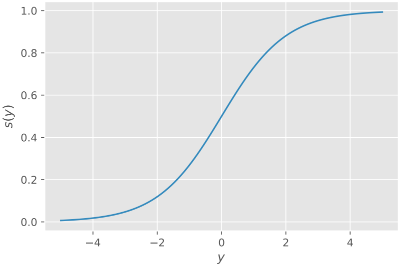
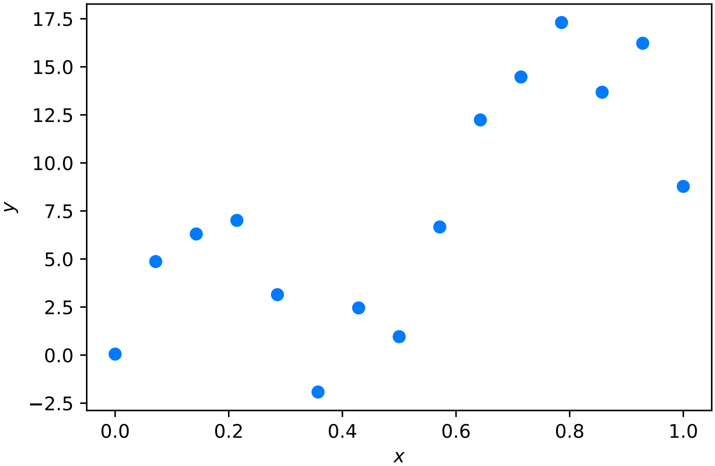


CSE 151A

Intro to Machine Learning

Lecture 08 – Part 01

Model Complexity


17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
−2.5
y
0.0
0.2
0.4
0.6
0.8
1.0
x

Empirical Risk Minimization

1. Pick a **model**.
   - E.g., linear prediction rules.

2. Pick a loss.
   - E.g., mean squared error.

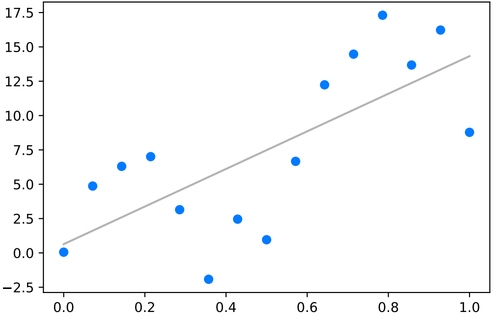
3. Find a prediction rule minimizing the **risk**.

Big Decision

- Pick a model.
- Picking the wrong model causes problems.

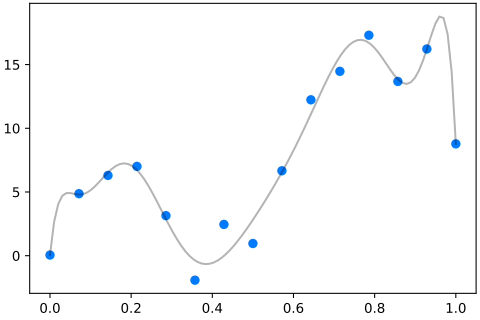
Underfitting

- Fit $H(x) = w_0 + w_1 x$?
  - We have **underfit** the data.



Overfitting

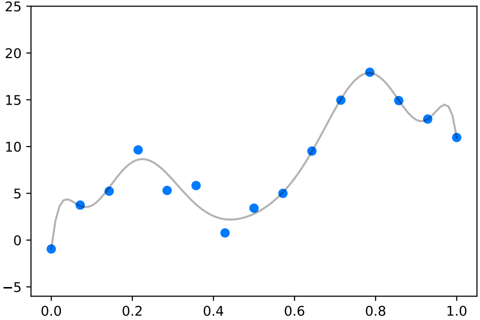
- Fit $H(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{10} x^{10}$?
  - We have **overfit** the data.



