Lecture 1: Course logistics, introduction, bias-variance tradeoff

STATS 202: Statistical Learning and Data Science

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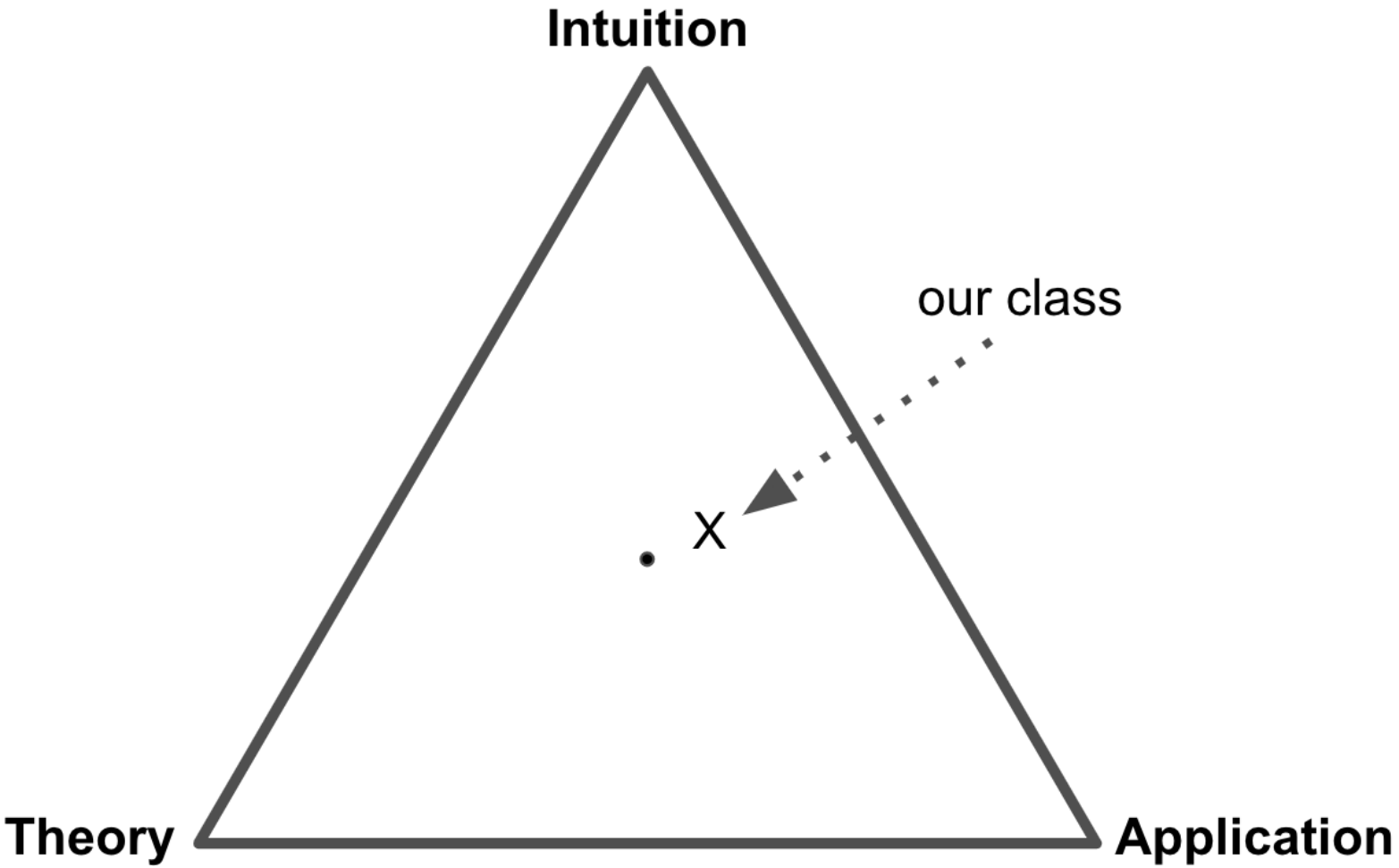
Syllabus

