Day 1: Introduction to the data science approach

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Day 1 Outline

- Data Science
  - Supervised Learning
  - Unsupervised Learning
- Course outline and logistics
- Machine Learning

Data Science

Data Scientist:

The Sexiest Job of the 21st Century

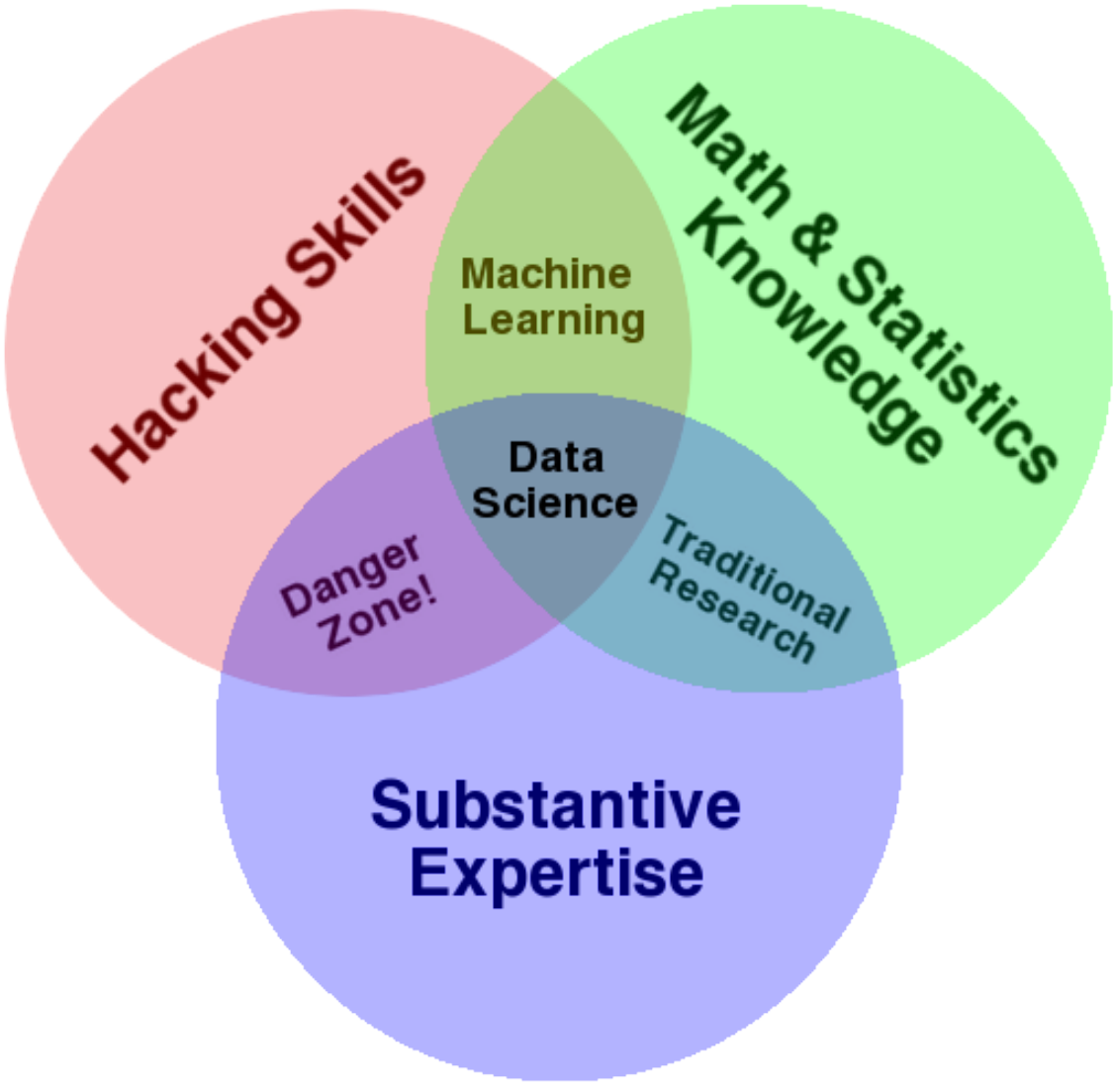
Meet the people who can coax treasure out of messy, unstructured data.

by Thomas H. Davenport and D.J. Patil

W

"I keep saying the sexy job in the next ten years will be statisticians. People think I'm joking, but who would've guessed that computer engineers would've been the sexy job of the 1990s?" Hal Varian (Chief Economist at Google, 2009).

What is data science?



Data Science Problems

- Predict an election outcome
- Identify the risk factors for various diseases (e.g. cancer).
- Predict whether someone will have a heart attack on the basis of demographic, diet and clinical measurements
- Identify the numbers in a handwritten post code
- Use mobile phone activity for disaster management during floods
- Identifying risk characters for Airbnb transactions
- Predict fares at Uber
- Asking Siri to make you a cup of coffee

Two main approaches to learning

- Supervised Learning
- Unsupervised Learning

The Supervised Learning Problem

Starting point:

- 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.

Philosophy

- It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
- One has to understand the simpler methods first, in order to grasp the more sophisticated ones.
- It is important to accurately assess the performance of a method, to know how well or how badly it is working (simpler methods often perform as well as fancier ones!).
- This is an exciting research area, having important applications in science, industry and policy.
- Machine learning is a fundamental ingredient in the training of a modern data scientist.

Unsupervised Learning

- No outcome variable, just a set of predictors (features) measured on a set of samples.
- Objective is more fuzzy – find groups of samples that behave similarly, find features that behave similarly, find linear combinations of features with the most variation.
- Difficult to know how well you are doing.
- Different from supervised learning, but can be useful as a pre-processing step for supervised learning.

Kaggle Competitions

- Higgs Boson Machine Learning Challenge.
- National Data Science Bowl – Assessing Ocean Health.
- Heritage Health Prize Competition.
- West Nile Virus Prediction.
- Predict Closed Questions on Stack Overflow.
- Flu Forecasting competition.
- Global Energy Forecasting Competition.

Statistical Learning versus Machine Learning

- Machine learning arose as a subfield of Artificial Intelligence.
- Statistical learning arose as a subfield of Statistics.
- There is much overlap.
- Successful MSc programs in Data Science are usually run jointly by Computer Science and Statistics departments.

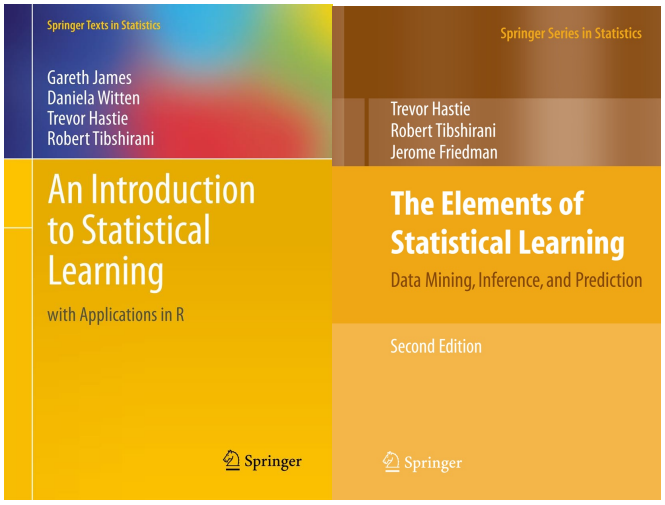
Course outline and logistics

Essential course resources

- On-line course resources

  GitHub repository `https://github.com/Classes-kbenoit/quants3`
- Using GitHub and forking the course repo
- RStudio and GitHub integration
- How to complete (and submit) assignments
  - For a brief on-line introduction to RMarkdown, which we will use for completing the exercises for the course, see `https://goo.gl/ZqOwUe`

Course Texts



- The course will cover most of the material in ISLR. Each chapter ends with an R lab, in which examples are developed. An electronic version of this book is available for free from the authors' websites.
- For statistical learning component of the course we closely follow ISLR, including figures and lecture materials, as made available by the authors.
- ESL is a more advanced treatment of similar topics, so may be useful for those who have previous data science training. Similarly, a free electronic version of the book is available from the authors' websites.