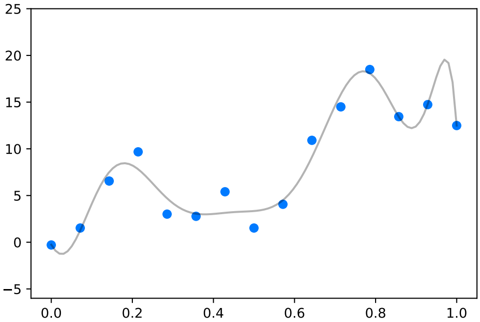
Model Complexity

- Difference? **Complexity**.
- Complex models are highly flexible.
  - They tend to **overfit**.
- Simple models are stiff.
  - They tend to **underfit**.

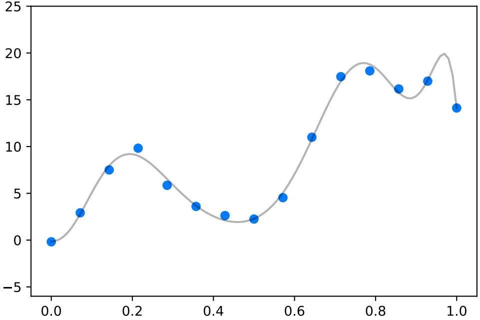
Degree 10 Polynomial



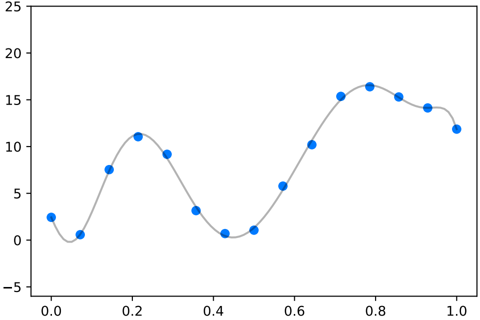
Degree 10 Polynomial



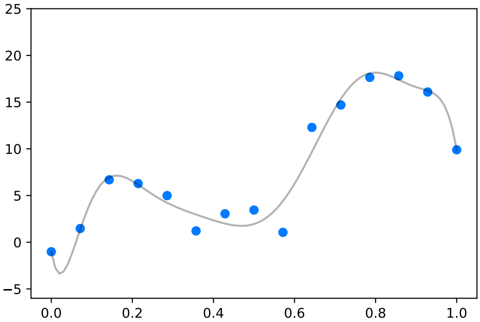
Degree 10 Polynomial



Degree 10 Polynomial



Degree 10 Polynomial



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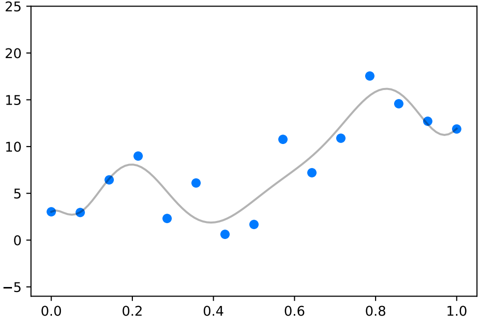

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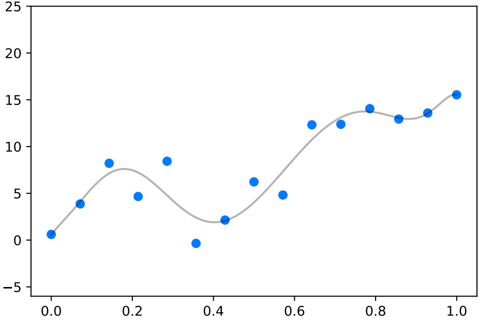

