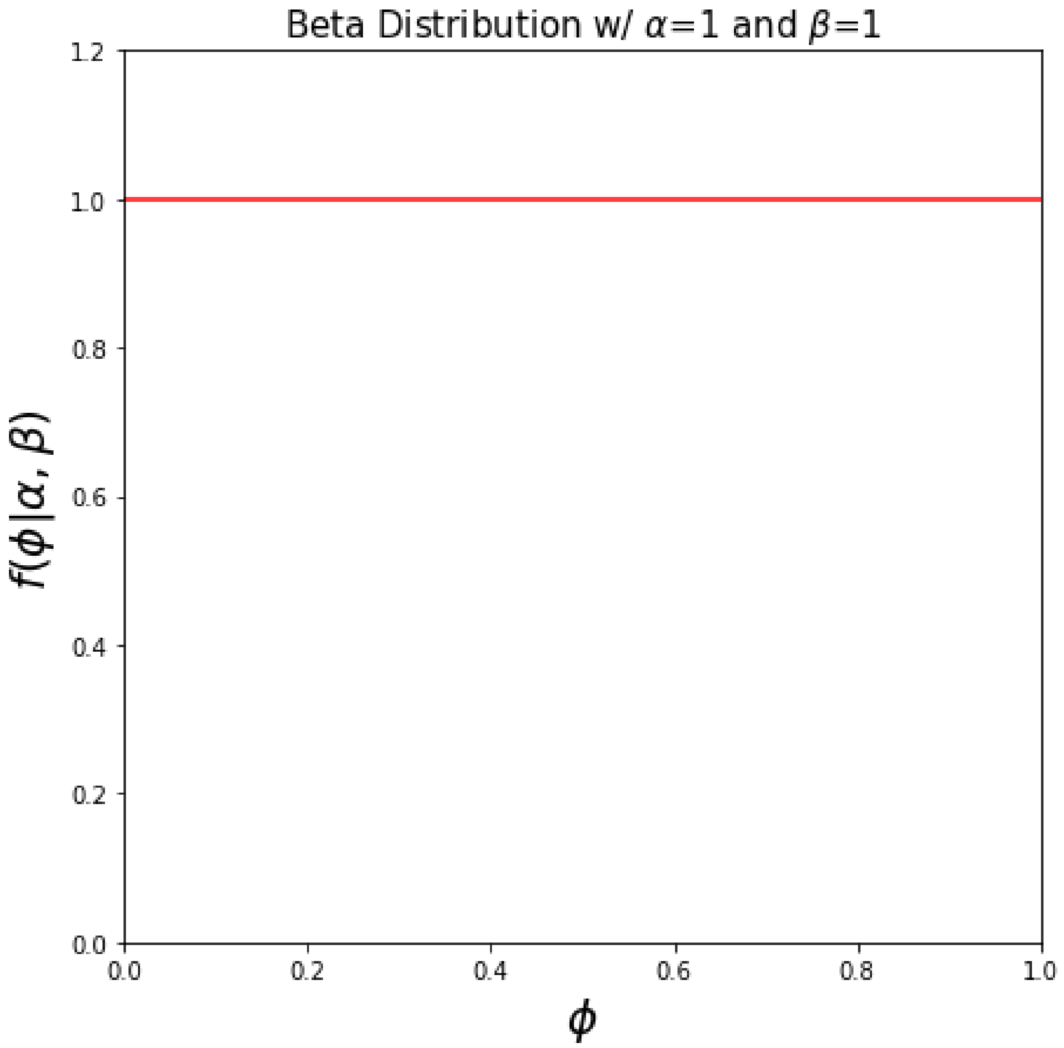
$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- Assume a Beta prior over the parameter ϕ, which has pdf

