Machine Learning

Lecture 02: Linear Regression and Basic ML Issues

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This set of notes is based on internet resources and
KP Murphy (2012). Machine learning: a probabilistic perspective. MIT Press. (Chapter 7)
Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning*. MIT press. www.deeplearningbook.org. (Chapter 5)
Andrew Ng. Lecture Notes on Machine Learning. Stanford.

Outline

Linear Regression: Problem Statement

- Given: A **training set** $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N$
  - Each $\mathbf{x}_i$ is a D-dimensional real-valued column vector: $\mathbf{x} = (x_1, \ldots, x_D)^\top$.
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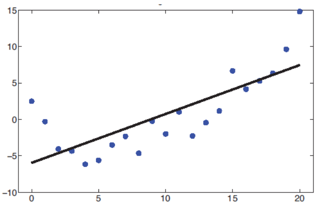
  - Each y_i is a real number
- To Learn: $$y = f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} = \sum_{j=0}^{D} w_j x_j$$
  - The **weights** $\mathbf{w} = (w_0, w_1, \ldots, w_D)^\top$ determine how important the features $(x_1, \ldots, x_D)$ are in predicting the response y.
  - Always set $x_0 = 1$, and w_0 is the **bias** term. Often it is denoted by b.



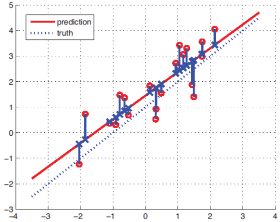
Linear Regression: Examples

Here are several examples from

http://people.sc.fsu.edu/∼jburkardt/datasets/regression/regression.html

- Predict brain weight of mammals based their body weight (x01.txt)
- Predict blood fat content based on age and weight (x09.txt)
- Predict death rate from cirrhosis based on a number of other factors (x20.txt)
- Predict selling price of houses based on a number of factors (X27.txt)

Linear Regression: Mean Squared Error



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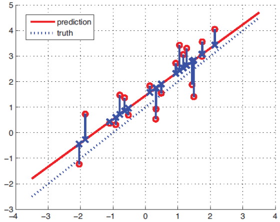

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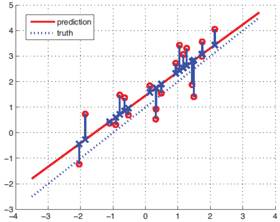

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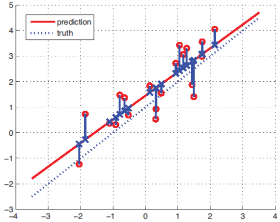

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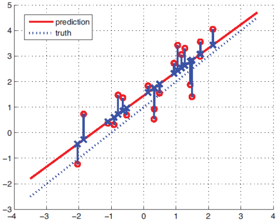

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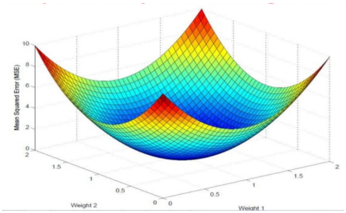

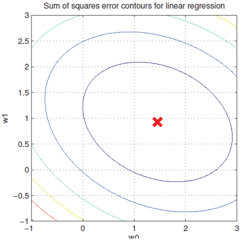

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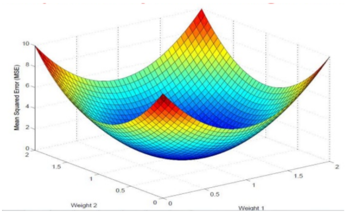

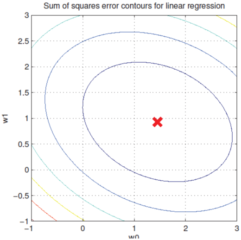

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- We can minimizing it by setting its gradient to 0

$$\nabla J(\mathbf{w}) = 0$$

Linear Regression: Matrix Representation

- We can represent the **training set** $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$ using the **design matrix** $\mathbf{X}$ and a column vector $\mathbf{y}$.

$$
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- Then, the MSE can be written as follows

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Linear Regression: The Normal Equation

- From the equation of the previous slide, we get (see Murphy Chapter 7) that

$$\nabla J(\mathbf{w}) = \frac{1}{N}(2\mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{X}^\top \mathbf{y})$$

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- The value of $\mathbf{w}$ that minimizes $J(\mathbf{w})$ is

$$\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$$

This is called the **ordinary least squares (OLS)** solution.