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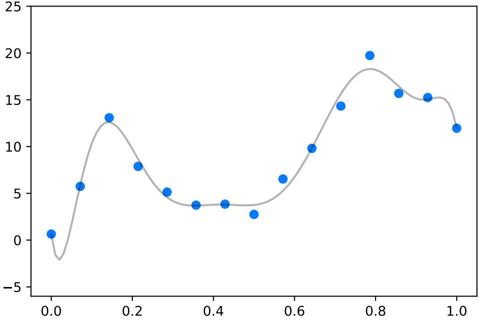
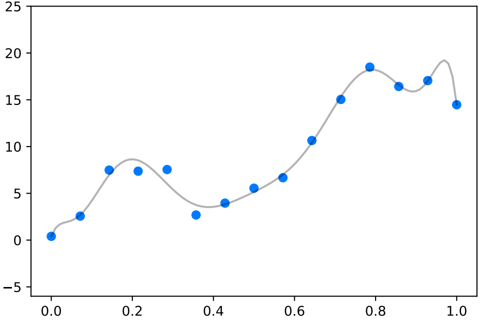
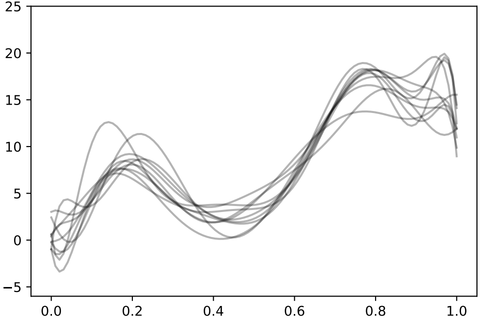


