Introduction to Machine Learning - CS725

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Lecture 5 - Bayesian Estimation and Bayesian Linear Regression

Recap: Least Squares, MLE and Regularization

- If solution $\Phi\mathbf{w} = \mathbf{y}$ exists, then least squares estimate $\mathbf{w}^*$ can be obtained by solving this linear system
- Additionally, if $n = m$ then Φ must be invertible and $\mathbf{w}^* = \Phi^{-1}\mathbf{y}$
- If $\mathbf{y}$ is NOT in the column space of Φ, then the least squares solution is obtained using the left-pseudoinverse of Φ:

$$\mathbf{w}^* = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{y} \tag{1}$$

- The Maximum Likelihood estimate $\mathbf{w}_{MLE}$ happens to be the same as the least squares estimate $\mathbf{w}^*$. That is, $\mathbf{w}_{MLE} = \mathbf{w}^*$
- Here $\Phi^T\Phi$ is invertible only if Φ has full column rank
- Bayesian Estimation and Regularization: (a) Encode prior belief on $\mathbf{w}$ and (b) Develop probabilistic distributions on $\mathbf{w}^*$

Building on questions on Least Squares Linear Regression

1. Is there a probabilistic interpretation?
   - Gaussian Error, Maximum Likelihood Estimate
2. Addressing overfitting
   - Bayesian and Maximum Aposteriori Estimates, Regularization
3. How to minimize the resultant and more complex error functions?
   - Level Curves and Surfaces, Gradient Vector, Directional Derivative, Gradient Descent Algorithm, Convexity, Necessary and Sufficient Conditions for Optimality

Bayesian Linear Regression

- The Bayesian interpretation of probabilistic estimation is a logical extension that enables reasoning with uncertainty **but in the light of some background belief**
- **Bayesian linear regression**: A Bayesian alternative to **Maximum Likelihood** least squares regression
- Continue with Normally distributed errors
- Model the **w** using a prior distribution and use the posterior over **w** as the result
- Intuitive Prior:

Bayesian Linear Regression

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- Intuitive Prior: Components of **w** should not become too large!
- Next: Illustration of Bayesian Estimation on a simple Coin-tossing example

Illustration through a Simple Coin Tossing Example: Maximum Likelihood Estimation vs. Bayesian Estimation

Case Study:

Suresh likes to toss coins. One day he decided to count the number of heads and tails in his coin tosses. Here is what he found. After tossing 1000 times (it took him a hours, but he likes to toss coins), he found that the coin landed on heads 400 times and tails 600 times. His reflection: If I were to toss the coin once more time, what is the probability that I get a heads?

Maximum Likelihood Estimation

- We are tempted to say that the probability of Heads in a subsequent toss is $400/1000 = 0.4$[1].
- But why?
- This is motivated by our wanting to maximize the probability of the occurance of the data we have. Or in other words, we want a **Maximum Likelihood Estimate**.

[1] This raises an important point, you can never know the probability of the coin giving a head, what you can give is only an estimate for it. So dont be confused with 0.4 as the probability of getting a head, it is only an intelligent guess

Revisiting Likelihood

- Let the observed data follow a distribution f_θ, with θ being the unknown parameter.
  1. Coin tossing expt: θ is probability of heads occurring in any given toss and corresponds to a bernoulli distribution.
  2. Logistic regression: θ is basically w
- Let $X_1, X_2, ..., X_n$ be the set of random variables governing the observation with a joint pdf/pmf denoted by:

$$f_\theta(x_1, x_2, ..., x_n) = f(x_1, x_2, ..., x_n|\theta)$$

Revisiting Likelihood: Continued

- Given observed values $X_1 = x_1, X_2 = x_2, ..., X_n = x_n$, the likelihood of θ is the function

$$L(\theta) = f(x_1, x_2, ..., x_n|\theta)$$

  treated as a function of θ.
- Thus, $L(\theta)$ is probability of observing the given data as a function of θ.
- The Maximum Likelihood Estimate (MLE) of θ is $\widehat{\theta}$ that maximises $L(\theta)$
- For an independent and identically distributed sample $X_1, X_2, \ldots, X_n$, this means:

$$MLE(\theta) : \hat{\theta} = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{n} f(x_i|\theta)$$

