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

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Front Matter

- Announcements:
	- · HW1 released 1/24, due 2
- Recommended Readings:
	- · Mitchell, Estimating Prob

Recall: Recipe for Linear Regression

- Define a model and model parameters
	- 1. Assume $y = w^T x$
	- 2. Parameters: $w = [w_0, w_1, ..., w_D]$
- 2. Write down an objective function 1. Minimize the mean squared error $\ell_{\mathcal{D}}(w) =$ 1 $\frac{1}{N}$ $\overline{n=1}$ \overline{N} $w^T x^{(n)} - y^{(n)}$
- 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

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

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

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

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

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

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

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

Recall: Closed Form Solution

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

- 1. Is $X^T X$ invertible?
	- When $N \gg D + 1$, X^TX 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

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• Suppose the current weight vector is $\boldsymbol{w}^{(t)}$

• Move some distance, η , in the "most downhill" direction, $\hat{\mathbf{\nu}}$: $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \eta \widehat{\mathbf{v}}$

Gradient Descent: Step Direction

- Suppose the current weight vector is $w^{(t)}$
- Move some distance, η , in the "most downhill" direction, $\hat{\mathbf{\nu}}$: $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \eta \widehat{\mathbf{v}}$
- The gradient points in the direction of steepest *increase …*
- \cdot ... so $\hat{\mathbf{v}}$ should point in the opposite direction:

 $-\nabla_{\mu}$ $\ell_{p}(\mu^{(t)})$

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

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

 \cdot Set $\eta^{(t)} = \eta^{(0)} \|\nabla_{\mathbf{w}} \ell_{\mathcal{D}} (\mathbf{w}^{(t)})\|$ $\cdot \|\nabla_{\bm{w}} \widehat{\ell}_{\mathcal{D}}\left(\bm{w}^{(t)}\right)\|$ decreases as $\ell_{\mathcal{D}}$ approaches its minimum $\rightarrow \eta^{(t)}$ (hopefully) decreases over time

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

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

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

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

- Input: $\mathcal{D} = \{(\pmb{x}^{(i)}, y^{(i)})\}$ $i=1$ \overline{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: $\nabla_{\mathbf{w}} \ell_{\mathcal{D}}(\mathbf{w}^{(t)}) = \frac{2}{N} \left(\chi^T X_{\mathcal{W}} - \chi^T \chi \right)$
	- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_w \ell_{\mathcal{D}}(w^{(t)})$
	- c. Increment $t: t \leftarrow t + 1$
- Output: $\boldsymbol{w}^{(t)}$

- Input: $\mathcal{D} = \{(\pmb{x}^{(i)}, y^{(i)})\}$ $i=1$ \overline{N} , η , ϵ
- 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: $\nabla_{\mathbf{w}} \ell_{\mathcal{D}}\left(\mathbf{w}^{(t)}\right)$
	- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_w \ell_{\mathcal{D}}(w^{(t)})$
	- c. Increment $t: t \leftarrow t + 1$
- \cdot Output: $w^{(t)}$

- Input: $\mathcal{D} = \{(\pmb{x}^{(i)}, y^{(i)})\}$ $i=1$ \overline{N} , η , \overline{T}
- 1. Initialize $w^{(0)}$ to all zeros and set $t = 0$
- 2. While $t < T$
	- a. Compute the gradient: $\nabla_{\mathbf{w}} \ell_{\mathcal{D}}\left(\mathbf{w}^{(t)}\right)$
	- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \eta \nabla_w \ell_{\mathcal{D}}(w^{(t)})$
	- c. Increment $t: t \leftarrow t + 1$
- \cdot Output: $\boldsymbol{w}^{(t)}$

Why Gradient Descent for linear regression? • Input: $\mathcal{D} = \{(\pmb{x}^{(i)}, y^{(i)})\}$ $i=1$ \overline{N} , η , \overline{T}

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

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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)
	- Works great if the objective function is convex!

 $H_w \ell_{\mathcal{D}}(w) =$) \overline{N} $X^T X$ 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, $c^* \colon \mathcal{X} \to \mathcal{Y}$
	- Classifier, $h: \mathcal{X} \rightarrow \mathcal{Y}$
	- Goal: find a classifier, h, that best approximates c^*
- Now:
	- \cdot (Unknown) Target *distribution*, $y \sim p^*(Y|\mathbf{x})$
	- Distribution, $p(Y|\mathbf{x})$
	- Goal: find a distribution, p , that best approximates p^*