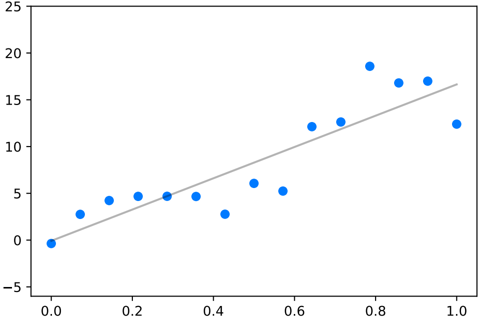
Degree 10 Polynomial



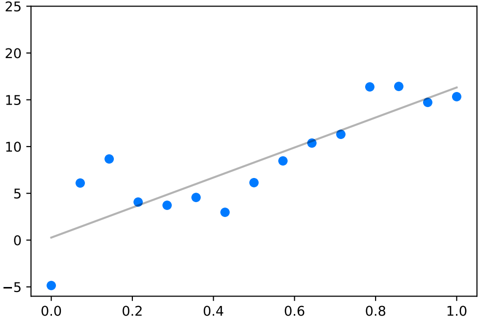
Degree 10 Polynomial



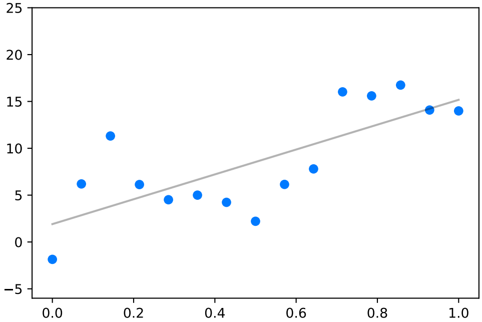
Degree 1 Polynomial



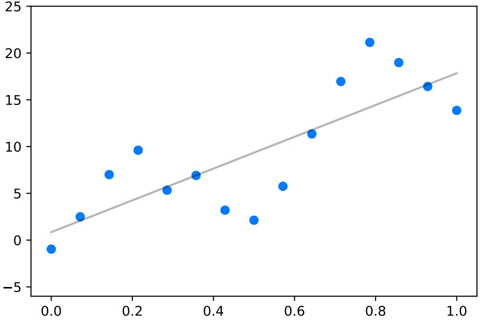
Degree 1 Polynomial



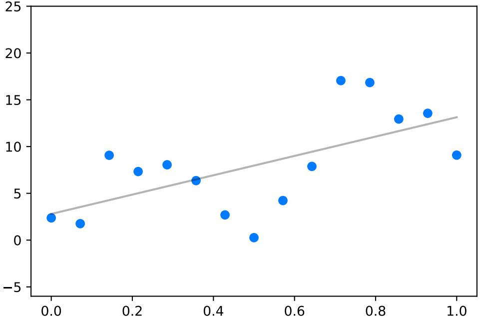
Degree 1 Polynomial



Degree 1 Polynomial



Degree 1 Polynomial



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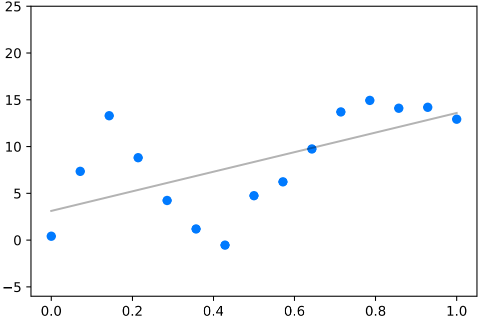
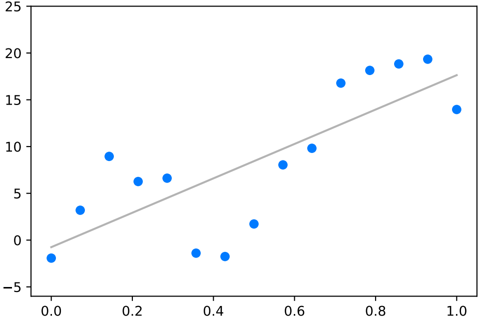
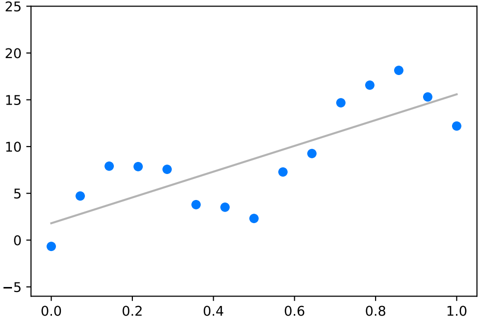


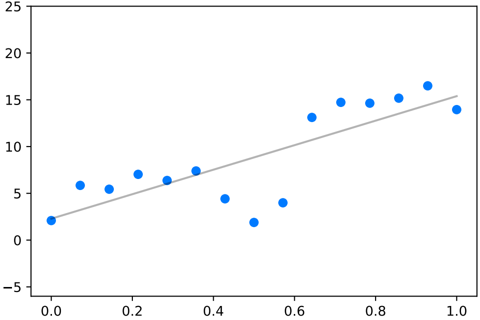
Degree 1 Polynomial



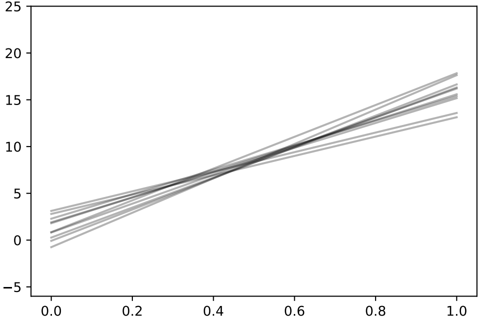
Degree 1 Polynomial



Degree 1 Polynomial



Degree 1 Polynomial



Example: kNN

- 1NN: complex model, likely to overfit.
- 20NN: less complex model, likely to underfit.

Choosing Model Complexity

- How do we choose between two models?
  - Between degree 10 and degree 1?
  - Between 1NN and 20NN?

- Not always obvious.

Bad Idea: Use training MSE

- Which has smaller MSE on training data?

Bad Idea: Use training MSE

- Which has smaller MSE on training data?
- **Problem**: Best 10-degree polynomial will **always** have smaller MSE on training data.

Good Idea: Use validation MSE

- We care about **generalization**.
- So keep a small amount of data hidden in a **validation set**.
- Fit model on training data, compute MSE on **validation set**.
- Pick whichever model has smaller validation error.

What do you expect?

- You fit a complex model on training data.
- Test it on a validation set.
- Likely: validation MSE > training MSE.

What do you expect?

- You fit a very simple model on training data.
- Test it on a validation set.
- Likely: validation MSE ≈ training MSE.

