CS 451/686-02 Data Mining
Statistical Learning

Fall 2016

Maria Daltayanni

part of the slides is credited to the ISL authors

The Supervised Learning Problem

• Outcome measurement Y (also called dependent variable, response, **target**).

• Vector of p predictor measurements X (also called inputs, regressors, covariates, **features**, independent variables).
  • In the **regression** problem, Y is quantitative (e.g price, blood pressure).
  • In the **classification** problem, Y takes values in a finite, unordered set (survived/died, digit 0-9, cancer class of tissue sample).

• We have **training data** $(x_1, y_1), \ldots (x_N, y_N)$. These are observations (examples, instances) of these measurements.

Objectives

On the basis of the training data we would like to:

- Accurately predict *unseen* **test** cases.
- Understand which inputs affect the outcome, and how.
- Assess the quality of our predictions and inferences.

Training and Testing in practice

- In practice, here is how training and testing works:

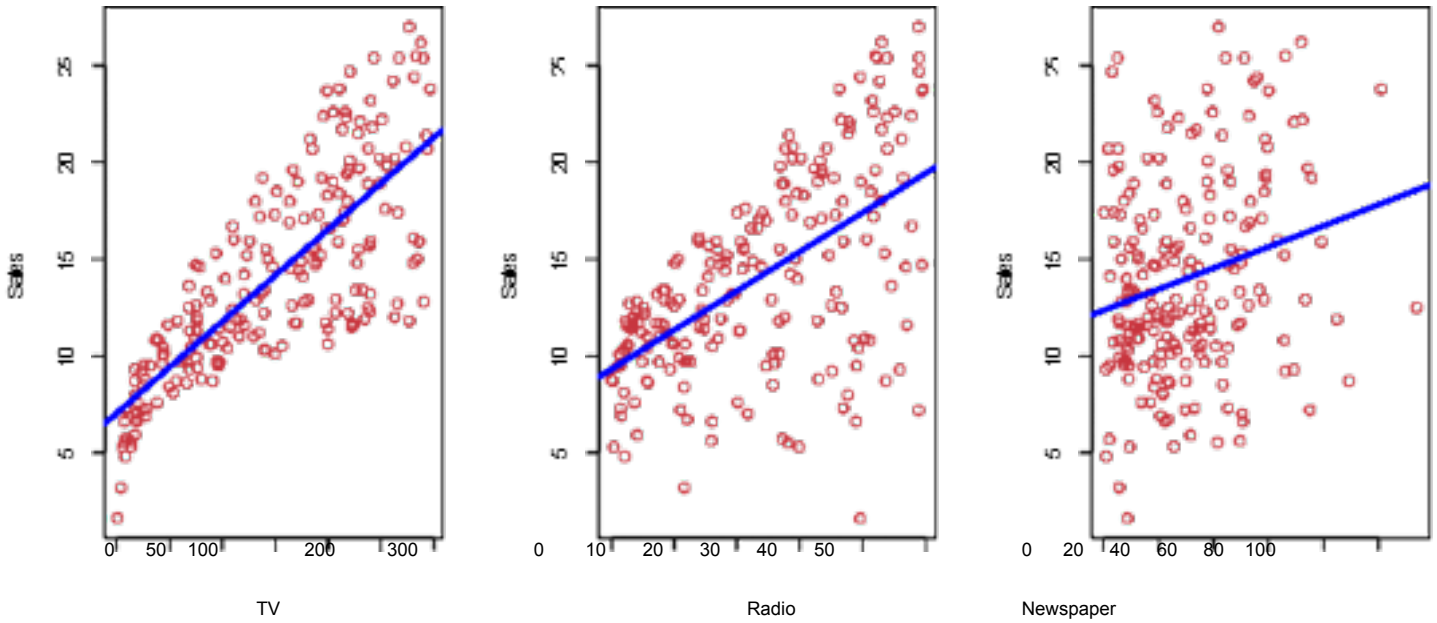
- Tr: training data (X and Y) are available to us, i.e. (x_1, y_1), … (x_N, y_N)
- Ts: test data (X, Y) are available to us (x_{N+1}, y_{N+1}), … (x_M, y_M)
- We use Tr to learn a model that predicts Y for the test data Ts.
- Then we measure how accurate our model is on Ts and we revise our model until we get a satisfactory accuracy.
- We use that model to new test data Ts'(X), for which we have never seen any Y, (x_{M+1}, y_{M+1}), … (x_L, y_L)
- We apply the model on the Y of Ts' and we wait until true Y becomes available.
- Then we can test how well our model did on the truly unknown data Ts'.

How can we evaluate and update our model?

- To revise our model, we need to know:

- Tr: training data (X and Y)
- Ts: test data (X, Y)
- We learn a model that predicts Y for the test data Ts
- The prediction is called Y^.
- Then we measure the different between the truth and the prediction, diff(Y, Y^).
- If diff(Y, Y^) < error, then we assume the model is good enough.
- Else, we modify our model, i.e. we use another f(X):
  - we may change f
  - we may change X
  - or both

Example: Sales



- Shown are Sales vs TV, Radio and Newspaper, with a blue linear-regression line fit separately to each.
- Can we predict Sales using these three? Perhaps we can do better using a model

- Sales $\approx f$ (TV, Radio, Newspaper)

Notation

- Here Sales is a *response* or *target* that we wish to predict. We generically refer to the response as Y .
- TV is a *feature*, or *input*, or *predictor*; we name it X_1. Likewise name Radio as X_2, and so on.
- We can refer to the *input vector* collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$

- Now we write our model as

$$Y = f(X) + \varepsilon$$

where ε captures measurement errors and other discrepancies.

What is f (X) good for?

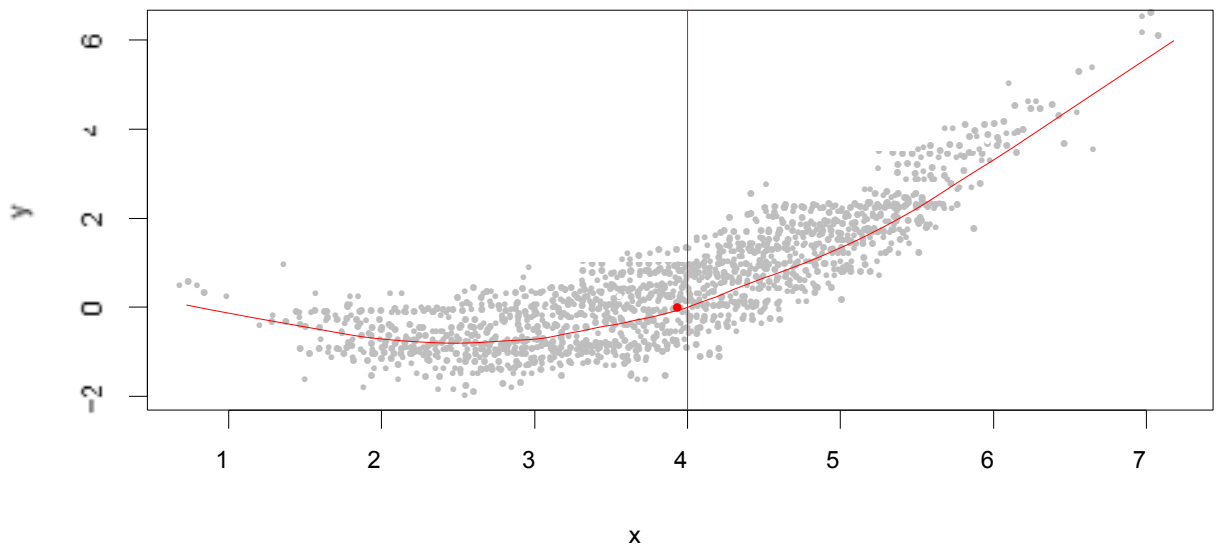
- With a good f we can make predictions of Y at new points

$X = x$.

- We can understand which components of

$X = (X_1, X_2, \ldots, X_p)$ are important in explaining Y, and which are irrelevant. e.g. Seniority and Years of Education have a big impact on Income, but Marital Status typically does not.

- Depending on the complexity of f, we may be able to understand how each component X_j of X affects Y.



- Is there an ideal $f(X)$? In particular, what is a good value for $f(X)$ at any selected value of X, say $X = 4$? There can be many Y values at $X = 4$. A good value is

$$f(4) = E(Y \mid X = 4)$$

- $E(Y \mid X = 4)$ means *expected value* (average) of Y given $X = 4$.
- This ideal $f(x) = E(Y \mid X = x)$ is called the *regression function*.

The regression function f (x)

- Is also defined for vector X; e.g.

