Computational Data Analysis

Machine Learning

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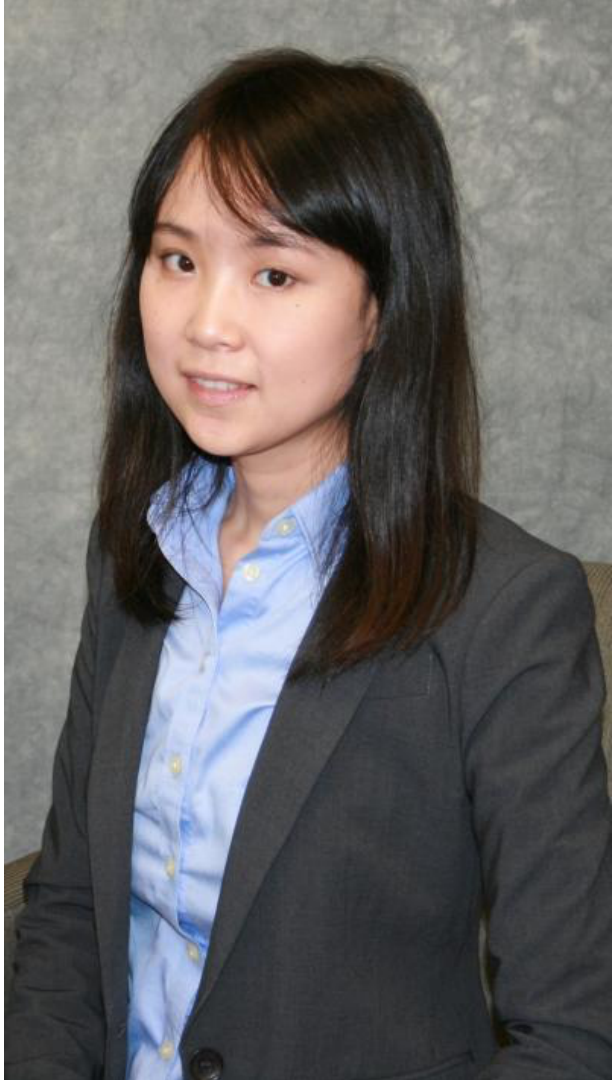
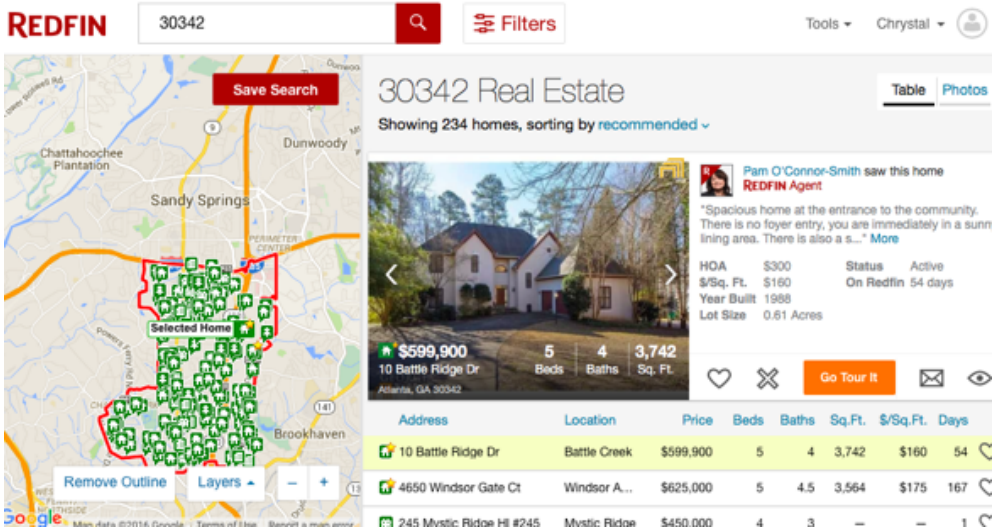


Cross Validation

Motivating example: real estate agent

Data was collected on 100 homes recently sold in a city. It consisted of the sale price, house size, the number of bedrooms, the number of bathrooms, the lot size, and the annual real estate tax. Use price as the response variable and determine which of the these factors should be included in the regression model.



Linear Regression Model

- Assume y is a linear function of x (features) plus noise ϵ

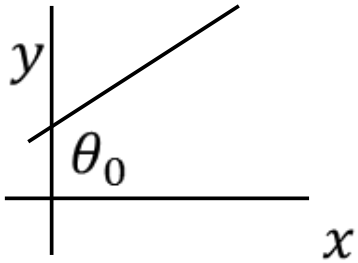
$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n + \epsilon$$

- where ϵ is an error term of unmodeled effects or random noise

- Let $\theta = (\theta_0, \theta_1, \ldots, \theta_n)^\top$, and augment data by one dimension

$$x \leftarrow (1, x)^\top$$

- Then $y = \theta^\top x + \epsilon$



Matrix version of the gradient

- $\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_i^m y^i x^i + \frac{2}{m}\sum_i^m x^i x^{i\top}\theta = 0$

- Equivalent to

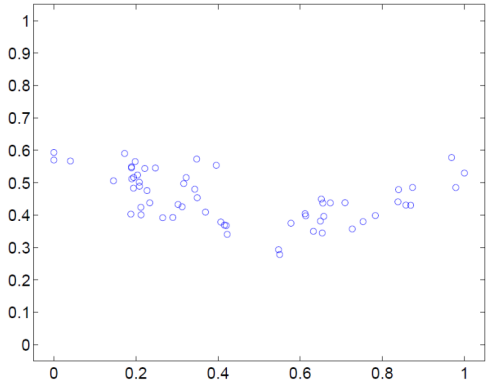
$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}(x^1 \dots, x^m)(y^1 \dots, y^m)^\top + \frac{2}{m}(x^1, \dots x^m)(x^1, \dots x^m)^\top\theta = 0$$

- Define $X = (x^1, x^2, \dots x^m), y = (y^1, y^2, \dots, y^m)^\top$, gradient becomes

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m} Xy + \frac{2}{m} XX^\top\theta$$

$$\Rightarrow \hat{\theta} = (XX^\top)^{-1}Xy$$

Nonlinear regression



- Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^n + \epsilon$$

- Let $\tilde{x} = (1, x, x^2, \ldots, x^n)^\top$ and $\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_n)^\top$

$$\mathrm{y} = \theta^\top \tilde{x}$$

Least mean square method

- Given m data points, find θ that minimizes the mean square error

$$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top \tilde{x}^i\right)^2$$

- Our usual trick: set gradient to 0 and find parameter

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i}^{m}\left(y^i - \theta^\top \tilde{x}^i\right)\tilde{x}^i = 0$$

$$\Leftrightarrow -\frac{2}{m}\sum_{i}^{m} y^i \tilde{x}^i + \frac{2}{m}\sum_{i}^{m} \tilde{x}^i \tilde{x}^{i\top}\theta = 0$$

Matrix version of the gradient

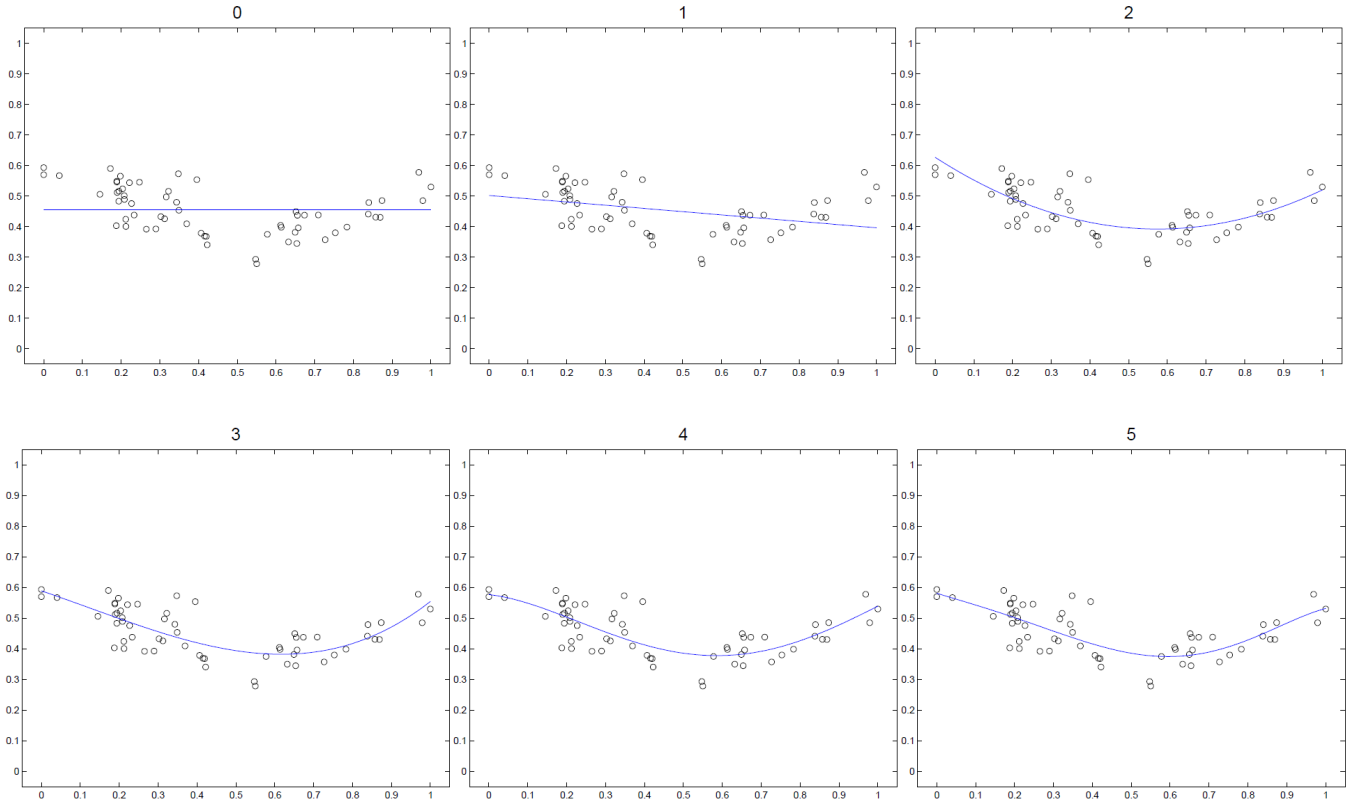
- Define $\tilde{X} = \left(\tilde{x}^{(1)}, \tilde{x}^{(2)}, \ldots \tilde{x}^{(m)}\right), y = \left(y^{(1)}, y^{(2)}, \ldots, y^{(m)}\right)^{\top}$, gradient becomes

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\tilde{X}y + \frac{2}{m}\tilde{X}\tilde{X}^{\top}\theta = 0$$
$$\Rightarrow \hat{\theta} = \left(\tilde{X}\tilde{X}^{\top}\right)^{-1}\tilde{X}y$$

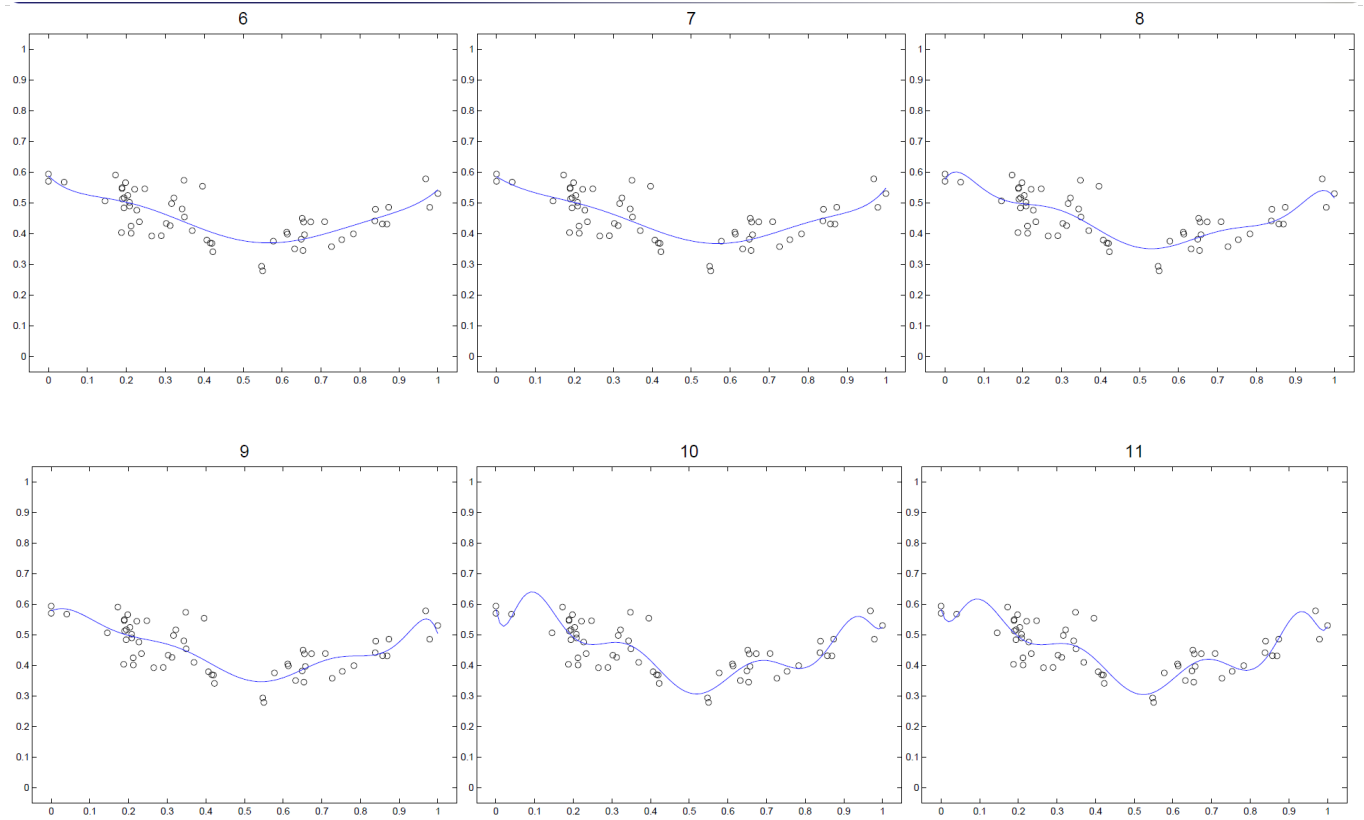
- Note that $\tilde{x} = (1, x, x^2, \ldots, x^n)^{\top}$

- If we choose a different maximal degree n for the polynomial, the solution will be different.

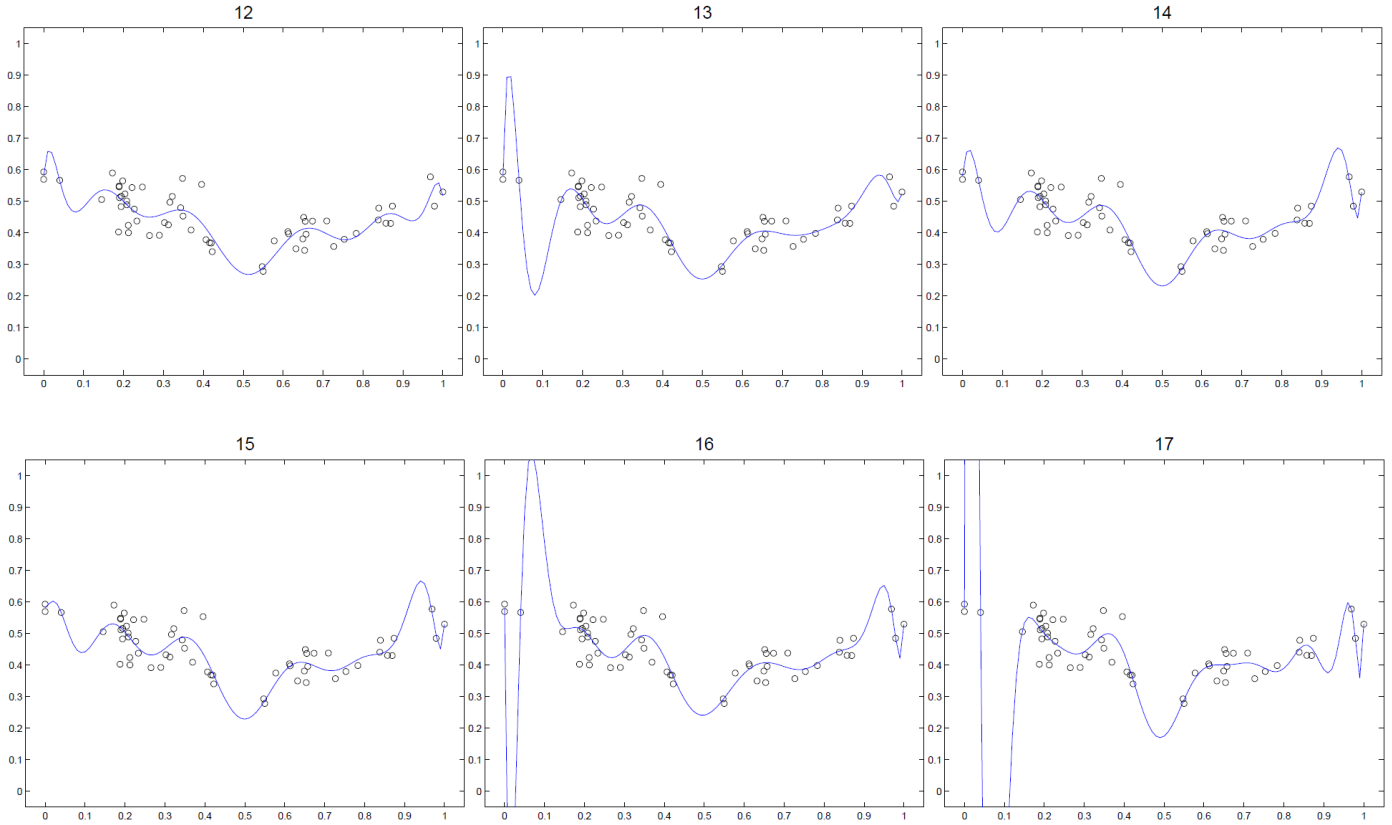
Increasing the maximal degree



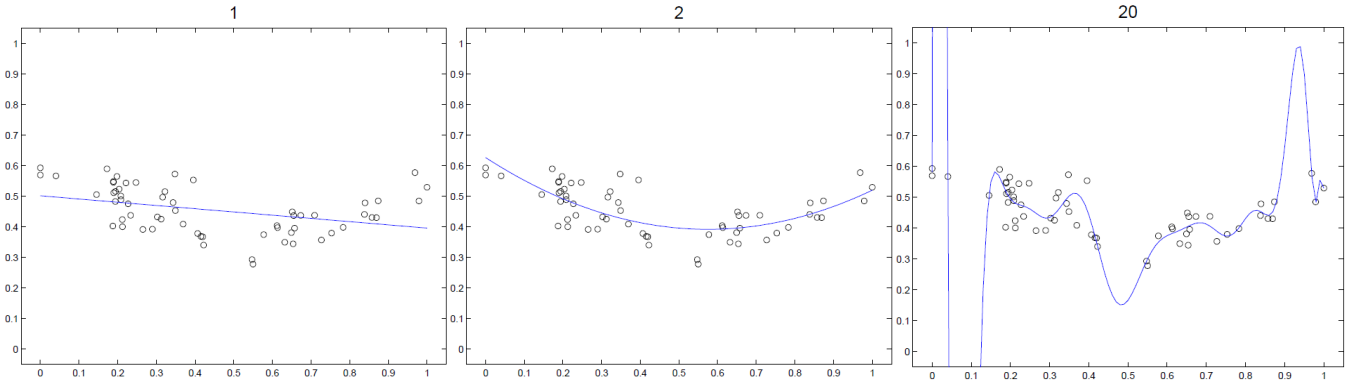
Increasing the maximal degree



Increasing the maximal degree



Which one is better?



