

# DSC 140A

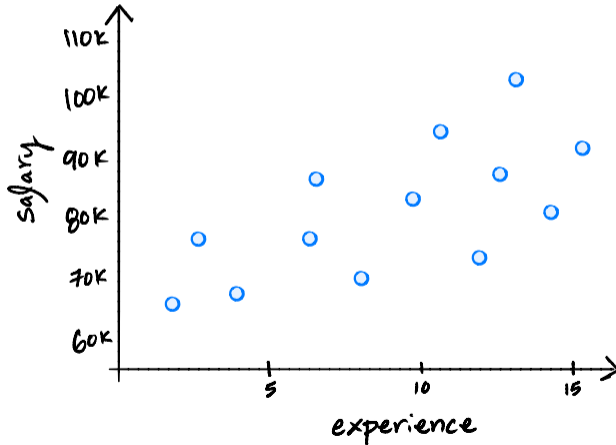
*Probabilistic Modeling & Machine Learning*

Lecture 16 | Part 1

**Recall: Regression**

# Recall

- ▶ We have seen the problem of regression.



# Recall

- ▶ Introduced **empirical risk minimization (ERM)**:
- ▶ Step 1: choose a **hypothesis class**
  - ▶ Let's assume we've chosen linear predictors
- ▶ Step 2: choose a **loss function**
  - ▶ Used square loss
- ▶ Step 3: minimize **expected loss (empirical risk)**
  - ▶ MSE (Mean Squared Error)

# Recall: Least Squares

- ▶ Goal: fit a function of the form  $H(\vec{x}; \vec{w}) = \text{Aug}(\vec{x}) \cdot \vec{w}$
- ▶ In (ordinary) least squares regression, we **minimized** the **mean squared error**:

$$\vec{w}^* = \arg \min_{\vec{w}} \frac{1}{n} \sum_{i=1}^n (H(\vec{x}^{(i)}; \vec{w}) - y_i)^2$$

- ▶ **Solution:**  $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$

# Observation

- ▶ This the “curve fitting” approach to regression.
- ▶ I.e., find a “line of best fit”.
- ▶ There was no consideration of the (random) process that generated the data.

# Today

- ▶ Take a probabilistic approach to regression.

# DSC 140A

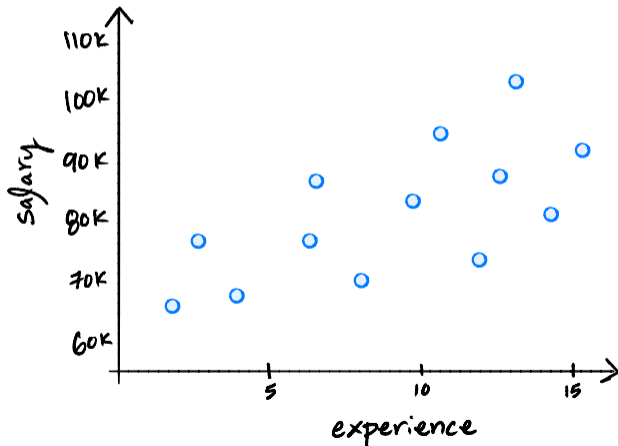
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Lecture 16 | Part 2

**Probabilistic View of Regression**

# Probabilistic View of Regression

- **Note:** There is **uncertainty** in the salary.



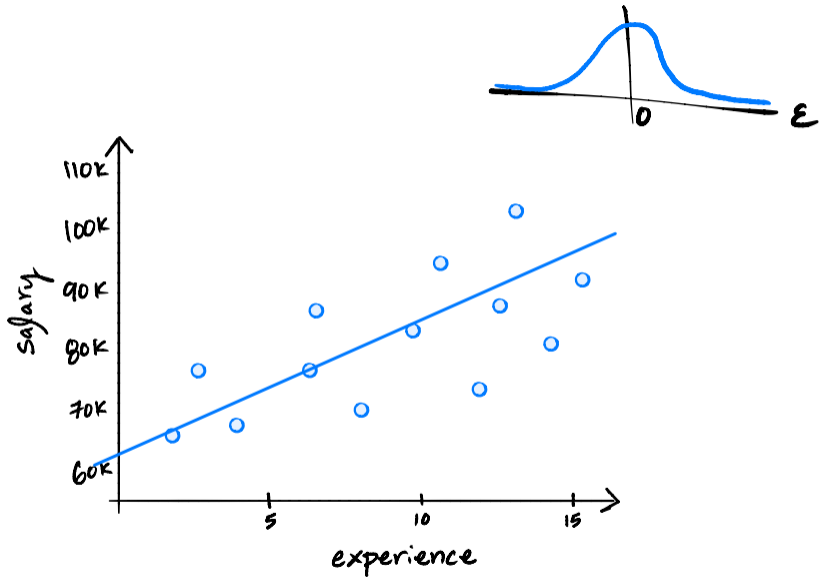


# Modeling Uncertainty

- ▶ We can model this uncertainty using probability.

$$\text{Salary} = w_0 + w_1 \times (\text{Experience}) + \varepsilon$$

- ▶ Here,  $\varepsilon$  is the (random) **error**.
- ▶ What is a reasonable choice of **distribution** for  $\varepsilon$ ?