$f(x) = f(x_1, x_2, x_3) = E(Y \mid X_1 = x_1, X_2 = x_2, X_3 = x_3)$

- Is the *ideal* or *optimal* predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y \mid X = x)$ is the function that minimizes $E[(Y - g(X))^2 \mid X = x]$ over all functions g at all points $X = x$.
- $\varepsilon = Y - f(x)$ is the *irreducible* error — i.e. even if we knew $f(x)$, we would still make errors in prediction, since at each $X = x$ there is typically a distribution of possible Y values.
- For any estimate $\hat{f}(x)$ of $f(x)$, we have

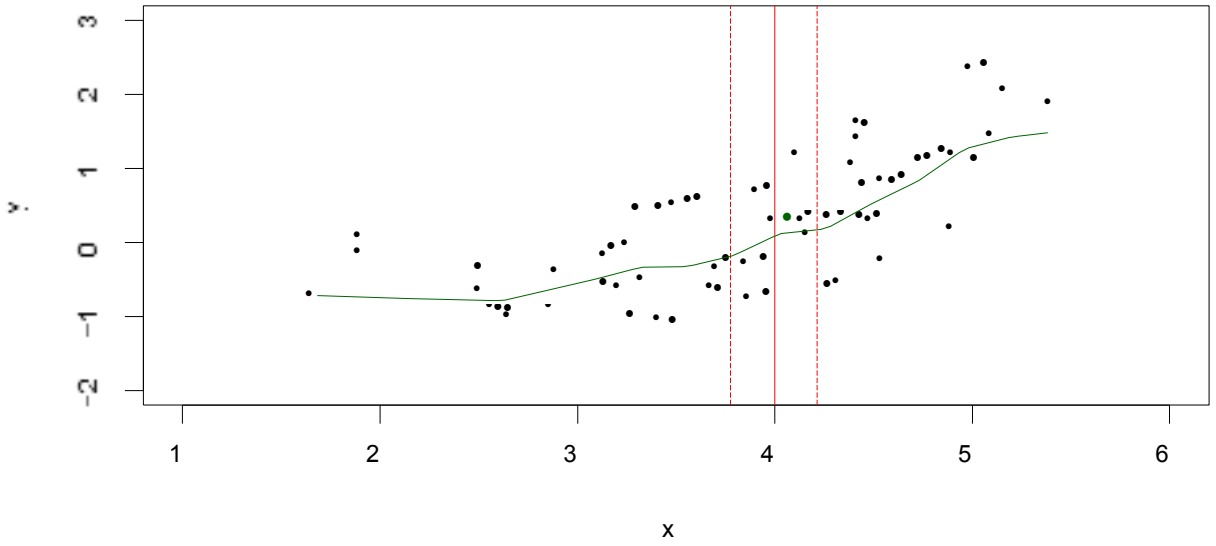
$$E[(Y - \hat{f}(X))^2 \mid X = x] = [f(x) - \hat{f}(x)]^2 + \mathrm{Var}(\varepsilon)$$

Reducible *Irreducible*

How to estimate f

- Typically we have few if any data points with $X = 4$ exactly.
- So we cannot compute $E(Y \mid X = x)$!

- Relax the definition and let
- $\hat{f}(x) = \text{Ave}(Y \mid X \in N(x))$ where $N(x)$ is some *neighborhood* of x.

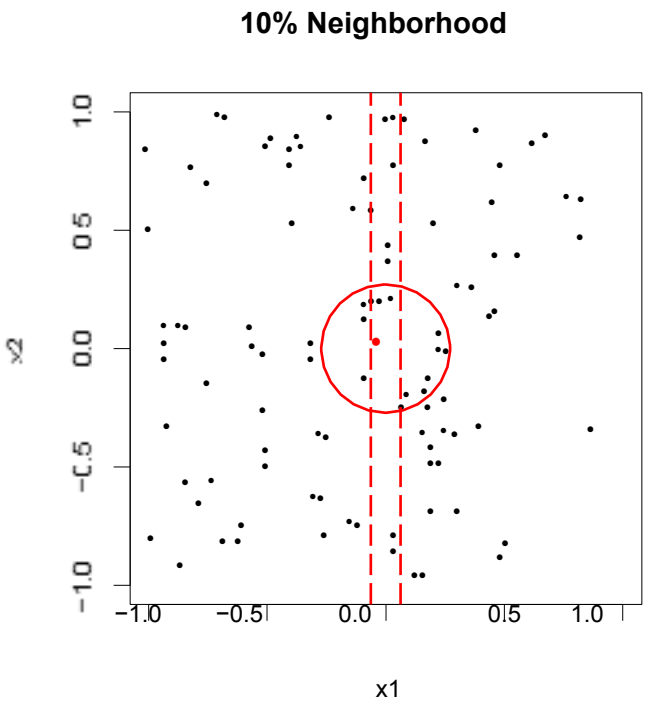


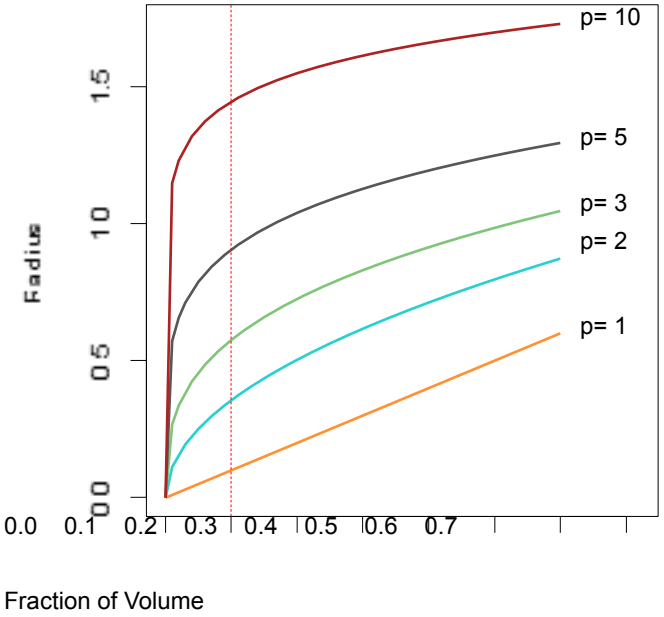
- Nearest neighbor averaging can be pretty good for small p — i.e. $p \leq 4$ and large-ish N .

- Nearest neighbor methods can be *lousy* when p is large. Reason: the *curse of dimensionality*. Nearest neighbors tend to be far away in high dimensions.

    - We need to get a reasonable fraction of the N values of y_i to average to bring the variance down—e.g. 10%.
    - A 10% neighborhood in high dimensions need no longer be local, so we lose the spirit of estimating $E(Y \mid X = x)$ by local averaging.

The curse of dimensionality





Parametric and structured models

- The *linear* model is an important example of a parametric model:

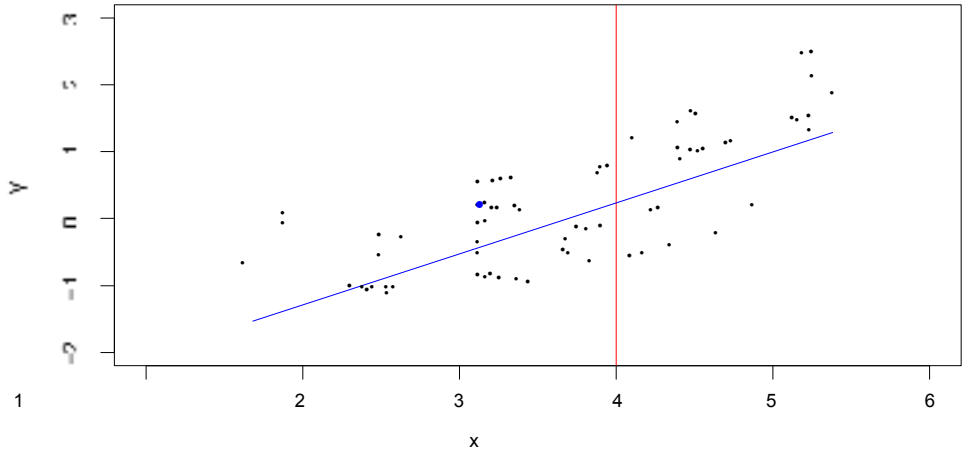
$$f_L(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots \beta_p X_p.$$

- A linear model is specified in terms of $p + 1$ parameters

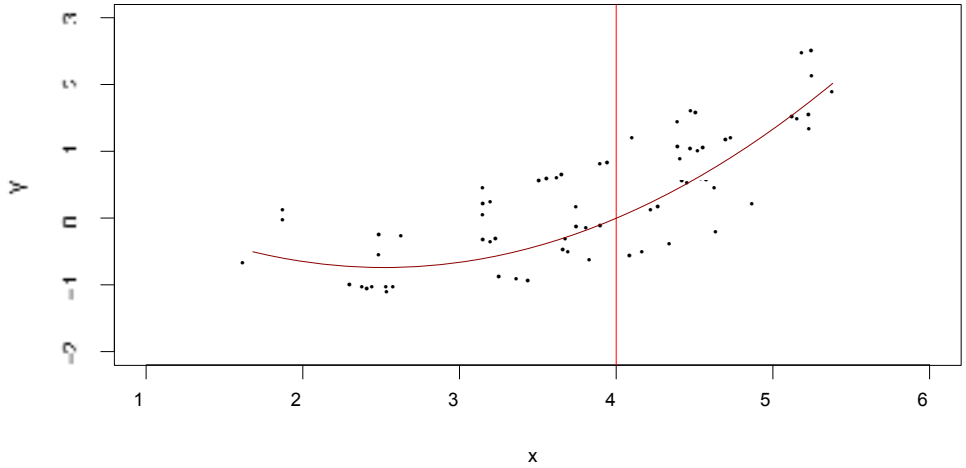
$$\beta_0, \beta_1, \ldots, \beta_p.$$

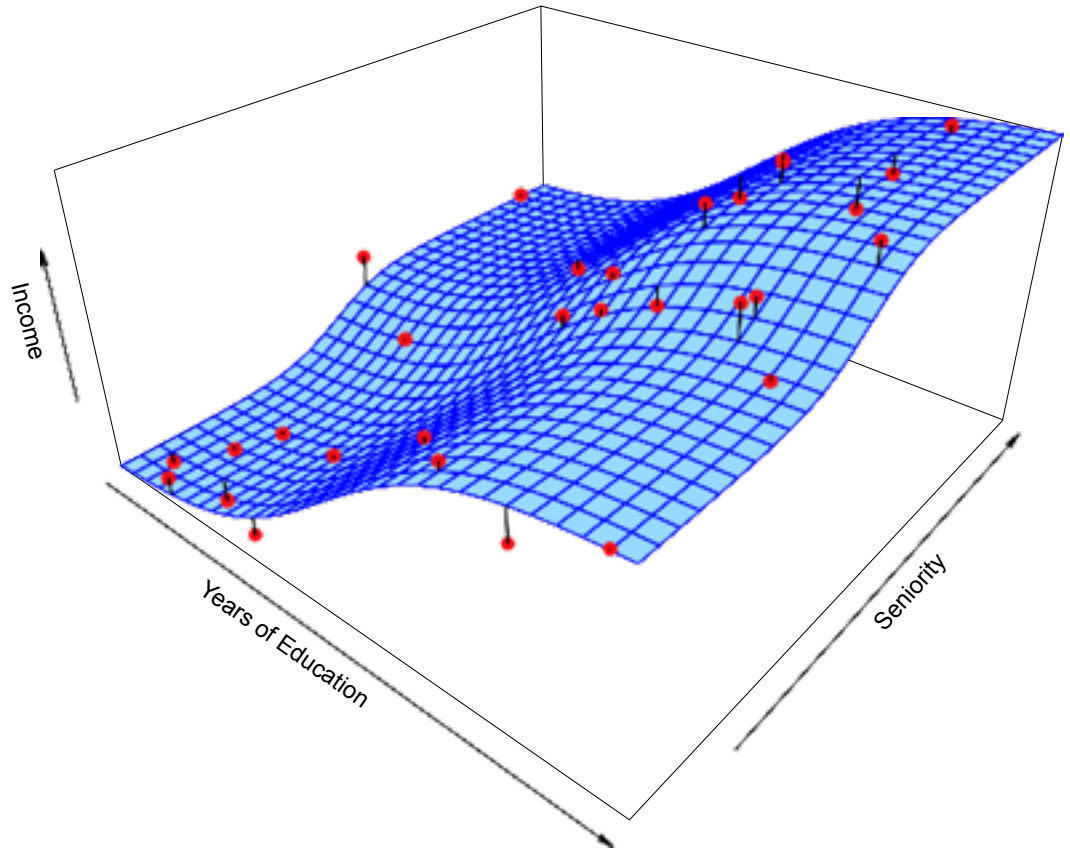
- We estimate the parameters by fitting the model to training data.
- Although it is *almost never correct*, a linear model often serves as a good and interpretable approximation to the unknown true function $f(X)$.

A linear model $\hat{f}_L(X) = \hat{\beta}_0 + \hat{\beta}_1 X$ gives a reasonable fit here



A quadratic model $\hat{f}_Q(X) = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 X^2$ fits slightly better.

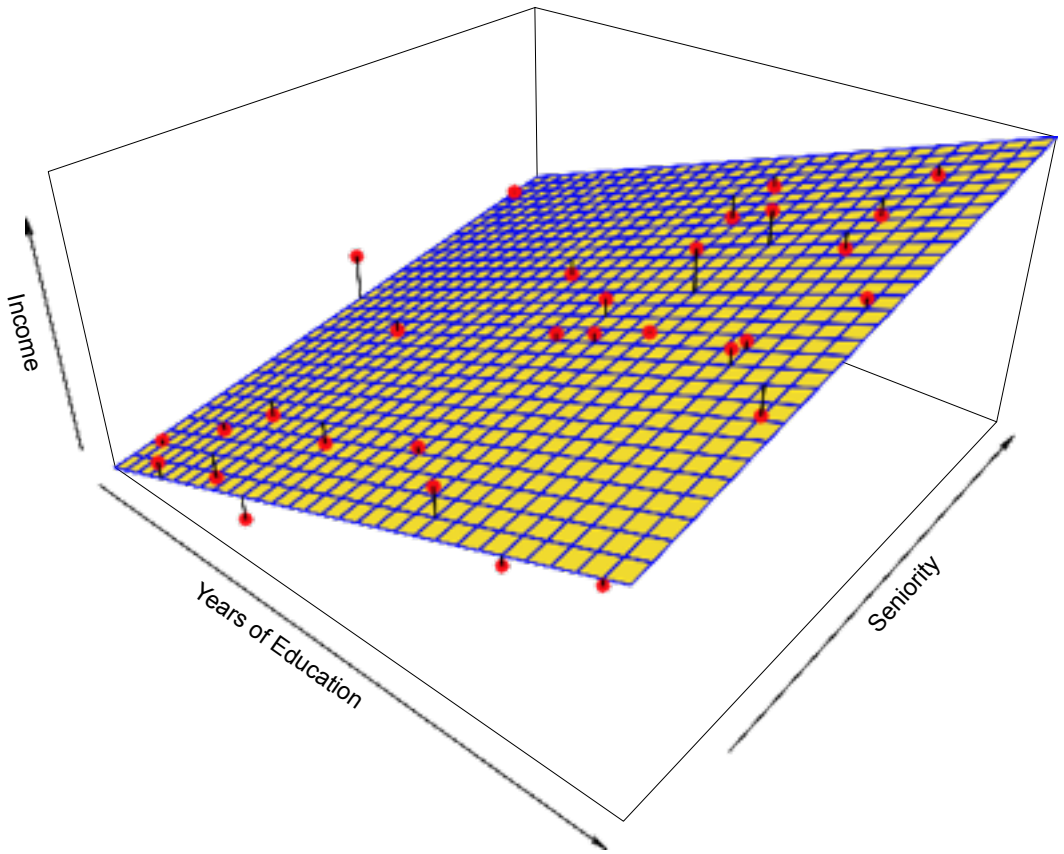




Simulated example. Red points are simulated values for income from the model

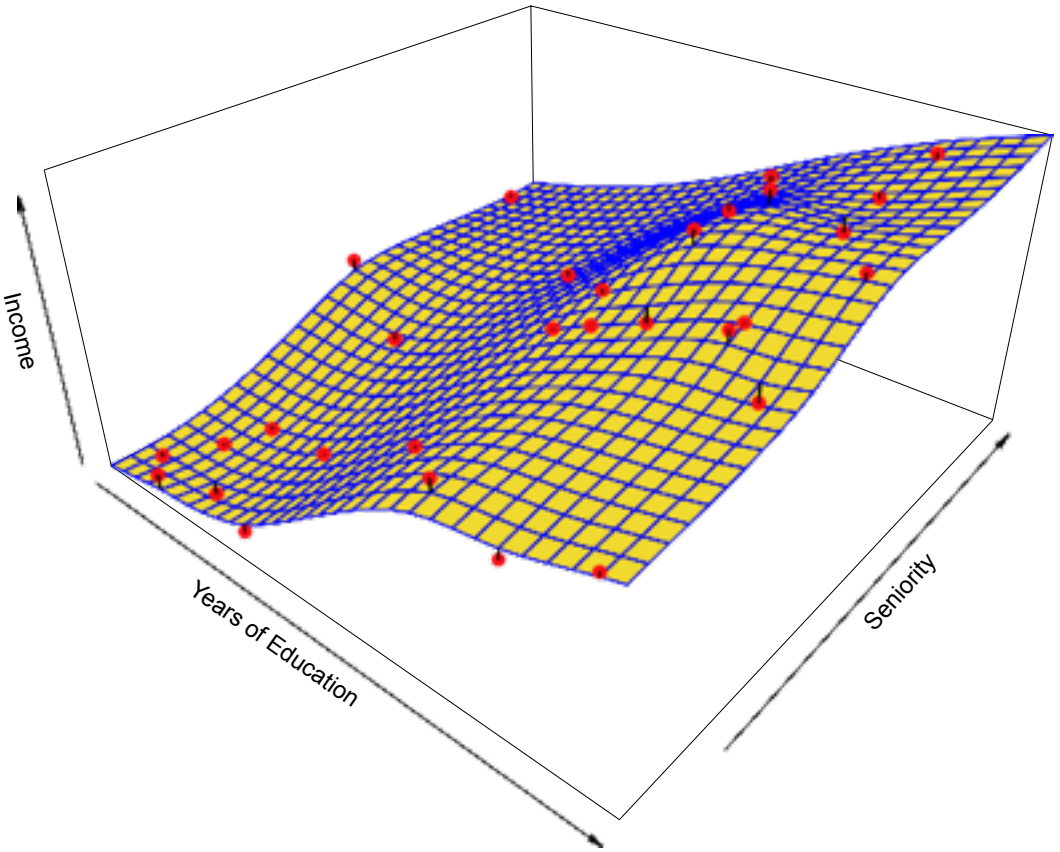
$$\text{income} = f(\text{education}, \text{seniority}) + \varepsilon$$

f is the blue surface.