Likelihood

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

 $n=1$

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

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

Log-Likelihood

 \cdot Given N independent, identically distribution (iid) samples $\mathcal{D} = \{ \mathcal{X}^{(1)}, ..., \mathcal{X}^{(N)} \}$ of a random variable X \cdot If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *log-likelihood* of D is $\ell(\theta) = \log |\cdot|$ $\overline{n}=\overline{1}$ \overline{N} $p(x^{(n)}|\theta) = \sum$ $\overline{n=1}$ \overline{N} $\log p(x^{(n)}|\theta)$ \cdot If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *log-likelihood* of D is \overline{N} \overline{N}

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

Maximum Likelihood Estimation (MLE)

- · Insight: every valid probability amount of probability mass a
- · Idea: set the parameter(s) so samples is maximized
- · Intuition: assign as much of the to the observed data *at the ex*
- Example: the exponential distribution

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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 likelihood is $\Lambda(\wedge)$ -(\therefore \log^{-10} $\overline{}$ \mathbf{t}_{max}

Exponential **Distribution** MLE

 The pdf of the exponential distribution is $f(x|\lambda) = \lambda e^{-\lambda x}$

M(C)LE for Linear Regression

• If we assume a linear model with additive Gaussian noise
\n
$$
y = \omega^T x + \epsilon
$$
 where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\omega^T x, \sigma^2)$...
\nthen given $X = \begin{bmatrix} 1 & x^{(1)^T} \\ 1 & x^{(2)^T} \\ \vdots & \vdots \\ 1 & x^{(N)^T} \end{bmatrix}$ and $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$, the MLE of ω is
\n $\hat{\omega} = \underset{\omega}{\text{argmax}} \log P(y|X, \omega)$
\n \vdots
\n $= (X^T X)^{-1} X^T y$

Bernoulli **Distribution** MLE

- \cdot A Bernoulli random variable takes value 1 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 $\{x^{(1)},...,x^{(N)}\}$, the log-likelihood is $2(\phi) =$ $\frac{1}{\sqrt{2}}$ \sum $log(P(X'))$ \mathbb{R}^N $\frac{1}{\sqrt{2}}$ log⁶ \$ 1 − #+6 \$ $\overline{}$ log + 1 − log 1 − \leq \geq \wedge \leq \leq \vee $= N, \log \emptyset + N_0$ log $(1-\beta)$ $\frac{1}{\sqrt{2}}$ number of $\frac{1}{\sqrt{2}}$ Henry Chai - 1/31/24 **48**

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

Maximum a **Posteriori** (MAP) Estimation

- **· Insight: sometimes we have** *prior* **information we want** to incorporate into parameter estimation
- \cdot Idea: use Bayes rule to reason about the *posterior* distribution over the parameters

 M_{\odot} \cap \parallel 8 \sum \sim arguments r \sim \mathbf{r} $M(A)^2$ finds C \overline{y} = \overline{y} $=$ argmex $P(D)$ $=$ argmax Γ Henry Chai - 1/31/24 **Prior** 52 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 $B(\alpha, \beta) = \int_0^1$ $\int_{0}^{1} \phi^{\alpha-1}(1-\phi)^{\beta-1} d\phi$ 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.

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

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
\n
$$
log(P(D|\theta)P(\theta)) = log(P(D|\theta)) + log(P(\theta))
$$
\n
$$
= M_1 log \phi + N_2 log(1-\phi)
$$
\n
$$
+ log \left(\frac{\phi^{\alpha-1}(1-\phi)}{\beta(\alpha/\beta)}\right)
$$
\n
$$
= M_1 log \phi + N_2 log(1-\phi)
$$
\n
$$
+ (\alpha-1) log \phi + (p-1) log(1-\phi) - log (B[1-\phi])
$$

Beta-Binomial MAP

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

$$
\frac{2}{20}\left((N_{1}+d-1)\log_{10}(N_{0}+B-1)\log_{11}\frac{1}{20}(1-\frac{1}{20})+\log_{10}\frac{1}{20}(B(d/3))\right)
$$

\n
$$
\frac{2}{20}\frac{N_{1}+d-1}{N_{1}+d-1}+\log_{10}\frac{1}{20}
$$

Coin **Flipping** MAP: Example • Suppose D consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails $(N_0 = 2)$: ϕ_{MLE} = 10 $10 + 2$ = 10 12

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

 φ _{*11AP*} =

Coin **Flipping** MAP: Example • Suppose D consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails $(N_0 = 2)$: ϕ_{MLE} = 10 $10 + 2$ = 10 12

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

Coin **Flipping** MAP: Example • Suppose D consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails $(N_0 = 2)$: ϕ_{MLE} = 10 $10 + 2$ = 10 12 • Using a Beta prior with $\alpha = 1$ and $\beta = 1$, then $\frac{1}{2}$ $\gamma_{\mu_{1,0}} - \gamma_{\mu_{1,0}} -$ = $\overline{}$ 12 $\sqrt{ }$

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