- **Topics:** Intro to statistical learning and methods for analyzing large amounts of data
- **Prereqs:** STATS 60, MATH 51, CS 105
- **Grades:** 3 components
  - *4 homework assignments* (50pts each)
    - Due by 4:30pm PDT of due date. Accepted up to 2-days late w/ 20% penalty after 1st day (2 total free late days)
    - Submit via Gradescope
  - Midterm on Wednesday, July 16 (100pts)
  - Final exam on Saturday, August 16 (200pts)
  - *Final project* (200pts)
    - Submissions due on Monday, August 11 at 12:00AM (i.e. Sunday night)
    - Write-up due on Wednesday, August 13
    - We take max(Final exam, Final project)

Class material



Programming

The course textbook uses both **R** and **Python**. You are free to choose between the two. Some thoughts:

- *R* (*style guide*)
  - Good visualizations
  - More detailed result outputs
  - Embraced by statistician community
  - Follow *Hadley Wickham's Style Guide*
- *Python* (*style guide*)
  - Good scalability
  - More detailed debugging logs
  - Embraced by ML community
  - Follow *PEP 8 style guide*

10% of your assignment grade is based upon the organization + style + readability of your code

Course Information

- **Class website:** *stats-202.github.io*
- **Videos:** In-person lectures will be recorded/uploaded to *Canvas*.
- **Textbook:** *An Introduction to Statistical Learning*
  - **Supplemental Textbook:** *The Elements of Statistical Learning*
- **Email policy:** Please use *ed stem* for most questions. Homeworks should be submitted via *Gradescope* (code: Y2JGKE).
- **Office hours:** Please refer to this *Google calendar*.

Motivation

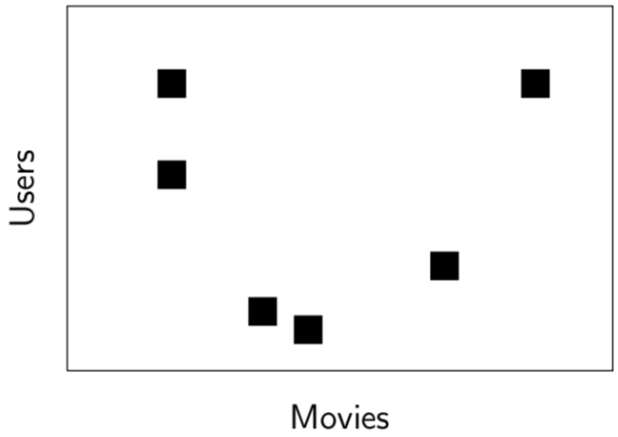
Companies are paying lots of money for statistical/ML models.

- *Netflix*
- *Heritage Provider Network*
- *Department of Homeland Security*
- *Zillow*
- Etc...

Netflix

Popularized prediction challenges by organizing an open, blind contest to improve its recommendation system.

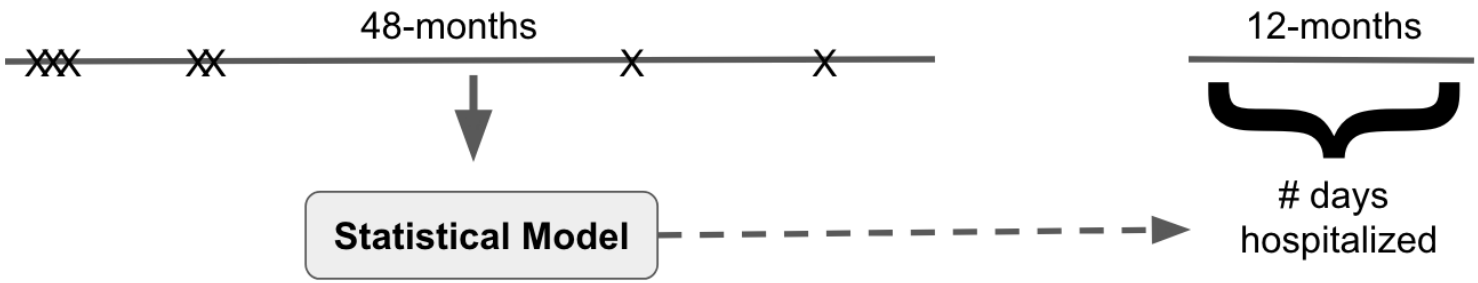
- **Prize:** $1 million
- **Features:** User ratings (1 to 5 stars) on previously watched films
- **Outcome:** User ratings (1 to 5 stars) for unwatched films



Heritage Provider Network

Ran for two years, with six milestone prizes during that span.