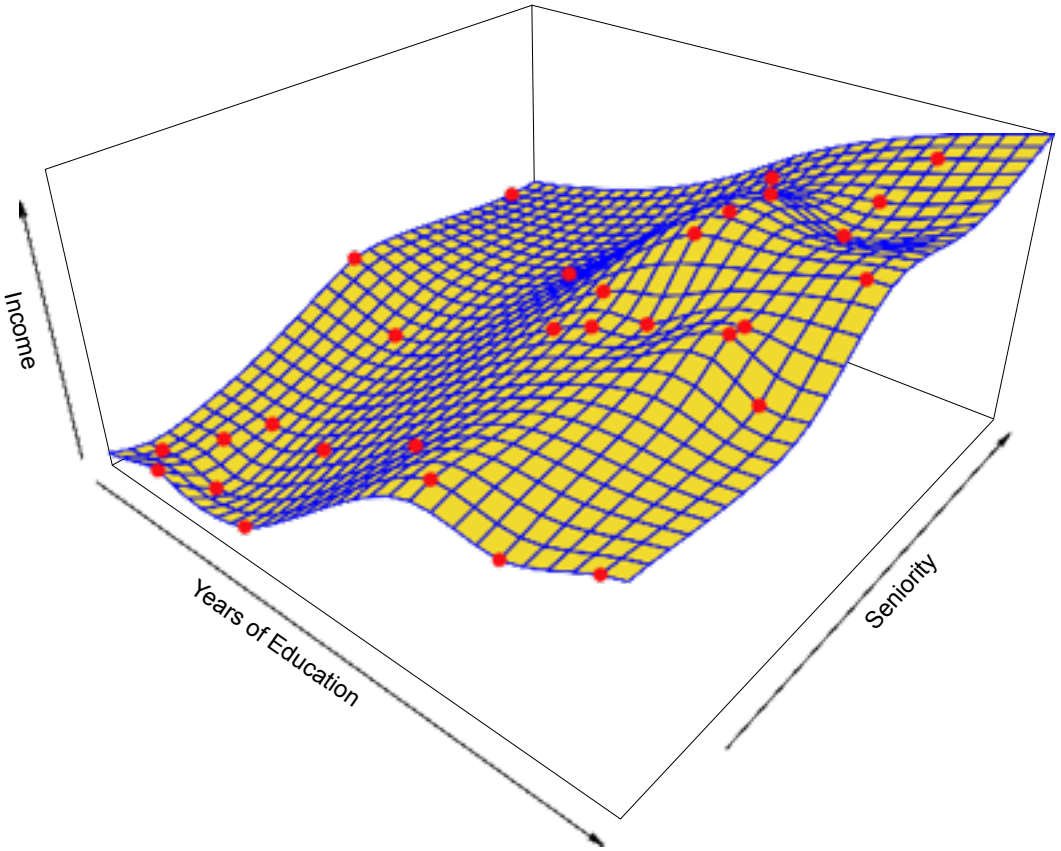


Linear regression model fit to the simulated data.

$\hat{f}_L(\text{education}, \text{seniority}) = \hat{\beta}_0 + \hat{\beta}_1 \times \text{education} + \hat{\beta}_2 \times \text{seniority}$



More flexible regression model $\hat{f}_S$(education, seniority) fit to the simulated data. Here we use a technique called a *thin-plate spline* to fit a flexible surface. We control the roughness of the fit (chapter 7).

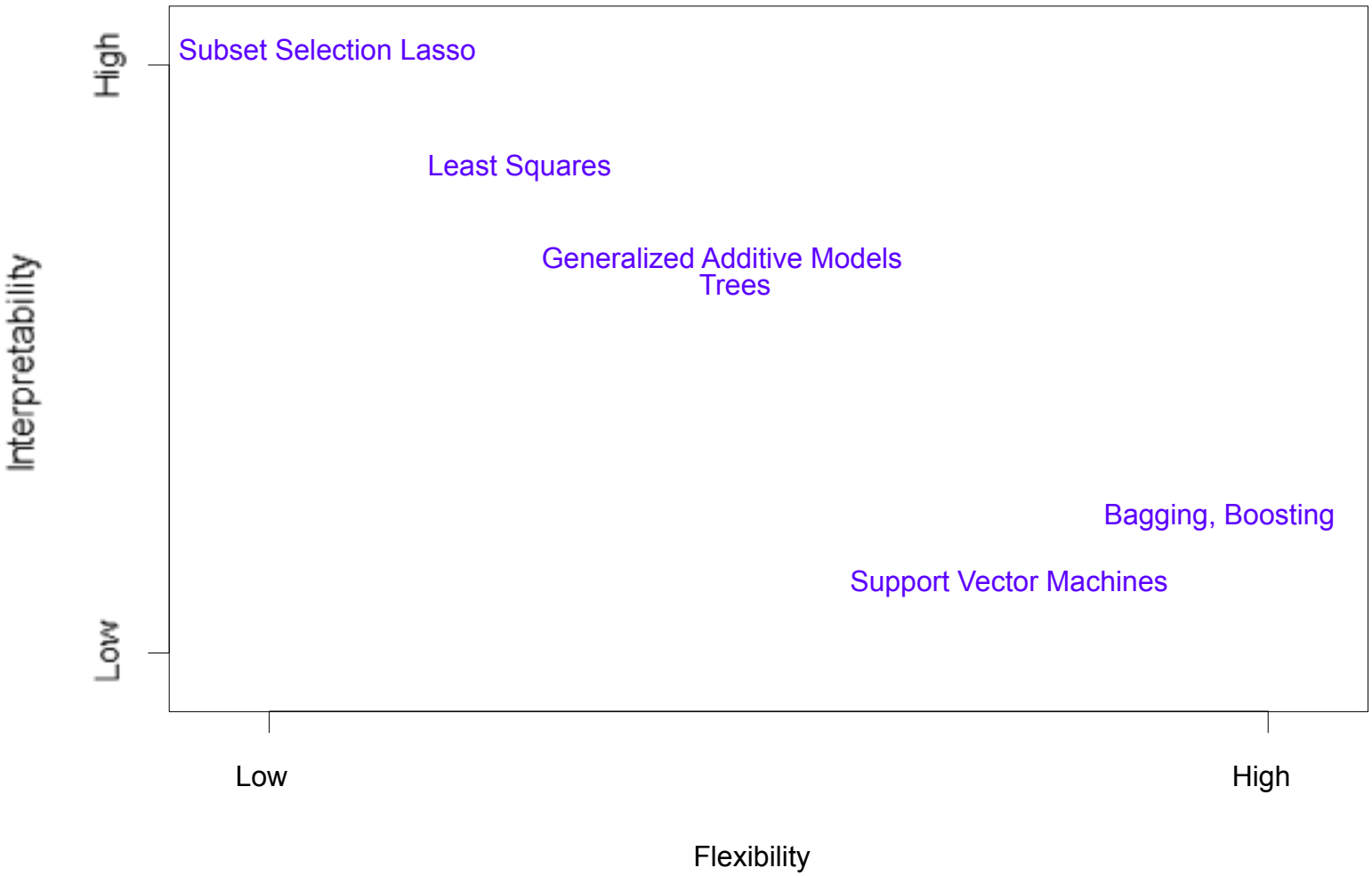


Even more flexible spline regression model

$\hat{f}$ s (education, seniority) fit to the simulated data. Here the fitted model makes no errors on the training data! Also known as *overfitting*.

Some trade-offs

- Prediction accuracy versus interpretability.
  —Linear models are easy to interpret; thin-plate splines are not.
- Good fit versus over-fit or under-fit.
  —How do we know when the fit is just right?
- Parsimony versus black-box.
  —We often prefer a simpler model involving fewer variables over a black-box predictor involving them all.


Subset Selection Lasso
Least Squares
Generalized Additive Models
Trees
Bagging, Boosting
Support Vector Machines
High
Low
Interpretability
Low
High
Flexibility

Assessing Model Accuracy

Suppose we fit a model $\hat{f}(x)$ to some training data $\text{Tr} = \{x_i, y_i\}_1^N$, and we wish to see how well it performs.

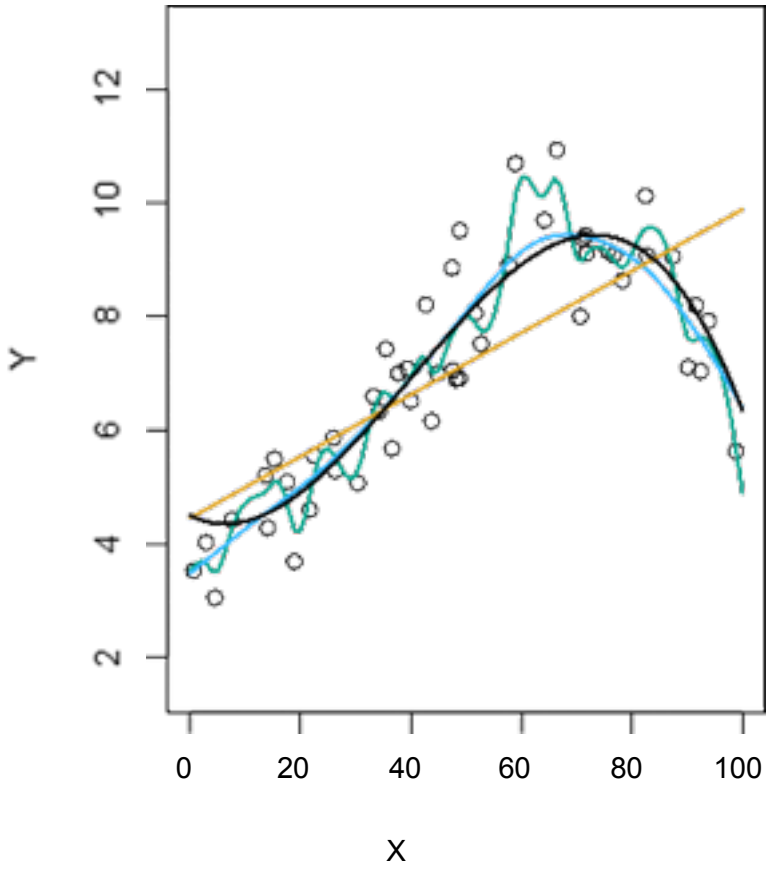
- We could compute the average squared prediction error over Tr:

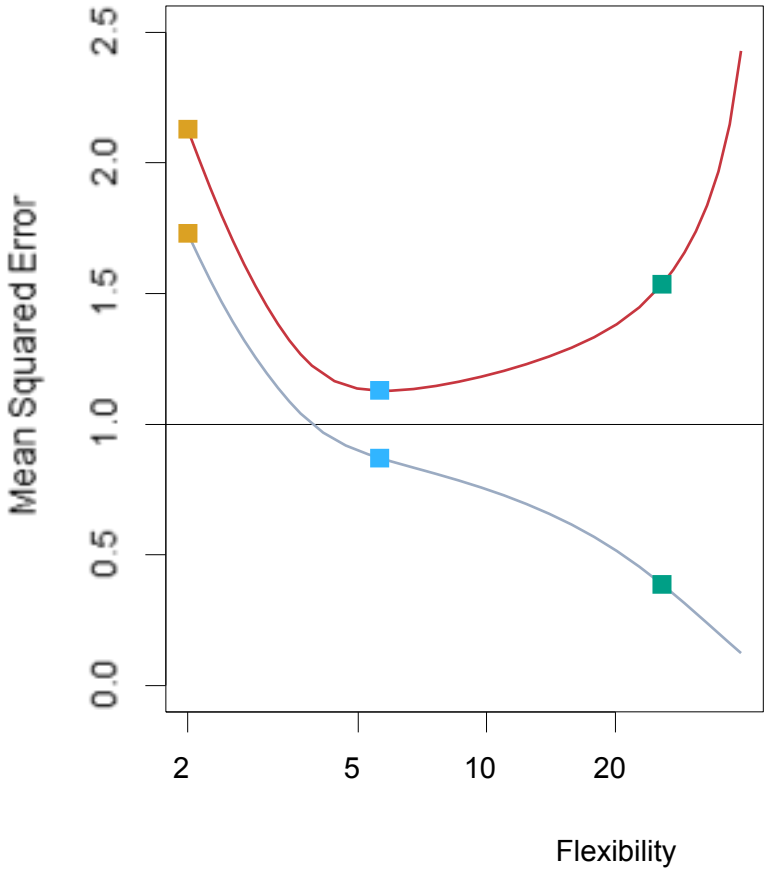
$$\text{MSE}_{\text{Tr}} = \text{Ave}_{i \in \text{Tr}}[y_i - \hat{f}(x_i)]^2$$

This may be biased toward more overfit models.

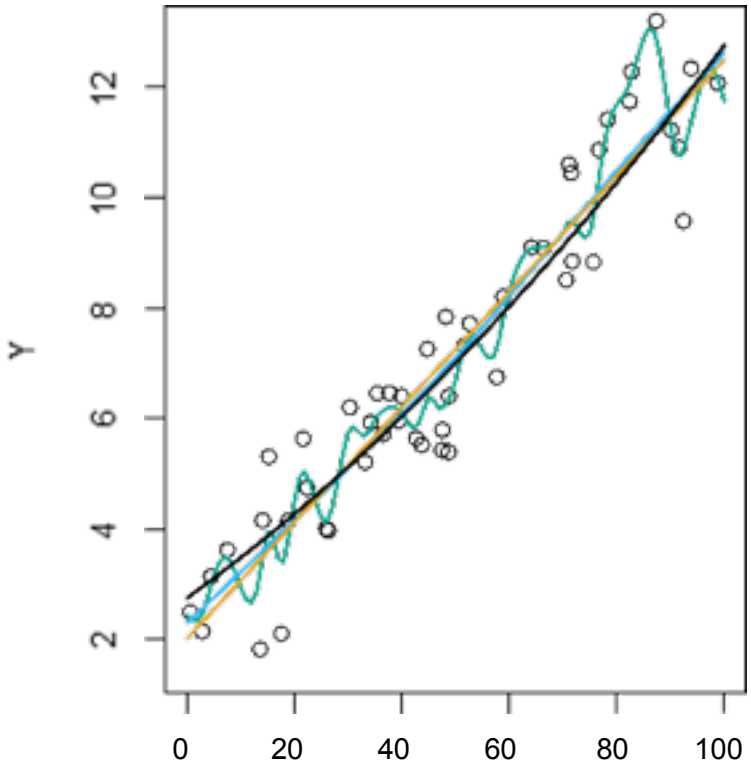
- Instead we should, if possible, compute it using fresh *test* data $\text{Te} = \{x_i, y_i\}_1^M$:

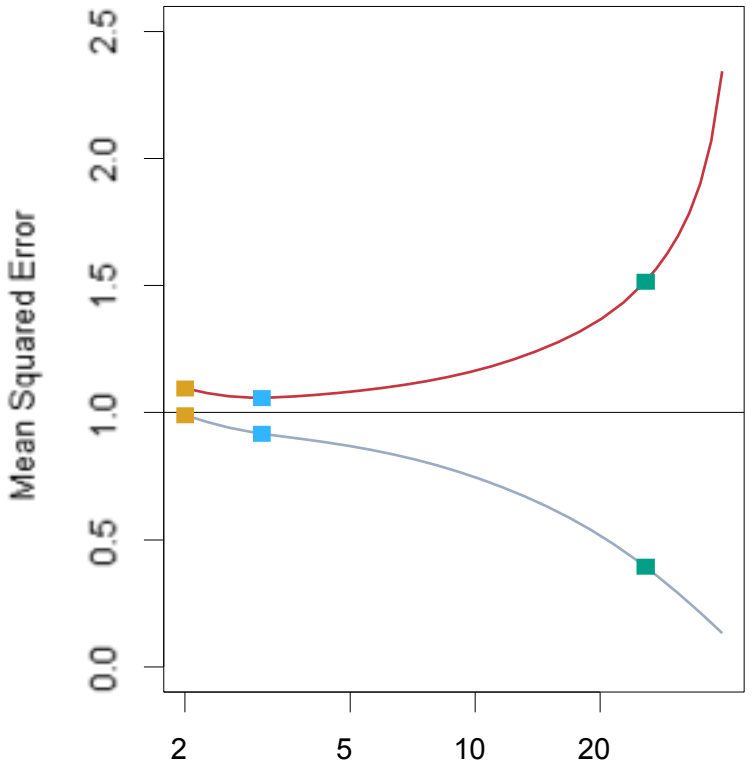
$$\text{MSE}_{\text{Te}} = \text{Ave}_{i \in \text{Te}}[y_i - \hat{f}(x_i)]^2$$



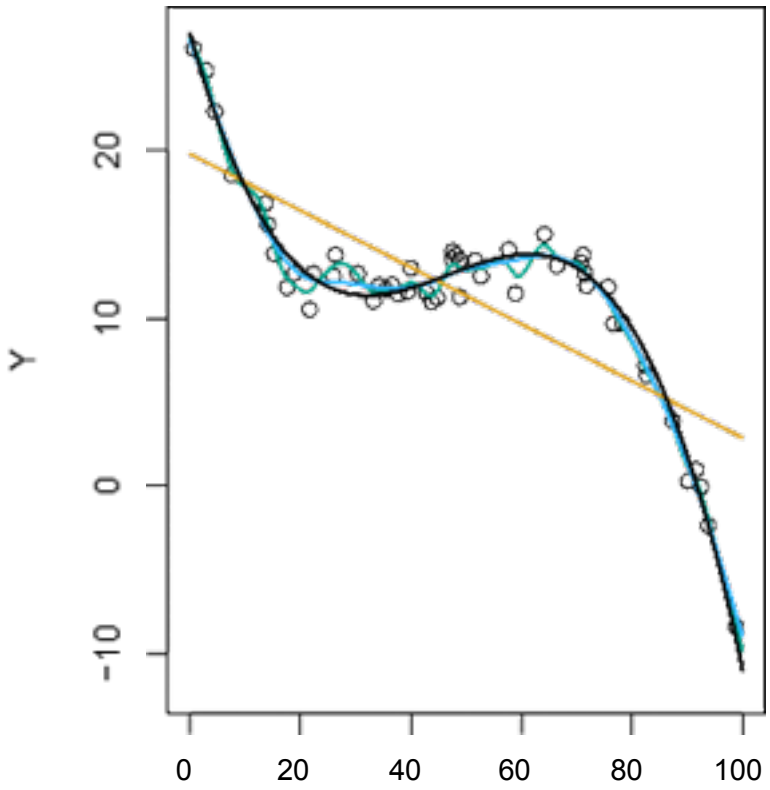


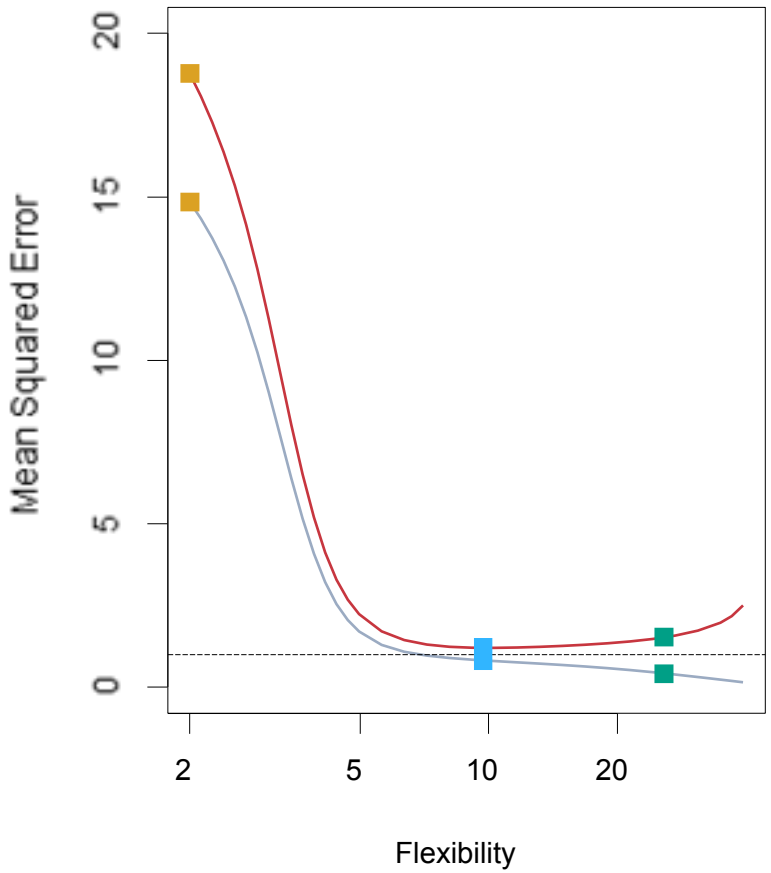
Black curve is truth. Red curve on right is MSE_{Te}, grey curve is MSE_{Tr}. Orange, blue and green curves/squares correspond to fits of different flexibility.





