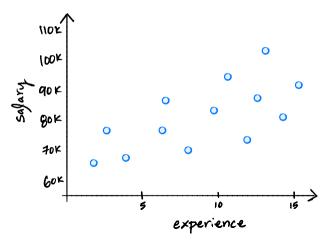
DSC 140A Probabilistic Modeling & Machine Kearning

Lecture 15 | 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**:

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

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.

100.0.

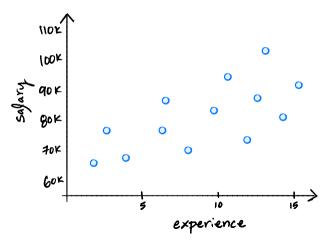
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Lecture 15 | Part 2

Probabilistic View of Regression

Probabilistic View of Regression

Note: There is uncertainty in the salary.

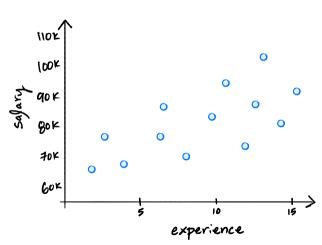


Modeling Uncertainty

We can model this uncertainty using probability.

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

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



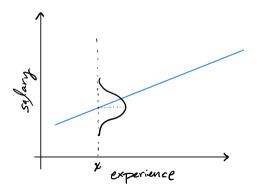
Error Distribution

- 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:

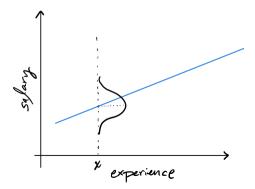
Salary =
$$w_0 + w_1 \times \text{(Experience)} + \underbrace{\mathcal{N}(0, \sigma^2)}_{\varepsilon}$$



Modeling Uncertainty

Equivalently:

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



In General

► In general:

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

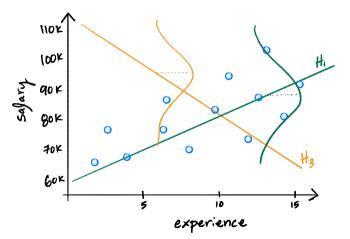
That is: for any feature vector \vec{x} , the target Y is drawn from a Gaussian centered at $\text{Aug}(\vec{x}) \cdot \vec{w}$.

Estimating Parameters

► We assume the model:

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

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



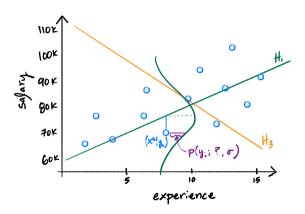
Likelihood

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

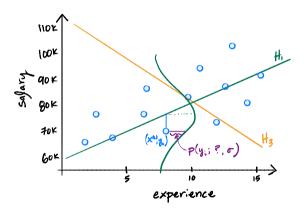
$$p(y; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(y-\mu)^2/(2\sigma^2)}$$

- ► 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,

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

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

Likelihood with respect to data set:

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

Log-Likelihood

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

Log-Likelihood

► The log-likelihood is:

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

We want to maximize this quantity.

Claim 1

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

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

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

Claim 2

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

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

Claim 3

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

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

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:

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

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

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Lecture 15 | 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: $\vec{w}^* = (X^TX + n\lambda I)^{-1}X^T\vec{y}$
- 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:

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

ightharpoonup 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:

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

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

 $\arg\max_{\vec{w}} \left[p_{\vec{w}}(\vec{w} \mid \vec{x}, y) \right] = \arg\max_{\vec{w}} \left[p_{y}(y \mid \vec{w}, \vec{x}) p_{\vec{w}}(\vec{w}) \right]$

= arg max ln $[p_y(y \mid \vec{w}, \vec{x})p_{\vec{w}}(\vec{w})]$

= $\arg\min_{\vec{w}} \left[MSE(\vec{w}) - \ln p_{\vec{w}}(\vec{w}) \right]$

= arg max $\left[\ln p_y(y \mid \vec{w}, \vec{x}) + \ln p_{\vec{w}}(\vec{w})\right]$

= arg min $\left[-\ln p_y(y \mid \vec{w}, \vec{x}) - \ln p_{\vec{w}}(\vec{w})\right]$

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

$$\underset{\vec{w}}{\operatorname{arg\,min}} \left[\operatorname{MSE}(\vec{w}) - \ln p_{\vec{w}}(\vec{w}) \right] = \underset{\vec{w}}{\operatorname{arg\,min}} \left[\operatorname{MSE}(\vec{w}) + \frac{1}{2\underline{s}^2} \|\vec{w}\|^2 \right]$$

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).