10-701: Introduction to Machine Learning Lecture 5 – MLE & MAP

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1/31/24

Front Matter

- Announcements:
 - HW1 released 1/24, due 2/2 (Friday) at 11:59 PM
- Recommended Readings:
 - Mitchell, <u>Estimating Probabilities</u>

Recall: Recipe for Linear Regression

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

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

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

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

Recall: Minimizing the Squared Error

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

$$= \frac{1}{N} ||X\mathbf{w} - \mathbf{y}||_{2}^{2} \text{ where } ||\mathbf{z}||_{2} = \sqrt{\sum_{d=1}^{D} z_{d}^{2}} = \sqrt{\mathbf{z}^{T}} \mathbf{z}$$

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

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

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

$$\to X^{T} X \widehat{\mathbf{w}} = X^{T} \mathbf{y}$$

$$\to \widehat{\mathbf{w}} = (X^{T} X)^{-1} X^{T} \mathbf{y}$$

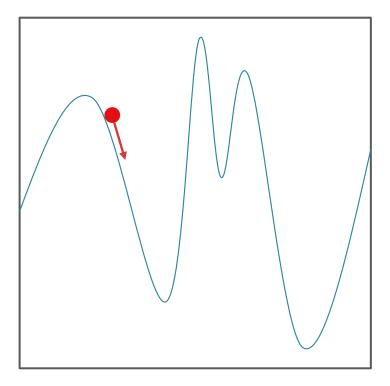
Recall: Closed Form Solution

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

- 1. Is X^TX invertible?
 - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible
 - If X^TX 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^TX ?
 - $X^TX \in \mathbb{R}^{D+1 \times D+1}$ so inverting X^TX takes $O(D^3)$ time...
 - Computing X^TX takes $O(ND^2)$ time
 - What alternative optimization method can we use to minimize the mean squared error?

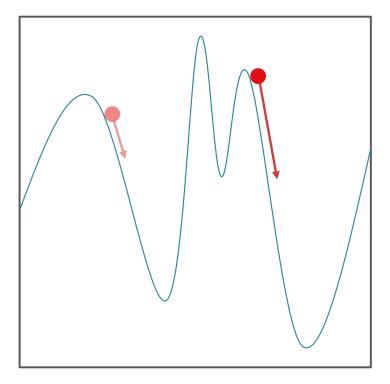
Gradient Descent: Intuition

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



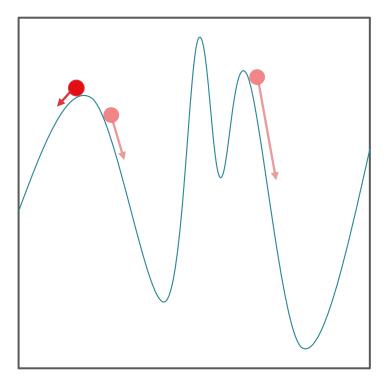
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Gradient Descent: Intuition

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



- Suppose the current weight vector is $\mathbf{w}^{(t)}$
- 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

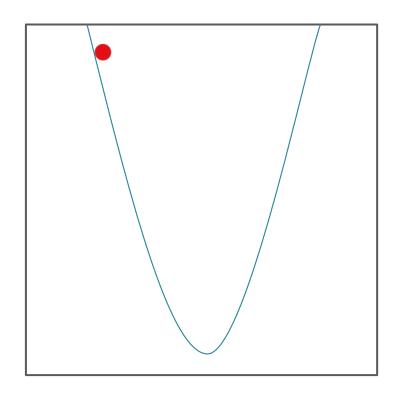
- Suppose the current weight vector is $\mathbf{w}^{(t)}$
- Move some distance, η , in the "most downhill" direction, \hat{v} :

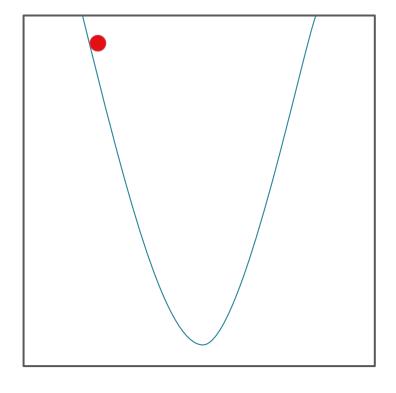
$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta \widehat{\boldsymbol{v}}$$