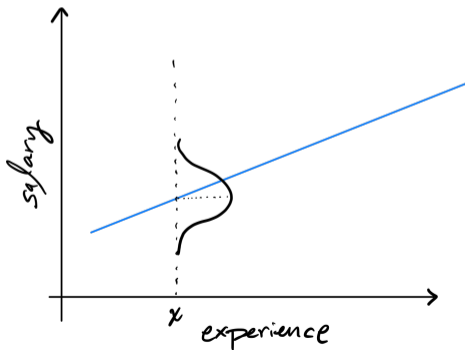
# Error Distribution

- ▶ It is reasonable to assume that the error distribution is:
  - ▶ **Symmetric:** equally as likely to predict high as to predict low
  - ▶ **Centered at zero:** mean error is zero
- ▶ The **Gaussian distribution** (with mean 0) satisfies this.

# Modeling Uncertainty

- ▶ Assuming a Gaussian (Normal) distribution:

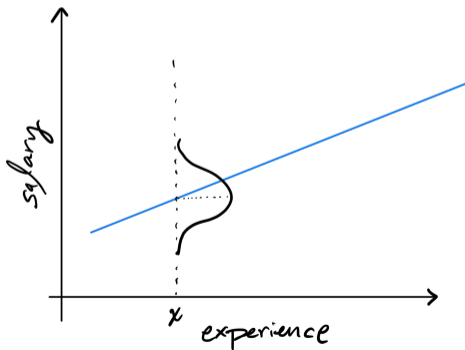
$$\text{Salary} = w_0 + w_1 \times (\text{Experience}) + \underbrace{\mathcal{N}(0, \sigma^2)}_{\varepsilon}$$



# Modeling Uncertainty

- ▶ Equivalently:

$$\text{Salary} \sim \mathcal{N}(w_0 + w_1 \times \text{Experience}, \sigma^2)$$



# In General

- ▶ In general:

$$Y \sim \mathcal{N}(\text{Aug}(\vec{x}) \cdot \vec{w}, \sigma^2)$$

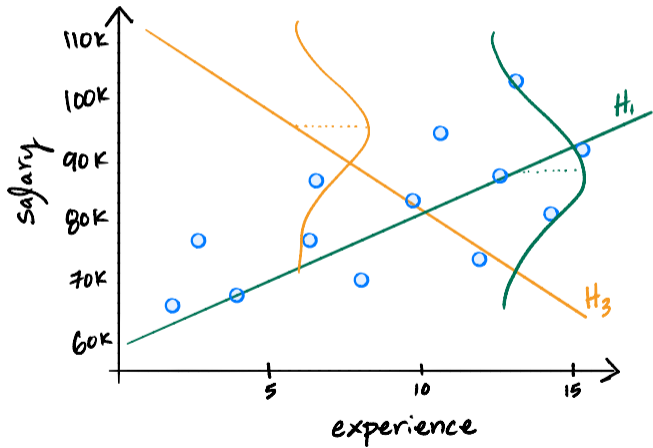
- ▶ That is: for any feature vector  $\vec{x}$ , the target  $Y$  is drawn from a Gaussian centered at  $\text{Aug}(\vec{x}) \cdot \vec{w}$ .

# Estimating Parameters

- ▶ We assume the model:

$$\text{Salary} \sim \mathcal{N}(w_0 + w_1 \times \text{Experience}, \sigma^2)$$

- ▶ Given some data, what parameters generated it?
  - ▶ What were  $w_0$ ,  $w_1$ ,  $\sigma$ ?
- ▶ **Estimate** them with maximum likelihood?