Course reading materials

- The R statistical package resources on https://cran.r-project.org/doc/manuals
- Key readings
- Additional readings – recommended if possible

Why R?

- R is the joint third (after SQL and Excel, and together with Python) top data science tool in use today according to 2015 O'Reilly Data Science Salary Survey.
- The 2016 KDnuggets survey of analytics/data science tools puts it first.
- IEEE Spectrum ranks it as the fifth most popular general programming language.
- The latest Rexer Data Miner survey shows that in the past eight years:
  - three-fold increase in respondents using R;
  - seven-fold increase in analysts/scientists using R as their primary tool.

Machine learning and this course

Machine learning

- Machine learning refers to a vast set of tools for *understanding data*.
- For a quantitative response Y and a set of predictors X:

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

- Here, f represents the *systematic* information that X provides about Y.
- Statistical learning refers to a set of approaches for estimating f.
- Most of the course we'll spend talking about different ways to estimate f and how to evaluate whether we've done a good job with it.

Where does this course fit in?

- Supervised versus unsupervised learning.
- Regression versus classification.
- No single *best* method. We'll spend a lot of time choosing the most appropriate tool for a given dataset using different measures of the quality of fit. E.g. MSE

$$MSE_{training} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

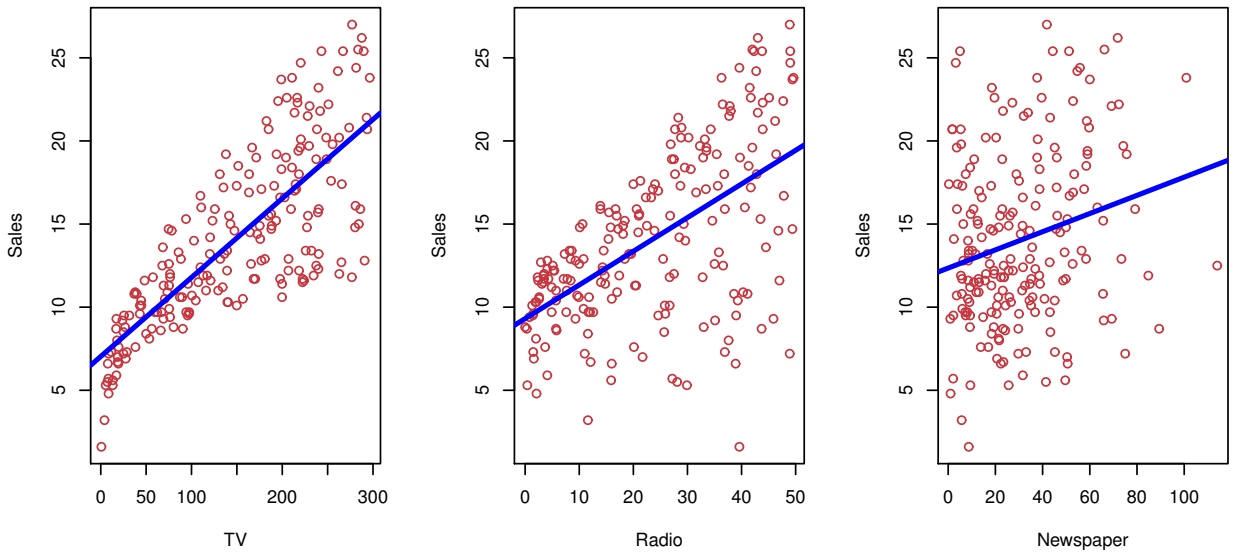
$$MSE_{test} = \mathrm{Ave}(\hat{f}(x_0) - y_0)^2$$

Why should we bother with f?

1. Prediction: $\hat{Y} = \hat{f}(X)$, where $\hat{f}$ is a *black box*.
2. Inference: How Y is changing as a function of X.

- Depending on whether the ultimate goal is prediction, inference or a mix of both, we may deploy different methods for estimating f.
- Also depending on the ultimate goal you may or may not care about evaluating the causal relationship between Y and X.

What is Machine Learning?



- Shown are `Sales` vs `TV`, `Radio` and `Newspaper`, with a blue linear-regression line fit separately to each.
- We can predict `Sales` 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

$$X = (X_1, X_2, X_3)$$

- Now we write our model as

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

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. For example, `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

$$f(4) = E(Y|X = 4)$$

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

The regression function $f(x)$

- Is also defined for vector X; e.g. $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$
- Is the ideal or optimal predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.
- $\epsilon = Y - f(x)$ 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

$$E[(Y - \hat{f}(X))^2|X = x] = \underbrace{[f(x) - \hat{f}(x)]^2}_{Reducible} + \underbrace{Var(\epsilon)}_{Irreducible}$$

How to estimate f

- Typically we have few if any data points with $X = 4$ exactly.
- So we cannot compute $E(Y|X = x)$!
- Relax the definition and let

$$\hat{f}(x) = Ave(Y|X \in N(x))$$

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.
- We will discuss smoother versions, such as kernel and spline smoothing later in the course.
- 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 $E(Y|X = x)$ by local averaging.