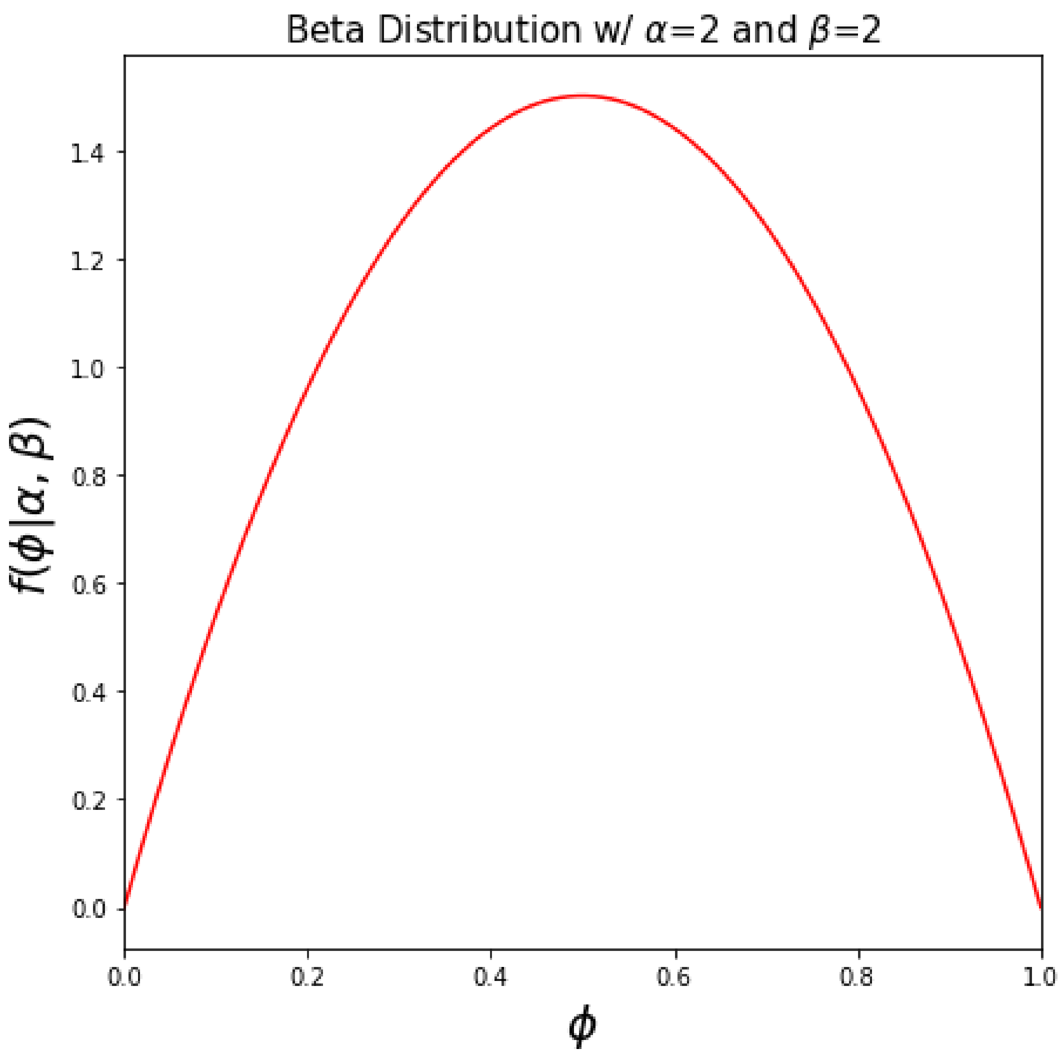
$$f(\phi|\alpha, \beta) = \frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}$$

where $\mathrm{B}(\alpha, \beta) = \int_0^1 \phi^{\alpha-1}(1-\phi)^{\beta-1} d\phi$ is a normalizing constant to ensure the distribution integrates to 1

