

Bayesian Regression

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Bayesian Statistics: Recap

The Bayesian Method

① Define the model:

- Choose a probability model or “**likelihood model**”:

$$\{p(\mathcal{D} \mid \theta) \mid \theta \in \Theta\}.$$

- Choose a distribution $p(\theta)$, called the **prior distribution**.

② After observing \mathcal{D} , compute the **posterior distribution** $p(\theta \mid \mathcal{D})$.

③ Choose **action** based on $p(\theta \mid \mathcal{D})$.

- e.g. $\mathbb{E}[\theta \mid \mathcal{D}]$ as point estimate for θ
- e.g. interval $[a, b]$, where $p(\theta \in [a, b] \mid \mathcal{D}) = 0.95$

The Posterior Distribution

- By Bayes rule, can write the posterior distribution as

$$p(\theta | \mathcal{D}) = \frac{p(\mathcal{D} | \theta)p(\theta)}{p(\mathcal{D})}.$$

- likelihood:** $p(\mathcal{D} | \theta)$
- prior:** $p(\theta)$
- marginal likelihood:** $p(\mathcal{D})$.
- Note: $p(\mathcal{D})$ is just a normalizing constant for $p(\theta | \mathcal{D})$. Can write

$$\underbrace{p(\theta | \mathcal{D})}_{\text{posterior}} \propto \underbrace{p(\mathcal{D} | \theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}}.$$

Summary

- Prior represents belief about θ before observing data \mathcal{D} .
- Posterior represents the **rationally “updated” beliefs** after seeing \mathcal{D} .
- All inferences and action-taking are based on posterior distribution.

Bayesian Gaussian Linear Regression

Bayesian Conditional Models

- Input space $\mathcal{X} = \mathbf{R}^d$ Output space $\mathcal{Y} = \mathbf{R}$
- **Conditional probability model, or likelihood model:**

$$\{p(y | x, \theta) \mid \theta \in \Theta\}$$

- Conditional here refers to the conditioning on the input x .
 - x 's are not governed by our probability model.
 - Everything conditioned on x means “ x is known”
- **Prior distribution:** $p(\theta)$ on $\theta \in \Theta$

Gaussian Regression Model

- Input space $\mathcal{X} = \mathbf{R}^d$ Output space $\mathcal{Y} = \mathbf{R}$
- **Conditional probability model, or likelihood model:**

$$y \mid x, w \sim \mathcal{N}(w^T x, \sigma^2),$$

for some known $\sigma^2 > 0$.

- **Parameter space?** \mathbf{R}^d .
- **Data:** $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$
 - **Notation:** $y = (y_1, \dots, y_n)$ and $x = (x_1, \dots, x_n)$.
 - Assume y_i 's are **conditionally independent**, given x and w .

Conditional Independence (Review)

Definition

We say W and S are **conditionally independent** given R , denoted

$$W \perp S \mid R,$$

if the conditional joint factorizes as

$$p(w, s \mid r) = p(w \mid r)p(s \mid r).$$

Also holds when W , S , and R represent **sets of random variables**.

- Can have conditional independence without independence.
- Can have independence without conditional independence.

Gaussian Likelihood and MLE

- The **likelihood** of $w \in \mathbf{R}^d$ for the data \mathcal{D} is

$$\begin{aligned} p(y \mid x, w) &= \prod_{i=1}^n p(y_i \mid x_i, w) \quad \text{by conditional independence.} \\ &= \prod_{i=1}^n \left[\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right) \right] \end{aligned}$$

- You should see **in your head**¹ that the **MLE** is

$$\begin{aligned} w_{\text{MLE}}^* &= \arg \max_{w \in \mathbf{R}^d} p(y \mid x, w) \\ &= \arg \min_{w \in \mathbf{R}^d} \sum_{i=1}^n (y_i - w^T x_i)^2. \end{aligned}$$

¹See <https://davidrosenberg.github.io/ml2015/docs/8.Lab.glm.pdf>, slide 5.

Priors and Posteriors

- Choose a Gaussian **prior distribution** $p(w)$ on \mathbf{R}^d :

$$w \sim \mathcal{N}(0, \Sigma_0)$$

for some **covariance matrix** $\Sigma_0 \succ 0$ (i.e. Σ_0 is spd).