MLE estimate for Coin Tossing

- We restate Suresh's problem as the MLE of the probability of getting a head. This is the value of p which maximizes the likelihood of observing 400 heads as outcomes.

$$\hat{p} = \underset{p}{\text{argmax}} \ {}^{1000}C_{400}p^{400}(1-p)^{600}$$

- $\hat{p} = 0.4$ as we had intuitively guessed. In general, the value of p which maximises the likelihood of observing h heads, given n coin tosses is.

$$\hat{p} = \underset{p}{\text{argmax}} \ {}^{n}C_{h}p^{h}(1-p)^{n-h}$$

Bayesian Inference/Estimation

Case Study:

Suresh now brings a newly minted coin to toss. He *believes* that the coin is fair and heads and tails are equally likely outcomes (since the coin is not worn out). Now like always he flips the coin 4 times, and finds out that heads appeared all the 4 times.

1. Is the MLE estimate $\hat{p} = 1$ intuitive? Is tails improbable?
2. Is there a way that Suresh could update his *belief* about the coin.

Bayesian Inference

- H: One of few competing hypotheses whose probability may be affected by observed data.
- $\Pr(H)$: The (prior) probability of H before data $\mathcal{D}$ is observed. This indicates one's previous *belief* in the hypothesis.
- The evidence $\mathcal{D}$: New data that were not used in computing the prior probability

$$p(H \mid \mathcal{D}) \propto p(\mathcal{D} \mid H)\ p(H)$$

Conjugate Prior

Let $\mathcal{D} \mid H$ follow a distribution d_1 and H follow a distribution d_2. The distribution d_2 is the conjugate prior of d_1 if the distribution of $\Pr(H \mid \mathcal{D})$ follows the distribution d_2.
Some Examples:

1. Bernoulli & Binomial - Beta
2. Geometric - Beta
3. Categorical - Dirichlet
4. Multinomial - Dirichlet
5. Poisson - Gamma
6. Normal - Inverse Gamma

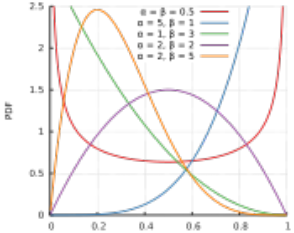
The Beta Conjugate Prior for Bernoulli/Binomial

Let $\mathcal{D} \mid H$ follow a distribution $Ber(p)$ (p is probability of heads) and p follow a distribution $Beta(p; \alpha, \beta) \sim \frac{p^{(\alpha-1)}(1-p)^{(\beta-1)}}{B(\alpha,\beta)}$,

1. *The beta normalization function:*
   $B(\alpha, \beta) = \int_{p=0}^{1} p^{(\alpha-1)}(1-p)^{(\beta-1)} dp = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$, where $\Gamma(.)$ behaves like the factorial function: $\Gamma(n) = (n-1)!$ if $n \in \mathbb{Z}^+$
2. $\Pr(H \mid \mathcal{D}) = \Pr(p \mid \mathcal{D}) = \frac{\Pr(\mathcal{D}|p)\Pr(p)}{\int_q \Pr(\mathcal{D} \mid q)\Pr(q)}$
   $= \frac{{}^nC_h p^h (1-p)^{n-h} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{(\alpha-1)}(1-p)^{(\beta-1)}}{\int_q {}^nC_h q^h (1-q)^{n-h} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} q^{(\alpha-1)}(1-q)^{(\beta-1)}} \propto p^{\alpha+h-1}(1-p)^{\beta+n-h-1}$
   $\sim Beta(p; \alpha + h, \beta + n - h)$

More on the $Beta(\alpha, \beta)$ distribution

1. $\mathbf{E}_{Beta(\alpha,\beta)}[p] = \frac{\alpha}{\alpha+\beta}$ and $\underset{p}{\operatorname{argmax}}\, Beta(p; \alpha, \beta) = \dfrac{\alpha - 1}{\alpha + \beta - 2}$ (the mode of the distribution)
2. $Beta(1, 1)$ is the uniform distribution!
3. Is the conjugate prior pdf for the Bernoulli, binomial, negative binomial and geometric distributions and has the following pdf plot:



The MAP Estimate for Bernoulli/Binoimal

Let $\mathcal{D} \mid H$ follow a distribution $Ber(p)$ (p is probability of heads) and p follow a distribution $Beta(p; \alpha, \beta) \sim \frac{p^{(\alpha-1)}(1-p)^{(\beta-1)}}{B(\alpha,\beta)}$,

1. *The Maximum Likelihood Estimate:* $\hat{p} = \underset{p}{\operatorname{argmax}} \ {}^{n}C_h p^h (1-p)^{n-h} = \frac{h}{n}$
2. *The Maximum a-Posterior (MAP) Estimate:* The mode of the posterior distribution $\tilde{p} = \underset{H}{\operatorname{argmax}} \Pr(H \mid \mathcal{D}) = \underset{p}{\operatorname{argmax}} \Pr(p \mid \mathcal{D})$
   $= \underset{p}{\operatorname{argmax}} \, Beta(p; \alpha + h, \beta + n - h) = \frac{\alpha + h - 1}{\alpha + \beta + n - 2}$

Case Study Continued

Coming back to the Suresh's case study, he observed 4 heads on 4 tosses, his MLE is

$$\hat{p} = \underset{p}{\text{argmax}} \ {}^4C_4 p^4 (1-p)^0 = 1$$

If his prior on p was $Beta(p; 3, 3)$, then his posterior will be $Beta(p; 3+4, 3+0) = Beta(p; 7, 3)$ and his MAP estimate will be

$$\hat{p} = \underset{p}{\text{argmax}} \ Beta(p; 7, 3) = \frac{7-1}{7+3-2} = 0.75$$

Prior Distribution for w for Linear Regression

$$y = \mathbf{w}^T \phi(\mathbf{x}) + \varepsilon$$
$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

- We saw that when we try to maximize log-likelihood we end up with $\hat{\mathbf{w}}_{MLE} = (\Phi^T \Phi)^{-1} \Phi^T y$
- We can use a Prior distribution on $\mathbf{w}$ to avoid over-fitting

  $$w_i \sim \mathcal{N}(0, \tfrac{1}{\lambda})$$

  (that is, each component w_i is approximately bounded within $\pm \frac{2}{\sqrt{\lambda}}$ by the $3 - \sigma$ rule)
- Q1: How do deal with Bayesian Estimation for Gaussian distribution?

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- Let $\Pr(X) \sim \mathcal{N}(\mu, \sigma^2)$ and let the data $\mathcal{D} = x_1 ... x_m$
- $\mu_{MLE} = \frac{1}{m} \sum_{i=1}^{m} x_i$ and $\sigma_{MLE} = \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu)^2$
- The conjugate prior for the (univariate) normally distributed random variable X in the case that σ^2 is not a random variable is $\Pr(\mu) = \mathcal{N}(\mu_0, \sigma_0^2)$, And the **posterior** is?

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- $\mu_m = (\frac{\sigma^2}{m\sigma_0^2 + \sigma^2} \mu_0) + (\frac{m\sigma_0^2}{m\sigma_0^2 + \sigma^2} \hat{\mu}_{ML})$
- $\frac{1}{\sigma_m^2} = \frac{1}{\sigma_0^2} + \frac{m}{\sigma^2}$