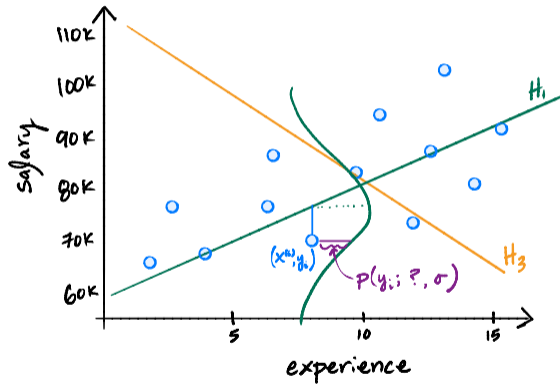
# Likelihood

- ▶ Let  $p(y; \mu, \sigma)$  be the Gaussian pdf:

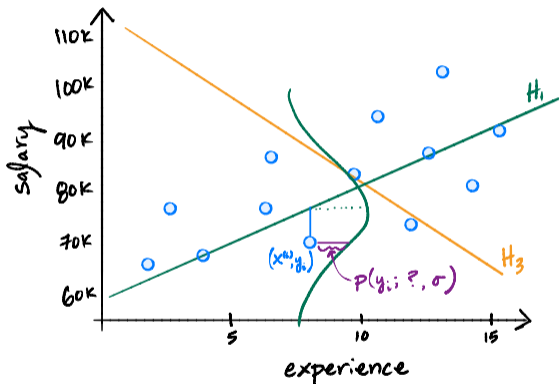
$$p(y; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(y-\mu)^2/(2\sigma^2)}$$

- ▶ We observe a data set  $\{(\vec{x}^{(i)}, y_i)\}$ .
- ▶ What is the likelihood of a choice of parameters  $\vec{w}, \sigma$ , with respect to the data?

# Likelihood wrt a Point



# Likelihood wrt a Point



- ▶  $p(y_i; w_0 + w_1 x^{(i)}, \sigma)$  measures likelihood with respect to  $(x^{(i)}, y_i)$ .

# Likelihood

- ▶ In general,

$$p(y_i; \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, \sigma)$$

measures likelihood with respect to single data point  $(\vec{x}^{(i)}, y_i)$ .

- ▶ Likelihood with respect to data set:

$$L(\vec{w}, \sigma) = \prod_{i=1}^n p(y_i; \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, \sigma)$$

# Log-Likelihood

Compute the log-likelihood from  $\prod_{i=1}^n p(y_i; \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, \sigma)$ .

$$p(y; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(y-\mu)^2}{\sigma^2}}$$

$$p(y_i; \vec{w}, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}}$$

$$Z(\vec{w}, \sigma) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}}$$

$$\tilde{Z}(\vec{w}, \sigma) = \ln \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}}$$

$$= \sum_{i=1}^n \ln \left[ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}} \right]$$

# Log-Likelihood

Compute the log-likelihood from

$$\prod_{i=1}^n p(y_i; \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, \sigma).$$

$$= \sum_{i=1}^n \ln \left[ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}\right\} \right]$$

$$= \sum_{i=1}^n \left[ \ln \frac{1}{\sqrt{2\pi\sigma^2}} + \ln \exp\left\{-\frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2}\right\} \right]$$

$$= \sum_{i=1}^n \left[ \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2} \frac{(y_i - \vec{w} \cdot \vec{x}^{(i)})^2}{\sigma^2} \right]$$

$$\ln \frac{1}{\sigma^2} = \ln 1 - \ln \sigma^2 = 0 - 2 \ln \sigma$$

## Log-Likelihood

- ▶ The log-likelihood is:

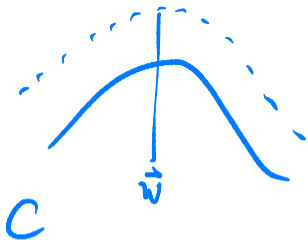
$$\tilde{L}(\vec{w}, \sigma) = -\frac{1}{2\sigma^2} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 + \frac{n}{2} \ln \frac{1}{\sigma^2} - \frac{n}{2} \ln(2\pi)$$

- ▶ We want to **maximize** this quantity.

$$\arg \max_{\vec{w}} f(\vec{w}) + C$$

$$= \arg \max_{\vec{w}} f(\vec{w})$$

## Claim 1



$$\arg \max_{\vec{w}} \left[ -\frac{1}{2\sigma^2} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 + \frac{n}{2} \ln \frac{1}{\sigma^2} - \frac{n}{2} \ln(2\pi) \right]$$

=

$$\arg \max_{\vec{w}} \left[ -\frac{1}{2\sigma^2} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 \right]$$



$$\arg \max_{\vec{w}} c_1 f(\vec{w})$$

$$= c_2, c_1 > 0$$

**Claim 2**

$$\arg \max_{\vec{w}} c_2 f(\vec{w})$$

$$\arg \max_{\vec{w}} \left[ -\frac{1}{2\sigma^2} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 \right]$$

=

$$\arg \max_{\vec{w}} \left[ -\frac{1}{n} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 \right]$$

$$\arg \max_{\vec{w}} -f(\vec{w})$$

$$= \arg \min_{\vec{w}} f(\vec{w})$$

## Claim 3

$$\arg \max_{\vec{w}} \left[ -\frac{1}{n} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 \right]$$

=

$$\arg \min_{\vec{w}} \left[ \frac{1}{n} \sum_{i=1}^n (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2 \right]$$

- ▶ That is, minimize the **mean squared error**.