- Can we increase the maximal polynomial degree to very large, such that the curve passes through all training points?

- The optimization does not prevent us from doing that

When maximal degree is very large

- Define $\tilde{X} = \left(\tilde{x}^{(1)}, \tilde{x}^{(2)}, \ldots \tilde{x}^{(m)}\right), y = \left(y^{(1)}, y^{(2)}, \ldots, y^{(m)}\right)^{\top}$, set gradient to zero, $\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\tilde{X}y + \frac{2}{m}\tilde{X}\tilde{X}^{\top}\theta = 0$

$$\Rightarrow \tilde{X}\tilde{X}^{\top}\theta = \tilde{X}y$$

- Each $\tilde{x} = (1, x, x^2, \ldots, x^n)^{\top}$ is a vector of polynomial features, the size of $\tilde{X}$ is $n \times m$, and $\tilde{X}\tilde{X}^{\top}$ is $n \times n$

- When $n > m$,

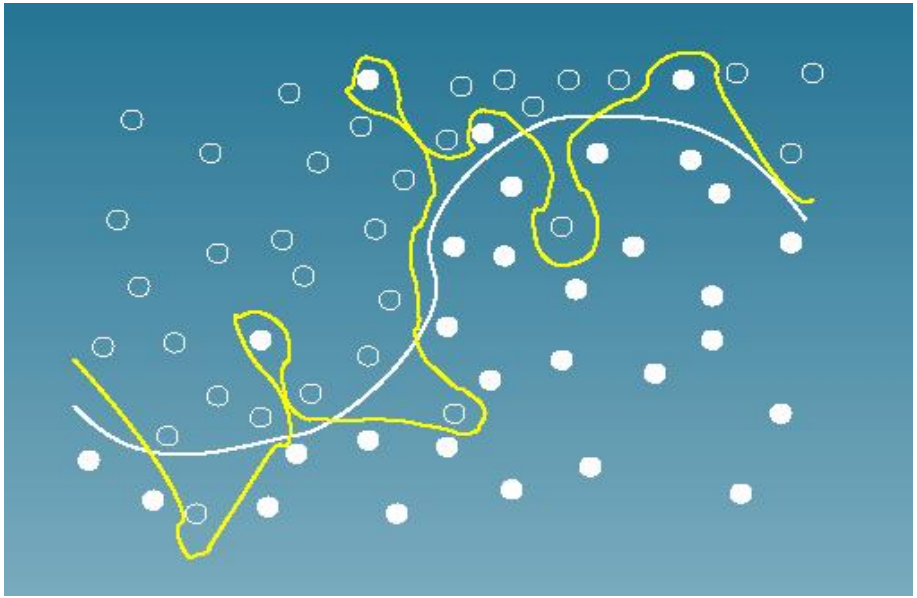
$\tilde{X}\tilde{X}^{\top}$ is not invertible; there are multiple solutions θ which give zero objective

$$L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^{\top}\tilde{x}^i\right)^2$$

Classification with polynomials

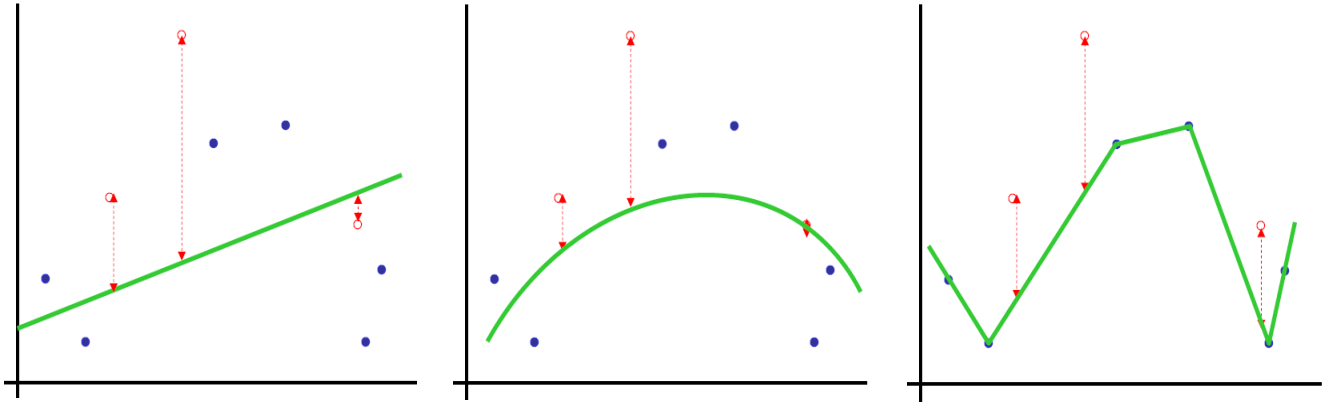
- Eg. Logistic regression with polynomial features

$$p(y = 1|x, \theta) = \frac{1}{1 + \exp(-\theta^{\top}\tilde{x})}$$



Overfitting/Underfitting

- Blue points: training data points, Red points: test data points
- The fit in the middle panel achieves a balance of small error in both training and test points.



Underfitting

Overfitting

What is the problem?

Suppose we have data points, and yi is going to be our response, and this xi is a square that go on top, representing our feature. It contains all of the linear and polynomial terms. So remember, the degree of the polynomial is going to determine the dimension of my axilla. If we have an end polynomial, this outer polynomial, then, your x is going to be a plus one dimensional vector that contains also the constant.

- Given m data points $D = \{(\tilde{x}^i, y^i)\}$, find θ that minimizes the mean square error

$$\hat{\theta} = argmin_\theta \hat{L}(\theta) := \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top \tilde{x}^i\right)^2$$

- But we really want to minimize the error for unseen data points, or with respect to the entire distribution of data

$$\theta^* = argmin_\theta L(\theta) \coloneqq \mathbb{E}_{(\tilde{x},y)\sim P(\tilde{x},y)}[(y - \theta^\top \tilde{x})^2]$$

- It is the finite number training point that creates the problem

Decomposition of expected loss

- Estimate your function from a finite data set D

$$\hat{f} = argmin_f \, \hat{L}(f) := \frac{1}{m}\sum_{i=1}^{m}\left(y^i - f\left(x^i\right)\right)^2$$

$\hat{f}$ is a random function, generally different for different data set

- Expected loss of $\hat{f}$

$$L\left(\hat{f}\right) := \mathbb{E}_D \mathbb{E}_{(x,y)}\left[\left(y - \hat{f}(x)\right)^2\right]$$

- Bias-variance decomposition

Expected loss = $(\text{bias})^2$ + variance + noise

What is the best we can do?

- The expected squared loss is

$$L(\hat{f}) := \mathbb{E}_D \mathbb{E}_{(x,y)} \left[\left(y - \hat{f}(x) \right)^2 \right]$$

$$= \mathbb{E}_D \left[\underbrace{\int \int \left(y - \hat{f}(x) \right)^2 p(x,y) dx dy}_{A} \right]$$

- Our goal is to choose $\hat{f}(x)$ that minimize $L(\hat{f})$. Calculus of variations

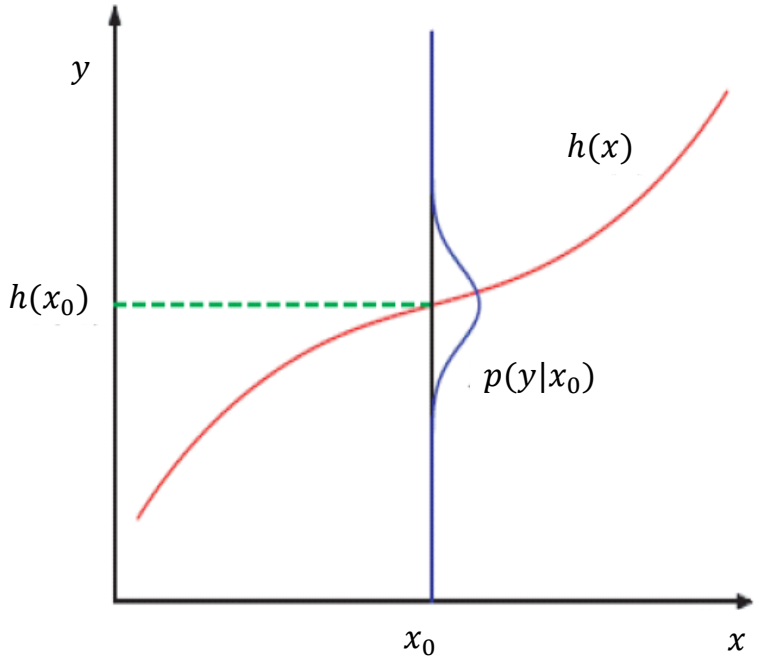
$$\frac{\partial A}{\partial f(x)} = 2 \int \big(y - f(x) \big) p(x,y) dy = 0$$

$$\Leftrightarrow \int f(x) p(x,y) dy = \int y p(x,y) dy$$

$$\Leftrightarrow h(x) := \int \frac{y p(x,y)}{p(x)} dy = \int y p(y|x) dt = \mathbb{E}_{y|x}[y] = \mathbb{E}[y|x]$$

The best predictor is the expected value

- The best you can do is $h(x) = \mathbb{E}_{y|x}[y]$: the expected value of y given a particular x



Noise term in the decomposition

- $h(x) = \mathbb{E}(y|x)$ is the **optimal** predictor, and $\hat{f}(x)$ our actual predictor, decompose the error a bit

$$\mathbb{E}_D \mathbb{E}_{(x,y)} \left[\left(y - \hat{f}(x) \right)^2 \right] = \mathbb{E}_D \left[\int \int \left(y - h(x) + h(x) - \hat{f}(x) \right)^2 p(x,y) dx dy \right]$$

$$= \mathbb{E}_D \left[\int \int \left(\left(\hat{f}(x) - h(x) \right)^2 + 2 \left(\hat{f}(x) - h(x) \right) (h(x) - y) \right. \right.$$

$$\left. \left. + (h(x) - y)^2 \right) p(x,y) dx dy \right]$$

$$= \underbrace{\mathbb{E}_D \left[\int \left(\hat{f}(x) - h(x) \right)^2 p(x) dx \right]}_{\text{Will decompose further}} + \underbrace{\int \int (h(x) - y)^2 p(x,y) dx dy}_{\text{Noise term. can not do better than this. a lower bound of the expected loss}}$$

Bias-variance decomposition

- $\hat{f}(x)$ is a random function, generally different for different dataset D
- $\mathbb{E}_D[\hat{f}(x)]$: expected value of $\hat{f}(x)$ with respected to random dataset

$$\mathbb{E}_D\left[\int \left(\hat{f}(x) - h(x)\right)^2 p(x)dx\right] = \mathbb{E}_D\mathbb{E}_x\left[\left(\hat{f}(x) - h(x)\right)^2\right]$$

$$= \mathbb{E}_x\mathbb{E}_D\left[\left(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)] + \mathbb{E}_D[\hat{f}(x)] - h(x)\right)^2\right]$$

$$= \mathbb{E}_x\mathbb{E}_D\left[\left(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)]\right)^2\right] + \mathbb{E}_x\mathbb{E}_D\left[\left(\mathbb{E}_D[\hat{f}(x)] - h(x)\right)^2\right]$$
$$-2\mathbb{E}_x\mathbb{E}_D\left[\left(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)]\right)\left(\mathbb{E}_D[\hat{f}(x)] - h(x)\right)\right]$$

$$= \underbrace{\mathbb{E}_x\mathbb{E}_D\left[\left(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)]\right)^2\right]}_{\text{variance}} + \underbrace{\mathbb{E}_x\left[\left(\mathbb{E}_D[\hat{f}(x)] - h(x)\right)^2\right]}_{\text{Bias}^2}$$

Overall decomposition of expected loss

- Putting things together

  Expected loss = (bias)^2 + variance + noise

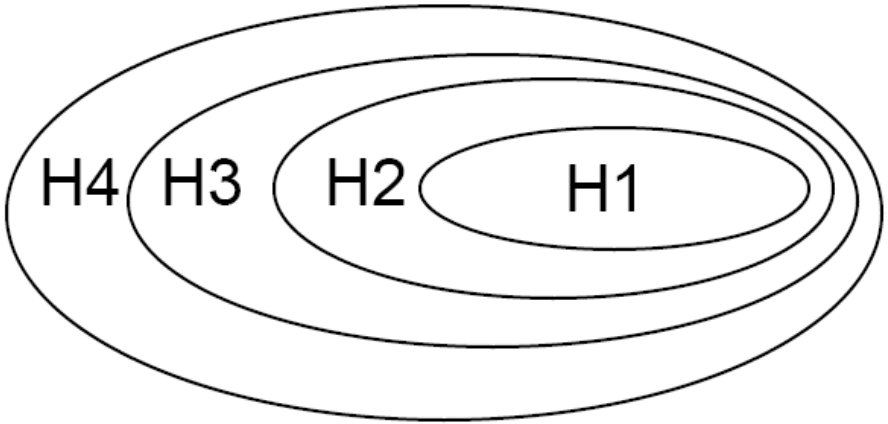
- In formula

$$\mathbb{E}_D \mathbb{E}_{(x,y)} \left[\left(y - \hat{f}(x) \right)^2 \right]$$
$$= \mathbb{E}_x \left[\left(\mathbb{E}_D \left[\hat{f}(x) \right] - h(x) \right)^2 \right] \ (bias^2)$$
$$+ \mathbb{E}_x \mathbb{E}_D \left[\left(\hat{f}(x) - \mathbb{E}_D \left[\hat{f}(x) \right] \right)^2 \right] \ (variance)$$
$$+ \mathbb{E}_{(x,y)} [(h(x) - y)^2] \ (noise)$$

- Key quantities
  - $\hat{f}(x)$: actual predictor
  - $\mathbb{E}_D \left[\hat{f}(x) \right]$: expected predictor
  - $h(x) = \mathbb{E}(y|x)$: **optimal** predictor

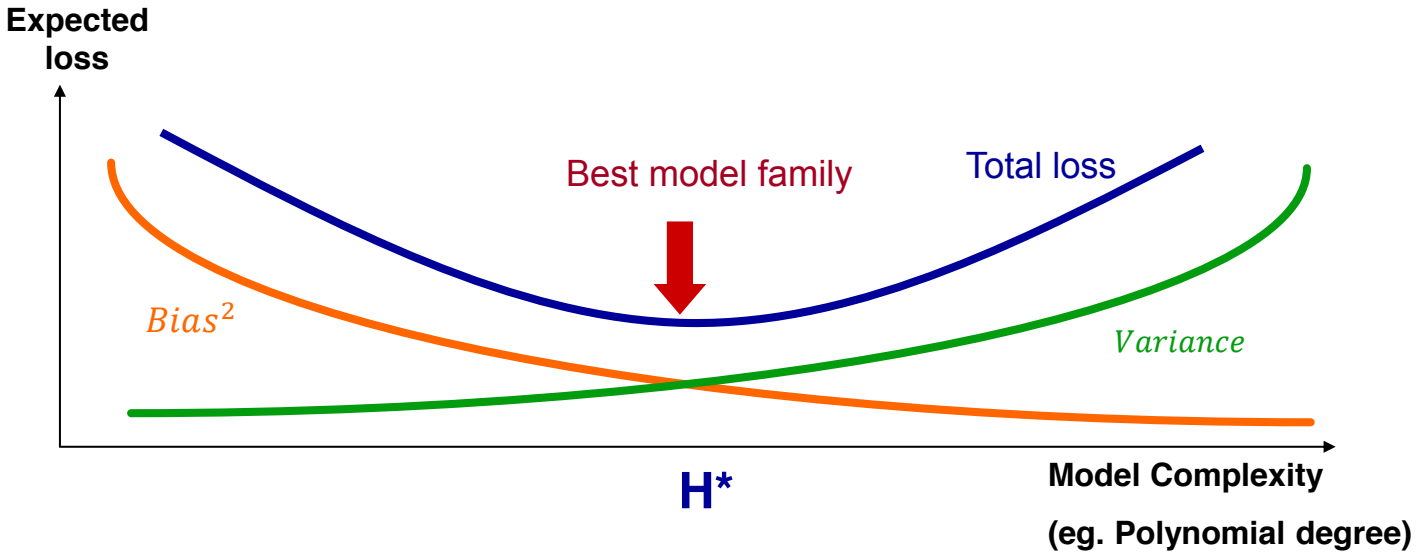
Model space

- Which model space should we choose?
- The more complex the model, the large the model space
- Eg. Polynomial function of degree 1, 2, … corresponds to space H1, H2 …



Intuition of model selection

Find the right model family s.t. expected loss becomes minimum



Other things that control model complexity

- Eg. In the case of linear models $y = \langle w, x \rangle + b$, one wants to make $\|w\|$ a controlled parameter

$$\|w\| < C$$

  - H_C the linear model function family satisfying the constraint
  - The large the C, the large the model family

- Eg. the larger the regularization parameter λ, the small the model family

  - $J(w) = \sum_i (w^\top x_i - y_i)^2 + \lambda \|w\|_2^2$
  - $J(w) = \sum_i (w^\top x_i - y_i)^2 + \lambda \|w\|_1$

- Eg. Early stopping in boosting

Ridge regression

- Given m data points, find θ that minimizes the regularized mean square error

$$\theta^r = argmin_\theta\, L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2 + \lambda\|\theta\|^2$$

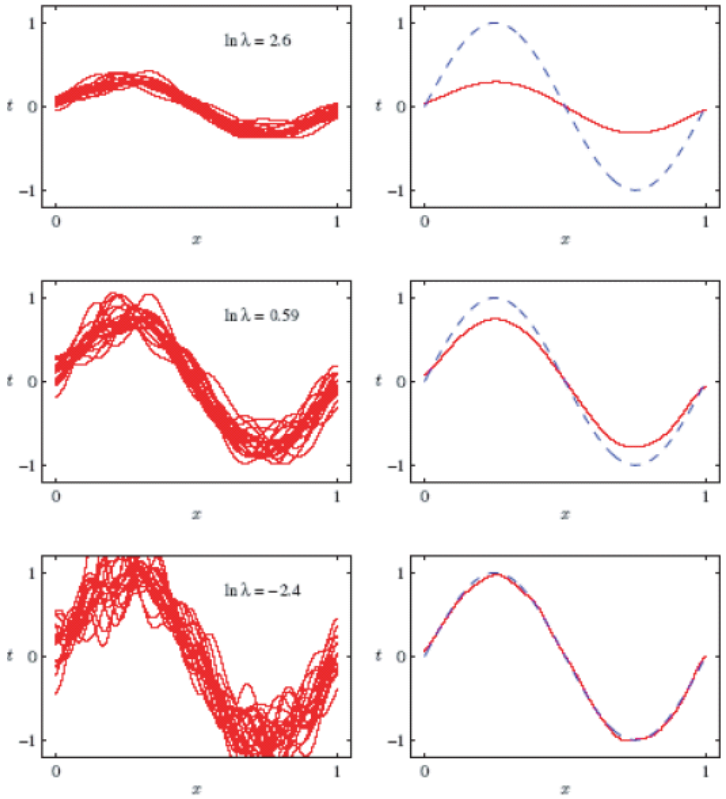
- gradient becomes

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}Xy + \frac{2}{m}XX^\top\theta + \frac{2\lambda}{m}\theta = 0$$

$$\Rightarrow \theta^r = (XX^\top + \lambda I)^{-1}Xy$$

If we choose a different λ, the solution will be different.