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where the error term ϵ captures unmodeled effects and random noise.
- We also assume that ϵ follow the Gaussian distribution with zero mean and variance σ: $\epsilon \sim \mathcal{N}(0, \sigma^2)$.
- The model parameters θ include $\mathbf{w}$ and σ. The conditional distribution of y given input $\mathbf{x}$ and parameters θ is a Gaussian
$$p(y|\mathbf{x}, \theta) = \mathcal{N}(y|\mu(\mathbf{x}), \sigma^2)$$
where $\mu(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$

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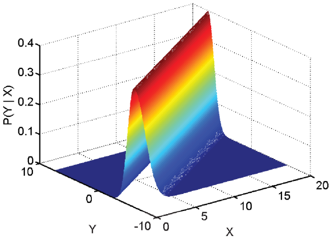
- For each input $\mathbf{x}$, we get a distribution of y, which is a Gaussian distribution.
- To get a **point estimation** of y, we can use the mean, i.e.,

$$\hat{y} = \mu(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$$



$$p(y|x, \boldsymbol{\theta}) = \mathcal{N}(y|w_0 + w_1 x, \sigma^2)$$

Parameter Estimation

- Determine $\theta = (\mathbf{w}, \sigma)$ by minimizing the cross entropy:

$$-\frac{1}{N}\sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \theta) = -\frac{1}{N}\sum_{i=1}^{N} \log[\frac{1}{\sqrt{2\pi\sigma}} \exp(-\frac{(y_i - \mathbf{w}^\top \mathbf{x}_i)^2}{2\sigma^2})]$$

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- Assume σ is fixed. This is the same as minimizing the MSE

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- **Summary**: Under some assumptions, least-squares regression can be justified as a very natural method that minimizes cross entropy, or maximize likelihood.

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Polynomial Regression

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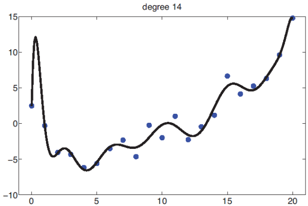
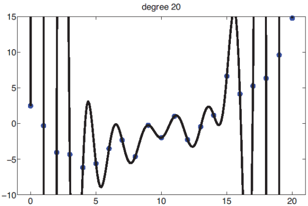
- The **hypothesis space** of a machine learning algorithm/model is the set of functions that it is allowed to select as being the solution.
- The "size" of the hypothesis space is called the **capacity** of the model.
- For polynomial regression, the larger the d, the higher the model capacity.
- Higher model capacity implies better fit to *training data*.
  - Two examples with $d = 14$ and 20 and one feature $\mathbf{x} = (x)$.





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- What we really care about is that it must perform well on new and previously unseen examples. This is called **generalization**.
- We use a the error on a **test set** to measure how well a model generalize:

$$J^{(test)}(\mathbf{w}) = \frac{1}{N^{(test)}}||\mathbf{y}^{(test)} - \mathbf{X}^{(test)}\mathbf{w}||_2^2$$

  This is called the **test error** or the **generalization error**

- In contrast, here is the **training error** we have been talking about so far:

$$J^{(train)}(\mathbf{w}) = \frac{1}{N^{(train)}}||\mathbf{y}^{(train)} - \mathbf{X}^{(train)}\mathbf{w}||_2^2$$

Test and Training Error

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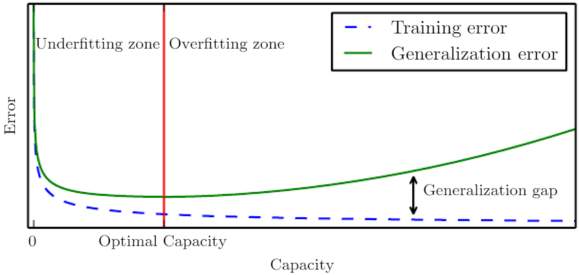
Overfitting and Underfitting

- Training and test error behave differently as model capacity increases.
- At the left end of the graph, training error and generalization error are both high. This is the **underfitting regime**.
- As we increase capacity, training error decreases, but the gap between training and generalization error increases. Eventually,the size of this gap outweighs the decrease in training error, and we enter the **overfitting regime**, where capacity is too large.