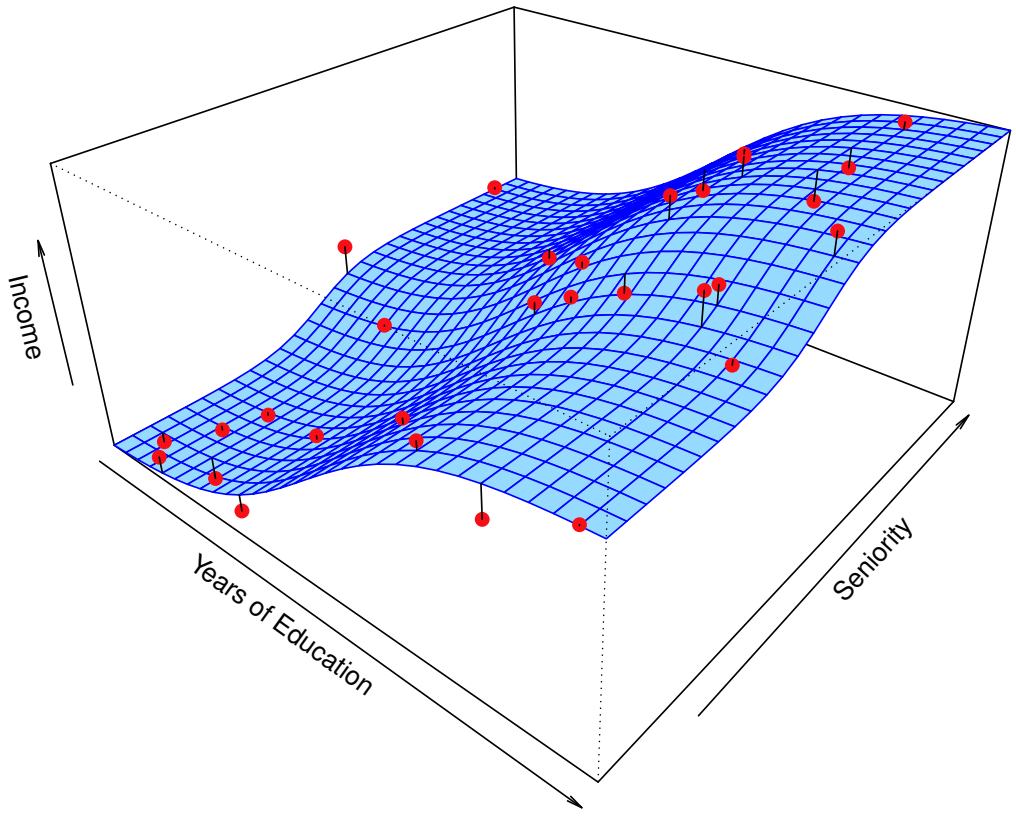
Parametric and structured models

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

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

- A linear model is specified in terms of $p + 1$ parameters $\beta_0, \beta_1, \beta_2, \ldots, \beta_p$.
- 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 $f(X)$.

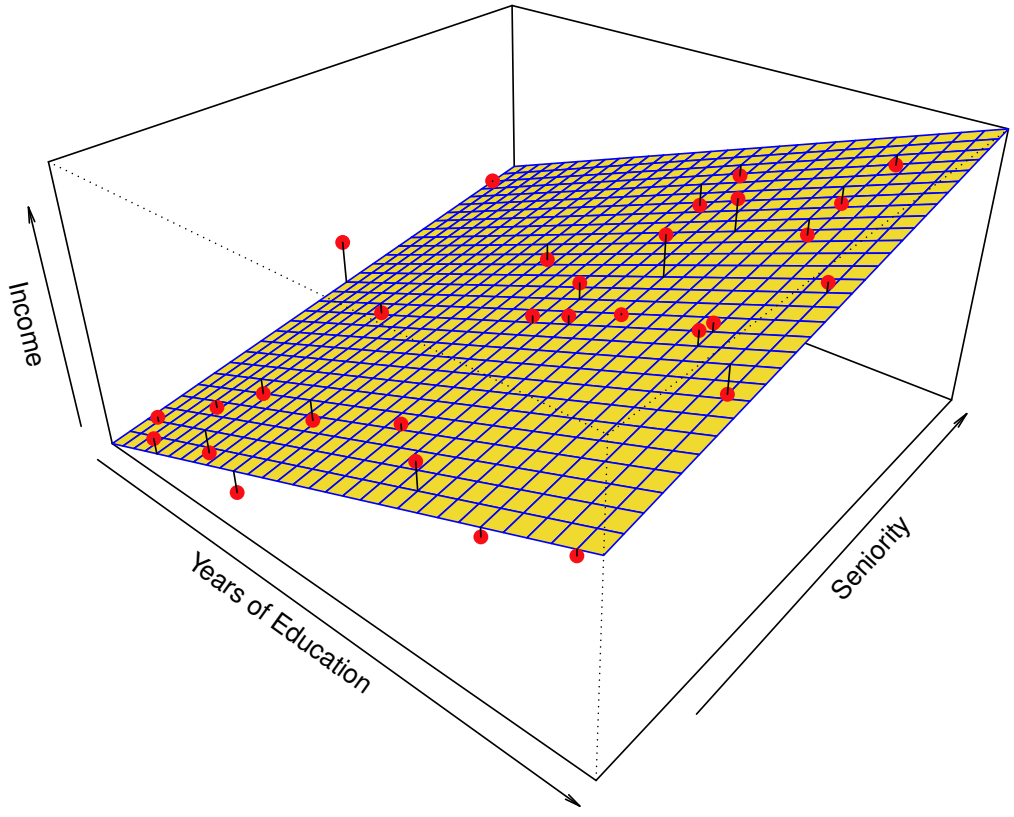
Simulated example



Red points are simulated values for `income` from the model

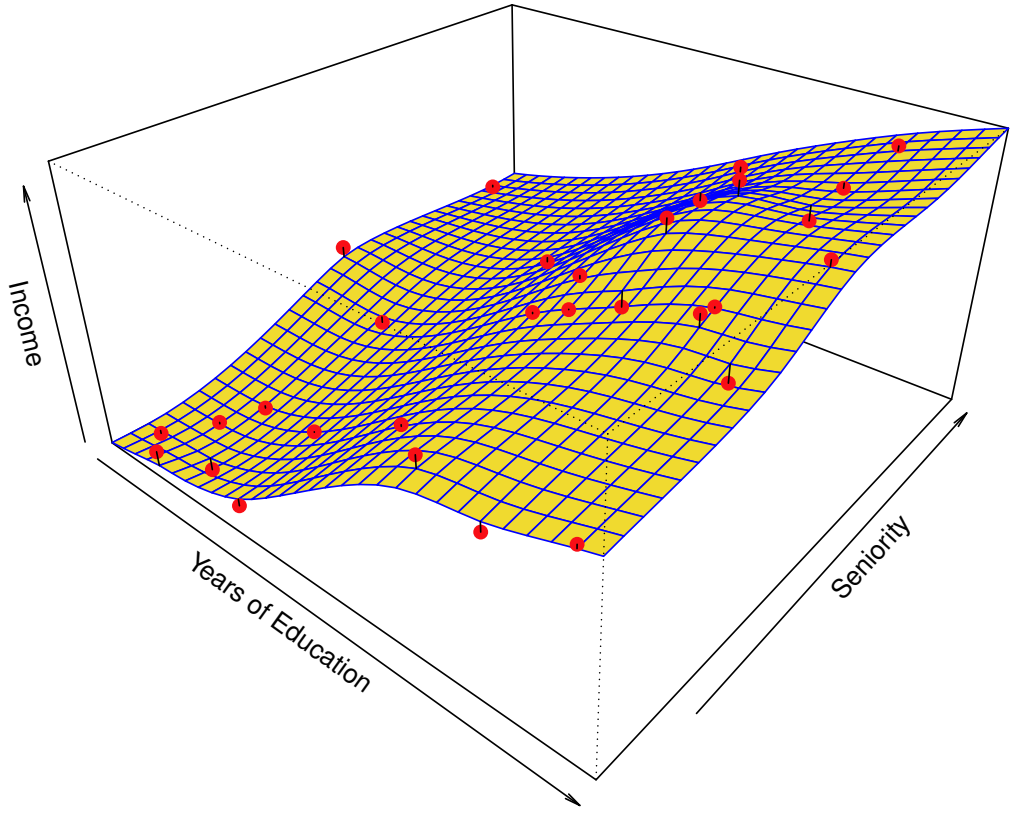
$$income = f(education, seniority) + \epsilon$$

f is the blue surface.

