

# Introduction to Machine Learning

Bayesian Regression

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## Outline

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## 1 Linear Regression

### 1.1 Problem Formulation

- There is one scalar **target** variable  $y$  (instead of hidden)

- There is one vector **input** variable  $x$

- Inductive bias:

$$y = \mathbf{w}^\top \mathbf{x}$$

### Linear Regression Learning Task

Learn  $\mathbf{w}$  given training examples,  $\langle \mathbf{X}, \mathbf{y} \rangle$ .

The training data is denoted as  $\langle \mathbf{X}, \mathbf{y} \rangle$ , where  $\mathbf{X}$  is a  $N \times D$  data matrix consisting of  $N$  data examples such that each data example is a  $D$  dimensional vector.  $\mathbf{y}$  is a  $N \times 1$  vector consisting of corresponding target values for the examples in  $\mathbf{X}$ .

- $y$  is assumed to be normally distributed

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

- or, equivalently:

$$y = \mathbf{w}^\top \mathbf{x} + \epsilon$$

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

- $y$  is a *linear combination* of the input variables
- Given  $\mathbf{w}$  and  $\sigma^2$ , one can find the probability distribution of  $y$  for a given  $\mathbf{x}$

### 1.2 Learning Parameters

- Find  $\mathbf{w}$  and  $\sigma^2$  that maximize the likelihood of training data

$$\begin{aligned}\hat{\mathbf{w}}_{MLE} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \\ \hat{\sigma}_{MLE}^2 &= \frac{1}{N} (\mathbf{y} - \mathbf{X} \hat{\mathbf{w}})^\top (\mathbf{y} - \mathbf{X} \hat{\mathbf{w}})\end{aligned}$$

The derivation of the MLE estimates can be done by maximizing the log-likelihood of the data set. The likelihood of the training data set is given by:

$$L(\mathbf{w}) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \mathbf{w}^\top \mathbf{x}_i)^2}{2\sigma^2}\right)$$

The log-likelihood is given by:

$$LL(\mathbf{w}) = -\frac{1}{2} \log 2\pi - \log \sigma - \frac{1}{2\sigma^2} \sum_{i=1}^N (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

This can be rewritten in matrix notation as:

$$LL(\mathbf{w}) = -\frac{1}{2} \log 2\pi - \log \sigma - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w})$$

To maximize the log-likelihood, we first compute its derivative with respect to  $\mathbf{w}$  and  $\sigma$ .

$$\begin{aligned} \frac{\partial LL(\mathbf{w})}{\partial \mathbf{w}} &= -\frac{1}{2\sigma^2} \frac{\partial}{\partial \mathbf{w}} (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= -\frac{1}{2\sigma^2} \frac{\partial}{\partial \mathbf{w}} (\mathbf{y}^\top \mathbf{y} + \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} - 2\mathbf{y}^\top \mathbf{X} \mathbf{w}) \end{aligned}$$

Note that, we use the fact that  $(\mathbf{X}\mathbf{w})^\top \mathbf{y} = \mathbf{y}^\top \mathbf{X}\mathbf{w}$ , since both quantities are scalars and the transpose of a scalar is equal to itself. Continuing with the derivative:

$$\frac{\partial LL(\mathbf{w})}{\partial \mathbf{w}} = -\frac{1}{2\sigma^2} (2\mathbf{w}^\top \mathbf{X}^\top \mathbf{X} - 2\mathbf{y}^\top \mathbf{X})$$

Setting the derivative to 0, we get:

$$\begin{aligned} 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{X} - 2\mathbf{y}^\top \mathbf{X} &= 0 \\ \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} &= \mathbf{y}^\top \mathbf{X} \\ (\mathbf{X}^\top \mathbf{X})^\top \mathbf{w} &= \mathbf{X}^\top \mathbf{y} \text{ (Taking transpose both sides)} \\ (\mathbf{X}^\top \mathbf{X}) \mathbf{w} &= \mathbf{X}^\top \mathbf{y} \\ \mathbf{w} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \end{aligned}$$