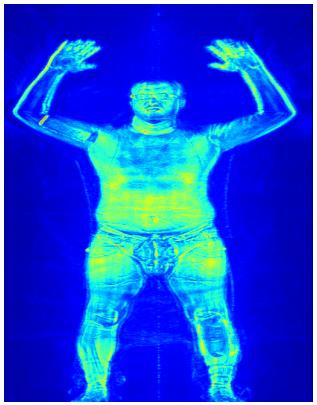
- **Prize:** $3 million ($500K)
- **Features:** Anonymized patient data over a 48 month period
- **Outcome:** How many days a patient will spend in a hospital in the next year

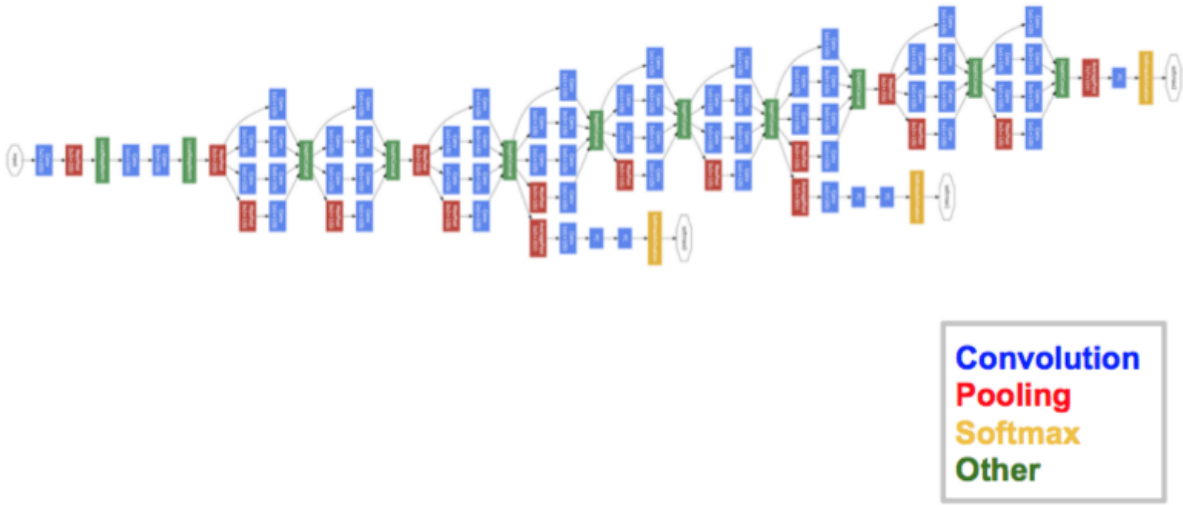


Department of Homeland Security

Improving the algorithms used by TSA to detect potential threats from body scans.

- **Prize:** \$1 million
- **Features:** Body scan images
- **Outcome:** Whether a given body zone has a threat present





OpenAI

Creator of ChatGPT (https://chat.openai.com)

- **Compensation:** $900K for Senior Engineers
- **Features:** Input text
- **Outcome:** Desired responses

Empirical vs true distributions

Common scenario: I have a data set. What do I do?
Common approaches:

- Fit a linear model and look at p-values
- Fit a non-parametric model and get predictions
- Calculate summary statistics and form a story around the answers