- Posterior distribution**

$$\begin{aligned} p(w \mid \mathcal{D}) &= p(w \mid x, y) \\ &= p(y \mid x, w) p(w) / p(y \mid x) \\ &\propto p(y \mid x, w) p(w) \\ &= \prod_{i=1}^n \left[\frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \right] \text{ (likelihood)} \\ &\quad \times |2\pi \Sigma_0|^{-1/2} \exp \left(-\frac{1}{2} w^T \Sigma_0^{-1} w \right) \text{ (prior)} \end{aligned}$$

Predictive Distributions

- **Likelihood model:** $y \mid x, w \sim \mathcal{N}(w^T x, \sigma^2)$
- If we knew w , best prediction function (for square loss) is

$$\hat{y}(x) = \mathbb{E}[y \mid x, w] = w^T x.$$

- In Bayesian statistics we have
 - **Prior distribution:** $w \sim \mathcal{N}(0, \Sigma_0)$, and
 - Given data, we can compute the **posterior distribution:** $p(w \mid \mathcal{D})$.
- Prior $p(w)$ and posterior $p(w \mid \mathcal{D})$ give **distributions over prediction functions**.

Gaussian Regression Example

Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathbb{R}$
- Given x , the world generates y as

$$y = w_0 + w_1 x + \varepsilon,$$

where $\varepsilon \sim \mathcal{N}(0, 0.2^2)$.

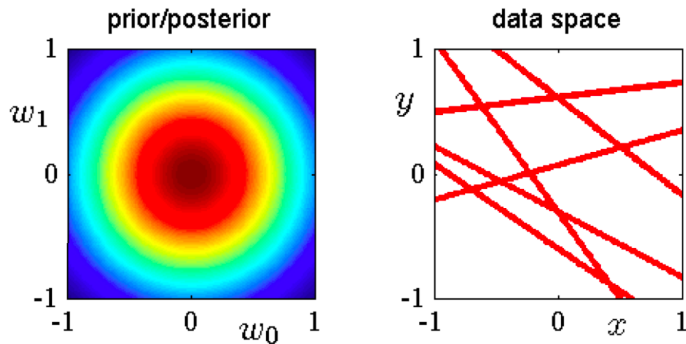
- Written another way, the **likelihood model** is

$$y \mid x, w_0, w_1 \sim \mathcal{N}(w_0 + w_1 x, 0.2^2).$$

- What's the parameter space? \mathbb{R}^2 .
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}(0, \frac{1}{2}I)$

Example in 1-Dimension: Prior Situation

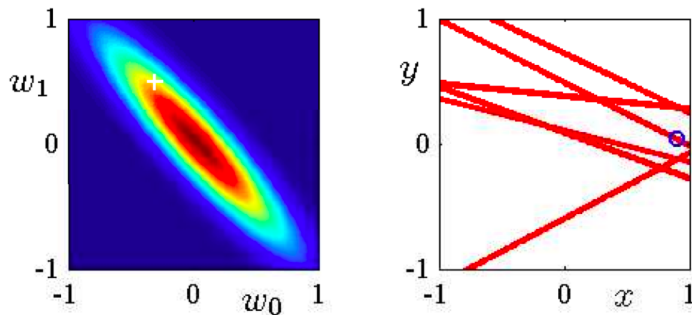
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}(0, \frac{1}{2}I)$ (Illustrated on left)



- On right, $y(x) = \mathbb{E}[y | x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}(0, \frac{1}{2}I)$.

Bishop's PRML Fig 3.7

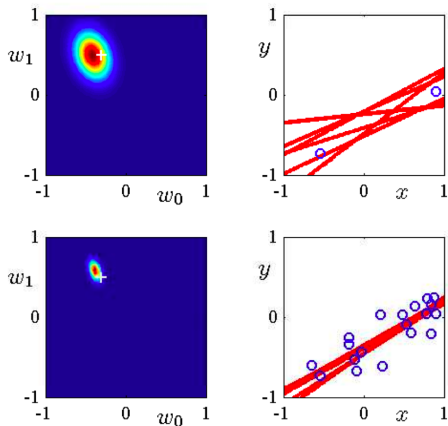
Example in 1-Dimension: 1 Observation



- On left: posterior distribution; white '+' indicates true parameters
- On right: blue circle indicates the training observation