Experiment with bias-variance tradeoff



- λ is a "regularization" terms in LR, the smaller the λ, is more complex the model
  - Simple (highly regularized) models have low variance but high bias.
  - Complex models have low bias but high variance.
- The actual $\mathbb{E}_D$ can not be computed
- You are inspecting an empirical average over 100 training set.

Cross-Validation

- K-fold cross-validation (CV)

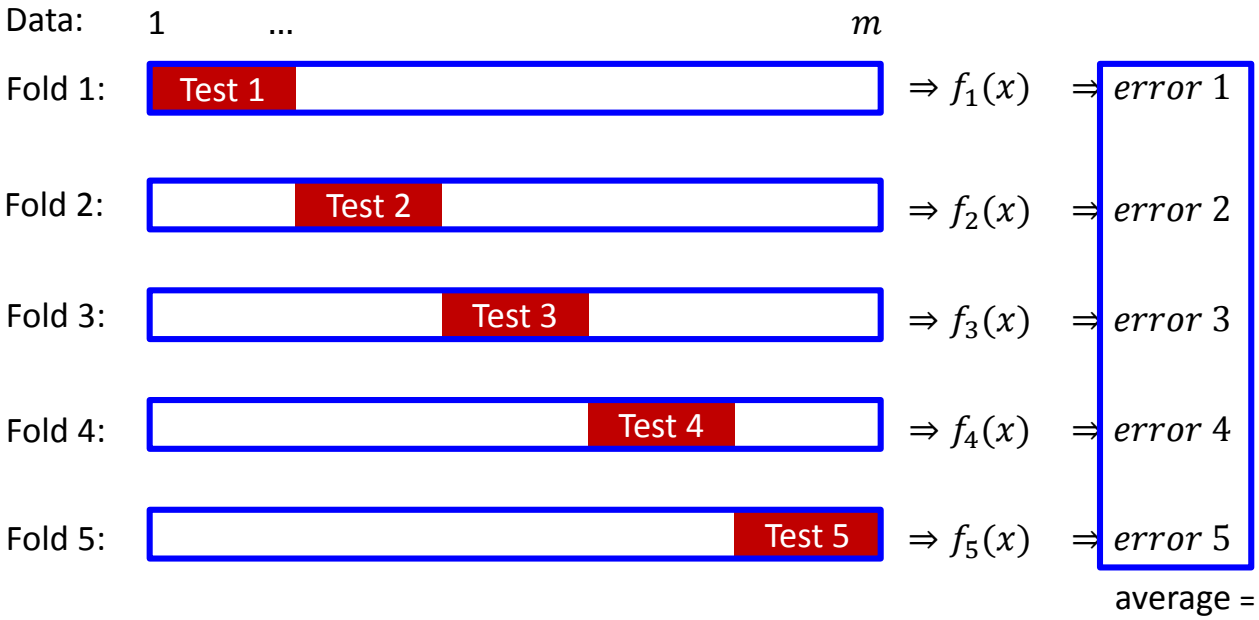
- For each fold i:
  - Set aside $\alpha \cdot m$ samples of D (where $m = |D|$) as the held-out data. They will be used to evaluate the error
  - Fit a model $f_i(x)$ to the remaining $(1-\alpha) \cdot m$ samples in D
  - Calculate the error of the model $f_i(x)$ on the held-out data.

- Repeat the above ***K* times**, choosing a **different** held-out data set each time, and the errors are averaged over the folds.

- For the polynomial degree with the lowest score, we use all of D to find the parameter values for $f(x)$.

Cross-Validation

- Eg. Want to select the maximal degree of polynomial
- 5-fold cross-validation (blank: training; red: test)



- Important: test data i is not used to fit model $f_i(x)$

Example: Cross validation error curve for ridge regression

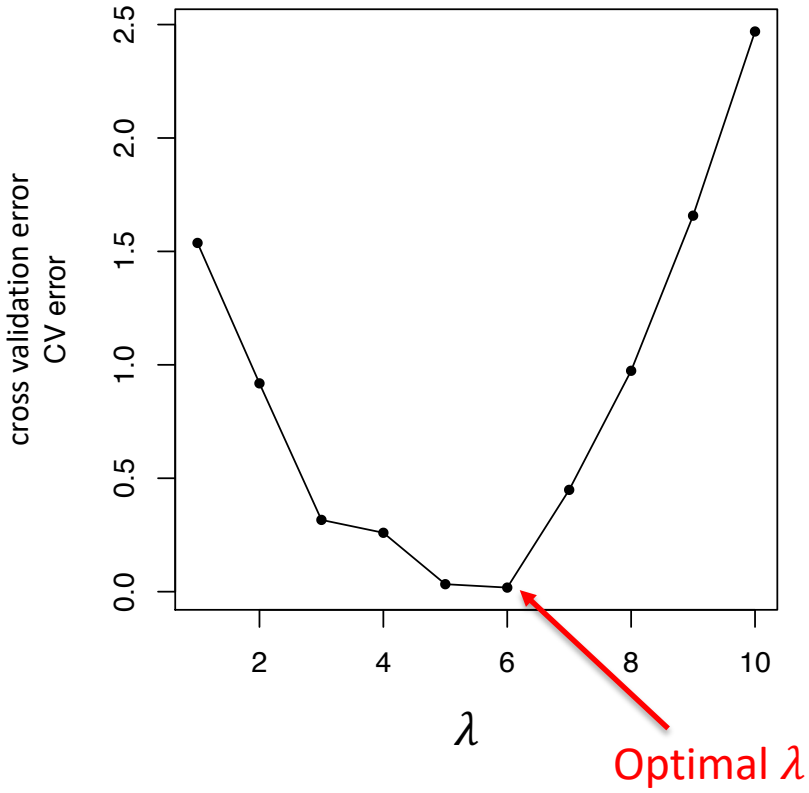
$$min_\theta\ L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2 + \lambda\|\theta\|^2$$

$$\Rightarrow \theta^r = (XX^\top + \lambda I)^{-1}Xy$$

Error (for each fold, L samples) =

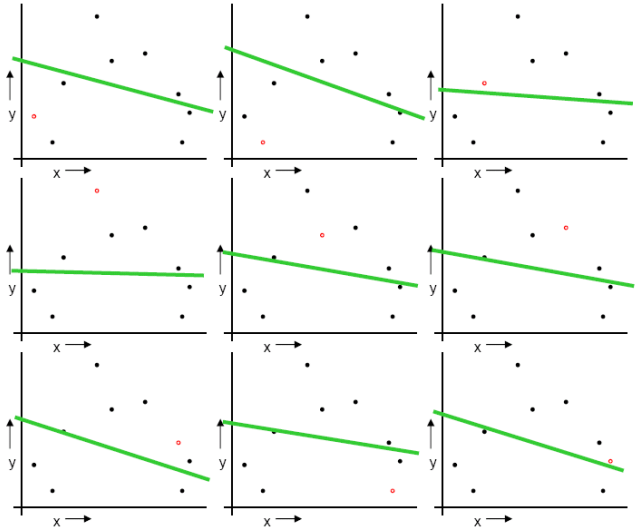
$$\frac{1}{L}\sum_{l=1}^{L}(\tilde{y}^l - (\theta^r)^T\tilde{x}^l)^2$$