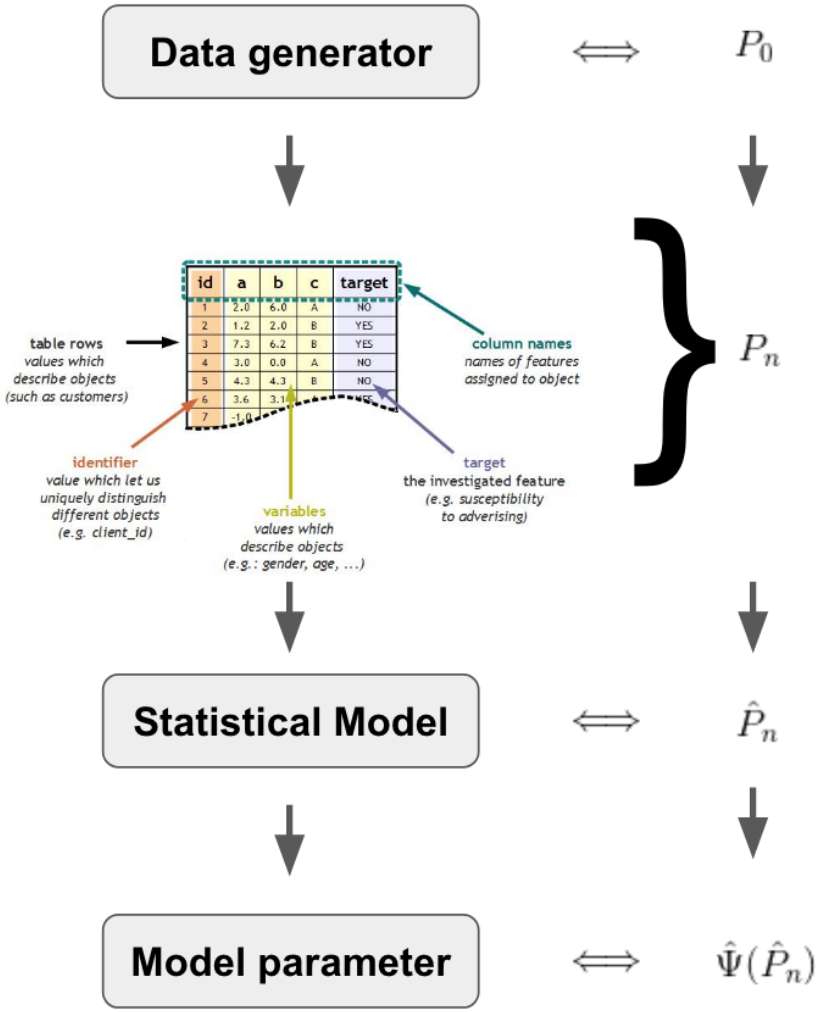
Empirical vs true distributions

Common scenario: I have a data set. What do I do?
Common approaches:

- Fit a linear model and look at p-values
- Fit a non-parametric model and get predictions
- Calculate summary statistics and form a story around the answers

Can result in significantly different answers!

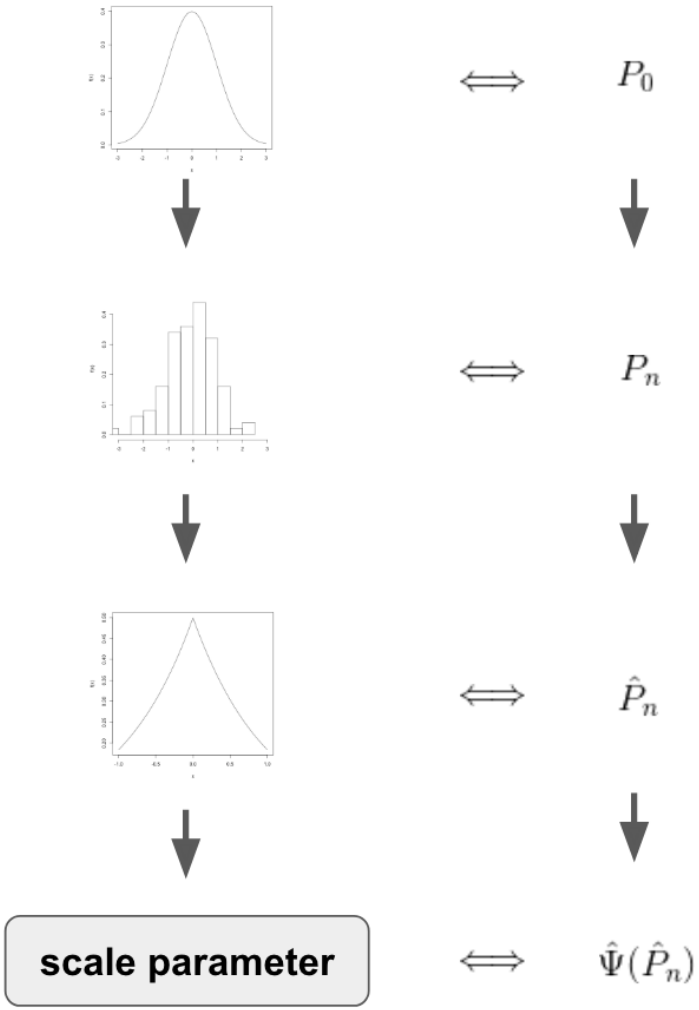
Empirical vs true distributions



Ideally, we want $\Psi(P_0)$.

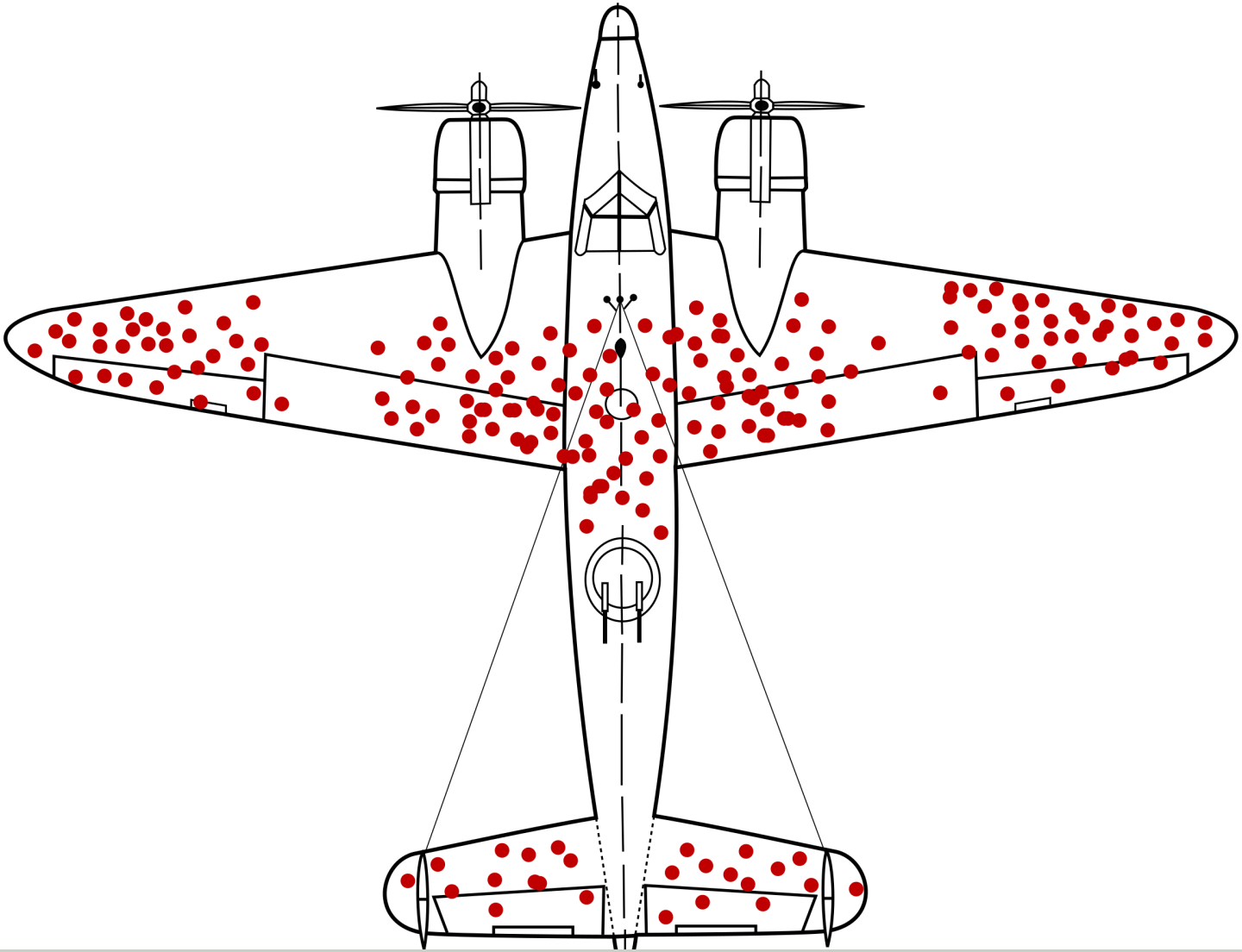
Empirical vs true distributions

Example: P_0 is Gaussian, while $\hat{P}_n$ is Laplace



Applied example

The World War II planes.