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

$$\widehat{\boldsymbol{v}}^{(t)} = -\frac{\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}} \left(\boldsymbol{w}^{(t)} \right)}{\left\| \nabla_{\boldsymbol{w}} \ell_{\mathcal{D}} \left(\boldsymbol{w}^{(t)} \right) \right\|_{2}}$$

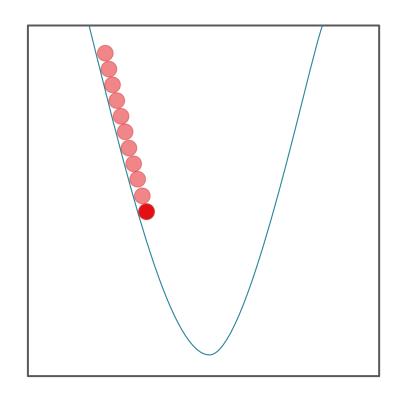
$$-\nabla_{\nu} \ell_{\mathcal{D}}(\omega^{(t)})$$

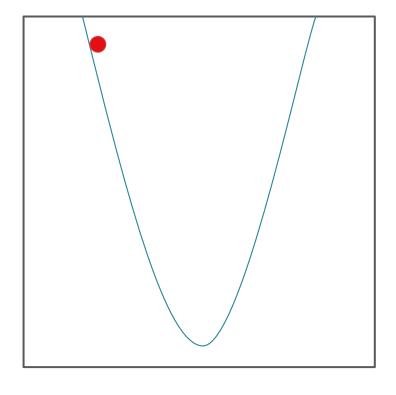




Small η

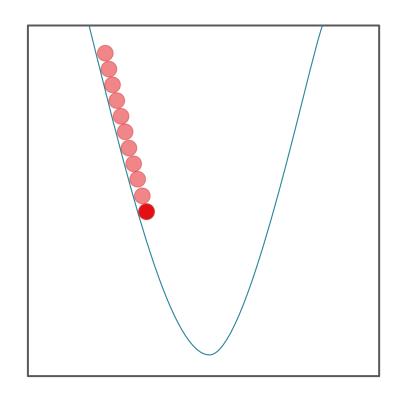
Large η

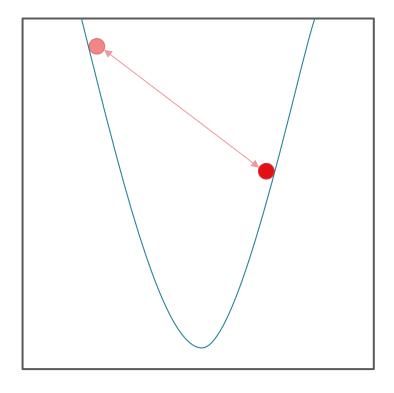




Small η

Large η

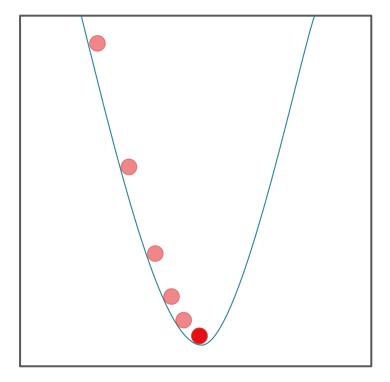




Small η

Large η

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



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

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

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

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

$$= \mathbf{w}^{(t)} + \left(-\frac{\sum_{i} l_{o}(\omega(t))}{\|\sum_{i} l_{o}(\omega(t))\|} \right) \eta^{(0)} \|\sum_{i} l_{o}(\omega(t))\|$$

$$= \mathbf{w}^{(t)} - \eta \quad \nabla_{\omega} l_{o}(\omega(t))$$

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

- 1. Initialize $\mathbf{w}^{(0)}$ to all zeros and set t=0
- 2. While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:

$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right) = \frac{2}{N}\left(\chi^{T}\chi_{\mathcal{W}} - \chi^{T}\gamma\right)$$

- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_{w} \ell_{\mathcal{D}} \left(w^{(t)} \right)$
- c. Increment $t: t \leftarrow t + 1$
- Output: $\mathbf{w}^{(t)}$

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

- 1. Initialize $\mathbf{w}^{(0)}$ to all zeros and set t=0
- 2. While $\|\nabla_{\mathbf{w}} \ell_{\mathcal{D}}(\mathbf{w}^{(t)})\| > \epsilon$
 - a. Compute the gradient:

$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right)$$

- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_w \ell_{\mathcal{D}} \left(w^{(t)} \right)$
- c. Increment $t: t \leftarrow t + 1$
- Output: $\mathbf{w}^{(t)}$

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

- 1. Initialize $\mathbf{w}^{(0)}$ 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 $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_{w} \ell_{\mathcal{D}} \left(w^{(t)} \right)$
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Why Gradient Descent for linear regression?