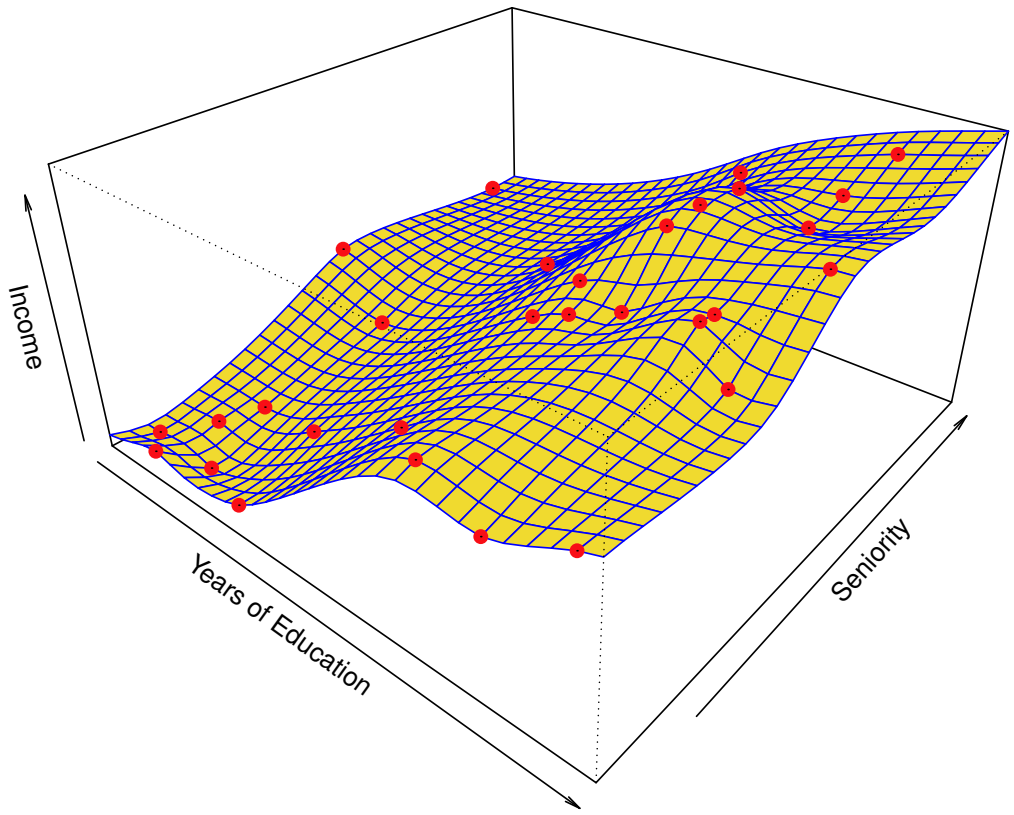


Linear regression model fit to the simulated data.

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



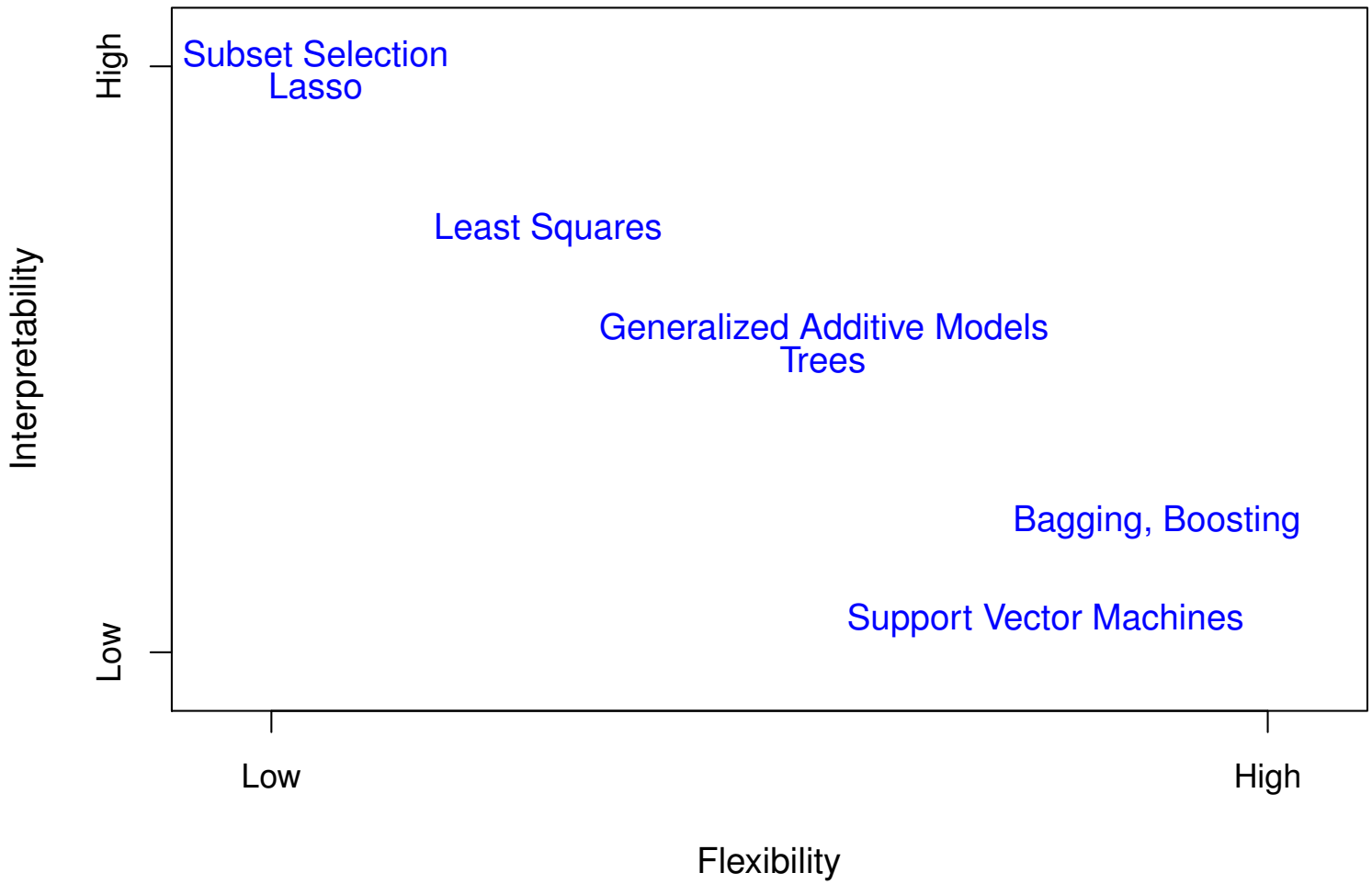
- More flexible regression model $\hat{f}_S(\mathit{education}, \mathit{seniority})$ fit to the simulated data.
- Here we use a technique called a thin-plate spline to fit a flexible surface.
- We control the roughness of the fit.