Applied example

- Let $O = (X_1, X_2, Y)$ be our data
  - e.g. X's are (horizontal/vertical) location of holes. Y is indicator that plane returned home.
- Generally want to estimate $\mathbb{P}_0[X_1, X_2 | Y = 0]$
- Two big issues:
  1. Need to condition on planes we don't observe
  2. Need to make assumption about the distribution of holes

Supervised vs unsupervised learning

Supervised: We have a clearly defined outcome of interest.

- Pro: More clearly defined
- Con: May take more resources to gather

Unsupervised: We don't have a clearly defined outcome of interest.

- Pro: Typically readily available
- Con: May be a more abstract problem

Unsupervised learning

Typically start with a data matrix, e.g.

id	weight	height	# children	education level	gender	profession	my life story
1							
2							
3							
.							

**n.b. The data may also be unstructured (e.g. text, pixels, etc).*

Unsupervised learning

id	weight	height	# children	education level	gender	profession	my life story
1							
2							
3							
.							

Two primary categories:

1. Quantitative:
   - Numerical
   - Ordinal
2. Qualitative:
   - Categorical
   - Free form

Unsupervised learning

Goal: Learn the overall structure of our data. e.g.

- Clustering: learn meaningful groupings of the data
  - e.g. k-means, Expectation Maximization, etc.
- Correlation: learn meaningful relationships between variables or units
  - e.g. concordance, Pearson's, etc.
- Dimension reduction: learn compression of data for downstream tasks
  - e.g. PCA, LDA, auto-encoding, etc.

We learn these using our data.

Supervised learning

Typically start with a data matrix **with an outcome**, e.g.

id	weight	height	# children	education level	gender	profession	my life story	**outcome**
1								
2								
3								
.								

Outcome can be quantitative or qualitative.

Supervised learning

Goal: We learn a mapping from input variables to output variables.

- If quantitative, then we refer to this as Regression
  - e.g. $\mathbb{E}_0[Y|X_1, X_2, ..., X_p]$
- If qualitative, then we refer to this as Classification
  - e.g. $\mathbb{P}_0[Y = y|X_1, X_2, ..., X_p]$

In both cases, we're interested in learning some function,

$$f_0(X_1, X_2, ..., X_p) \tag{1}$$

We estimate f_0 using our data.

Supervised learning

Motivation: Why learn f_0?

Prediction

- Useful when we can readily get $X_1, X_2, ..., X_p$, but not Y.
- Allows us to predict what Y likely is.
- Example: Predict stock prices next month using data from last year.

Inference

- Allows us to understand how differences in $X_1, X_2, ..., X_p$ might affect Y.
- Example: What is the influence of genetic variations on the incidence of heart disease.

