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

- Is there a probabilistic interpretation?
 - Gaussian Error, Maximum Likelihood Estimate
- Addressing overfitting
 - Bayesian and Maximum Aposteriori Estimates, Regularization
- Mow 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 $Beta(p; \alpha, \beta) \sim \frac{p^{(\alpha-1)}(1-p)^{(\beta-1)}}{B(\alpha, \beta)}$,

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

$$= \mathop{\mathsf{argmax}}_{m{p}} \mathcal{B}$$
eta $(m{p}; lpha + m{h}, eta + m{n} - m{h}) = rac{lpha + m{h} - 1}{lpha + eta + m{n} - 2}$

Intuition for Bayesian Linear Regression

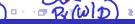
- The Bayesian interpretation of probabilistic estimation is a logical extension that enables reasoning with uncertainty but in the light of some background belief
- Bayesian linear regression: A Bayesian alternative to Maximum Likelihood least squares regression
- Continue with Normally distributed errors
- ullet Model the ullet using a prior distribution and use the posterior over ullet as the result
- Intuitive Prior: Components of w should not become too large!

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 **w** to avoid over-fitting $w_i \sim \mathcal{N}(0, \frac{1}{\lambda})$ $\mathcal{N}(0, \frac{1}{\lambda})$ $\mathcal{N}(0, \frac{1}{\lambda})$ $\mathcal{N}(0, \frac{1}{\lambda})$ 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?

 Q: How to estimate distr for W & WD





$$P_{i}(\omega) = P_{i}(\omega, \omega_{2} ... \omega_{n})$$

$$St P_{i}(\omega_{i}) = \frac{\sqrt{\lambda}}{\sqrt{2\pi}} e^{-\lambda \omega_{i}^{2}/2} = N(0, \frac{1}{\lambda})$$

$$P_{i}(\omega) = N([0, ... o], \frac{1}{\lambda} [0, ... o])$$

$$Density fn shown as concentric arcles in 2-D$$

Q: What to do abt Pr(WID) ? We will start with the simpler setting! X~ N(M, -2) 9r (x1D) ~ 7 Evolve tricks in simpler setting

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

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
- Let $\mathsf{Pr}(X) \sim \mathcal{N}(\mu, \sigma^2)$ and let the data $\mathcal{D} = x_1...x_m$
- $\mu_{MLE} = \frac{1}{m} \sum_{i=1}^{m} x_i$ and $\sigma_{MLE}^2 = \frac{1}{m} \sum_{i=1}^{m} (x_i \mu_{MLE})^2$
 - 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?

How: Set
$$\frac{\partial}{\partial M} = 0$$
 4 $\frac{\partial}{\partial \sigma^2} = 0$

Conjugate Prior for (univariate) Gaussian

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



$$P(M|X_{1}...X_{m}) = P(X_{1}...X_{m}|M)P(M)$$

$$P(X_{1}...X_{m})$$

$$Will be accounted for through marmalization factors
$$= \frac{1}{Z} P(X_{1}...X_{m}|M)P(M)$$

$$= \frac{1}{Z} \left(\frac{1}{\sqrt{12}\pi} \left(\frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} \left(\frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} \right) \right) - \frac{1}{\sqrt{2}\sqrt{2}\pi}$$

$$= \frac{1}{Z} \left(\frac{1}{\sqrt{12}\pi} \left(\frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} \right) \right) = \frac{1}{\sqrt{2}\sqrt{2}}$$

$$= \frac{1}{Z} \left(\frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} + \frac{1}{\sqrt{2}\sqrt{2}} \right)$$$$

Detailed derivation

$$\Pr(\mu) = \frac{1}{\sqrt{2\pi\sigma_0^2}} \exp\left(\frac{-(\mu-\mu_0)^2}{2\sigma_0^2}\right) \qquad \text{Trick: Determine params}$$

$$\Pr(x_i|\mu;\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(x_i-\mu)^2}{2\sigma^2}\right) \qquad \text{Of Tandom Variable (4)}$$

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

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

$$\exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^m (x_i-\mu)^2 - \frac{(\mu-\mu_0)^2}{2\sigma_0^2}\right) = \exp\left(\frac{-1}{2\sigma_m^2}(\mu-\mu_m)^2\right) \sim \mathcal{N}(\mathcal{M}_{M_0}, \mathcal{O}_{M_0})$$