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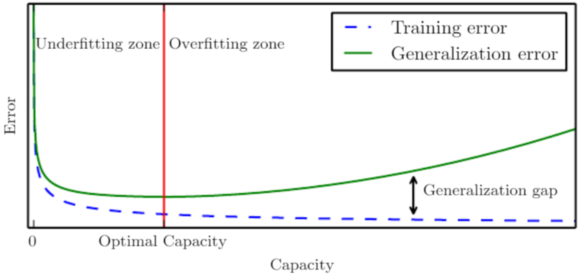

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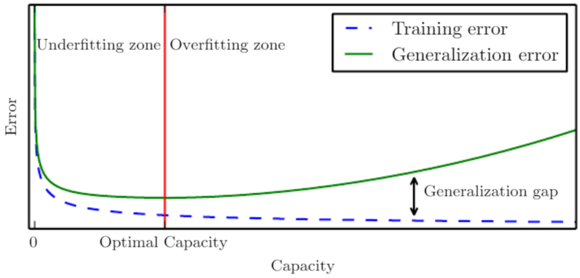

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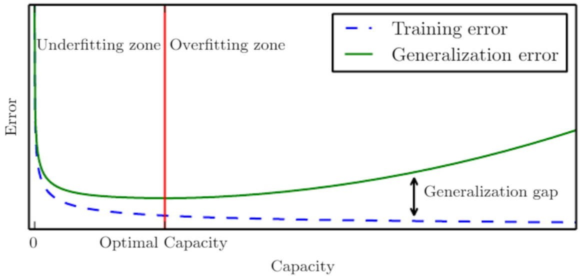

- **Choosing a model with the appropriate capacity is important.**

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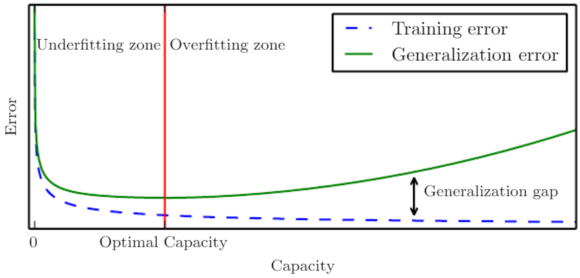

- **Choosing a model with the appropriate capacity is important**.
  - This can be achieved by either validation or regularization.

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    - For each possible value of d, train the model on the training set, and measure the error on the validation set. This is called the **validation error**.
    - Pick the value that has the minimum validation error.

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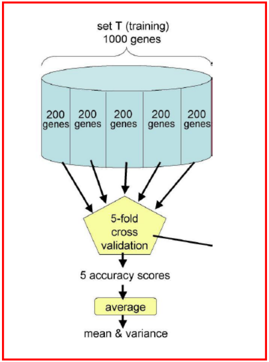

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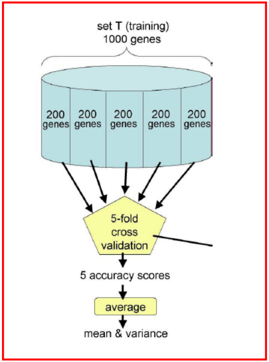

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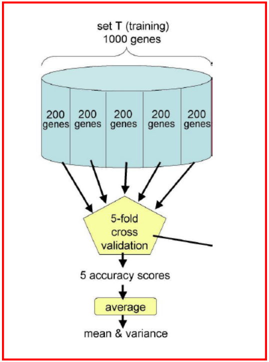

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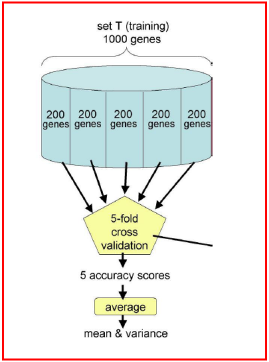

