CS 446/ECE 449: Machine Learning

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Logistics:

- **Signup:** Campuswire and Gradescope. (https://campuswire.com/p/G47CE41F1, Code: 0662)
- **Tutorial:** Amnon will host a Probability / Numpy / PyTorch tutorial soon. Stay tuned for more information.
- **HW1 Update:** We will release it on Wednesday (January 24), and the due date is February 6.
- **Slides:** Slides will be uploaded before the class begins. Handwritten notes (if any) will be uploaded after the class ends.

L3: Linear Regression

Goals of this lecture

- Math Intro
- Getting to know linear regression
- Understanding how linear regression works
- Examples for linear regression

Reading Material

- K. Murphy; Machine Learning: A Probabilistic Perspective; Chapter 7

Math Intro:

- Vector: $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n$
- Matrix: $\mathbf{X} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,m} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,m} \end{bmatrix} \in \mathbb{R}^{n \times m}$
- Norm: $\|x^{(1)} - x^{(2)}\|_2^2 = \sum_{i=1}^n (x_i^{(1)} - x_i^{(2)})^2$ distance between two points in n dimensions
- Transpose: $\mathbf{X}^T = \begin{bmatrix} x_{1,1} & \cdots & x_{n,1} \\ \vdots & \ddots & \vdots \\ x_{1,m} & \cdots & x_{m,n} \end{bmatrix} \in \mathbb{R}^{m \times n}$

$$\boldsymbol{x}^T = \left[\begin{array}{ccc} x_1 & \cdots & x_n \end{array} \right] \in \mathbb{R}^{1 \times n}$$

- Matrix multiplication: $\mathbf{X}^T \boldsymbol{x}$ or $\mathbf{X}\boldsymbol{x}$?

Discrete Probability: $y \in \{1, \dots, 6\}$

- Discrete probability distribution: $p(Y = y) \in [0, 1]$ with $\sum_{y \in \{1,\dots,6\}} p(Y = y) = 1$
- Abbreviation: $p(Y = y) = p(y) \in [0, 1]$
- Expectation: $\mathbb{E}_{p(y)}[f(y)] = \sum_{y \in \{1,\dots,6\}} p(y)f(y)$

Continuous probability: $y \in \mathbb{R}$

- $p(Y = 1) = 0$
- Probability density function: $p(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y - \mu)^2\right)$
- Mean: $\mathbb{E}_{p(y)}[y] = \int_{-\infty}^{\infty} yp(y)dy = \mu$
- Variance: $\mathbb{E}_{p(y)}[(y - \mu)^2] = \sigma^2$

Multivariate continuous probability: $\boldsymbol{y} \in \mathbb{R}^n$ $\mu \in \mathbb{R}^n$

- n-dimensional density: $p(\boldsymbol{y}) = p(y_1, \ldots, y_n) = \frac{1}{\sqrt{(2\pi)^n|\Sigma|}} \exp\left(-\frac{1}{2}(\boldsymbol{y} - \mu)^T \Sigma^{-1} (\boldsymbol{y} - \mu)\right)$
- Covariance matrix: Σ

Petersen & Pedersen; The Matrix Cookbook

Multivariate calculus: $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{w} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{n \times n}$

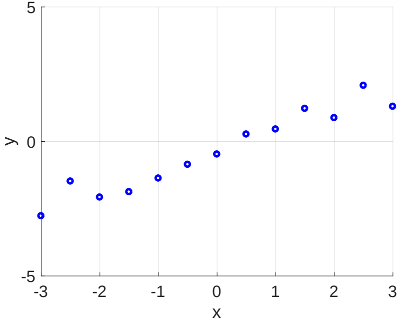
- Multivariate function: $f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$
- Derivative: $\frac{\partial f}{\partial \boldsymbol{x}} = \boldsymbol{w}$
- Multivariate function: $f(\boldsymbol{x}) = \boldsymbol{x}^T \mathbf{A} \boldsymbol{x}$
- Derivative: $\frac{\partial f}{\partial \boldsymbol{x}} = (\mathbf{A} + \mathbf{A}^T)\boldsymbol{x}$

Recap: What we have learned so far?

- Lecture 1: KNN
- Lecture 2: Naive Bayes
- Parameteric or Non-parametric?
- What are the key underlying assumptions?
- Linear or non-linear decision boundaries?
- Key pros and cons?