Cross-Validation

- We want all the training data we can get.
- Reserving some of it is wasteful.
- Idea: **split** data into pieces, each takes turn as validation set.

k-Fold Cross Validation

1. Split data set into k pieces, $S_1, \ldots, S_k$.

2. Loop k times; on iteration i:
   - Use S_i as validation set; rest as training.
   - Compute validation error ϵ_i

3. Overall error: $\frac{1}{k} \sum \epsilon_i$

Leave-One-Out Cross Validation

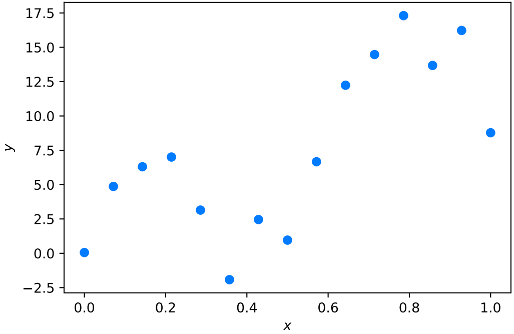
- Suppose we have n labeled data points.
- LOOCV: k-fold CV with $k = n$.

Another Approach

- We can control complexity by choosing model.
- Also: via **regularization**.

Regularization

- Let's fit a complex model: $w_0 + w_x x + \ldots + w_{10} x^{10}$.
- But impose a budget on weights, $w_0, \ldots, w_d$.



Budgeting Weights

- One way to budget: ask that $\|\vec{w}\|^2$ is small.

- Before: minimize

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (\vec{w} \cdot \vec{x}^{(i)} - y_i)^2$$

- Now: minimize

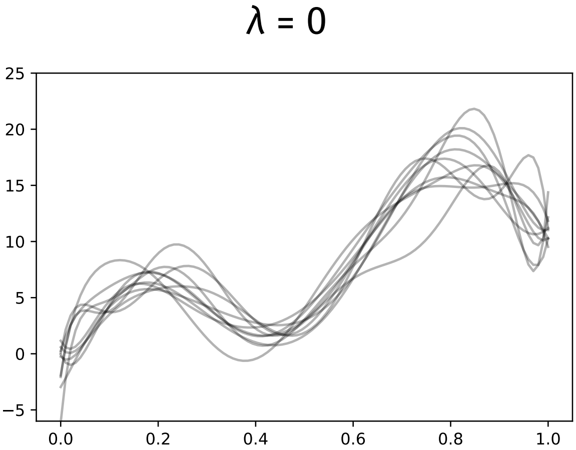
$$\tilde{R}_{\text{sq}}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (\vec{w} \cdot \vec{x}^{(i)} - y_i)^2 + \lambda \|\vec{w}\|^2$$

Solution

- The **regularized** Normal Equations:

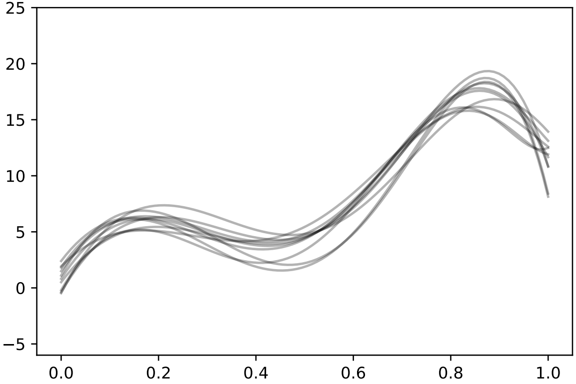
$$(X^T X + \lambda I)\vec{w} = X^T \vec{y}$$