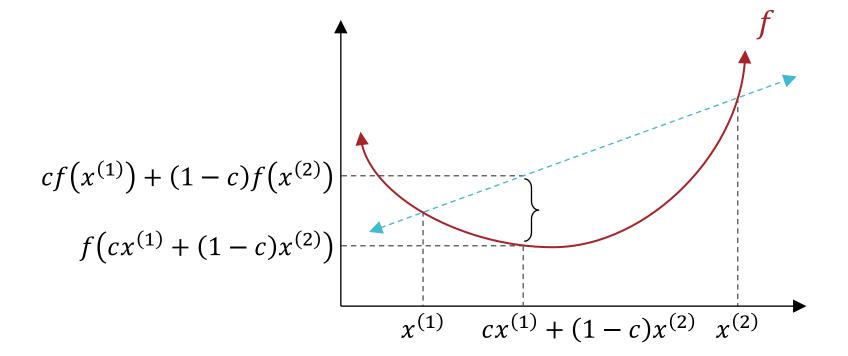
• Input:
$$\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}, \eta, T$$

- 1. Initialize $\mathbf{w}^{(0)}$ to all zeros and set t=0
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 - a. Compute the gradient:

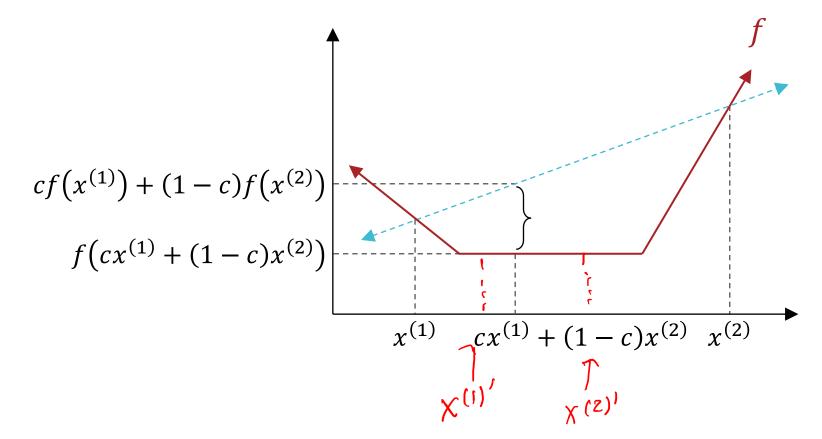
$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right) = \frac{Z}{N}\left(\boldsymbol{\chi}^{\mathsf{T}}\boldsymbol{\chi}\sim -\boldsymbol{\chi}^{\mathsf{T}}\boldsymbol{\gamma}\right)$$

- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_{w} \ell_{\mathcal{D}} \left(w^{(t)} \right)$
- c. Increment $t: t \leftarrow t + 1$
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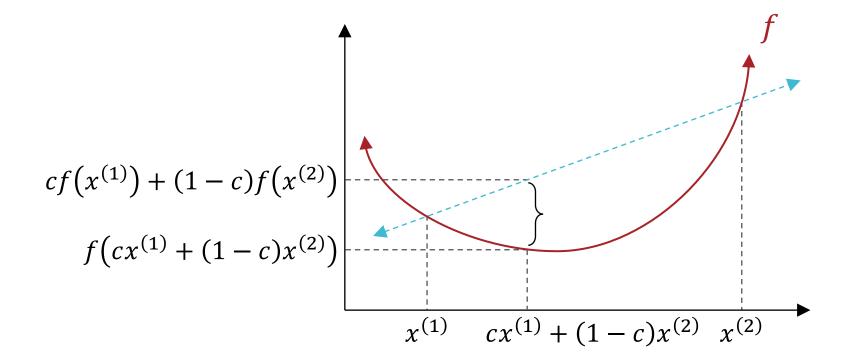
• A function $f: \mathbb{R}^D \to \mathbb{R}$ is convex if $\forall \ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D \text{ and } 0 \le c \le 1$ $f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \le cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$