Our reference equality:

$$\exp\left(\frac{-1}{2\sigma^2}\sum_{i=1}^{m}(x_i - \mu)^2 - \frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right) = \exp\left(\frac{-1}{2\sigma_m^2}(\mu - \mu_m)^2\right),$$
Matching coefficients of μ_i^2 , we get
$$-\frac{1}{2\sigma^2}m - \frac{1}{2\sigma_0^2} = \frac{1}{2\sigma_m^2} = \frac{1}{2\sigma_m^2}$$
The provided as μ_i^2 and μ_i^2 and μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 and μ_i^2 are μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 are μ_i^2 and μ_i^2 are μ_i^2 are μ_i^2 and μ_i^2 are $\mu_i^$

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Matching coefficients of μ^2 , we get

$$rac{-\mu^2}{2\sigma_m^2}=rac{-\mu^2}{2}(rac{m}{\sigma^2}+rac{1}{\sigma_0^2})\Rightarrow$$

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Matching coefficients of μ , we get
$$\frac{-1}{2\sigma^2}\left(2\sum_{i=1}^m x_i\right)-\frac{1}{2\sigma_0^2}\stackrel{\times}{}^{2M_0}=\frac{-1}{2\sigma_m^2}+\frac{2M_m}{\sigma^2}$$

$$\frac{2\sigma^2}{2\sigma_m^2}=\frac{2\sigma_m^2}{2\sigma_m^2}+\frac{$$

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, we get
$$\frac{-\mu^2}{2\sigma_m^2} = \frac{-\mu^2}{2} \left(\frac{m}{\sigma^2} + \frac{1}{\sigma_0^2}\right) \Rightarrow \frac{1}{\sigma_m^2} = \frac{1}{\sigma_0^2} + \frac{m}{\sigma^2}$$

Matching coefficients of μ , we get

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

Our reference equality:

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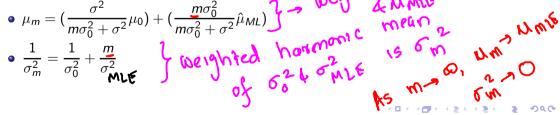
$$\frac{2\mu\mu_{m}}{2\sigma_{m}^{2}} = \mu\left(\frac{2\sum_{i=1}^{m}x_{i}}{2\sigma^{2}} + \frac{2\mu_{0}}{2\sigma_{0}^{2}}\right) \Rightarrow \mu_{m} = \sigma_{m}^{2}\left(\frac{\sum_{i=1}^{m}x_{i}}{\sigma^{2}} + \frac{\mu_{0}}{\sigma_{0}^{2}}\right) \text{ or } \mu_{m} = \sigma_{m}^{2}\left(\frac{m\hat{\mu}_{ML}}{\sigma^{2}} + \frac{\mu_{0}}{\sigma_{0}^{2}}\right) \Rightarrow \mu_{m} = \left(\frac{\sigma^{2}}{m\sigma_{0}^{2} + \sigma^{2}}\mu_{0}\right) + \left(\frac{m\sigma_{0}^{2}}{m\sigma_{0}^{2} + \sigma^{2}}\hat{\mu}_{ML}\right)$$

Summary: Conjugate Prior for (univariate) Gaussian

- Let $\Pr(X) \sim \mathcal{N}(\mu, \sigma^2)$ and let the data $\mathcal{D} = x_1...x_m$
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- 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?
- Answer: $\Pr(\mu|x_1...x_m) = \mathcal{N}(\mu_m, \sigma_m^2)$ such that

Summary: Conjugate Prior for (univariate) Gaussian

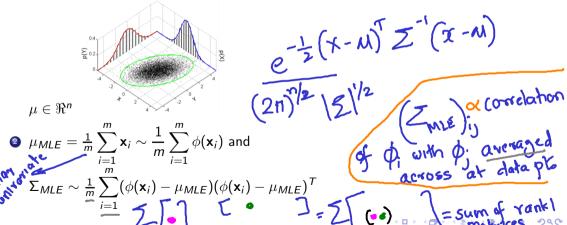
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- Suppose you are told that the conjugate prior for the (univariate) normally distributed random variable X in the case that σ^2 is not a random variable is $\mu_m = (\frac{\sigma^2}{m\sigma_0^2 + \sigma^2}\mu_0) + (\frac{m\sigma_0^2}{m\sigma_0^2 + \sigma^2}\hat{\mu}_{ML})$ weighted mean is the sum of the sum of



Multivariate Normal Distribution and MLE estimate

The multivariate Gaussian (Normal) Distribution is:

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



Summary for MAP estimation with Normal Distribution

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

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

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 uncertainty in μ

• For the Bayesian setting for the multivariate case with fixed Σ $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma), \ \mu \sim \mathcal{N}(\mu_0, \Sigma_0) \ \& \ p(\mathbf{x}|D) \sim \mathcal{N}(\mu_m, \Sigma_m)$

$$Z_{m}^{-1} = m Z_{ml} + Z_{\delta}$$

Summary for MAP estimation with Normal Distribution

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

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 \bullet For the Bayesian setting for the multivariate case with fixed Σ

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

$$\Sigma_{m}^{-1} = m\Sigma^{-1} + \Sigma_{0}^{-1}$$

$$\Sigma_{m}^{-1}\mu_{m} = m\Sigma^{-1}\hat{\mu}_{mle} + \Sigma_{0}^{-1}\mu$$

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



Prior Distribution for w for Linear Regression

$$P(\omega) = \mathcal{N}(\omega) | O_{1} \frac{1}{\lambda} \mathbf{I}$$

$$y = \mathbf{w}^{T} \phi(\mathbf{x}) + \varepsilon$$

$$\varepsilon \sim \mathcal{N}(0, \sigma^{2})$$

$$P_{1}(\omega) \mathcal{D} ?$$

- We saw that when we try to maximize log-likelihood we end up with $\hat{\mathbf{w}}_{MLE} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$
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$$w_i \sim \mathcal{N}(0, \frac{1}{\lambda})$$

..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

Recall.
$$x \sim N(N, \Sigma)$$
 $N \sim N(N_0, \Sigma_0)$ $Y = \Phi w + \epsilon \{ \} \}$
Here: $\epsilon \sim N(0, \sigma^2)$ $W \sim N(0, \frac{1}{2}\Sigma)$ $Y = \omega^{T} \phi(x) + \epsilon$
of $w = N(0, \frac{1}{2})$ then $w \sim N(0, \frac{1}{2}L)$ where L is an $n \times n$ identity matrix

- 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
- **3** We will specifically consider Bayesian Estimation for multivariate Gaussian (Normal) Distribution on \mathbf{w} : $\frac{1}{(2\pi)^{\frac{n}{2}}(\frac{1}{\lambda})^{\frac{1}{2}}}e^{-\frac{\lambda}{2}\|w\|_2^2}$

$$Z_{o} = \frac{1}{\lambda} I \quad M_{o} = 0 \quad P_{1}(\omega | D) = W(M_{m}, Z_{m})$$

$$Z_{m}^{-1} = \lambda I + \Phi^{T} \Phi^{*} \frac{1}{\sigma^{2}} \quad Z_{m}^{M_{m}} = Z_{o}^{M_{o}} + \Phi^{T} y/\sigma^{2}$$

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

(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: $P(\omega)$

Prior Distribution for w for Linear Regression

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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:

$$\Sigma_{m}^{-1}\mu_{m} = \Sigma_{0}^{-1}\mu_{0} + \Phi^{T}y/\sigma^{2}$$
$$\Sigma_{m}^{-1} = \Sigma_{0}^{-1} + \frac{1}{\sigma^{2}}\Phi^{T}\Phi$$



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

$$\Sigma_{m}^{-1}\mu_{m} = \Phi^{T}\mathbf{y}/\sigma^{2}$$

$$\Sigma_{m}^{-1} = \lambda I + \Phi^{T}\Phi/\sigma^{2}$$

$$\mu_{m} = \frac{(\lambda I + \Phi^{T}\Phi/\sigma^{2})^{-1}\Phi^{T}\mathbf{y}}{\sigma^{2}}$$

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 ⇒

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

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

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

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	$\hat{ heta}_{ extit{MLE}} = \operatorname{argmax}_{ heta} extit{LL}(D heta)$	$p(x \theta_{MLE})$
Bayes Estimator	$\hat{\theta}_B = E_{p(\theta D)}E[\theta]$	$p(x \theta_B)$
MAP	$\mid \hat{ heta}_{MAP} = \operatorname{argmax}_{ heta} p(heta D)$	$p(x \theta_{MAP})$
Pure Bayesian	[y x,w,x) = N(nop(x) +)	$p(\theta D) = rac{p(D \theta)p(\theta)}{\int\limits_{m} p(D \theta)p(\theta)d\theta}$ $p(D \theta) = \prod_{i=1} p(x_i \theta)$ $p(x D) = \int\limits_{\theta} p(x \theta)p(\theta D)d\theta$

where θ is the parameter