Learning f_0

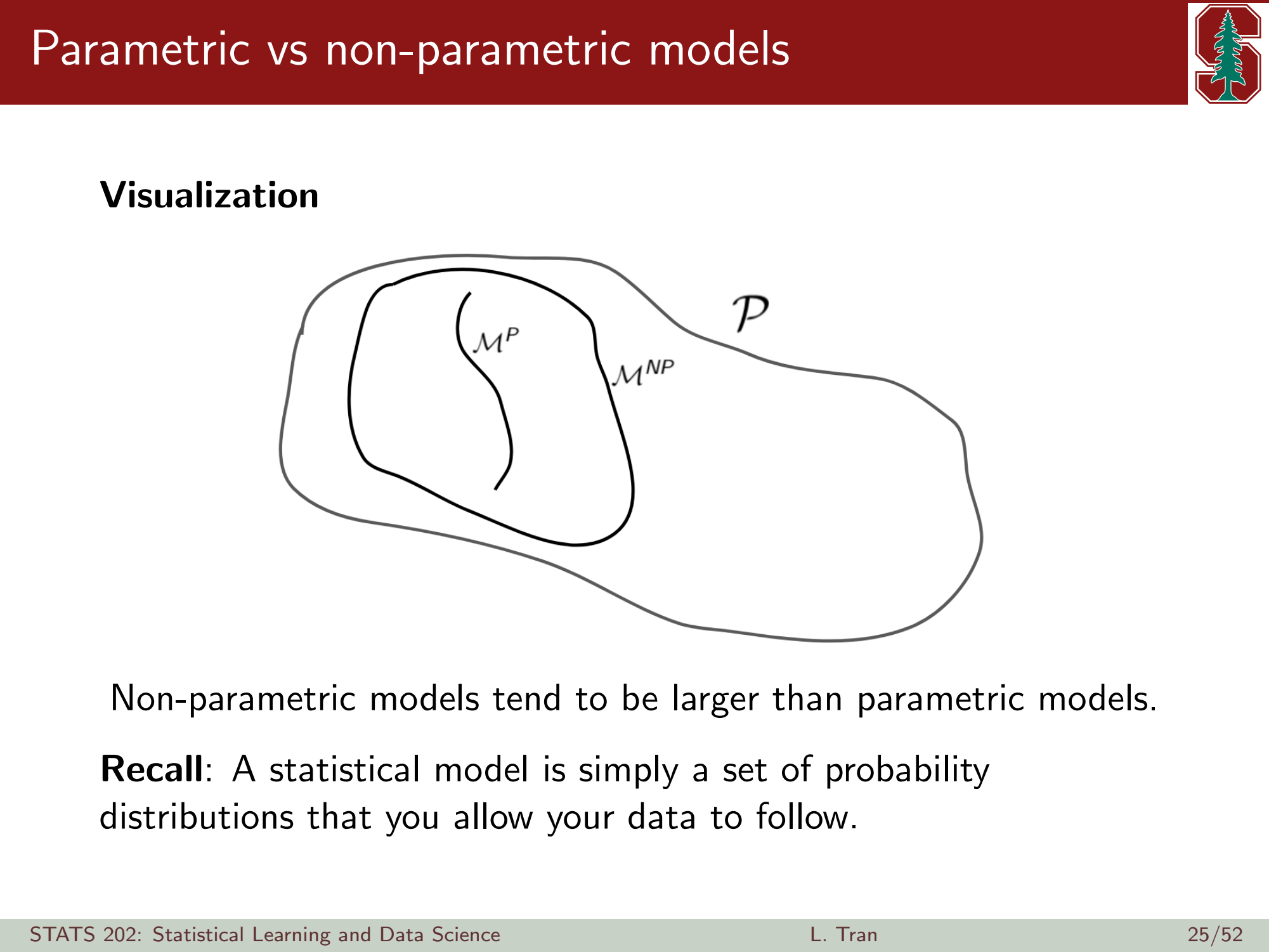
How do we estimate f_0? Two classes of methods:

- **Parametric models**: We assume that f_0 takes a specific form. For example, a linear form:

$$f_0(X_1, X_2, ..., X_p) = X_1\beta_1 + X_2\beta_2 + ... + X_p\beta_p \tag{2}$$

- **Non-parametric models**: We don't make any assumptions on the form of f_0, but we restrict how "wiggly" or "rough" the function can be. For example, using loess.