- Even more flexible spline regression model $\hat{f}_S(\mathit{education}, \mathit{seniority})$ 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

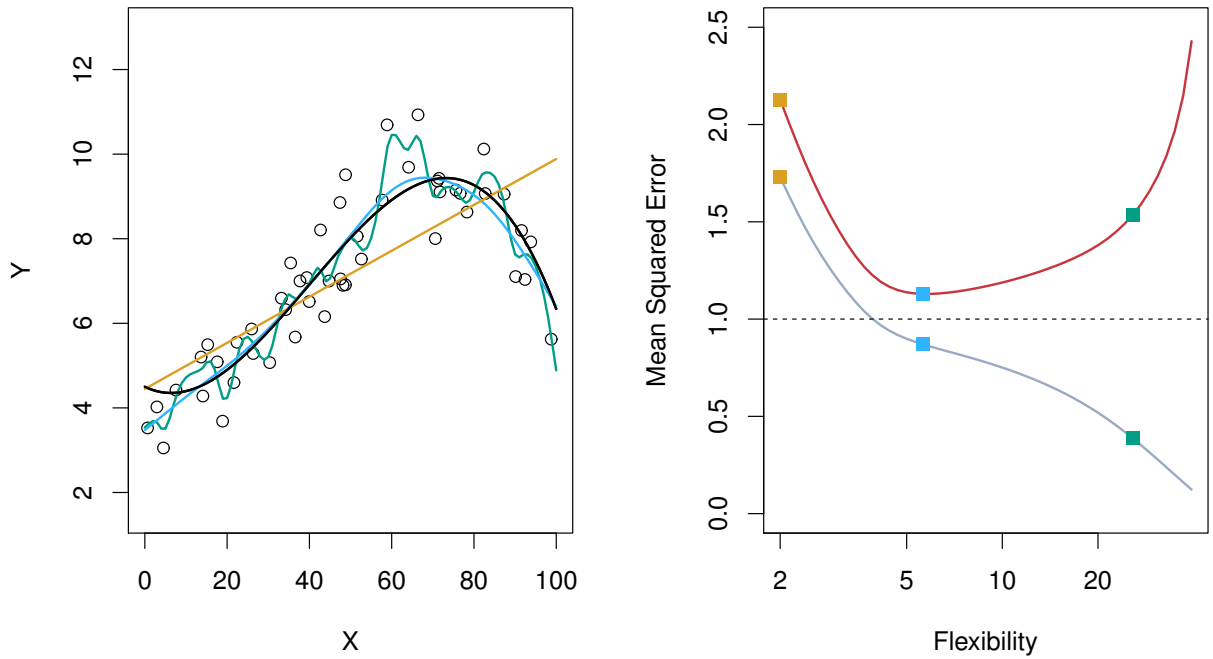
Assessing Model Accuracy

- Suppose we fit a model $\hat{f}(x)$ to some training data $Tr = \{x_i, y_i\}_1^N$, and we wish to see how well it performs.
- We could compute the average squared prediction error over Tr:

$$MSE_{Tr} = Ave_{i \in Tr}[y_i - \hat{f}(x_i)]^2$$

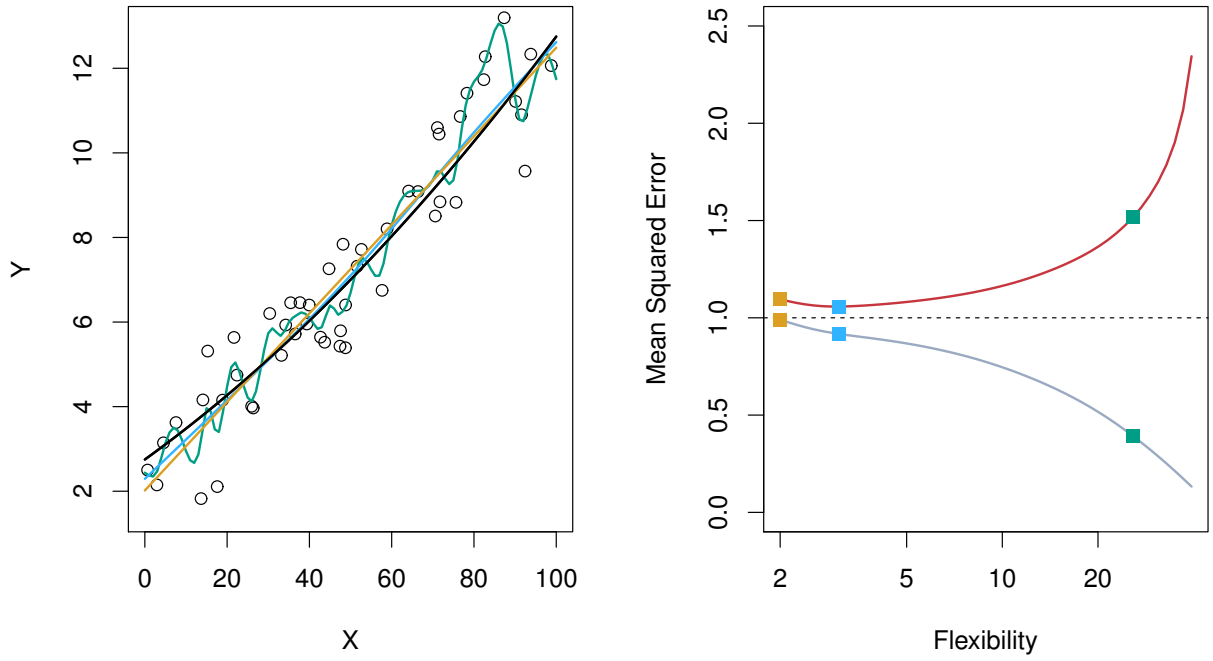
  This may be biased toward more overfit models.
- Instead we should, if possible, compute it using fresh test data $Te = \{x_i, y_i\}_1^M$:

$$MSE_{Te} = Ave_{i \in Te}[y_i - \hat{f}(x_i)]^2$$

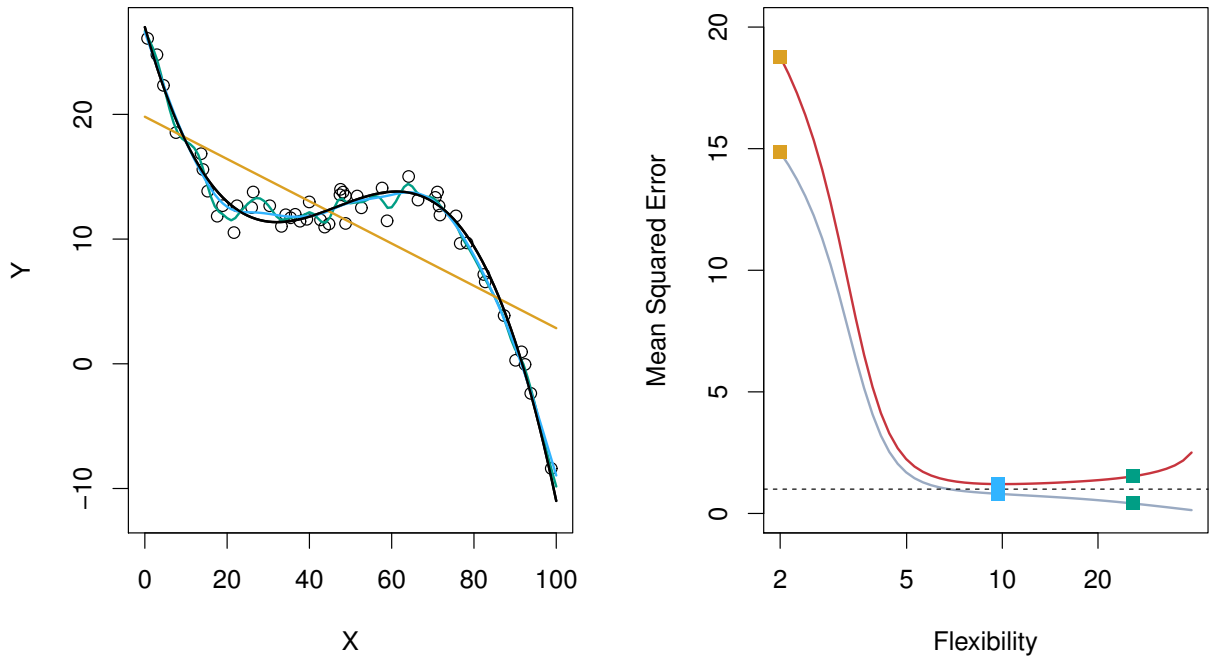


Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two smoothing splines.