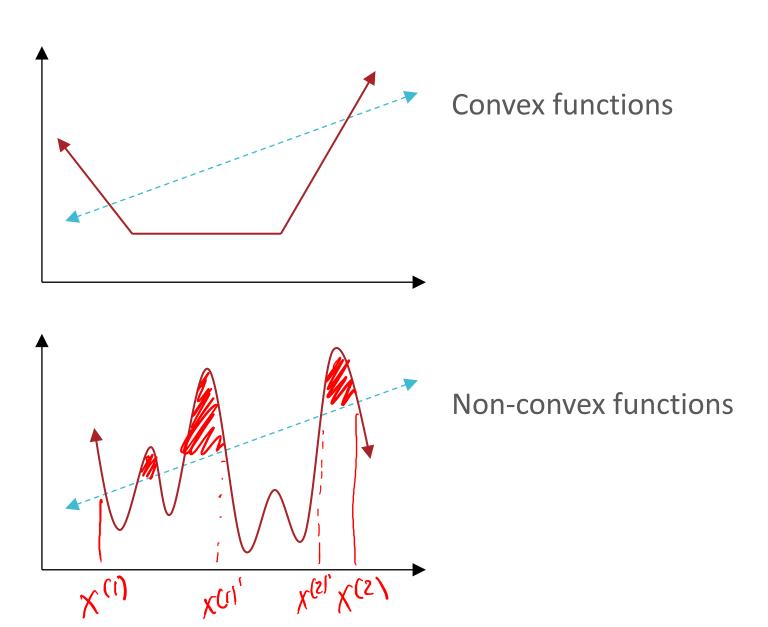


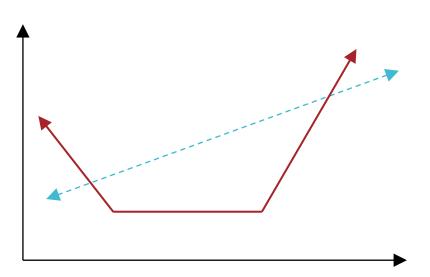
• A function $f: \mathbb{R}^D \to \mathbb{R}$ is convex if $\forall x^{(1)} \in \mathbb{R}^D, x^{(2)} \in \mathbb{R}^D$ and $0 \le c \le 1$ $f(cx^{(1)} + (1-c)x^{(2)}) \le cf(x^{(1)}) + (1-c)f(x^{(2)})$



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

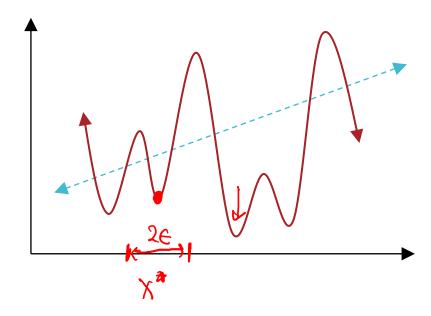




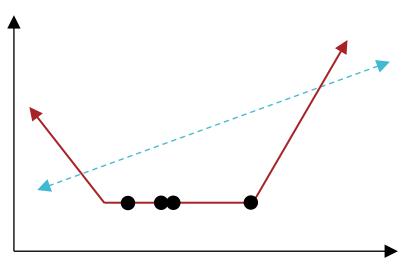


Given a function $f: \mathbb{R}^D \to \mathbb{R}$

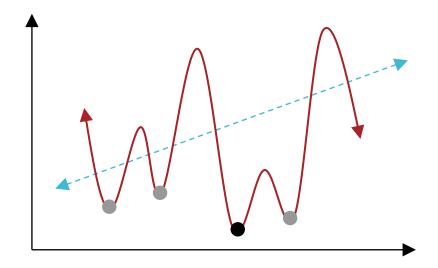
• x^* is a *global* minimum iff $f(x^*) \le f(x) \ \forall \ x \in \mathbb{R}^D$



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

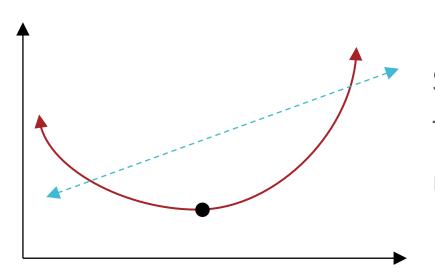


Convex functions:
Each local minimum is a global minimum!

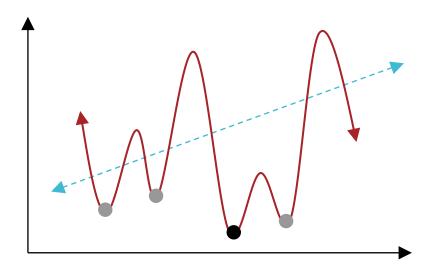


Non-convex functions:

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



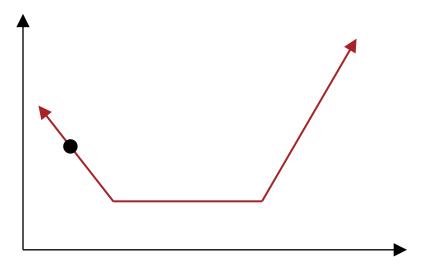
Strictly convex functions:
There exists a unique global minimum!



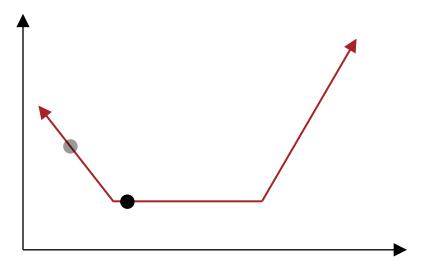
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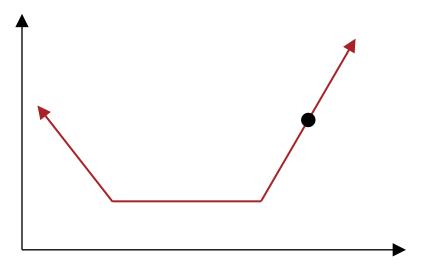
- Gradient descent is a local optimization algorithm it will converge to a local minimum (if it converges)
 - Works great if the objective function is convex!



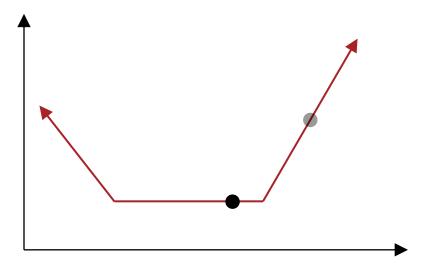
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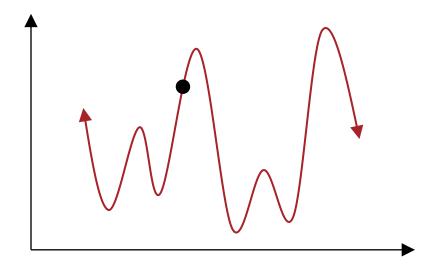
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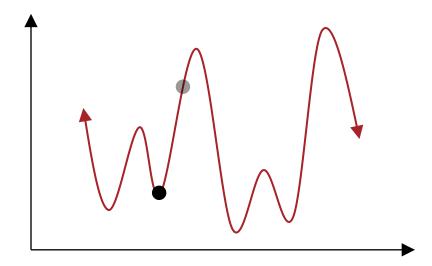
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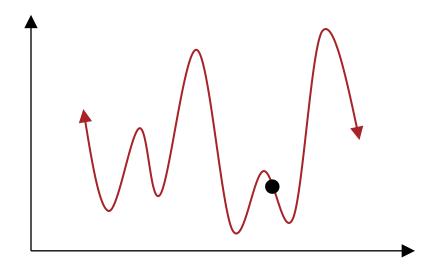
- Gradient descent is a local optimization algorithm it will converge to a local minimum (if it converges)
 - Not ideal if the objective function is non-convex...



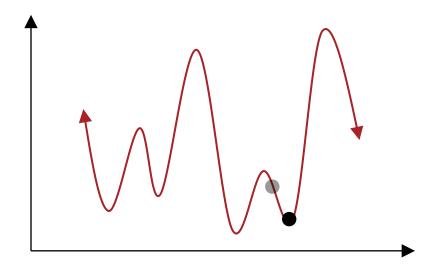
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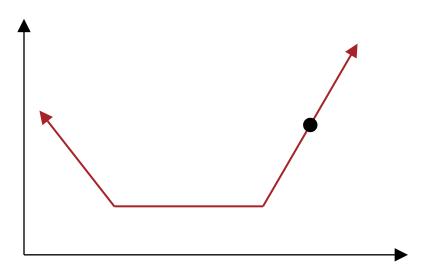


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The squared error for linear regression is convex (but not strictly convex)!