Here the truth is smoother, so the smoother fit and linear model do really well.





Here the truth is wiggly and the noise is low, so the more flexible fits do the best.

Bias-Variance Trade-off

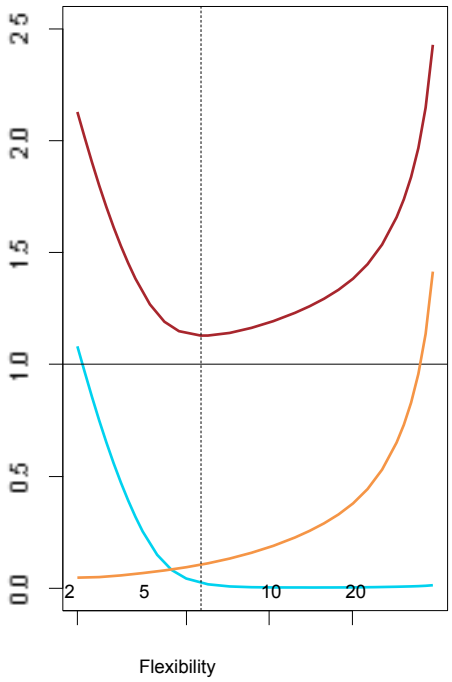
- Suppose we have fit a model $\hat{f}(x)$ to some training data Tr, and let (x_0, y_0) be a test observation drawn from the population. If the true model is $Y = f(X) + \varepsilon$ (with $f(x) = E(Y \mid X = x)$), then

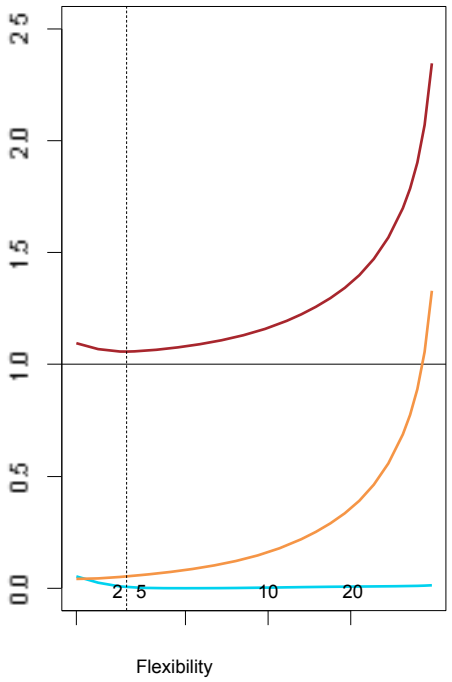
- $E\,(y_0 - \hat{f}(x_0))^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + \mathrm{Var}(\varepsilon)$.

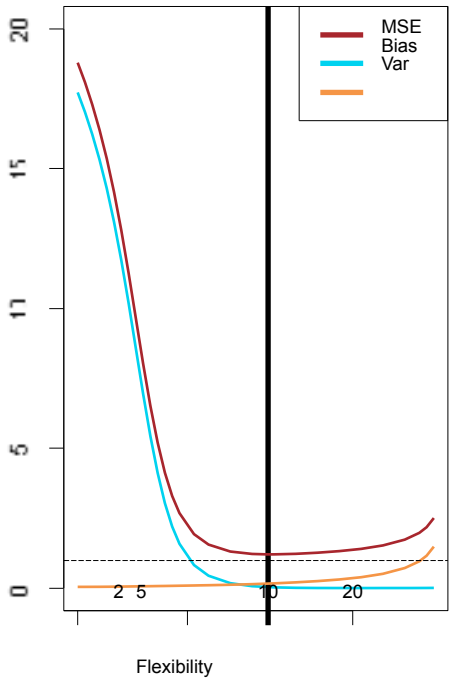
- The expectation averages over the variability of y_0 as well as the variability in Tr. Note that $\mathrm{Bias}(\hat{f}(x_0))] = E[\hat{f}(x_0)] - f(x_0)$.

- Typically as the *flexibility* of $\hat{f}$ increases, its variance increases, and its bias decreases. So choosing the flexibility based on average test error amounts to a *bias-variance trade-off*.

Bias-variance trade-off for the three examples



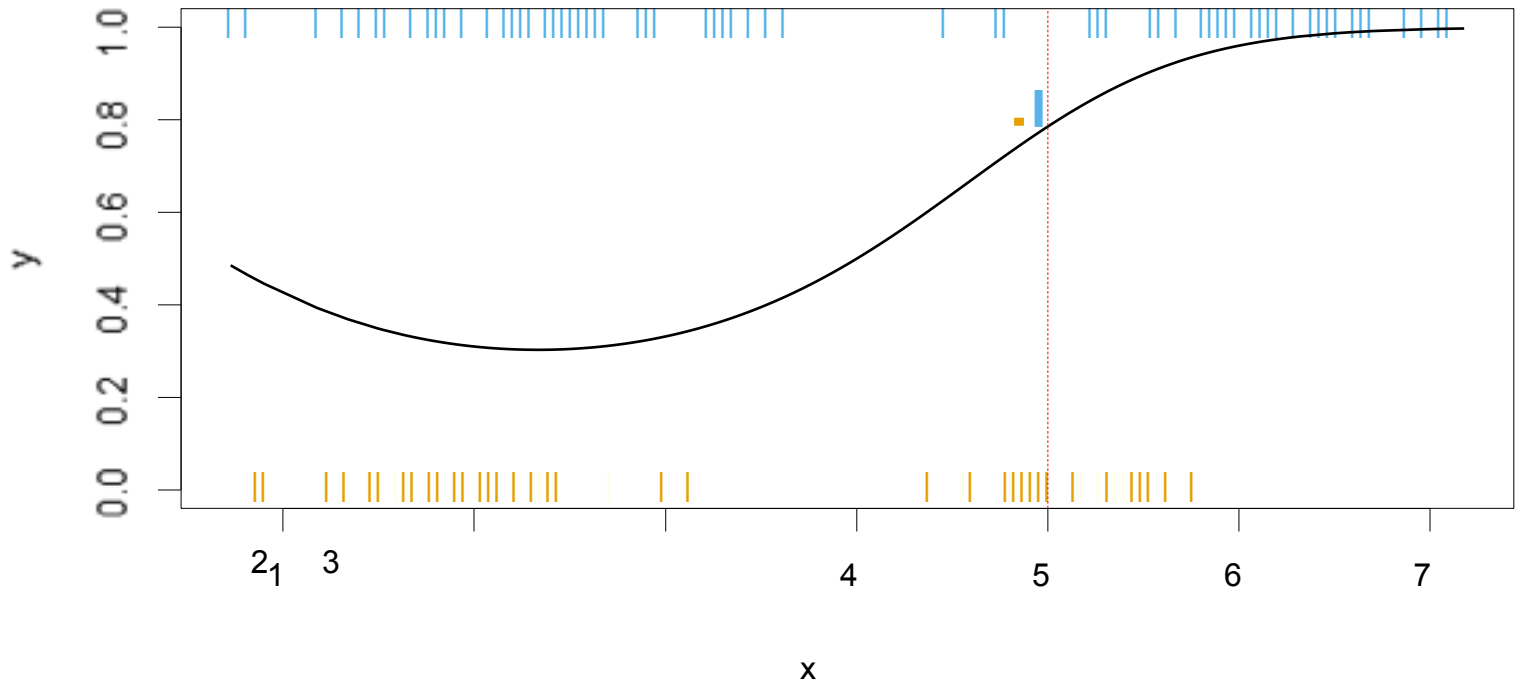




Classification Problems

Here the response variable Y is *qualitative* — e.g. email is one of C = (spam, ham) (ham=good email), digit class is one of $C = \{0, 1, \ldots, 9\}$. Our goals are to:

- Build a classifier $C(X)$ that assigns a class label from C to a future unlabeled observation X.
- Assess the uncertainty in each classification
- Understand the roles of the different predictors among $X = (X_1, X_2, \ldots, X_p)$.