Classification problem (output is category)

Regression - The Problem:



Given continuous-valued outcomes $y^{(i)} \in \mathbb{R}$ for covariates $x^{(i)} \in \mathbb{R}$ (e.g. predict housing price based on area's annual family income),

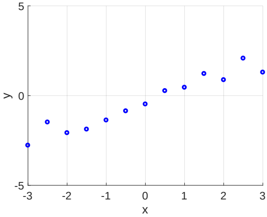
- How do we parametrize the model?
- What loss / objective function should we use to judge the fit?
- How do we optimize fit to unseen test data (generalization)?

Linear Regression:
Let's assume a linear model with parameters $w_1 \in \mathbb{R}$ and $w_2 \in \mathbb{R}$

$$y = w_1 \cdot x + w_2$$

Given a dataset of N pairs (x, y):

$$\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$$



How do we find the parameters w_1, w_2?

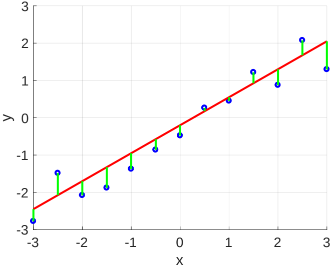
Assuming model

$$y = w_1 \cdot x + w_2$$

Find parameters w_1, w_2 such that the squared error is small

$$\arg\min_{w_1, w_2} \frac{1}{2} \sum_{i=1}^{N} \left(y^{(i)} - w_1 \cdot x^{(i)} - w_2 \right)^2$$

What exactly is the error?



Program:

$$\underset{w_1, w_2}{\arg\min} \frac{1}{2} \sum_{i=1}^{N} \left(y^{(i)} - w_1 \cdot x^{(i)} - w_2 \right)^2$$

Vector notation:

$$\underset{w_1, w_2}{\arg\min} \frac{1}{2} \left\| \underbrace{\begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}}_{\mathbf{Y} \in \mathbb{R}^N} - \underbrace{\begin{bmatrix} x^{(1)} & 1 \\ \vdots & \vdots \\ x^{(N)} & 1 \end{bmatrix}}_{\mathbf{X}^\top \in \mathbb{R}^{N \times 2}} \cdot \underbrace{\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}}_{\mathbf{w} \in \mathbb{R}^2} \right\|_2^2$$

Program:

$$\arg\min_{\boldsymbol{w}} \underbrace{\frac{1}{2}\|\boldsymbol{Y} - \boldsymbol{X}^\top \boldsymbol{w}\|_2^2}_{\text{loss function}}$$

How to solve the program:

- Take derivative w.r.t. $\boldsymbol{w}$ of loss function
- Set derivative w.r.t. $\boldsymbol{w}$ to zero
- Solve for $\boldsymbol{w}$

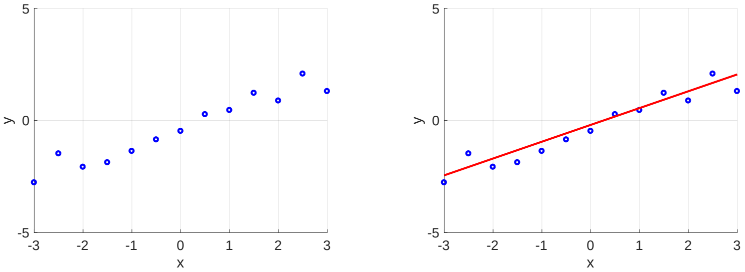
Derivative:

$$\boldsymbol{X}\boldsymbol{X}^\top \boldsymbol{w}^* - \boldsymbol{X}\boldsymbol{Y} = 0$$

Solution:

$$\boldsymbol{w}^* = \left(\boldsymbol{X}\boldsymbol{X}^\top\right)^{-1} \boldsymbol{X}\boldsymbol{Y}$$

Linear regression:



Extensions:

- Higher dimensional problems ($\boldsymbol{x}^{(i)} \in \mathbb{R}^d$)
- Regularization
- Higher order polynomials

Higher dimensional problems ($\boldsymbol{x}^{(i)} \in \mathbb{R}^d$, $y^{(i)} \in \mathbb{R}$)
Model:

$$y^{(i)} = w_0 + \sum_{k=1}^{d} \boldsymbol{x}_k^{(i)} w_k$$

Program:

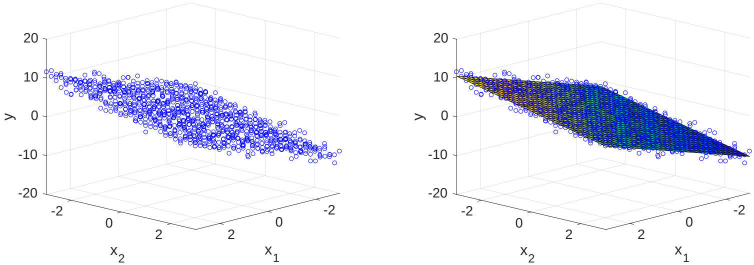
$$\arg\min_{\boldsymbol{w}} \frac{1}{2} \| \underbrace{\boldsymbol{Y}}_{\in \mathbb{R}^N} - \underbrace{\boldsymbol{X}^\top}_{\in \mathbb{R}^{N \times (d+1)}} \underbrace{\boldsymbol{w}}_{\in \mathbb{R}^{d+1}} \|_2^2$$

Solution: (obviously the same as before)

$$\boldsymbol{w}^* = \left(\boldsymbol{X}\boldsymbol{X}^\top \right)^{-1} \boldsymbol{X}\boldsymbol{Y}$$

Example:

$$\boldsymbol{w}^* = \left(\boldsymbol{X}\boldsymbol{X}^\top\right)^{-1}\boldsymbol{X}\boldsymbol{Y}$$



What if $N < d + 1$?

Regularization:

we want to make sure that the parameters are not too large

we want to make sure we can invert the matrix

Program:

$$\arg\min_{\boldsymbol{w}} \underbrace{\frac{1}{2}\|\boldsymbol{Y} - \boldsymbol{X}^\top \boldsymbol{w}\|_2^2 + \frac{C}{2}\|\boldsymbol{w}\|_2^2}_{\text{cost function}}$$

Solution:

$$\boldsymbol{w}^* = \left(\boldsymbol{X}\boldsymbol{X}^\top + C\boldsymbol{I}\right)^{-1} \boldsymbol{X}\boldsymbol{Y}$$

Higher order polynomials ($x^{(i)} \in \mathbb{R}$, $y^{(i)} \in \mathbb{R}$)

Model:

$$y^{(i)} = w_2 \cdot \left(x^{(i)}\right)^2 + w_1 \cdot x^{(i)} + w_0$$

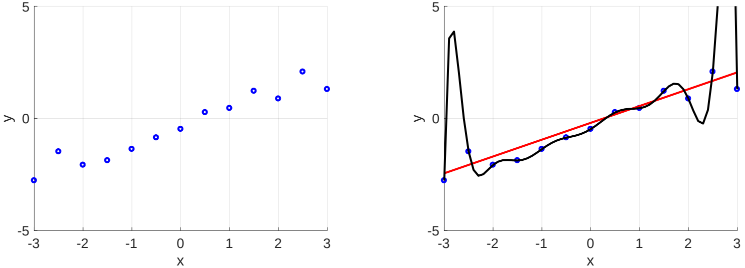
Program:

$$\arg\min_{w_0,w_1,w_2} \frac{1}{2} \left\| \underbrace{\begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}}_{\mathbf{Y} \in \mathbb{R}^N} - \underbrace{\begin{bmatrix} \left(x^{(1)}\right)^2 & x^{(1)} & 1 \\ \vdots & \vdots & \vdots \\ \left(x^{(N)}\right)^2 & x^{(N)} & 1 \end{bmatrix}}_{\Phi^\top \in \mathbb{R}^{N \times M}} \cdot \underbrace{\begin{bmatrix} w_2 \\ w_1 \\ w_0 \end{bmatrix}}_{\mathbf{w} \in \mathbb{R}^M} \right\|_2^2$$

Solution:

$$\boldsymbol{w}^* = \left(\Phi\Phi^\top\right)^{-1} \Phi \boldsymbol{Y}$$

Example:



Which model is more reasonable?

Generalizing all aforementioned cases:

- $x^{(i)}$ is some data (e.g., images)
- $\phi(x^{(i)}) \in \mathbb{R}^M$ is a transformation into a feature vector

Model:

$$y^{(i)} = \phi(x^{(i)})^\top \boldsymbol{w}$$

Program:

$$\arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(y^{(i)} - \phi(x^{(i)})^\top \boldsymbol{w} \right)^2$$

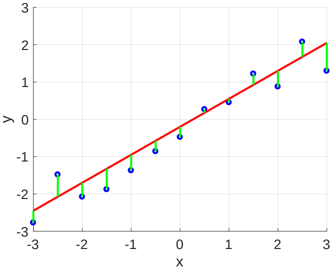
Solution:

$$\boldsymbol{w}^* = \left(\Phi \Phi^\top \right)^{-1} \Phi \boldsymbol{Y} \quad \text{where} \quad \Phi = \left[\phi(x^{(1)}), \cdots, \phi(x^{(N)}) \right] \in \mathbb{R}^{M \times N}$$