- Gradient descent is a local optimization algorithm it will converge to a local minimum (if it converges)
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$$H_{\mathbf{w}}\ell_{\mathcal{D}}(\mathbf{w}) = \frac{2}{N}X^TX$$
 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, $c^*: \mathcal{X} \to \mathcal{Y}$
 - Classifier, $h: \mathcal{X} \to \mathcal{Y}$
 - Goal: find a classifier, h, that best approximates c^*
- Now:
 - (Unknown) Target distribution, $y \sim p^*(Y|x)$
 - Distribution, p(Y|x)
 - Goal: find a distribution, p, that best approximates p^*

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 *likelihood* of \mathcal{D} is

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

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

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

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

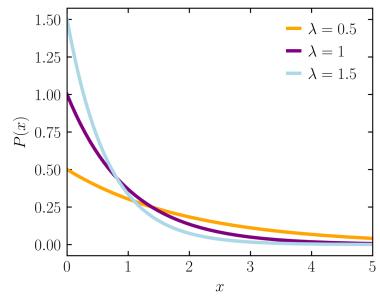
$$\ell(\theta) = \log \prod_{n=1}^{N} p(x^{(n)}|\theta) = \sum_{n=1}^{N} \log p(x^{(n)}|\theta)$$

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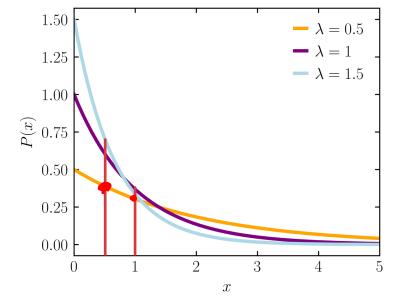
Maximum Likelihood Estimation (MLE)

- 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



Maximum Likelihood Estimation (MLE)

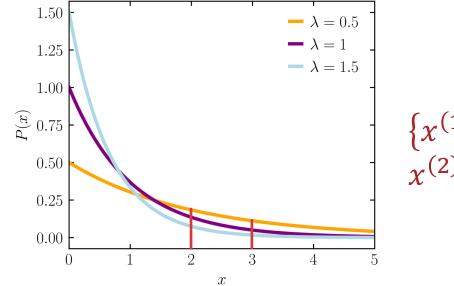
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$$\begin{cases} x^{(1)} = 0.5, \\ x^{(2)} = 1 \end{cases}$$

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

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

samples
$$\{x^{(1)}, ..., x^{(N)}\}$$
, the likelihood is
$$\lambda \left(\lambda\right) = \prod_{n=1}^{N} \lambda e^{-\lambda x^{(n)}}$$

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)}, ..., x^{(N)}\}\$$
, the log-likelihood is

samples
$$\{x^{(1)}, ..., x^{(N)}\}\$$
, the log-likelihood is
$$\begin{array}{cccc}
\downarrow (\gamma) &= & \sum_{n \geq 1} \log (\lambda) e^{-\lambda x^{(n)}} \\
&= & \sum_{n \geq 1} \log (\lambda) + (-\lambda x^{(n)}) \\
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M(C)LE for Linear Regression

If we assume a linear model with additive Gaussian noise

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

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 $\boldsymbol{y} = \begin{bmatrix} \boldsymbol{y^{(1)}} \\ \boldsymbol{y^{(2)}} \\ \vdots \\ \boldsymbol{y^{(N)}} \end{bmatrix}$, the MLE of $\boldsymbol{\omega}$ is

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

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

Bernoulli Distribution MLE

- A Bernoulli random variable takes value 1 with probability ϕ and value 0 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 $\{x^{(1)}, ..., x^{(N)}\}$, the log-likelihood is

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

$$= \sum_{N=1}^{N} \log \left(\phi^{(n)} (1-\phi)^{1-x^{(n)}} \right)$$

$$= \sum_{N=1}^{N} x^{(n)} \log (\phi) + (1-x^{(n)}) \log (1-\phi)$$

$$= N_1 \log \phi + N_2 \log (1-\phi)$$
where $N_1 = \emptyset$ of its in \mathbb{D}

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

$$\frac{\partial l}{\partial \phi} = \frac{N_1}{\phi} - \frac{N_2}{1-\phi}$$

$$\Rightarrow \frac{N_1}{\phi} - \frac{N_2}{1-\phi} \Rightarrow N_1 (1-\phi) = \frac{N_2}{1-\phi}$$

$$\Rightarrow \frac{N_1}{\phi} = \frac{N_2}{1-\phi} \Rightarrow N_2 (1-\phi) = \frac{N_2}{1-\phi}$$

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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
$$\hat{\Theta} = \underset{\bullet}{\text{argmax}} L(\hat{\Theta}) = P(D|\hat{\Theta})$$