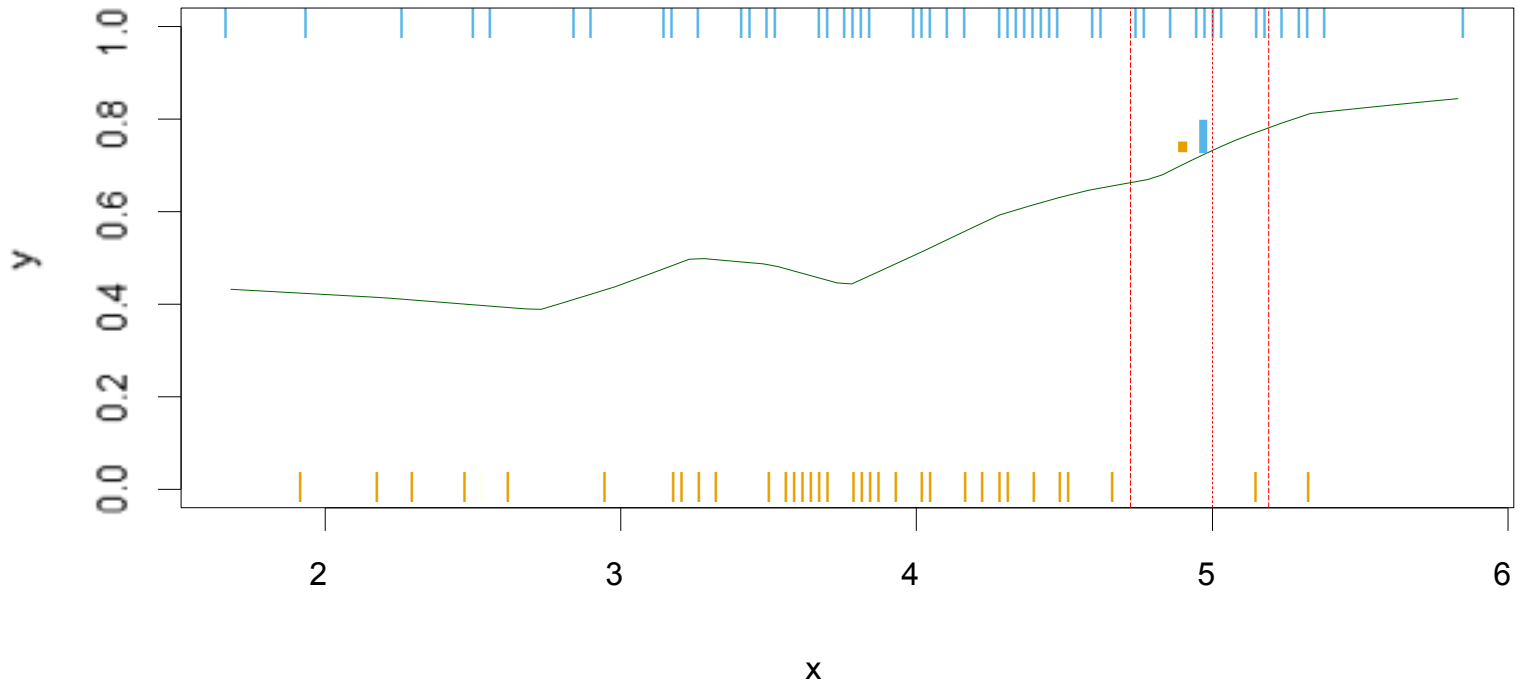


Is there an ideal $C(X)$? Suppose the K elements in C are numbered 1, 2, . . . , K. Let

$$p_k(x) = \Pr(Y = k | X = x), \quad k = 1, 2, \ldots, K.$$

These are the *conditional class probabilities* at x; e.g. see little barplot at $x = 5$. Then the *Bayes optimal* classifier at x is

$$C(x) = j \text{ if } p_j(x) = \max\{p_1(x), p_2(x), \ldots, p_K(x)\}$$



Nearest-neighbor averaging can be used as before.
Also breaks down as dimension grows. However, the impact on $\hat{C}(x)$ is less than on $\hat{p}_k(x)$, $k = 1, \ldots, K$.

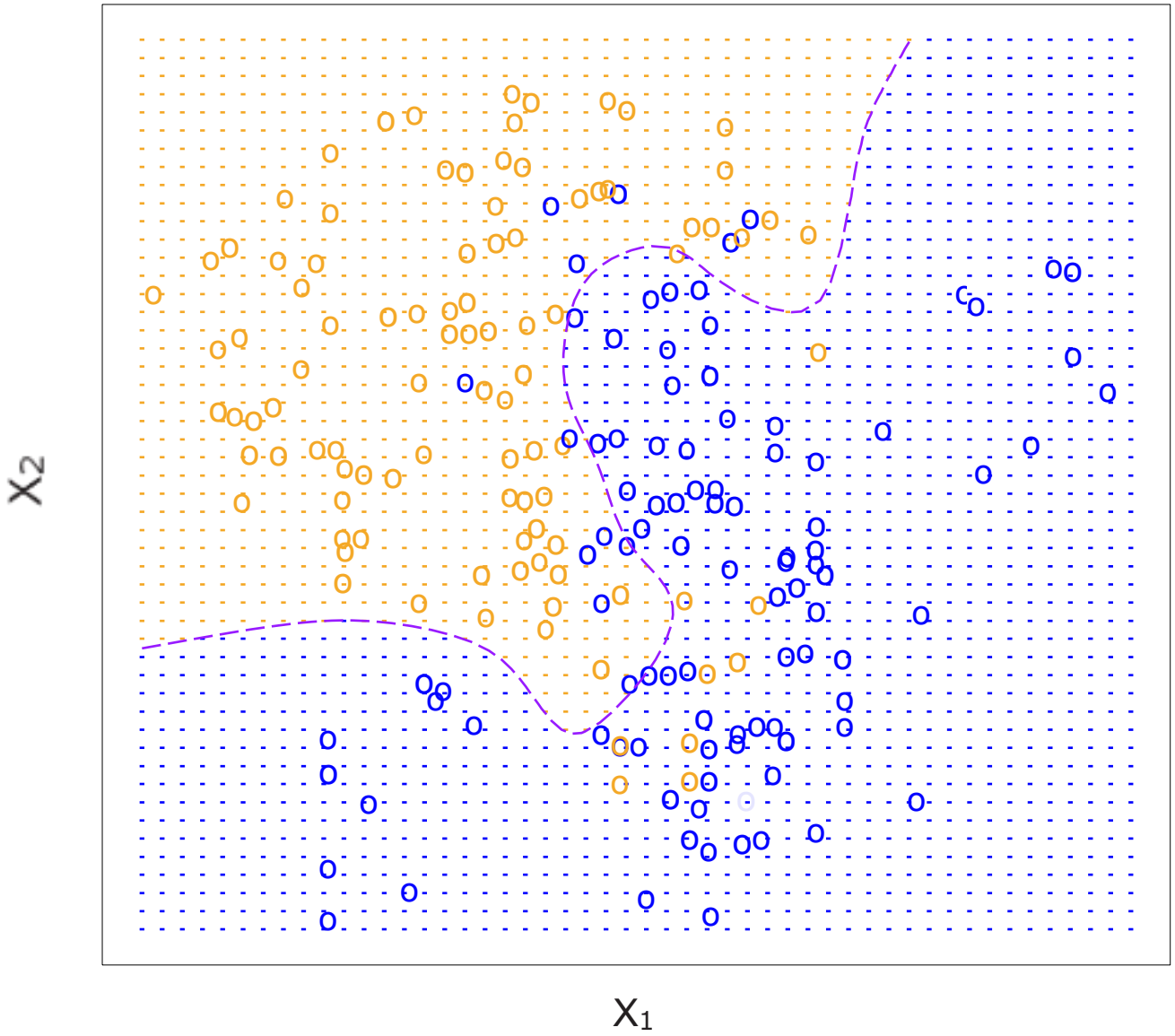
Classification: some details

- Typically we measure the performance of $\hat{C}(x)$ using the misclassification error rate:

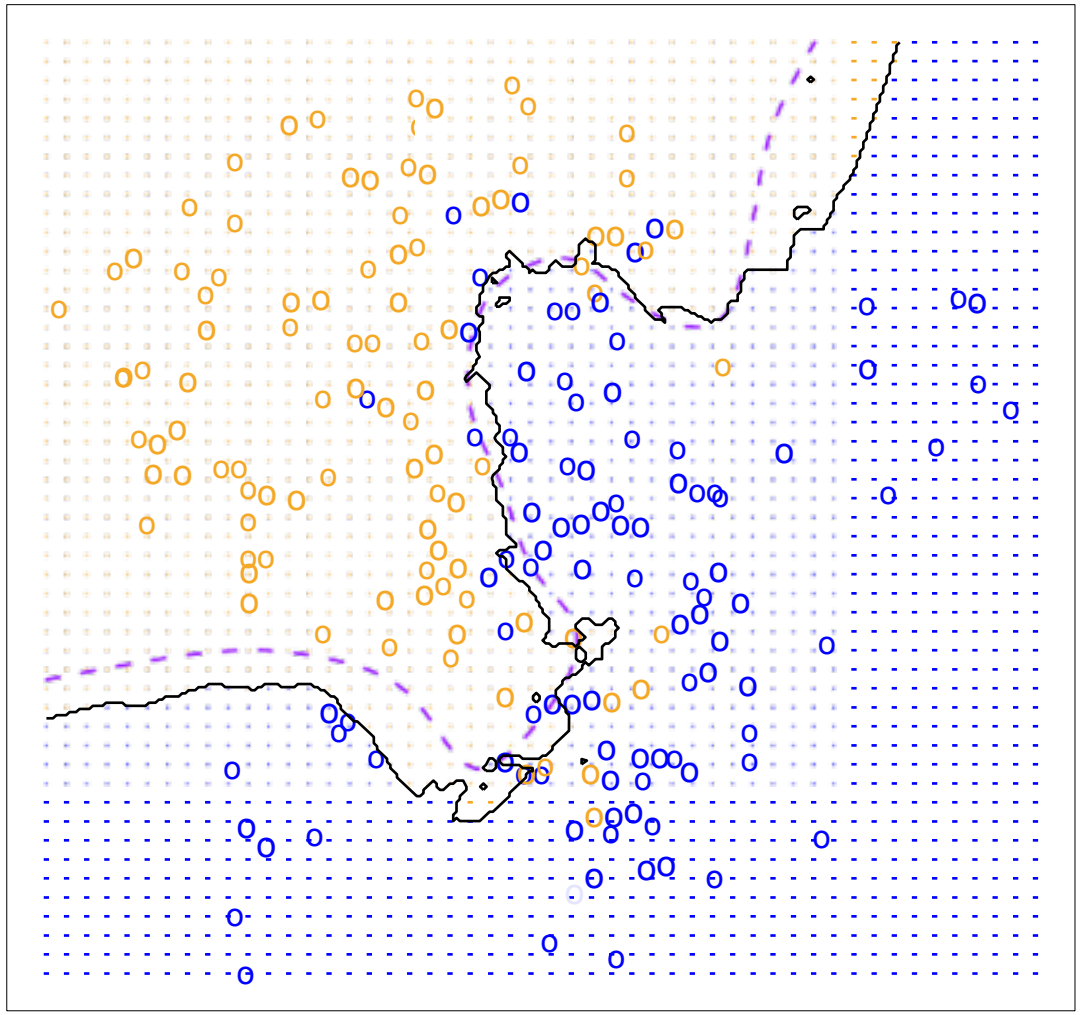
$$\text{Err}_{\text{Te}} = \text{Ave}_{i \in \text{Te}} \; I[y_i \; != \hat{C}(x_i)]$$

- The Bayes classifier (using the true $p_k(x)$) has smallest error (in the population).
- Support-vector machines build structured models for $C(x)$.
- We will also build structured models for representing the $p_k(x)$. e.g. Logistic regression, generalized additive models.

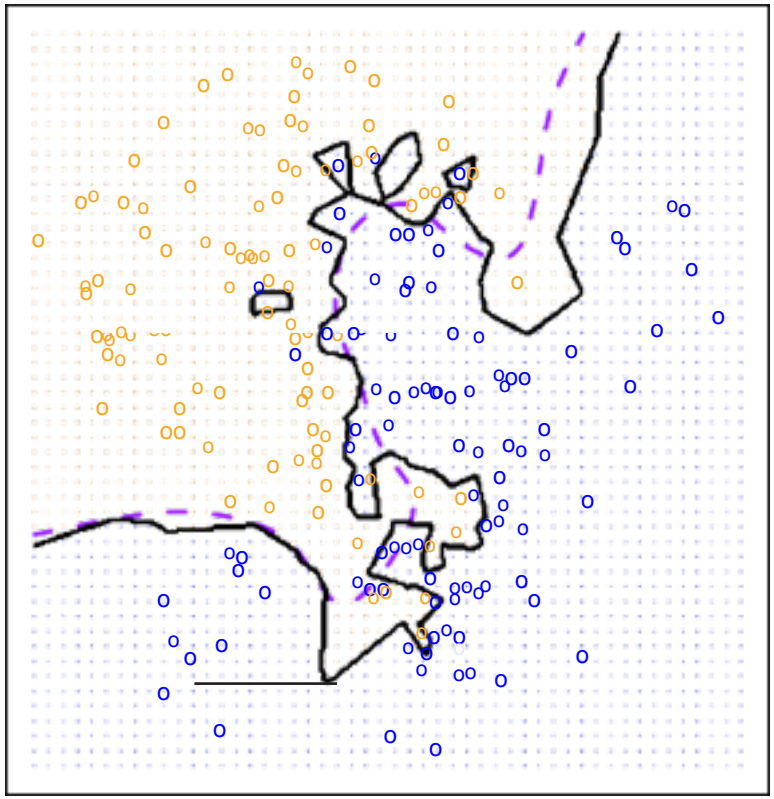
Example: K-nearest neighbors in two dimensions



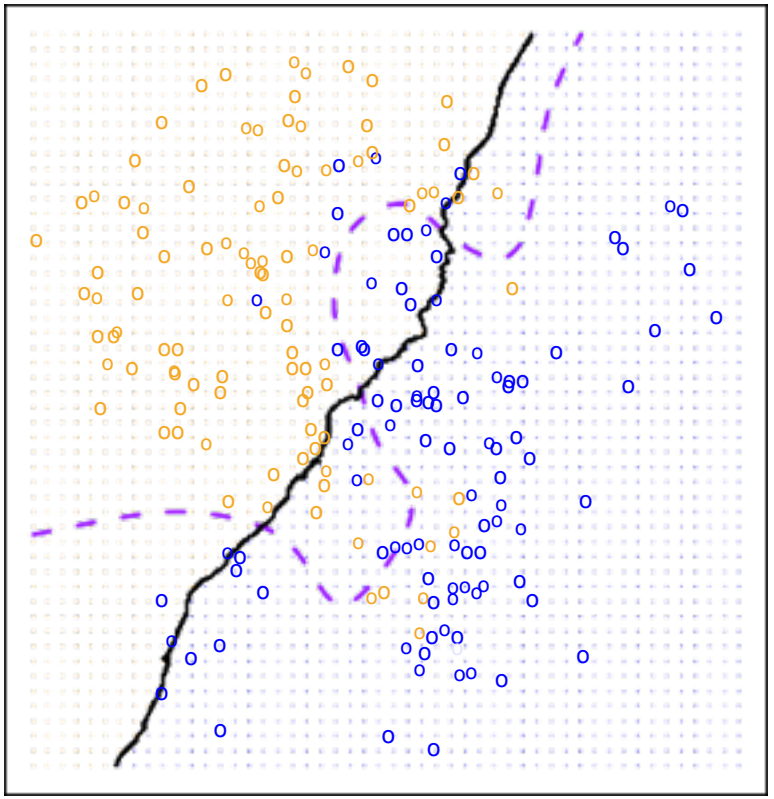
KNN: K=10

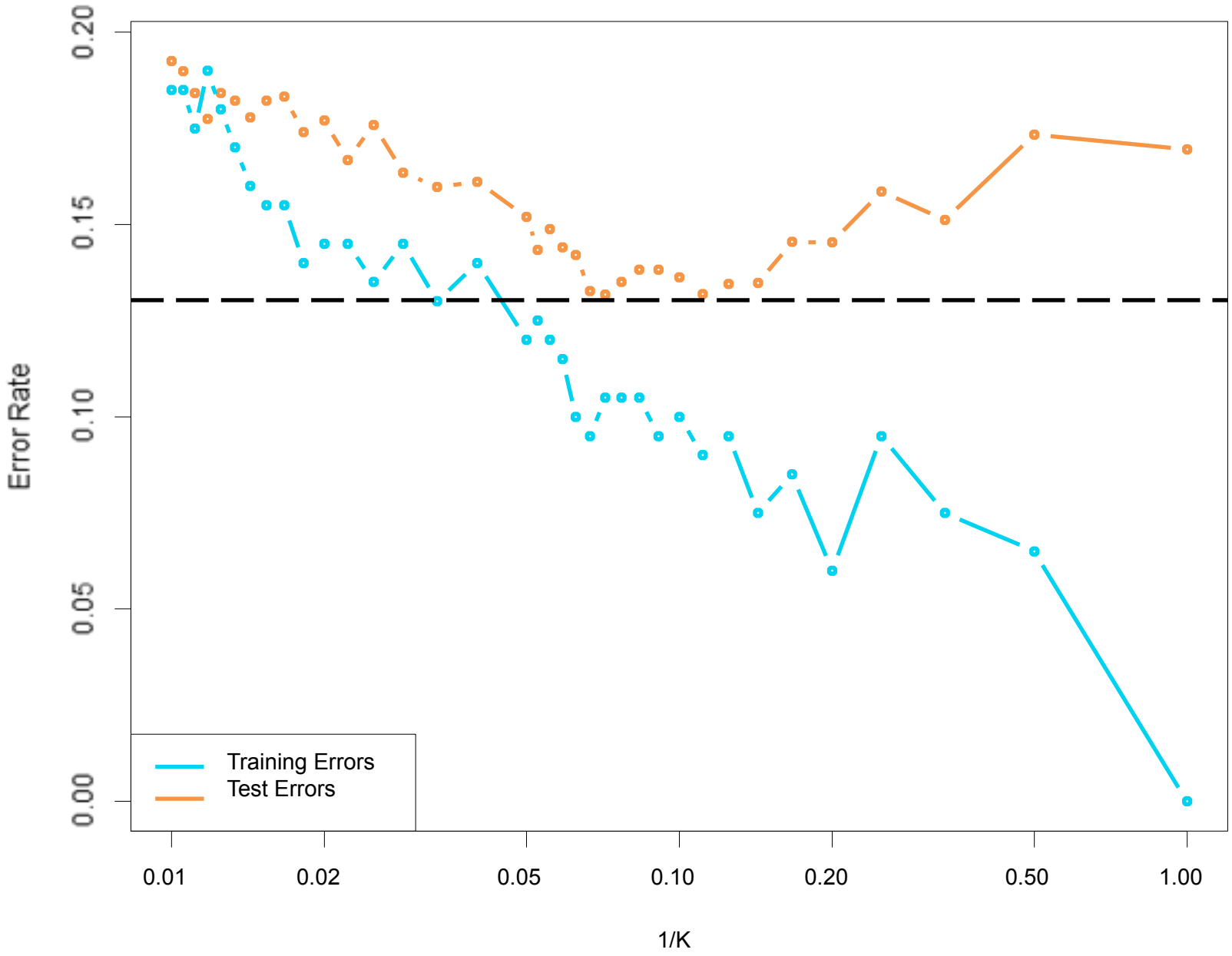


KNN: K=1



KNN: K=100




Error Rate
0.00
0.05
0.10
0.15
0.20
0.01
0.02
0.05
0.10
0.20
0.50
1.00
1/K
Training Errors
Test Errors