- 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.



- The setup as before, using a different true f that is much closer to linear. In this setting, linear regression provides a very good fit to the data.
- Here the truth is smoother, so the smoother fit and linear model do really well.



- Setup as above, using a different f that is far from linear.
- In this setting, linear regression provides a very poor fit to the data.
- Here the truth is wiggly and the noise is low, so the more flexible fits do the best.

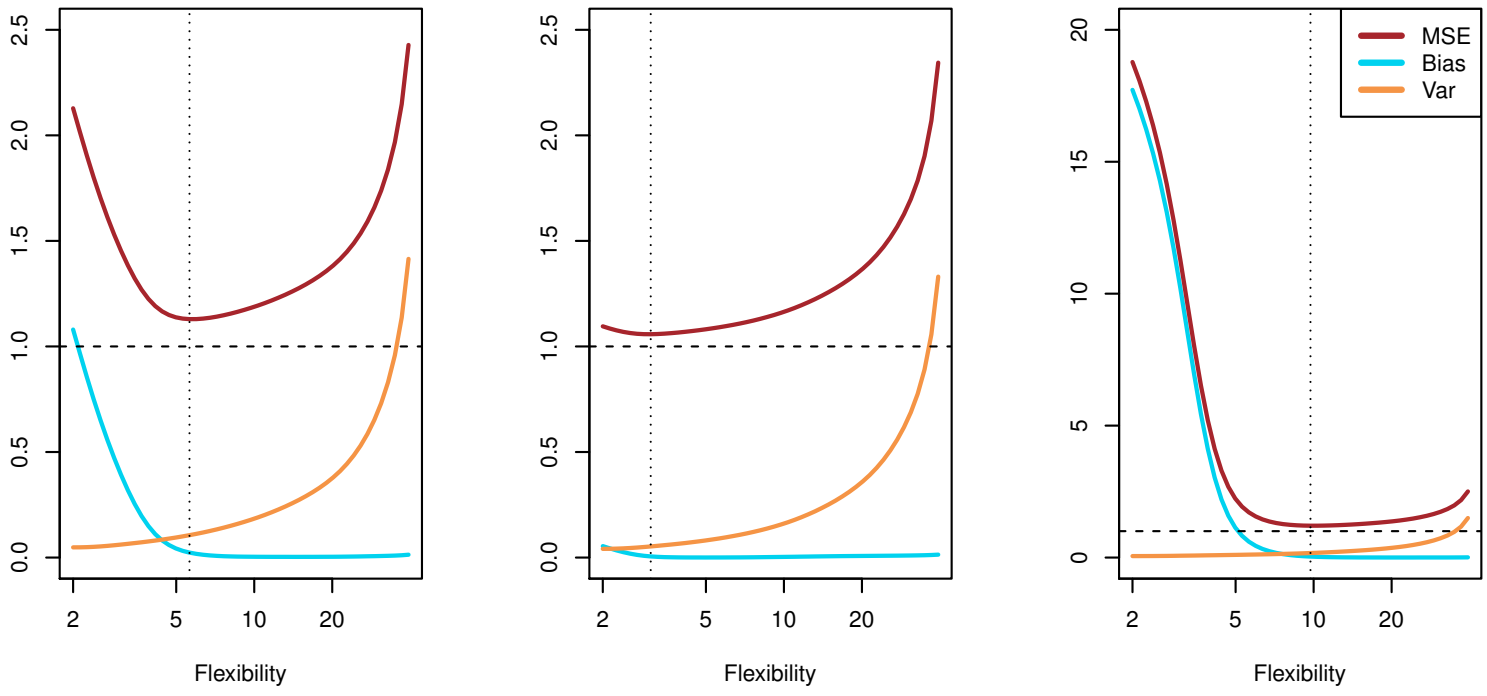
Bias-Variance Trade-off

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

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

- The expectation averages over the variability of y_0 as well as the variability in Tr. Note that $\text{Bias}(\hat{f}(x_0)) = E[\hat{f}(x_0)] - f(x_0)$.
- 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 $\mathcal{C} = (spam, ham)$ ($ham = godemail$), digitclass is one of $\mathcal{C} = \{0, 1, \ldots, 9\}$. Our goals are to:

- Build a classifier $\mathcal{C}(X)$ that assigns a class label from $\mathcal{C}$ 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 $\mathcal{C}(X)$? Suppose the K elements in $\mathcal{C}$ are numbered $1, 2, \ldots, K$. Let

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

- These are the conditional class probabilities at x. Then the Bayes optimal classifier at x is