MAP finds $\hat{\Theta} = \underset{\bullet}{\text{argmax}} P(D|\hat{\Theta})$

$$= \underset{\bullet}{\text{argmax}} P(D|\hat{\Theta})P(\hat{\Theta})$$

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Coin Flipping MAP

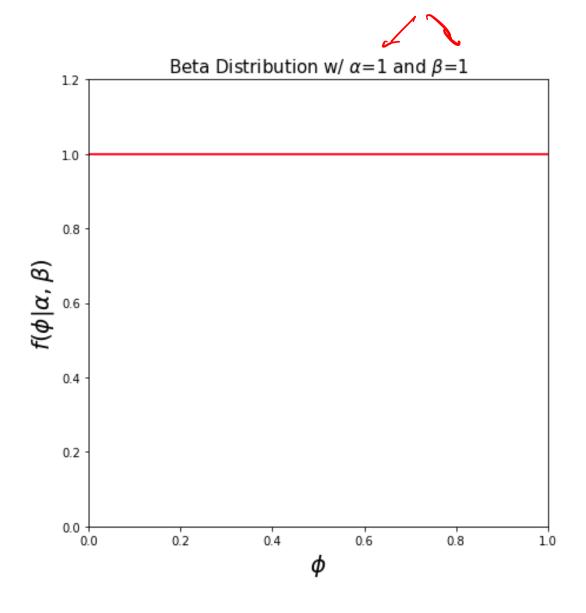
- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1-\phi$
- The pmf of the Bernoulli distribution is

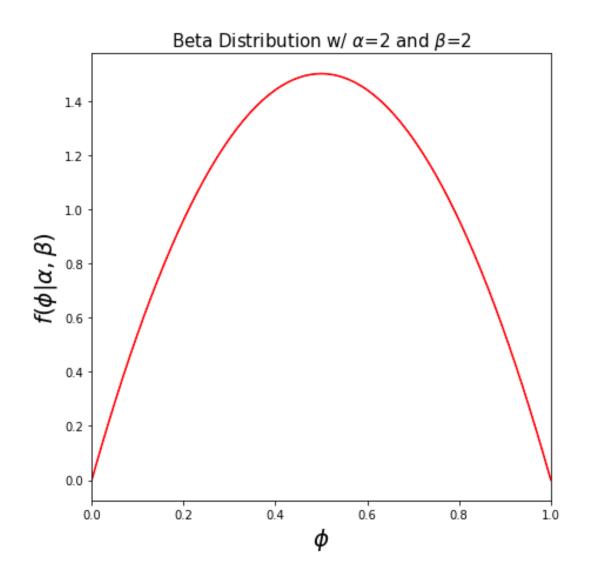
$$p(x|\phi) = \phi^x (1-\phi)^{1-x}$$

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

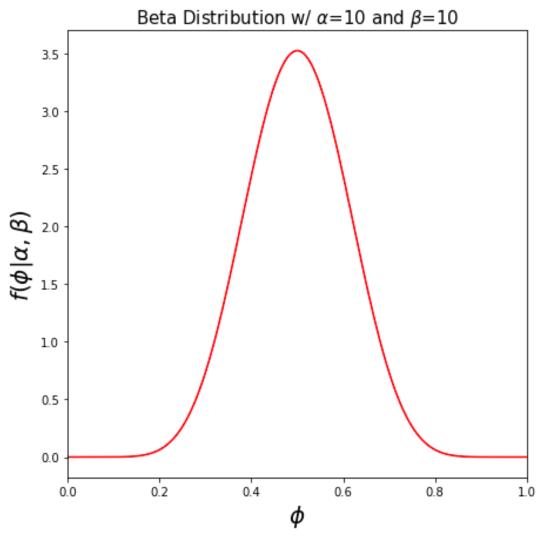
$$f(\phi|\alpha,\beta) = \frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{B(\alpha,\beta)}$$