Example

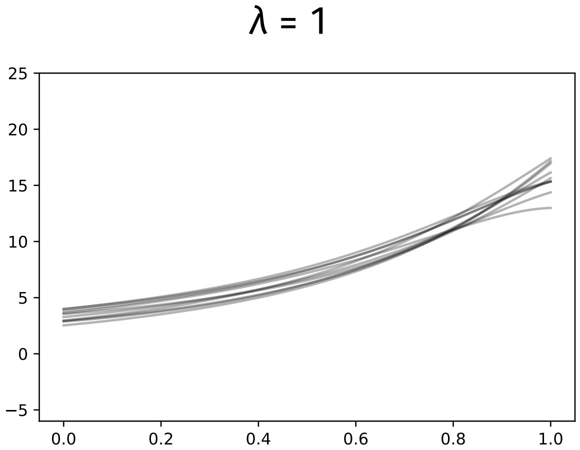


Example

$\lambda = 1 \times 10^{-4}$



Example

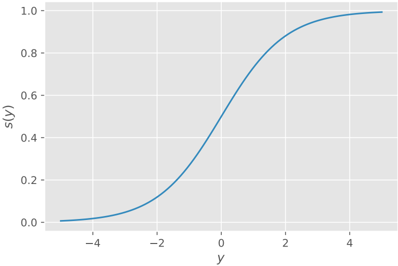


Regularization

- As λ increases, simpler models preferred.
- Pick λ using cross-validation.

Other Penalizations

- $\|\vec{w}\|_2^2$ is ℓ_2 regularization (explicit solution)
  - a.k.a., **ridge regression**
- $\|\vec{w}\|_1$ is ℓ_1 regularization (no explicit solution)
  - a.k.a., **the LASSO**
  - encourages **sparse** $\vec{w}$



CSE 151A
Intro to Machine Learning

Lecture 08 – Part 02
Logistic Regression

Note

- The midterm will cover everything up to right now.
- Regularization: **yes**.
- Logistic regression: **no**.

Predicting Heart Disease

- **Classification problem**: Does a patient have heart disease?
- **Features**: blood pressure, cholesterol level, exercise amount, maximum heart rate, sex

Better idea…

- Instead of predicting **yes/no**…
- Give a **probability** that they have heart disease.
  - 1 = definitely yes
  - 0 = definitely no
  - 0.75 = probably, yes
  - …

Associations

- If cholesterol is high, increased likelihood.
  - Positive association.

- If exercise is low, increased likelihood.
  - Negative association.

The Model

- Measure cholesterol (x_1), exercise (x_2), etc.
- **Idea**: weighted[1] "vote" for heart disease:

$$w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

- Convention:
  - A positive number = vote for yes
  - A negative number = vote for no

[1]We'll learn weights later.

The Model

- Add a “bias” term:

$$
\begin{aligned}
&w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d \\
&= \vec{w} \cdot \text{Aug}(\vec{x})
\end{aligned}
$$

- The more positive $\vec{w} \cdot \text{Aug}(\vec{x})$, the more likely.

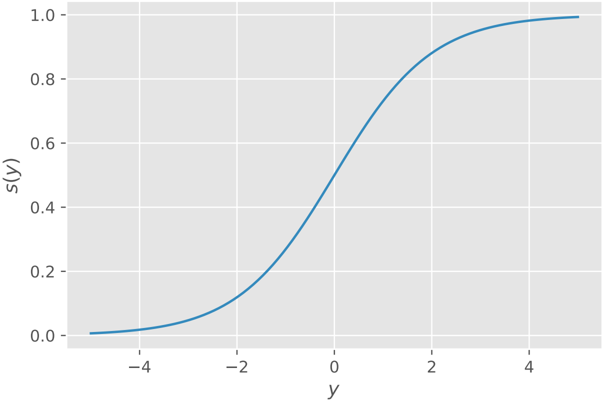
- The more negative $\vec{w} \cdot \text{Aug}(\vec{x})$, the less likely.

Converting to a Probability

- Probabilities are between 0 and 1.
- **Problem**: $\vec{w} \cdot \text{Aug}(\vec{x})$ can be anything in $(-\infty, \infty)$
- We need to convert it to a probability.

The Logistic Function

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$



The Model

- Our simplified model for probability of heart disease:
$$H(\vec{x}) = \sigma(\vec{w} \cdot \text{Aug}(\vec{x}))$$

- What should $\vec{w}$ be?

- To find $\vec{w}$, use principle of **maximum likelihood**.