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations



Bishop's PRML Fig 3.7

Gaussian Regression Continued

Closed Form for Posterior

- Model:

$$w \sim \mathcal{N}(0, \Sigma_0)$$

$$y_i | x, w \text{ i.i.d. } \mathcal{N}(w^T x_i, \sigma^2)$$

- Design matrix X ; Response column vector y
- Posterior distribution is a **Gaussian distribution**:

$$w | \mathcal{D} \sim \mathcal{N}(\mu_P, \Sigma_P)$$

$$\mu_P = (X^T X + \sigma^2 \Sigma_0^{-1})^{-1} X^T y$$

$$\Sigma_P = (\sigma^{-2} X^T X + \Sigma_0^{-1})^{-1}$$

- Posterior Variance Σ_P gives us a natural uncertainty measure.**

See Rasmussen and Williams' *Gaussian Processes for Machine Learning*, Ch 2.1. <http://www.gaussianprocess.org/gpml/chapters/RW2.pdf>

Closed Form for Posterior

- Posterior distribution is a **Gaussian distribution**:

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$$\Sigma_P = (\sigma^{-2} X^T X + \Sigma_0^{-1})^{-1}$$

- The **MAP estimator** and the **posterior mean** are given by

$$\mu_P = (X^T X + \sigma^2 \Sigma_0^{-1})^{-1} X^T y$$

- For the prior variance $\Sigma_0 = \frac{\sigma^2}{\lambda} I$, we get

$$\mu_P = (X^T X + \lambda I)^{-1} X^T y,$$

which is of course the ridge regression solution.

Posterior Variance vs. Traditional Uncertainty

- Traditional regression: OLS estimator (also the MLE) is a random variable – why?
 - Because estimator is a function of data \mathcal{D} and data is random.
- Common assumption: data are iid with Gaussian noise: $y = w^T x + \varepsilon$, with $\varepsilon \sim \mathcal{N}(0, \sigma^2)$.

- Then OLS estimator \hat{w} has a **sampling distribution** that is Gaussian with mean w and

$$\text{Cov}(\hat{w}) = (\sigma^{-2} X^T X)^{-1}$$

- By comparison, the posterior variance is

$$\Sigma_P = (\sigma^{-2} X^T X + \Sigma_0^{-1})^{-1}.$$

- When we take $\Sigma_0^{-1} = 0$, we get back $\text{Cov}(\hat{\theta})$ (i.e. like our prior variance goes to ∞ .)
- Σ_P is “smaller” than $\text{Cov}(\hat{w})$ because we’re using a “more informative” prior.

Posterior Mean and Posterior Mode (MAP)

- Posterior density for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w | \mathcal{D}) \propto \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2} \|w\|^2\right)}_{\text{prior}} \underbrace{\prod_{i=1}^n \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\text{likelihood}}$$

- To find **MAP**, sufficient to minimize the negative log posterior:

$$\begin{aligned} \hat{w}_{\text{MAP}} &= \arg \min_{w \in \mathbf{R}^d} [-\log p(w | \mathcal{D})] \\ &= \arg \min_{w \in \mathbf{R}^d} \underbrace{\sum_{i=1}^n (y_i - w^T x_i)^2}_{\text{log-likelihood}} + \underbrace{\lambda \|w\|^2}_{\text{log-prior}} \end{aligned}$$

- Which is the ridge regression objective.

Predictive Distribution

- Given a new input point x_{new} , how to predict y_{new} ?
- **Predictive distribution**

$$\begin{aligned} p(y_{\text{new}} | x_{\text{new}}, \mathcal{D}) &= \int p(y_{\text{new}} | x_{\text{new}}, w, \mathcal{D}) p(w | \mathcal{D}) dw \\ &= \int p(y_{\text{new}} | x_{\text{new}}, w) p(w | \mathcal{D}) dw \end{aligned}$$

- For Gaussian regression, predictive distribution has closed form.

Closed Form for Predictive Distribution

- Model:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i | x, w &\text{ i.i.d. } \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- Predictive Distribution

$$p(y_{\text{new}} | x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} | x_{\text{new}}, w) p(w | \mathcal{D}) dw.$$

- Averages over prediction for each w , weighted by posterior distribution.

- Closed form:

$$\begin{aligned} y_{\text{new}} | x_{\text{new}}, \mathcal{D} &\sim \mathcal{N}(\eta_{\text{new}}, \sigma_{\text{new}}) \\ \eta_{\text{new}} &= \mu_P^T x_{\text{new}} \\ \sigma_{\text{new}} &= \underbrace{x_{\text{new}}^T \Sigma_P x_{\text{new}}}_{\text{from variance in } w} + \underbrace{\sigma^2}_{\text{inherent variance in } y} \end{aligned}$$

Predictive Distributions

- With predictive distributions, can give mean prediction with error bands:

