Introduction to Machine Learning - CS725
Instructor: Prof. Ganesh Ramakrishnan
Lecture 5 - Linear Regression - Bayesian Inference and Regularization

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

Recap: Bayesian Inference with Coin Tossing

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

Intuition for 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 $\mathbf{w}$ using a prior distribution and use the posterior over $\mathbf{w}$ as the result
- Intuitive Prior: Components of $\mathbf{w}$ should not become too large!

Prior Distribution for $\mathbf{w}$ 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
$$w_i \sim \mathcal{N}(0, \tfrac{1}{\lambda})$$
Each component w_i is approximately bounded within $\pm \frac{3}{\sqrt{\lambda}}$. λ is also called the precision of the Gaussian
- Q1: How do deal with Bayesian Estimation for Gaussian distribution?

Conjugate Prior for (univariate) Gaussian

- We will temporarily generalize the discussion with x taking the place of ε and μ taking the place of w_i

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

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- Answer: $\Pr(\mu | x_1 ... x_m) = \mathcal{N}(\mu_m, \sigma_m^2)$ such that $\mu_m = ...$ and $\dfrac{1}{\sigma_m^2} = ...$
- Helpful tip: Product of Gaussians is always a Gaussian

Detailed derivation

$$\Pr(\mu) = \frac{1}{\sqrt{2\pi\sigma_0^2}} exp\left(\frac{-(\mu - \mu_0)^2}{2\sigma_0^2}\right)$$

$$\Pr(x_i|\mu;\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left(\frac{-(x_i - \mu)^2}{2\sigma^2}\right)$$

$$\Pr(\mathcal{D}|\mu) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^m exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^{m}(x_i - \mu)^2\right)$$

$$\Pr(\mu|\mathcal{D}) \propto \Pr(\mathcal{D}|\mu)\Pr(\mu) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^m \frac{1}{\sqrt{2\pi\sigma_0^2}} exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^{m}(x_i - \mu)^2 - \frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right) \propto$$

$$exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^{m}(x_i - \mu)^2 - \frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right) = exp\left(\frac{-1}{2\sigma_m^2}(\mu - \mu_m)^2\right)$$

Detailed derivation (contd.)

Our reference equality:

$$exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^{m}(x_i-\mu)^2-\frac{(\mu-\mu_0)^2}{2\sigma_0^2}\right)=exp\left(\frac{-1}{2\sigma_m^2}(\mu-\mu_m)^2\right),$$

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Matching coefficients of μ, we get

$\frac{2\mu\mu_m}{2\sigma_m^2}=\mu\left(\frac{2\sum_{i=1}^{m}x_i}{2\sigma^2}+\frac{2\mu_0}{2\sigma_0^2}\right)\Rightarrow$

Detailed derivation (contd.)

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

Summary: Conjugate Prior for (univariate) Gaussian

- Let $\Pr(X) \sim \mathcal{N}(\mu, \sigma^2)$ and let the data $\mathcal{D} = x_1 \dots x_m$
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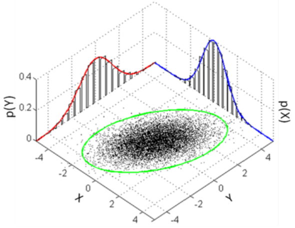
- Answer: $\Pr(\mu | x_1 ... x_m) = \mathcal{N}(\mu_m, \sigma_m^2)$ such that
- $\mu_m = (\frac{\sigma^2}{m\sigma_0^2 + \sigma^2}\mu_0) + (\frac{m\sigma_0^2}{m\sigma_0^2 + \sigma^2}\hat{\mu}_{ML})$
- $\frac{1}{\sigma_m^2} = \frac{1}{\sigma_0^2} + \frac{m}{\sigma^2}$

Multivariate Normal Distribution and MLE estimate

1. The multivariate Gaussian (Normal) Distribution is:
   $\mathcal{N}(\mathbf{x}; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)}$ when $\Sigma \in \Re^{n\times n}$ is positive-definite and



   $\mu \in \Re^n$

2. $\mu_{MLE} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i \sim \frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_i)$ and
   $\Sigma_{MLE} \sim \frac{1}{m}\sum_{i=1}^{m}(\phi(\mathbf{x}_i) - \mu_{MLE})(\phi(\mathbf{x}_i) - \mu_{MLE})^T$

Summary for MAP estimation with Normal Distribution

- Summary: With $\mu \sim \mathcal{N}(\mu_0, {\sigma^2}_0)$ and $x \sim \mathcal{N}(\mu, \sigma^2)$

$$\frac{1}{\sigma_m^2} = \frac{m}{\sigma^2} + \frac{1}{\sigma_0^2}$$
$$\frac{\mu_m}{\sigma_m^2} = \frac{m}{\sigma^2}\hat{\mu}_{mle} + \frac{\mu_0}{\sigma_0^2}$$

  such that $p(x|D) \sim \mathcal{N}(\mu_m, {\sigma_m}^2)$. Here m/σ^2 is due to noise in observation while $1/\sigma_0^2$ is due to uncertainity in μ

- For the Bayesian setting for the multivariate case with fixed Σ

$$\mathbf{x} \sim \mathcal{N}(\mu, \Sigma),\ \mu \sim \mathcal{N}(\mu_0, \Sigma_0)\ \&\ p(\mathbf{x}|D) \sim \mathcal{N}(\mu_m, \Sigma_m)$$

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$$\Sigma_m^{-1} = m\Sigma^{-1} + \Sigma_0^{-1}$$
$$\Sigma_m^{-1}\mu_m = m\Sigma^{-1}\hat{\mu}_{mle} + \Sigma_0^{-1}\mu$$

- We now conclude our discussion on Bayesian Linear Regression..