Maximum Likelihood

- Suppose you have an unfair coin.
- Probability of heads is p, unknown.
- Flip 8 times and see: H, H, T, H, H, H, H, T
- Which is more **likely**: $p = 0.5$ or $p = 0.75$?

Maximum Likelihood

- Assume coin flips are independent.
- The **likelihood** of H, H, T, H, H, H, H, T is:

$$\begin{aligned}\mathcal{L}(p) &= p \cdot p \cdot (1 - p) \cdot p \cdot p \cdot p \cdot p \cdot (1 - p) \\ &= p^6 (1 - p)^2\end{aligned}$$

- Idea: find p maximizing $\mathcal{L}(p)$
  - Equivalently, find p maximizing $\log \mathcal{L}(p)$

Maximum Likelihood

Find p maximizing $\log \mathcal{L}(p) = \log p^6(1 - p)^2$:

Maximum Likelihood

- In general, given n_1 observed heads, n_2 observed tails, maximize:

$$\log\left[P(F_1 = f_1) \cdot P(F_2 = f_2) \cdots \cdot P(F_n = f_n)\right]$$

$$= \sum_{i=1}^{n} \log P(F_1 = f_1)$$

Back to Logistic Regression

- The probability that person i has heart disease:

$$H(\vec{x}^{(i)}) = \vec{w} \cdot \text{Aug}(\vec{x}^{(i)})$$

- Gather a data set, $(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)$.
- What is the most **likely** $\vec{w}$?

Maximum Likelihood

- Suppose 3 people, (+,-,+).
- Likelihood:

$$
\begin{aligned}
&H(\vec{x}^{(1)}) \cdot (1 - H(\vec{x}^{(2)})) \cdot H(\vec{x}^{(3)}) \\
&\quad = \sigma(\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(1)})) \cdot \left(1 - \sigma(\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(2)}))\right) \cdot \sigma(\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(3)})) \\
&\quad = \frac{1}{1 + e^{-\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(1)})}} \cdot \left(1 - \frac{1}{1 + e^{-\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(2)})}}\right) \cdot \frac{1}{1 + e^{-\vec{w} \cdot \operatorname{Aug}(\vec{x}^{(3)})}}
\end{aligned}
$$

Observation

- Note:

$$1 - \frac{1}{1 + e^{-t}} = \frac{1}{1 + e^{t}}$$

Maximum Likelihood

- The likelihood:

$$\frac{1}{1 + e^{-\vec{w} \cdot \text{Aug}(\vec{x}^{(1)})}} \cdot \frac{1}{1 + e^{\vec{w} \cdot \text{Aug}(\vec{x}^{(2)})}} \cdot \frac{1}{1 + e^{-\vec{w} \cdot \text{Aug}(\vec{x}^{(3)})}}$$

- Suppose $y_i = 1$ if positive, $y_i = -1$ if negative:

$$\frac{1}{1 + e^{-y_1 \vec{w} \cdot \text{Aug}(\vec{x}^{(1)})}} \cdot \frac{1}{1 + e^{-y_2 \vec{w} \cdot \text{Aug}(\vec{x}^{(2)})}} \cdot \frac{1}{1 + e^{-y_3 \vec{w} \cdot \text{Aug}(\vec{x}^{(3)})}}$$

Maximum Likelihood

- In general, the likelihood is:

$$\mathcal{L}(\vec{w}) = \prod_{i=1}^{n} \frac{1}{1 + e^{-y_i \vec{w} \cdot \text{Aug}(\vec{x}^{(i)})}}$$

- The **log likelihood** is:

$$\log \mathcal{L}(\vec{w}) = -\sum_{i=1}^{n} \log\left[1 + e^{-y_i \vec{w} \cdot \text{Aug}(\vec{x}^{(i)})}\right]$$

Maximizing Likelihood

- **Goal**: find $\vec{w}$ maximizing $\log \mathcal{L}$
- Take gradient, set to zero, solve?
- **Problem**: try it, you'll get stuck.
- Unlike least-squares regression, there is no explicit solution.

Next Time

How to maximize the log loss with gradient descent.