DSC 140A

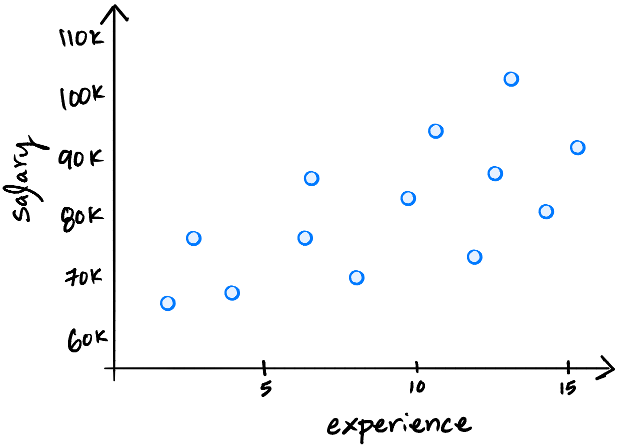
Probabilistic Modeling & Machine Learning

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.

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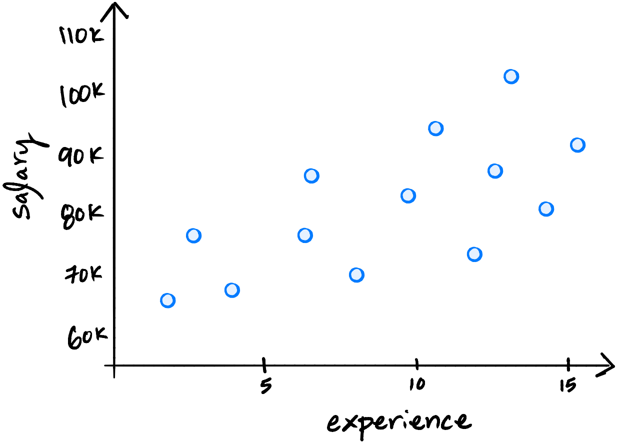
Probabilistic Modeling & Machine Learning

Lecture 16 | Part 2

Probabilistic View of Regression

Probabilistic View of Regression

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

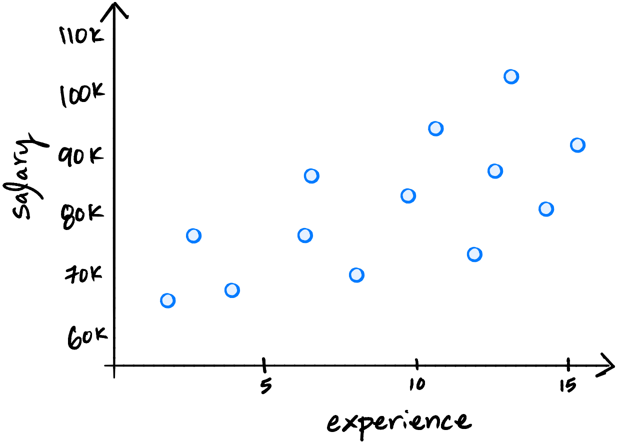


Modeling Uncertainty

- We can model this uncertainty using probability.

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

- Here, ε is the (random) **error**.
- What is a reasonable choice of **distribution** for ε?



110K
100K
90K
80K
70K
60K
salary
5
10
15
experience

Error Distribution

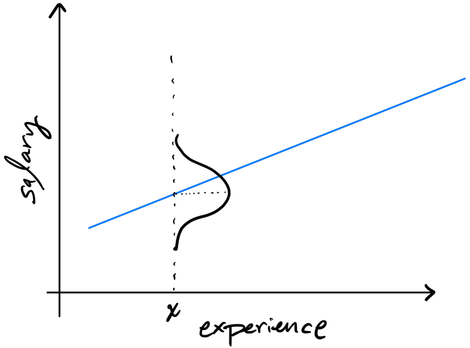
- It is reasonable to assume that the error distribution is:
  - **Symmetric:** equally as likely to predict high as to predict low
  - **Centered at zero:** mean error is zero

- The **Gaussian distribution** (with mean 0) satisfies this.

Modeling Uncertainty

- Assuming a Gaussian (Normal) distribution:

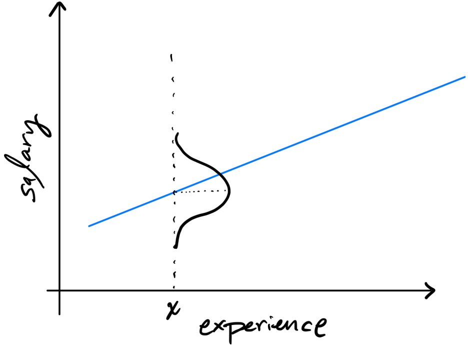
$$\text{Salary} = w_0 + w_1 \times (\text{Experience}) + \underbrace{\mathcal{N}(0, \sigma^2)}_{\varepsilon}$$



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 $\text{Aug}(\vec{x}) \cdot \vec{w}$.

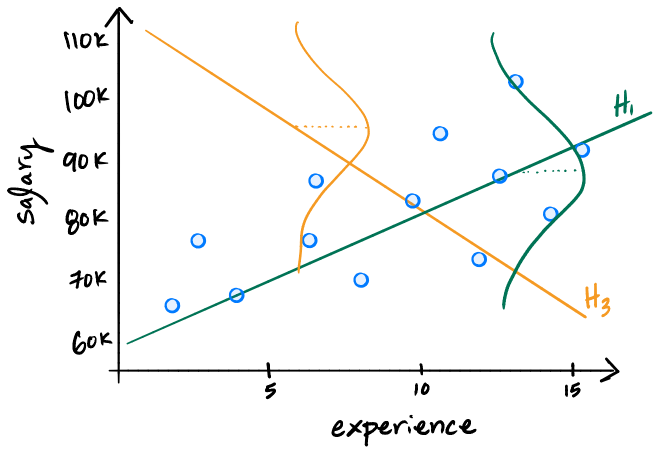
Estimating Parameters

- 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, σ?

- **Estimate** them with maximum likelihood?


110K
100K
90K
80K
70K
60K
salary
5
10
15
experience
H_1
H_3

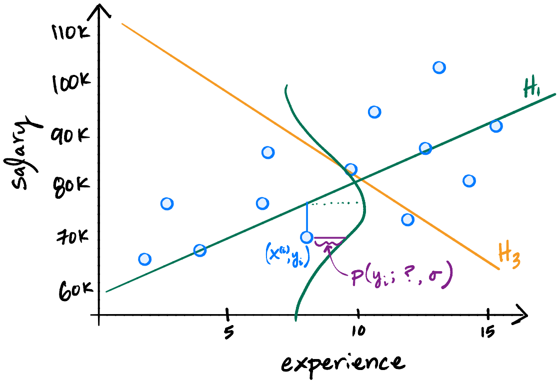
Likelihood

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

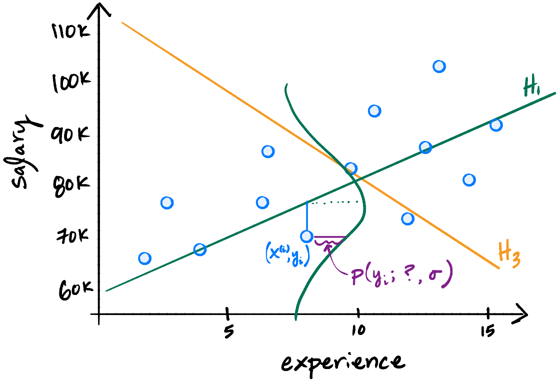
$$p(y; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(y-\mu)^2/(2\sigma^2)}$$

- We observe a data set $\{(\vec{x}^{(i)}, y_i)\}$.
- What is the likelihood of a choice of parameters $\vec{w}$, σ, 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 $\prod_{i=1}^{n} p(y_i; \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, \sigma)$.

Log-Likelihood

- The log-likelihood is:

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

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

Claim 1

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

$$=$$

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

Claim 2

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

$$=$$

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

Claim 3

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

$$=$$

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

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

Main Idea

Mazimizing 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.

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Probabilistic Modeling & Machine Learning

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:

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

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

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

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

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

Main Idea

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