CV Error = Average of error over all folds

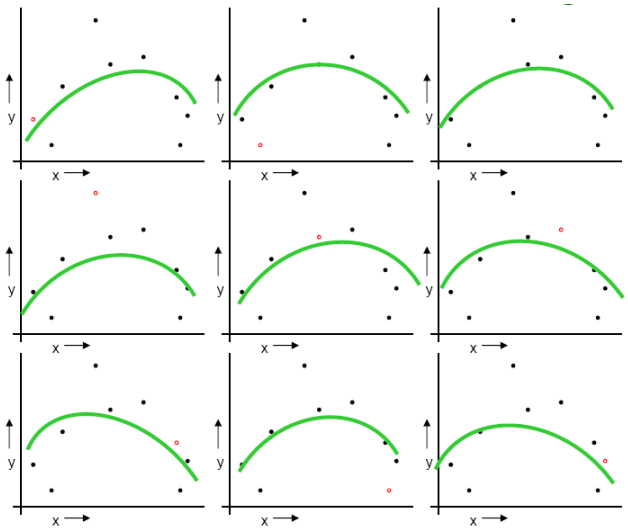


Example:

- When $\alpha = 1/N$, the algorithm is known as Leave-One-Out-Cross-Validation (LOOCV)



MSELOOCV(M_1)=2.12



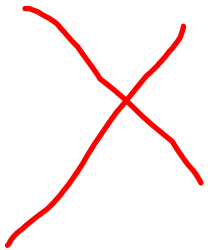
MSELOOCV(M_2)=0.962

Practical issues for K-fold CV

- How to decide the values for K (or α)
  - Commonly used $K = 10$ or $(\alpha = 0.1)$.
  - Large K makes it time-consuming.
  - Bias-variance trade-off
    - Large K usually leads to low bias. In principle, *LOOCV* provides an almost unbiased estimate of the generalization ability of a classifier, but it can also have high variance.
    - Small K can reduce variance, but will lead to under-use of data, and causing high-bias.

- One important point is that the test data D_{test} is never used in CV, because doing so would result in overly (indeed dishonest) optimistic accuracy rates during the testing phase.

Ridge regression



- Given m data points, find θ that minimizes the regularized mean square error

$$\theta^r = argmin_\theta \, L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2 + \lambda\|\theta\|^2$$

- gradient becomes

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}Xy + \frac{2}{m}XX^\top\theta + \frac{2\lambda}{m}\theta = 0$$

$$\Rightarrow \theta^r = (XX^\top + \lambda I)^{-1}Xy$$

If we choose a different λ, the solution will be different.

Regularization in maximum likelihood

- Regularize the likelihood objective (also known as penalized likelihood, shrinkage, smoothing, etc.)

$$\hat{\theta}_{shrinkage} = \arg\max_{\theta}[l(\theta; D) - \lambda\|\theta\|]$$

where $\lambda > 0$ and $\|\theta\|$ might be the L_1 or L_2 norm.

- The choice of norm has an effect
  - using the L_2 norm pulls directly towards the origin,
  - while using the L_1 norm pulls towards the coordinate axes, i.e it tries to set some of the coordinates to 0.

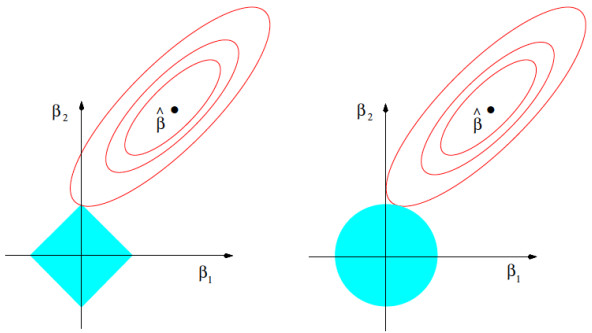
Lasso for variable selection

- Least square method

$$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{m}\sum_{i}^{m}\left(y^{i} - \theta^{\top}x^{i}\right)^{2}$$

- Encourage θ to be sparse, i.e., having very few number of non-zeros, while having a good "fit"

$$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{m}\sum_{i}^{m}\left(y^{i} - \theta^{\top}x^{i}\right)^{2} + \|\theta\|_{1}$$



Lasso

The lasso estimate

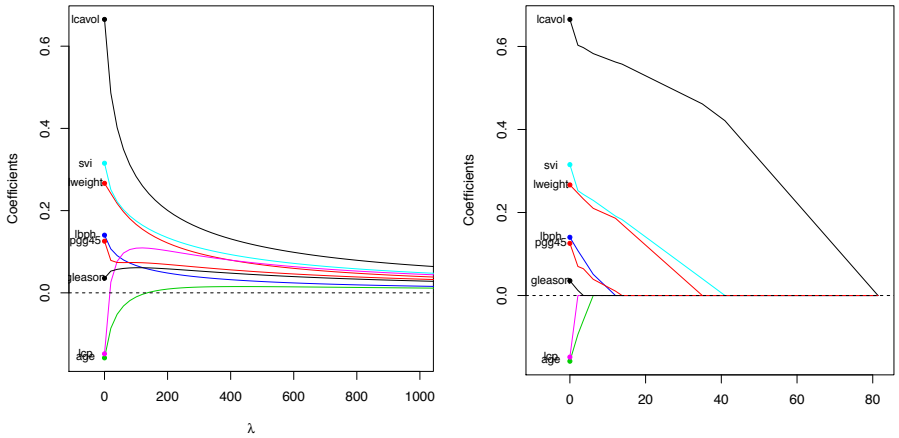
$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda\|\beta\|_1$$

- The penalty term $\|\beta\|_2^2$ is replace by ℓ_1 norm $\|\beta\|_1$
- λ controls the strength of the penalty
- lasso is able to perform model selection in the linear model
- As λ increases, more coefficients are set to 0 (less variables are selected)
- Among the nonzero coefficients, more shrinkage is employed

R. Tibshirani, 1996, Regression shrinkage and selection via the lasso.

Example: prostate data

- We are interested in the level of prostate-specific antigen (PSA) elevated in men who has prostate cancer.
- Measure PSA on $n = 97$ patients, $p = 8$ clinical variables



Ridge Lasso

- If we want the 3 leading factors, we report "cancer volume", "seminal sesicle invasion", "prostate weight"


SUMMARY