In a similar fashion, one can set the derivative to 0 with respect to  $\sigma$  and plug in the the optimal value of  $\mathbf{w}$

### 1.3 Issues with Linear Regression

1. Not truly Bayesian
2. Susceptible to outliers

3. *Too simplistic* - Underfitting
4. No way to control overfitting
5. Unstable in presence of correlated input attributes
6. Gets “confused” by unnecessary attributes

## 2 Bayesian Linear Regression

### 3 Bayesian Regression

- “Penalize” large values of  $\mathbf{w}$
- A zero-mean Gaussian prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \tau^2 I)$$

- What is posterior of  $\mathbf{w}$

$$p(\mathbf{w}|\mathcal{D}) \propto \prod_i \mathcal{N}(y_i|\mathbf{w}^\top \mathbf{x}_i, \sigma^2) p(\mathbf{w})$$

- Posterior is also Gaussian
- Regularized least squares estimate of  $\mathbf{w}$

$$\arg \max_{\mathbf{w}} \sum_{i=1}^N \log \mathcal{N}(y_i|\mathbf{w}^\top \mathbf{x}_i, \sigma^2) + \log \mathcal{N}(\mathbf{w}|0, \tau^2 I)$$

#### 3.1 Estimating Bayesian Regression Parameters

- Prior for  $\mathbf{w}$

$$\mathbf{w} \sim \mathcal{N}(\mathbf{w}|0, \tau^2 \mathbf{I}_D)$$

- Posterior for  $\mathbf{w}$

$$\begin{aligned} p(\mathbf{w}|\mathbf{y}, \mathbf{X}) &= \frac{p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})} \\ &= \mathcal{N}(\bar{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + \frac{\sigma^2}{\tau^2} \mathbf{I}_N)^{-1} \mathbf{X}^\top \mathbf{y}, \sigma^2 (\mathbf{X}^\top \mathbf{X} + \frac{\sigma^2}{\tau^2} \mathbf{I}_N)^{-1}) \end{aligned}$$

- Posterior distribution for  $\mathbf{w}$  is also Gaussian
- What will be MAP estimate for  $\mathbf{w}$ ?

The denominator term in the posterior above can be computed as the marginal likelihood of data by marginalizing  $\mathbf{w}$ :

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})d\mathbf{w}$$

One can compute the posterior for  $\mathbf{w}$  as follows. We first show that the likelihood of  $\mathbf{y}$ , i.e., all target values in the training data, can be jointly modeled as a Gaussian as follows:

$$\begin{aligned} p(\mathbf{y}|\mathbf{X}, \mathbf{w}) &= \prod_{i=1}^N \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2\right) \\ &= \frac{1}{(2\pi\sigma^2)^{N/2}} \exp\left(-\frac{1}{2\sigma^2}|\mathbf{y} - \mathbf{X}\mathbf{w}|^2\right) \\ &= \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I}_N) \end{aligned}$$

Ignoring the denominator which does not depend on  $\mathbf{w}$ :

$$\begin{aligned} p(\mathbf{w}|\mathbf{y}, \mathbf{X}) &\propto \exp\left(-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w})\right) \exp\left(-\frac{1}{2\tau^2}\mathbf{w}^\top \mathbf{w}\right) \\ &\propto \exp\left(-\frac{1}{2}(\mathbf{w} - \bar{\mathbf{w}})^\top \left(\frac{1}{\sigma^2}\mathbf{X}^\top \mathbf{X} + \frac{1}{\tau^2}\mathbf{I}_N\right)(\mathbf{w} - \bar{\mathbf{w}})\right) \end{aligned}$$

where  $\bar{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + \frac{\sigma^2}{\tau^2}\mathbf{I}_N)^{-1}\mathbf{X}^\top \mathbf{y}$ .