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 $\hat{\mathbf{w}}_{MLE} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$
- We can use a Prior distribution on $\mathbf{w}$ to avoid over-fitting

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

..Each component w_i is approximately bounded within $\pm \frac{3}{\sqrt{\lambda}}$. λ is also called the precision of the Gaussian

- Q1: How do deal with Bayesian Estimation for Gaussian distribution?
- Q2: Then what is the (collective) prior distribution of the n-dimensional vector $\mathbf{w}$?

Multivariate Normal Distribution and MAP estimate

1. If $w_i \sim \mathcal{N}(0, \frac{1}{\lambda})$ then $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \frac{1}{\lambda}I)$ where I is an $n \times n$ identity matrix
2. $\Rightarrow$ That is, $\mathbf{w}$ has a multivariate Gaussian distribution $\Pr(\mathbf{w}) = \frac{1}{(\frac{2\pi}{\lambda})^{\frac{n}{2}}} e^{-\frac{\lambda}{2}\|w\|_2^2}$ with $\mu_0 = \mathbf{0}$. $\Sigma_0 = \frac{1}{\lambda}I$
3. We will specifically consider Bayesian Estimation for multivariate Gaussian (Normal) Distribution on $\mathbf{w}$: $\frac{1}{(2\pi)^{\frac{n}{2}}(\frac{1}{\lambda})^{\frac{1}{2}}} e^{-\frac{\lambda}{2}\|w\|_2^2}$

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- We can use a Prior distribution on w to avoid over-fitting
$$w_i \sim \mathcal{N}(0, \frac{1}{\lambda})$$
(that is, each component w_i is approximately bounded within $\pm \frac{1}{\sqrt{\lambda}}$ by the $3 - \sigma$ rule)
- We want to find $P(\mathbf{w}|D) = \mathcal{N}(\mu_m, \Sigma_m)$
Invoking the Bayes Estimation results from before:

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  $$w_i \sim \mathcal{N}(0, \tfrac{1}{\lambda})$$
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- We want to find $P(\mathbf{w}|D) = \mathcal{N}(\mu_m, \Sigma_m)$
  Invoking the Bayes Estimation results from before:
  $$\Sigma_m^{-1} \mu_m = \Sigma_0^{-1} \mu_0 + \Phi^T y / \sigma^2$$
  $$\Sigma_m^{-1} = \Sigma_0^{-1} + \frac{1}{\sigma^2} \Phi^T \Phi$$

Finding μ_m & Σ_m for $\mathbf{w}$

Setting $\Sigma_0 = \frac{1}{\lambda} I$ and $\mu_0 = \mathbf{0}$

$$
\begin{aligned}
\Sigma_m^{-1} \mu_m &= \Phi^T \mathbf{y} / \sigma^2 \\
\Sigma_m^{-1} &= \lambda I + \Phi^T \Phi / \sigma^2 \\
\mu_m &= \frac{(\lambda I + \Phi^T \Phi / \sigma^2)^{-1} \Phi^T \mathbf{y}}{\sigma^2}
\end{aligned}
$$

or

$$
\mu_m = (\lambda \sigma^2 I + \Phi^T \Phi)^{-1} \Phi^T \mathbf{y}
$$

MAP and Bayes Estimates

- $\Pr(\mathbf{w} \mid \mathcal{D}) = \mathcal{N}(\mathbf{w} \mid \mu_m, \Sigma_m)$
- The **MAP estimate** or mode under the Gaussian posterior is the mode of the posterior $\Rightarrow$

$$\hat{w}_{MAP} = \operatorname*{argmax}_{\mathbf{w}} \mathcal{N}(\mathbf{w} \mid \mu_m, \Sigma_m) = \mu_m$$

- Similarly, the **Bayes Estimate**, or the expected value under the Gaussian posterior is the mean $\Rightarrow$

$$\hat{w}_{Bayes} = E_{\Pr(\mathbf{w}|\mathcal{D})}[\mathbf{w}] = E_{\mathcal{N}(\mu_m, \Sigma_m)}[\mathbf{w}] = \mu_m$$

- Summarily:

$$\mu_{MAP} = \mu_{Bayes} = \mu_m = (\lambda\sigma^2 I + \Phi^T\Phi)^{-1}\Phi^T\mathbf{y}$$

$$\Sigma_m^{-1} = \lambda I + \frac{\Phi^T\Phi}{\sigma^2}$$

From Bayesian Estimates to (Pure) Bayesian Prediction

	Point?	$p(x\|D)$
MLE	$\hat{\theta}_{MLE} = \text{argmax}_\theta\, LL(D\|\theta)$	$p(x\|\theta_{MLE})$
Bayes Estimator	$\hat{\theta}_B = E_{p(\theta\|D)} E[\theta]$	$p(x\|\theta_B)$
MAP	$\hat{\theta}_{MAP} = \text{argmax}_\theta\, p(\theta\|D)$	$p(x\|\theta_{MAP})$
Pure Bayesian		$p(\theta\|D) = \frac{p(D\|\theta)p(\theta)}{\int_m p(D\|\theta)p(\theta)d\theta}$ $p(D\|\theta) = \prod_{i=1} p(x_i\|\theta)$ $p(x\|D) = \int_\theta p(x\|\theta)p(\theta\|D)d\theta$

where θ is the parameter