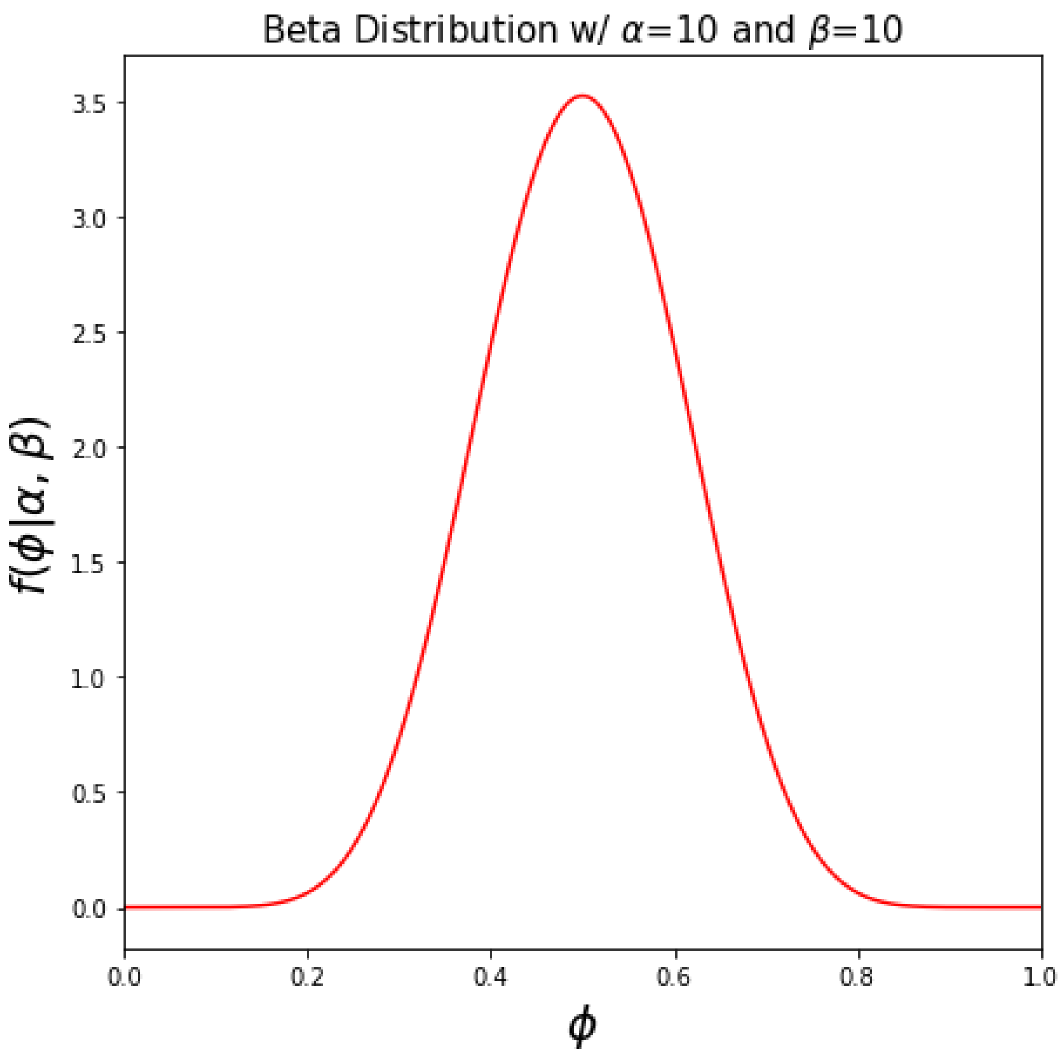
Beta Distribution



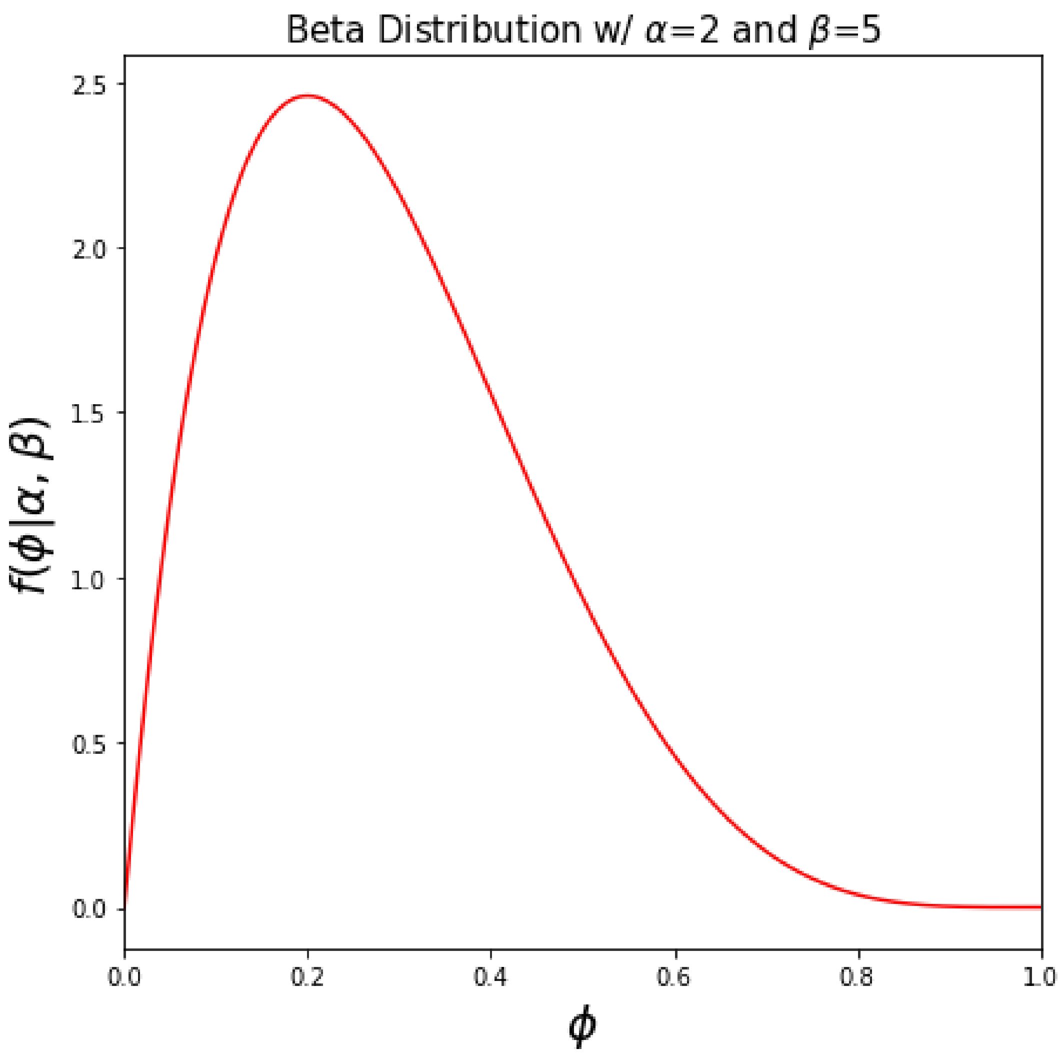
Beta Distribution



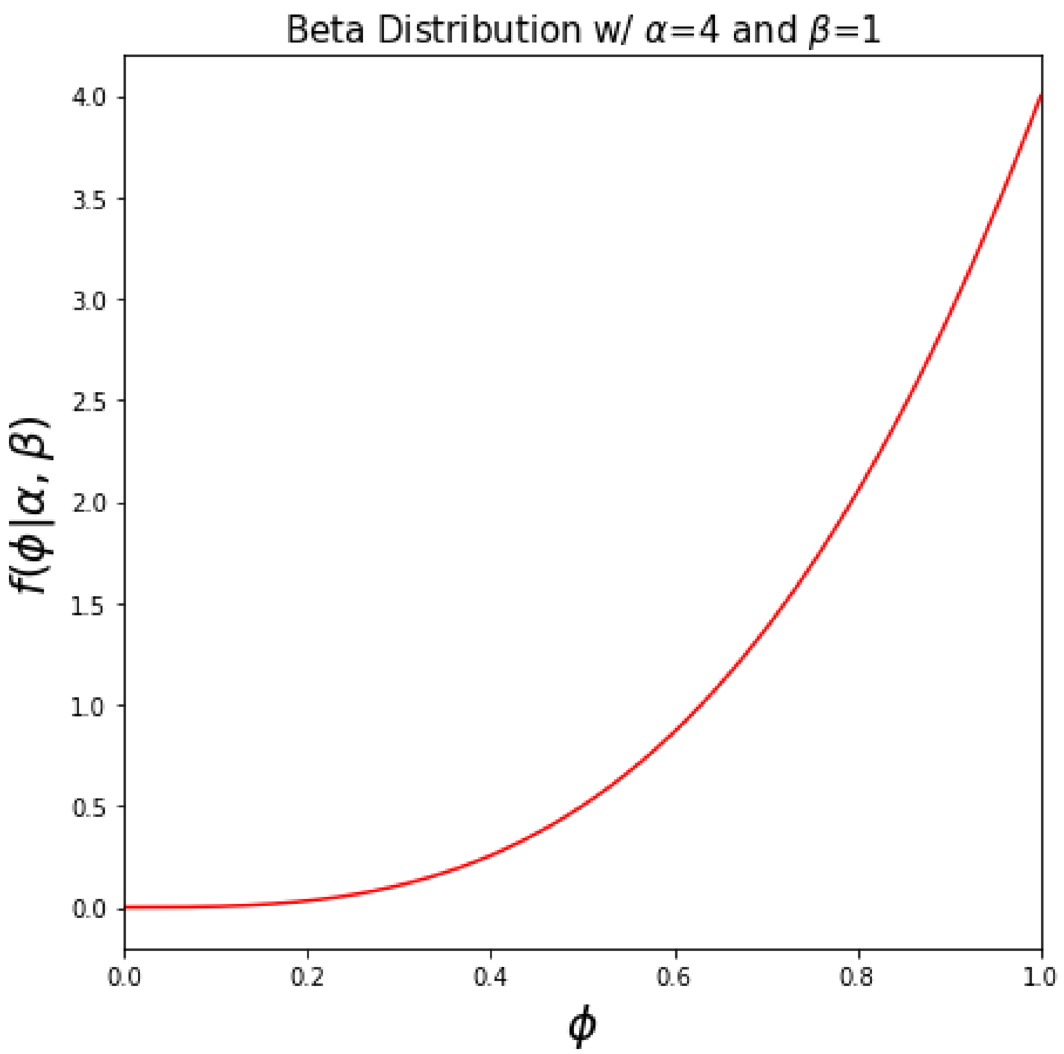
Beta Distribution



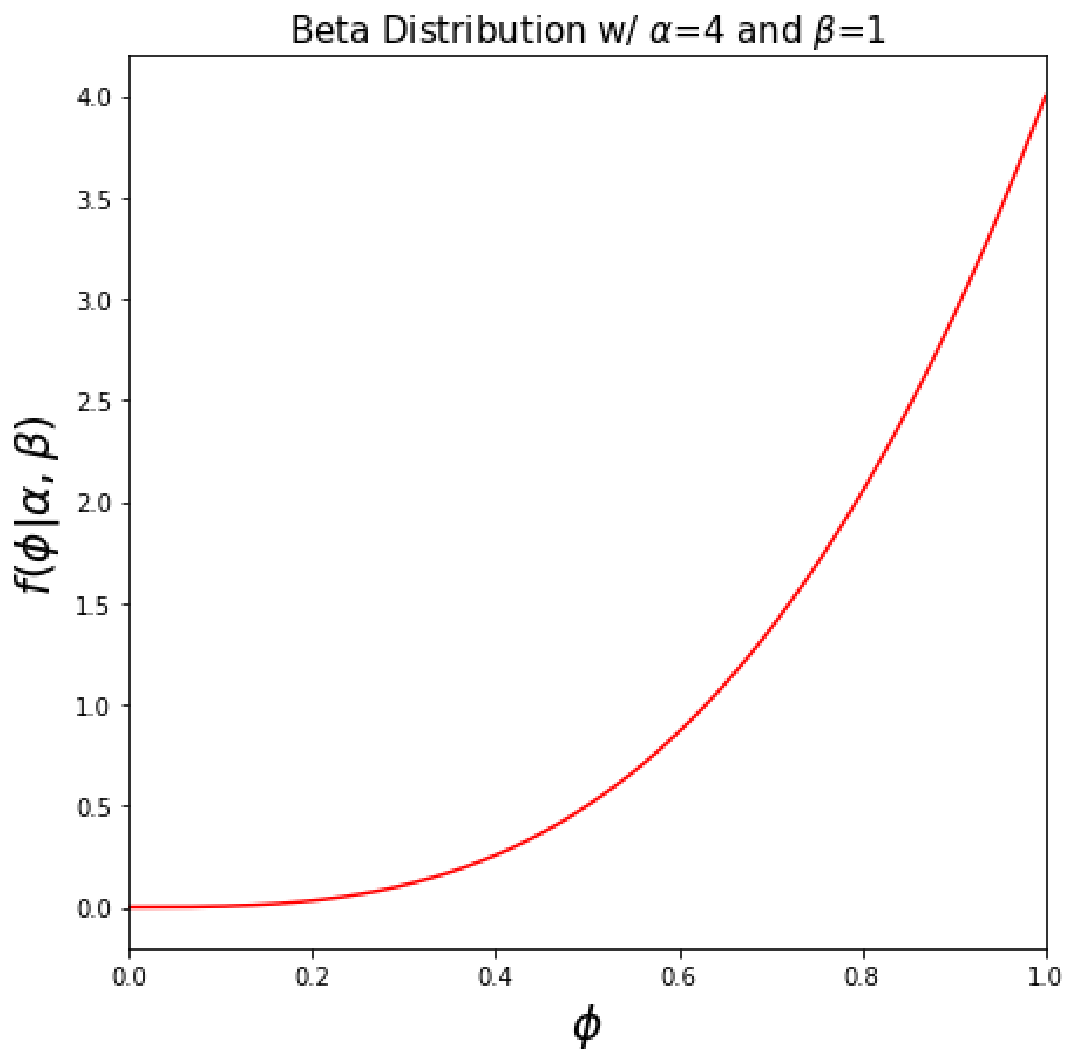
Beta Distribution



Beta Distribution



Okay, but why should we use this strange distribution as a prior?



Conjugate Priors

- For a given likelihood function $p(\mathcal{D}|\theta)$, a prior $p(\theta)$ is called a *conjugate prior* if the resulting posterior distribution $p(\theta|\mathcal{D})$ is in the same family as $p(\theta)$ i.e., $p(\theta|\mathcal{D})$ and $p(\theta)$ are the same type of random variable just with different parameters
  - We like conjugate priors because they are mathematically convenient
  - However, we do not **have** to use a conjugate prior if it doesn't align with our actual prior belief.