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

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

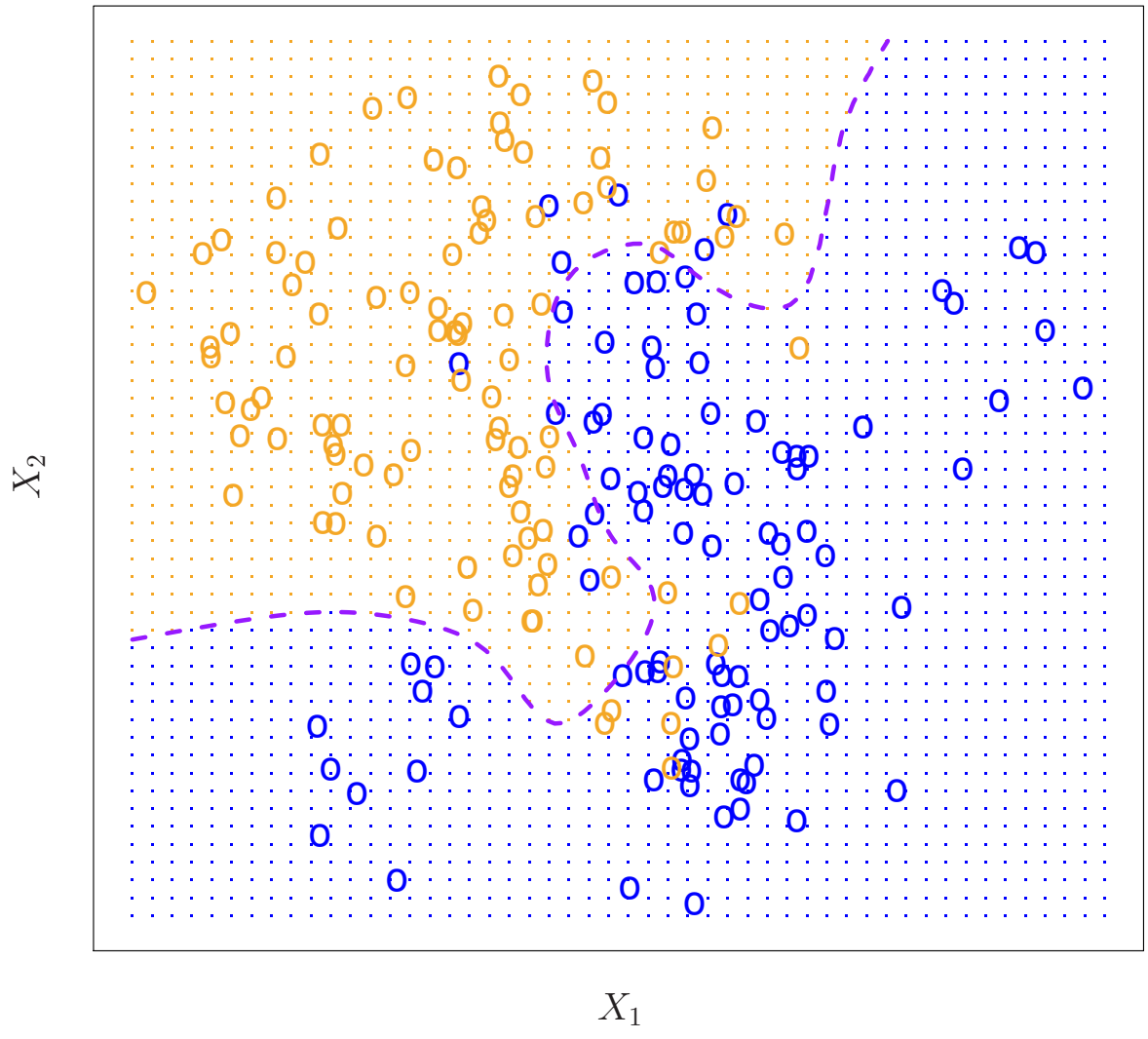
Classification: some details

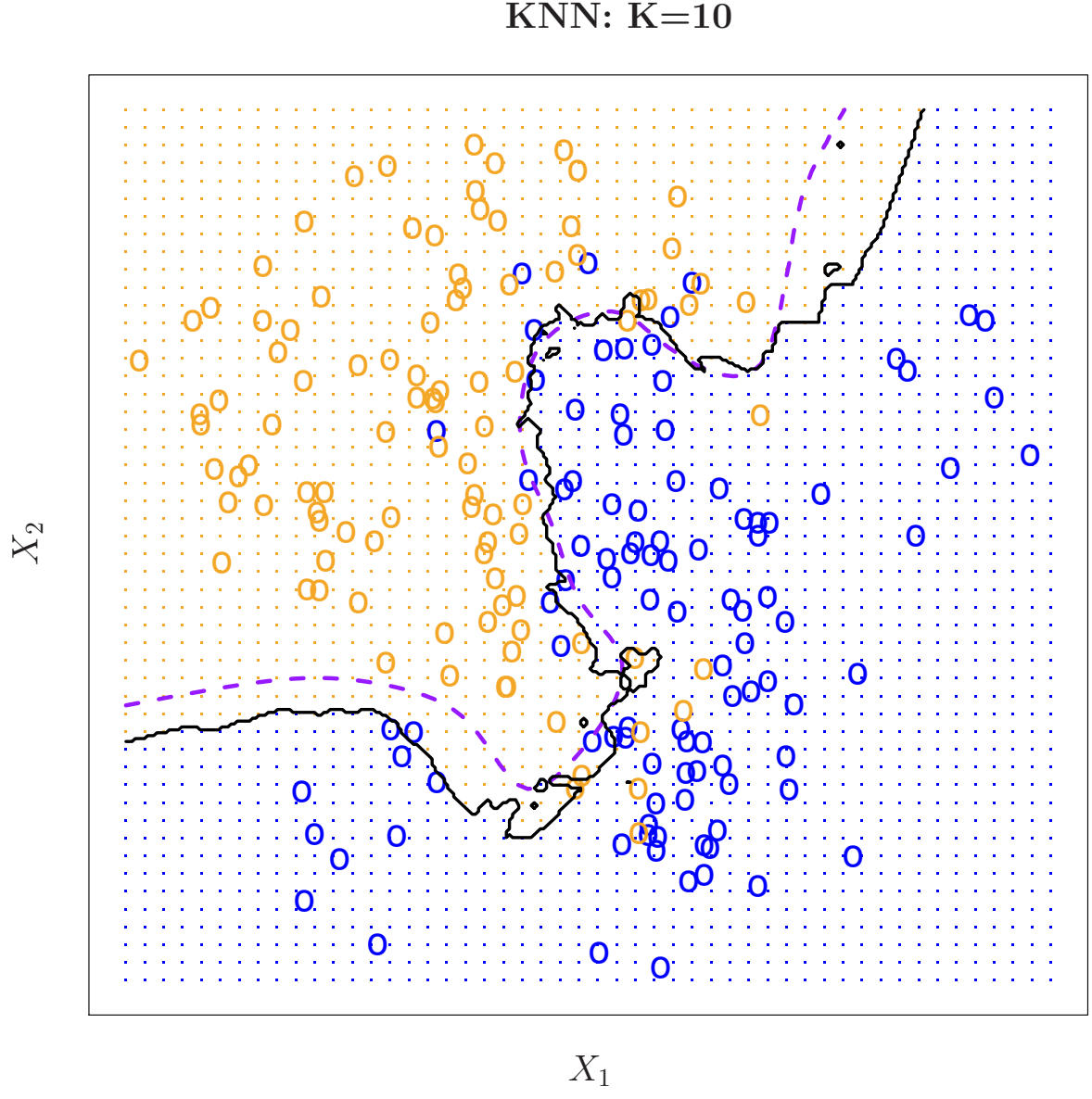
- Typically we measure the performance of $\hat{\mathcal{C}}(x)$ using the misclassification error rate:

$$Err_{Te} = Ave_{i \in Te} \mathcal{I}[y_i \neq \hat{\mathcal{C}}(x_i)]$$

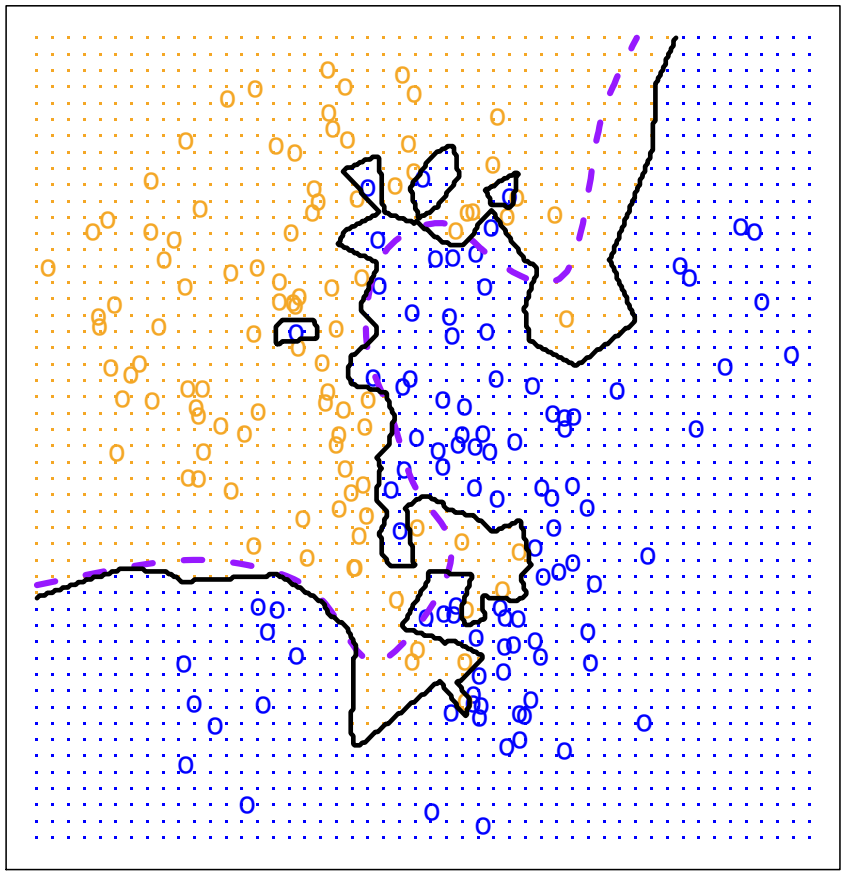
- The Bayes classifier (using the true $p_k(x)$) has smallest error (in the population).
- Support-vector machines build structured models for $\mathcal{C}(x)$.
- We will also build structured models for representing the $p_k(x)$. For example, logistic regression, generalized additive models.