### 3.2 Prediction with Bayesian Regression

- For a new  $\mathbf{x}^*$ , predict  $y^*$
- Point estimate of  $y^*$

$$y^* = \hat{\mathbf{w}}_{MLE}^\top \mathbf{x}^*$$

- Treating  $y$  as a Gaussian random variable

$$\begin{aligned} p(y^*|\mathbf{x}^*) &= \mathcal{N}(\hat{\mathbf{w}}_{MLE}^\top \mathbf{x}^*, \hat{\sigma}_{MLE}^2) \\ p(y^*|\mathbf{x}^*) &= \mathcal{N}(\hat{\mathbf{w}}_{MAP}^\top \mathbf{x}^*, \hat{\sigma}_{MAP}^2) \end{aligned}$$

- Treating  $y$  and  $\mathbf{w}$  as random variables

$$p(y^*|\mathbf{x}^*) = \int p(y^*|\mathbf{x}^*, \mathbf{w})p(\mathbf{w}|\mathbf{X}, \mathbf{y})d\mathbf{w}$$

- This is also *Gaussian*!

## 4 Handling Outliers in Regression

- Linear regression training gets impacted by the presence of outliers
- The square term in the exponent of the Gaussian pdf is the culprit
  - Equivalent to the square term in the loss
- How to handle this (*Robust Regression*)?
- Probabilistic:
  - Use a different distribution instead of Gaussian for  $p(y|\mathbf{x})$
  - Robust regression uses Laplace distribution

$$p(y|\mathbf{x}) \sim \text{Laplace}(\mathbf{w}^\top \mathbf{x}, b)$$

- Geometric:
  - *Least absolute deviations* instead of least squares

$$J(\mathbf{w}) = \sum_{i=1}^N |y_i - \mathbf{w}^\top \mathbf{x}_i|$$

## 5 Generative vs. Discriminative Classifiers

- Probabilistic classification task:

$$p(Y = \text{benign}|\mathbf{X} = \mathbf{x}), p(Y = \text{malicious}|\mathbf{X} = \mathbf{x})$$

- How do you estimate  $p(y|\mathbf{x})$ ?

$$p(y|\mathbf{x}) = \frac{p(y, \mathbf{x})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$$

- Two step approach - Estimate generative model and then posterior for  $y$  (Naïve Bayes)
- Solving a more general problem [2, 1]
- Why not directly model  $p(y|\mathbf{x})$ ? - **Discriminative approach**
- Number of training examples needed to learn a PAC-learnable classifier  $\propto VC\text{-dimension of the hypothesis space}$
- VC-dimension of a probabilistic classifier  $\propto$  Number of parameters [2] (or a small polynomial in the number of parameters)
- Number of parameters for  $p(y, \mathbf{x}) >$  Number of parameters for  $p(y|\mathbf{x})$

Discriminative classifiers need lesser training examples to for PAC learning than generative classifiers

## 6 Bayesian Logistic Regression

- $y|\mathbf{x}$  is a *Bernoulli* distribution with parameter  $\theta = \text{sigmoid}(\mathbf{w}^\top \mathbf{x})$
- When a new input  $\mathbf{x}^*$  arrives, we toss a coin which has  $\text{sigmoid}(\mathbf{w}^\top \mathbf{x}^*)$  as the probability of heads
- If outcome is heads, the predicted class is 1 else 0
- Learns a linear boundary

### Learning Task for Logistic Regression

Given training examples  $\langle \mathbf{x}_i, y_i \rangle_{i=1}^D$ , learn  $\mathbf{w}$

## References

## References

- [1] A. Y. Ng and M. I. Jordan. On discriminative vs. generative classifiers: A comparison of logistic regression and naive bayes. In T. G. Dietterich, S. Becker, and Z. Ghahramani, editors, *NIPS*, pages 841–848. MIT Press, 2001.

- [2] V. Vapnik. *Statistical learning theory*. Wiley, 1998.