Linear regression:

- So far: Error view

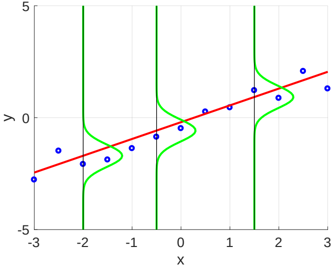
$$\left(y^{(i)} - \phi(x^{(i)})^\top \boldsymbol{w}\right)^2$$



- Alternatively: Probabilistic view

A probabilistic interpretation of linear regression:
Model: Gaussian distribution

$$p(y^{(i)}|x^{(i)}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y^{(i)} - \boldsymbol{w}^\top \phi(x^{(i)}))^2\right)$$



How to find $\boldsymbol{w}$?

Maximize likelihood of dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$ assuming samples to be drawn independently from an identical distribution (i.i.d.).

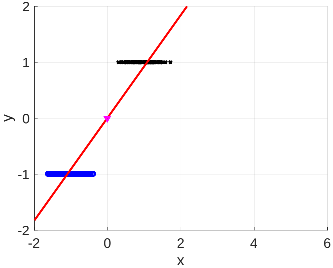
$$
\begin{aligned}
\arg\max_{\boldsymbol{w}} p(\mathcal{D}) &= \arg\max_{\boldsymbol{w}} \prod_i^N p(y^{(i)}|x^{(i)}) \quad \text{(i.i.d.)} \\
&= \arg\max_{\boldsymbol{w}} \sum_i^N \log p(y^{(i)}|x^{(i)}) \quad \text{(log of prod)} \\
&= \arg\max_{\boldsymbol{w}} \sum_i^N \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y^{(i)} - \boldsymbol{w}^\top \phi(x^{(i)}))^2\right) \\
&= \arg\max_{\boldsymbol{w}} \sum_i^N \left(-\frac{1}{2\sigma^2}(y^{(i)} - \boldsymbol{w}^\top \phi(x^{(i)}))^2\right) + C \quad \text{(log-exp)} \\
&= \arg\min_{\boldsymbol{w}} \sum_{i=1}^N \left(y^{(i)} - \phi(x^{(i)})^\top \boldsymbol{w}\right)^2 \quad \text{(take out minus sign)}
\end{aligned}
$$

Linear regression for classification?

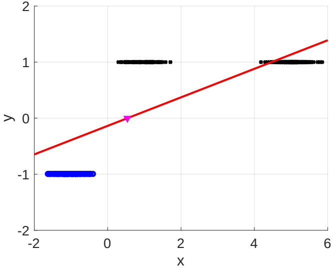
$$y^{(i)} \in \{-1, 1\}$$

Model:

$$y = w_1 x + w_0 \qquad \text{threshold at } y = 0$$



perfect classification



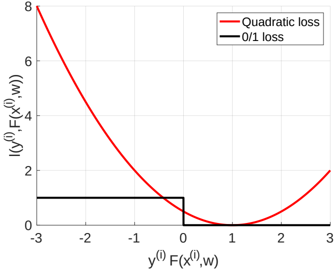
decision boundary shifted

Why is this?

Linear regression: Quadratic loss (recall $y^{(i)} \in \{-1, 1\}$)

$$\ell(y_i, \phi(x^{(i)})^\top \boldsymbol{w}) \quad = \quad \frac{1}{2}(y^{(i)} - \phi(x^{(i)})^\top \boldsymbol{w})^2$$

$$\overset{(y^{(i)})^2=1}{=} \quad \frac{1}{2}(\underbrace{1 - y^{(i)} \underbrace{\phi(x^{(i)})^\top \boldsymbol{w}}_{F(x^{(i)},\boldsymbol{w})}}_{F(x^{(i)},\boldsymbol{w},y^{(i)})})^2$$



We penalize samples that are 'very easy to classify.'

How to fix this?
Next lecture...

Quiz

- Linear regression optimizes what loss function?
- How can we optimize this loss function?
- What are the assumptions?
- What are issues of linear regression applied to classification?

Important topics of this lecture

- We learned about linear regression
- We saw how to solve linear regression problems
- We got to know examples of where to use linear regression
- We understood some shortcomings

What's next:

- Understanding shortcomings of linear classification
- Fixing those shortcomings (logistic regression)

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