Example: Beta-Binomial Conjugacy

$$f(\phi|x,\alpha,\beta) = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{p(x|\alpha,\beta)}$$

$$p(x|\alpha,\beta) = \int p(x|\phi)f(\phi|\alpha,\beta)d\phi$$

$$= \int \phi^x(1-\phi)^{1-x}\frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{\mathrm{B}(\alpha,\beta)}d\phi$$

$$= \frac{1}{\mathrm{B}(\alpha,\beta)}\int \phi^{\alpha+x-1}(1-\phi)^{\beta-x}d\phi = \frac{\mathrm{B}(\alpha+x,\beta-x+1)}{\mathrm{B}(\alpha,\beta)}$$

Example: Beta-Binomial Conjugacy

$$f(\phi|x,\alpha,\beta) = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{p(x|\alpha,\beta)} = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{\int p(x|\phi)f(\phi|\alpha,\beta)d\phi}$$

$$f(\phi|x,\alpha,\beta) = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{\left(\frac{\mathrm{B}(\alpha+x,\beta-x+1)}{\mathrm{B}(\alpha,\beta)}\right)}$$

$$= \frac{\phi^{x}(1-\phi)^{1-x}\frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{\mathrm{B}(\alpha,\beta)}}{\left(\frac{\mathrm{B}(\alpha+x,\beta-x+1)}{\mathrm{B}(\alpha,\beta)}\right)}$$

$$= \frac{\phi^{\alpha+x-1}(1-\phi)^{\beta-x}}{\mathrm{B}(\alpha+x,\beta-x+1)} = f(\phi|\alpha+x,\beta-x+1)$$

$$= f(\phi|\alpha+x,\beta+(1-x))$$

Beta-Binomial MAP

- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the log-posterior is

Beta-Binomial MAP

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-posterior is

$$\ell(\phi) = \log f\Big(\phi \Big| \alpha + x^{(1)} + x^{(2)} + \cdots x^{(N)},$$
$$\Big(\beta + \big(1 - x^{(1)}\big) + \big(1 - x^{(2)}\big) + \cdots + \big(1 - x^{(N)}\big)\Big)$$

$$= \log f(\phi | \alpha + N_1, \beta + N_0)$$

where N_i is the number of i's observed in the samples

$$= \log \frac{\phi^{\alpha + N_1 - 1}(1 - \phi)^{\beta + N_0 - 1}}{\mathrm{B}(\alpha, \beta)}$$
$$= (\alpha + N_1 - 1) \log \phi + (\beta + N_0 - 1) \log 1 - \phi - \log \mathrm{B}(\alpha, \beta)$$

Beta-Binomial MAP

- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the partial derivative of the log-posterior is

$$\frac{\partial \ell}{\partial \phi} = \frac{(\alpha + N_1 - 1)}{\phi} - \frac{(\beta + N_0 - 1)}{1 - \phi}$$

$$\vdots$$

$$\rightarrow \hat{\phi}_{MAP} = \frac{(N_1 + \alpha - 1)}{(N_0 + \beta - 1) + (N_1 + \alpha - 1)}$$

- $\alpha - 1$ is a "pseudocount" of the number of 1's you've "observed"
- $\beta - 1$ is a "pseudocount" of the number of 0's you've "observed"

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 2$ and $\beta = 5$, then

$$\phi_{MAP} = \frac{(2-1+10)}{(2-1+10)+(5-1+2)} = \frac{11}{17} < \frac{10}{12}$$

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10 + 2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 101$ and $\beta = 101$, then

$$\phi_{MAP} = \frac{(101 - 1 + 10)}{(101 - 1 + 10) + (101 - 1 + 2)} = \frac{110}{212} \approx \frac{1}{2}$$

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 1$ and $\beta = 1$, then

$$\phi_{MAP} = \frac{(1-1+10)}{(1-1+10)+(1-1+2)} = \frac{10}{12} = \phi_{MLE}$$

Key Takeaways

- Two ways of estimating the parameters of a probability distribution given samples of a random variable:
  - Maximum likelihood estimation – maximize the (log-)likelihood of the observations
  - Maximum a posteriori estimation – maximize the (log-)posterior of the parameters conditioned on the observations
    - Requires a prior distribution, drawn from background knowledge or domain expertise