## Main Idea

Maximizing the likelihood of  $\vec{w}$  with respect to the data (assuming Gaussian error term) is **equivalent** to minimizing mean squared error.

# Solution

- ▶ The maximum likelihood estimate for  $\vec{w}$  is therefore:

$$\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$$

- ▶ That is, the exact same as we obtained by empirical risk minimization with the square loss.

# DSC 140A

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Lecture 16 | Part 3

**A Probabilistic View of Regularization**

# Recall: Ridge Regression

- ▶ In **ridge regression**, we added a regularization term:  $\|\vec{w}\|^2$ .

$$\vec{w}^* = \arg \min_{\vec{w}} \frac{1}{n} \sum_{i=1}^n (H(\vec{x}^{(i)}; \vec{w}) - y_i)^2 + \lambda \|\vec{w}\|^2$$

- ▶ **Solution:**  $\vec{w}^* = (X^T X + n\lambda I)^{-1} X^T \vec{y}$
- ▶ Helps control overfitting.

# Probabilistic View

- ▶ Regularization term  $\|\vec{w}\|^2$  was motivated by observing that  $\|\vec{w}\|$  tends to be large when overfitting.
- ▶ Now: motivate same term, probabilistically.
- ▶ Will adopt a **Bayesian** perspective.

# A Prior on Weights

- ▶ Imagine we have yet to see the data.
- ▶ There is no reason to believe that a given weight  $w_i$  is positive or negative.
- ▶ We believe it is more likely to be small (close to zero) than large.



# A Prior on Weights

- ▶ This **prior belief** is captured by assuming:

$$w_i \sim \mathcal{N}(0, s^2)$$

- ▶ Note that in truth,  $w_i$  is **not** random.
- ▶ We are adopting a **Bayesian** view of probability; it expresses level of belief.

# A Prior on Weights

- ▶ If each weight has distribution  $\mathcal{N}(0, s^2)$ , then:

$$\vec{w} \sim \mathcal{N}(\vec{0}, s^2 \cdot I)$$

- ▶ That is, the distribution of  $\vec{w}$  has density:

$$p_{\vec{w}}(\vec{w}) = \frac{1}{(2\pi s^2)^{d/2}} e^{-\frac{1}{2} \frac{\|\vec{w}-\vec{0}\|^2}{s^2}}$$

# Distribution of $\vec{w}$

- ▶ Using Bayes' Rule:

$$p_{\vec{w}}(\vec{w} | \vec{x}, y) \propto p_y(y | \vec{w}, \vec{x})p_{\vec{w}}(\vec{w})$$

- ▶ What is the most probable value of  $\vec{w}$ ?

$$\begin{aligned}\arg \max_{\vec{w}} [p_{\vec{w}}(\vec{w} | \vec{x}, y)] &= \arg \max_{\vec{w}} [p_y(y | \vec{w}, \vec{x})p_{\vec{w}}(\vec{w})] \\ &= \arg \max_{\vec{w}} \ln [p_y(y | \vec{w}, \vec{x})p_{\vec{w}}(\vec{w})] \\ &= \arg \max_{\vec{w}} [\ln p_y(y | \vec{w}, \vec{x}) + \ln p_{\vec{w}}(\vec{w})] \\ &= \arg \min_{\vec{w}} [-\ln p_y(y | \vec{w}, \vec{x}) - \ln p_{\vec{w}}(\vec{w})] \\ &= \arg \min_{\vec{w}} [\text{MSE}(\vec{w}) - \ln p_{\vec{w}}(\vec{w})]\end{aligned}$$

# Deriving the Regularizer

► Since

$$p_{\vec{w}}(\vec{w}) = \frac{1}{(2\pi s^2)^{d/2}} e^{-\frac{1}{2} \frac{\|\vec{w}-\vec{0}\|^2}{s^2}}$$

we have:

$$-\ln p_{\vec{w}}(\vec{w}) = c + \frac{1}{2s^2} \|\vec{w}\|^2$$

► So

$$\arg \min_{\vec{w}} [\text{MSE}(\vec{w}) - \ln p_{\vec{w}}(\vec{w})] = \arg \min_{\vec{w}} \left[ \text{MSE}(\vec{w}) + \underbrace{\frac{1}{2s^2}}_{\lambda} \|\vec{w}\|^2 \right]$$

## Main Idea

Placing a  $\mathcal{N}(0, s^2)$  prior on each weight and maximizing  $p_{\vec{w}}(\vec{w} | \vec{x}, y)$  is equivalent to minimizing the  $\|\vec{w}\|^2$ -regularized mean squared error (**ridge regression**).