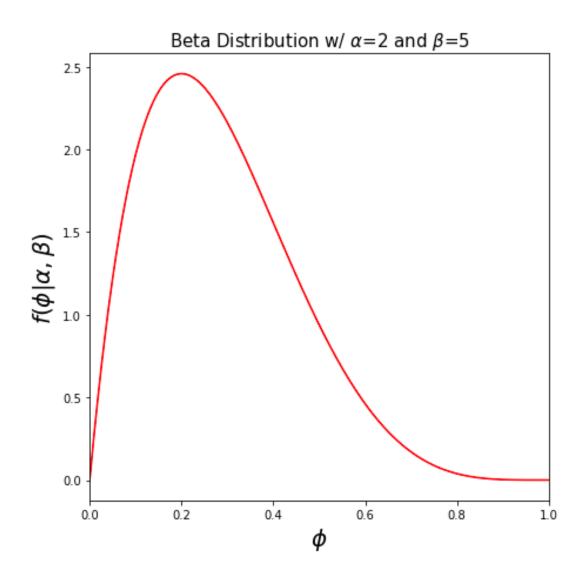
where $B(\alpha,\beta)=\int_0^1\phi^{\alpha-1}(1-\phi)^{\beta-1}d\phi$ is a normalizing constant to ensure the distribution integrates to 1

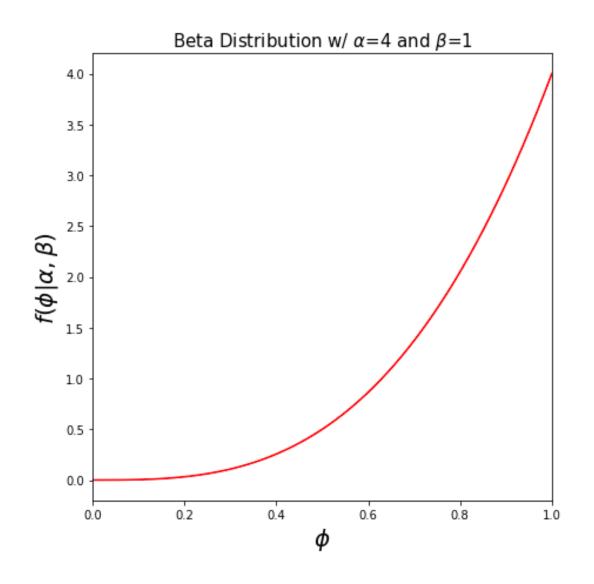




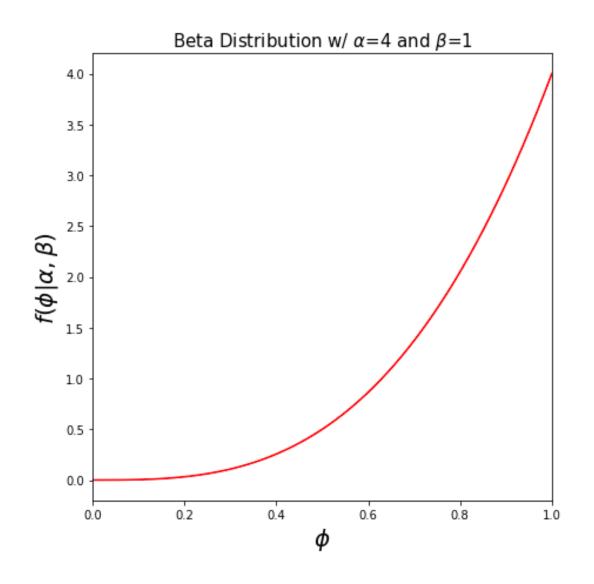








Okay, but why should we use this strange distribution as a prior?



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.

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

Example: Beta-Binomial Conjugacy

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

Example: Beta-Binomial Conjugacy

Beta-Binomial MAP

• Given N iid samples
$$\{x^{(1)}, ..., x^{(N)}\}$$
, the log-posterior is
$$\log (P(D|\Theta)P(\Theta)) = \log (P(D|\Theta)) + \log (P(\Theta))$$

$$= N, \log \beta + N_0 \log (1-\beta)$$

$$+ \log \left(\frac{\beta^{\alpha-1}(1-\beta)^{\beta-1}}{\beta(\alpha,\beta)}\right)$$

$$= N, \log \beta + N_0 \log (1-\beta)$$

$$+ (\alpha-1)\log \beta + (\beta-1)\log (1-\beta) - \log (\beta(\alpha,\beta))$$

Beta-Binomial MAP

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

$$\frac{2}{20}$$
 ((N,+d-1) log Ø + (No+B-1) log (1-Ø)
+ log (B(a,B))

$$\frac{\partial^{2}}{\partial x^{2}} = \frac{N_{1} + \lambda - 1}{N_{1} + \lambda - 1 + N_{0} + \beta - 1}$$

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



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

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

$$\phi_{MAP} = \phi_{MLE} = \frac{N_1 + 1}{N_1 + 1 + 1}$$

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