Example: K-nearest neighbors in two dimensions

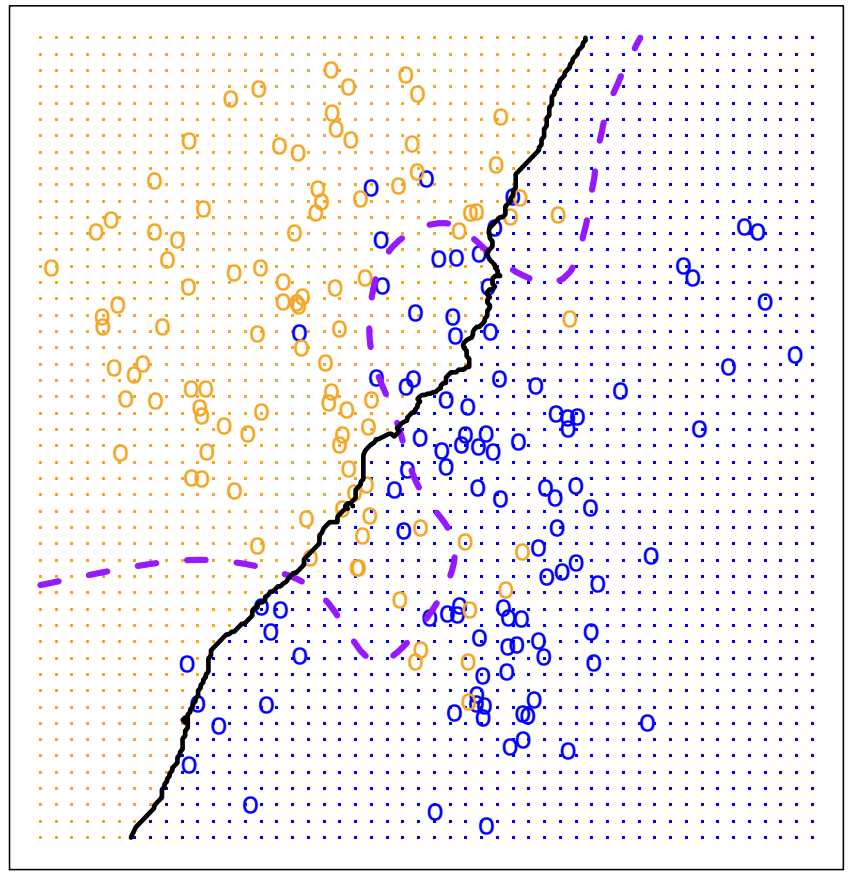


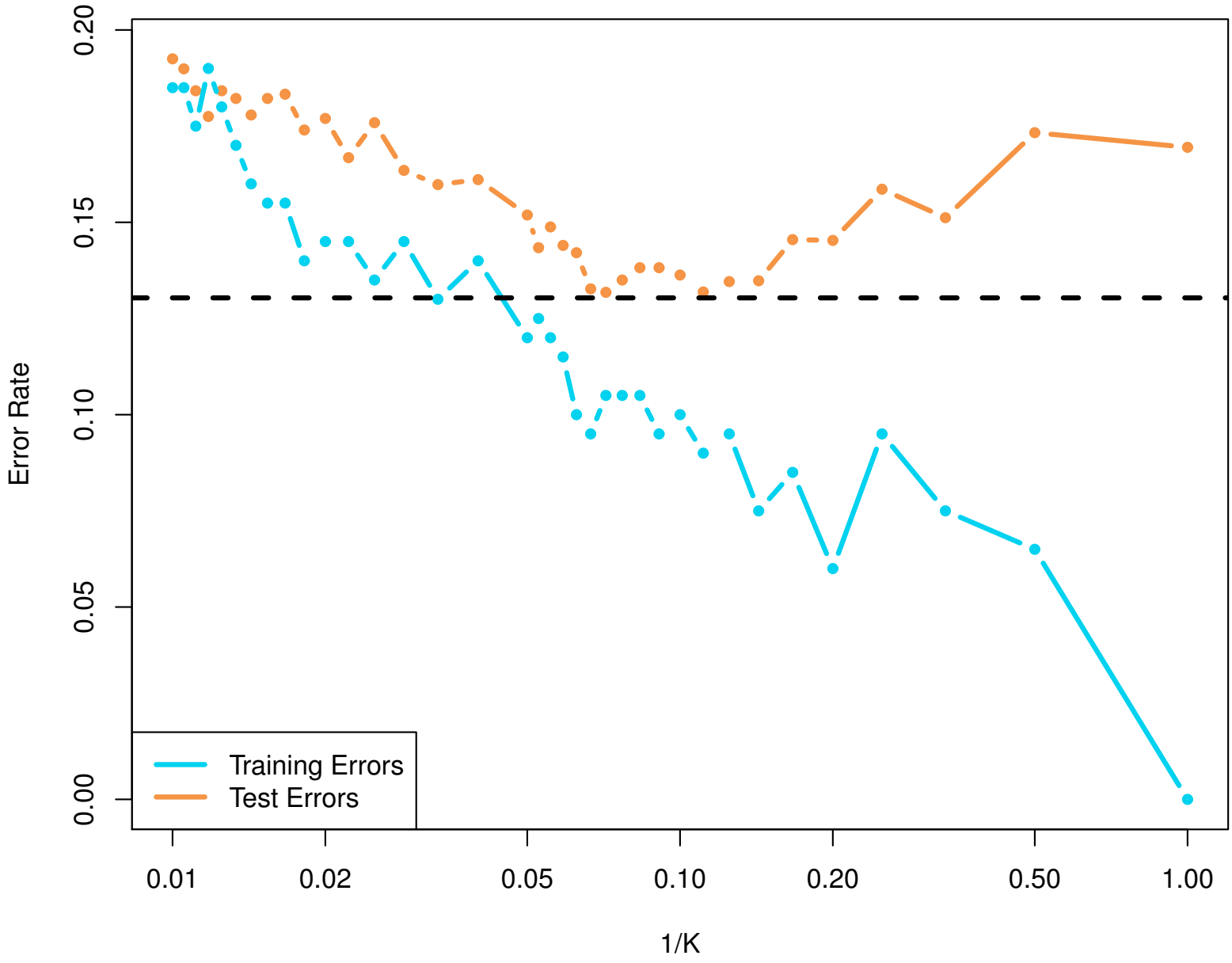

KNN: K=10
X_2
X_1

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