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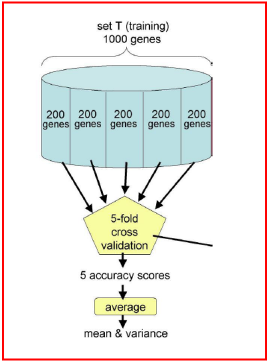

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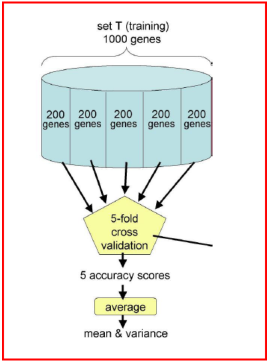

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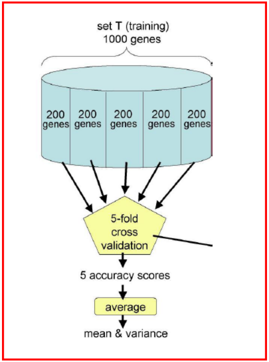

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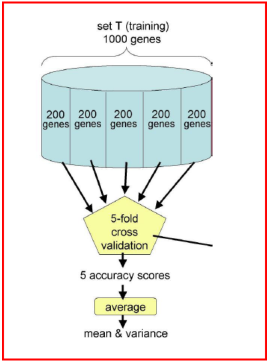

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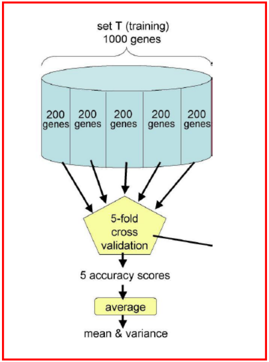

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4. Typically $k = 10$.

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  - Let $\mathbf{w} = (w_1, w_2, \ldots, w_K)^\top$. The bias w_0 is separated from $\mathbf{w}$.

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- Note that w_0 is not regularized as it does not influence model complexity.

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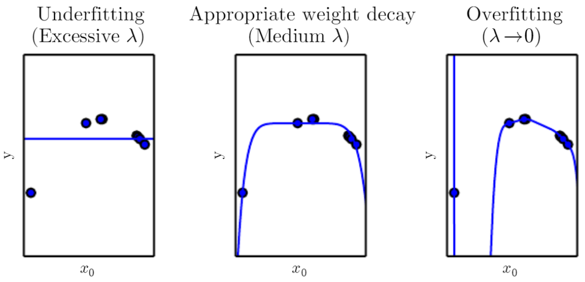
- CENTER: With a medium value of λ, the learning algorithm recovers a curve with the right general shape.



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- Compare this with the ordinary least squares solution:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}$$

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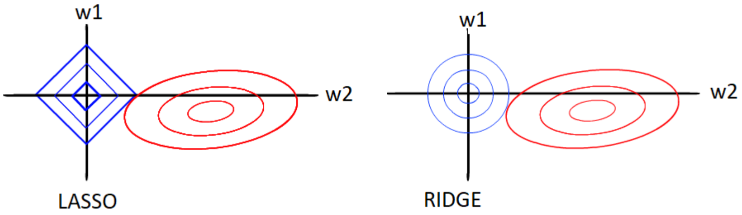

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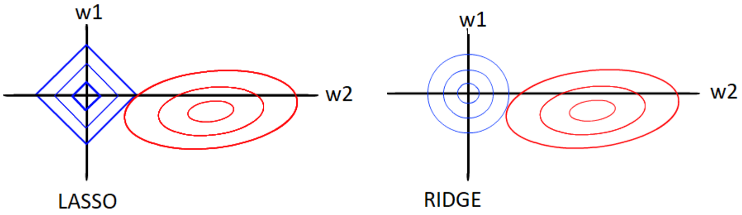

- Red circles represent contours of the error function $\mathit{error}(\mathbf{w})$; Blue lines represent contours of the regularization term $\mathit{regularization}(\mathbf{w})$; Minimum is at the center.
- With Lasso, the sum $\mathit{error}(\mathbf{w}) + \mathit{regularization}(\mathbf{w})$ usually achieves minimum at some corners, which lie on the axes.This means some of the weights are set to 0, and the corresponding features not used.
- With Ridge regression, the minimum is usually not achieved on the axes. Weights are seldom 0.