Parametric vs non-parametric models

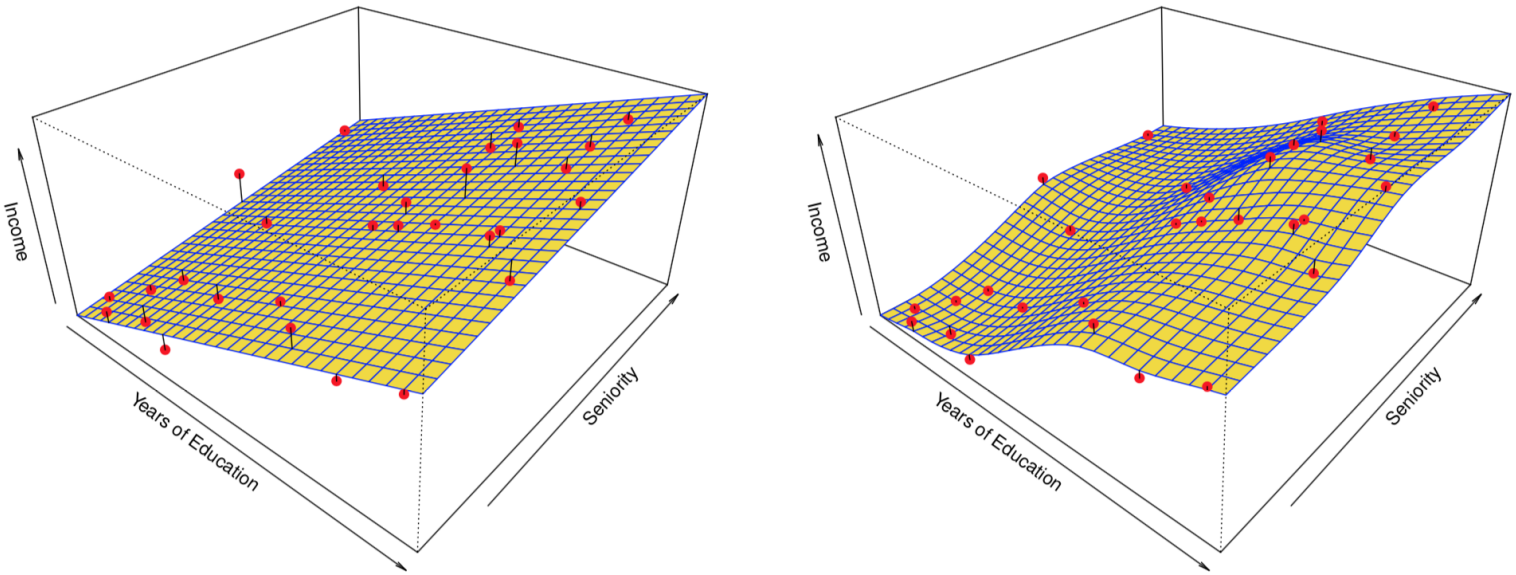


Visualization

Non-parametric models tend to be larger than parametric models.

Recall: A statistical model is simply a set of probability distributions that you allow your data to follow.

Parametric vs non-parametric fit



Non-parametric models tend to be more flexible.

Parametric vs non-parametric models

Question: Why don't we just always use non-parametric models?

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1. Interpretability: parametric models are simpler to interpret

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Parametric vs non-parametric models

Question: Why don't we just always use non-parametric models?

1. Interpretability: parametric models are simpler to interpret
2. Convenience: less computation, more reproducibility, better behavior
3. Overfitting: non-parametric models tend to overfit (aka. high variance)

Prediction error

Training data: $(x_i, y_i) : i = 1, 2, ..., n$
Goal: Estimate f_0 with our data, resulting in $\hat{f}_n$

Typically: we get $\hat{f}_n$ by minimizing a prediction error

- Assumes $(x_i, y_i) \overset{iid}{\sim} P_0$

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Standard prediction error functions:

- Classification: Cross-entropy

$$CE(\hat{f}_n) = \mathbb{E}_0[-\mathbf{y}_i \cdot \log \hat{\mathbf{f}}_n(x_i)] \tag{3}$$

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Standard prediction error functions:

- Classification: Cross-entropy

$$CE(\hat{f}_n) = \mathbb{E}_0[-\mathbf{y}_i \cdot \log \hat{\mathbf{f}}_n(x_i)] \tag{3}$$

- Regression: Mean squared error

$$MSE(\hat{f}_n) = \mathbb{E}_0[y_i - \hat{f}_n(x_i)]^2 \tag{4}$$

Prediction error

Cross entropy:

$$CE(\hat{f}_n) = \mathbb{E}_0[-\mathbf{y}_i \cdot \log \hat{\mathbf{f}}_n(x_i)] \tag{5}$$

n.b. We can't directly calculate this, since P_0 is unknown.

Prediction error

Cross entropy:

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n.b. We can't directly calculate this, since P_0 is unknown.

But:
We do have P_n, i.e. our training data $(x_i, y_i) : i = 1, 2, ..., n$.

Prediction error

Cross entropy:

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But:
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Estimating cross entropy

$$\begin{aligned} \widehat{CE}(\hat{f}_n) &= \mathbb{E}_n[-\mathbf{y}_i \cdot \log \hat{\mathbf{f}}_n(x_i)] && (6) \\ &= \frac{1}{n}\sum_{i=1}^{n} -\mathbf{y}_i \cdot \log \hat{\mathbf{f}}_n(x_i) && (7) \end{aligned}$$

Prediction error

Similarly:

We estimate the mean squared error using our data.

Estimating mean squared error

$$\widehat{MSE}(\hat{f}_n) = \mathbb{E}_n[y_i - \hat{f}_n(x_i)]^2 \quad (8)$$

$$= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}_n(x_i))^2 \quad (9)$$

Prediction error

There are two common problems with prediction errors:

1. A high prediction error could mean underfitting.
    - e.g. You could have the wrong functional form

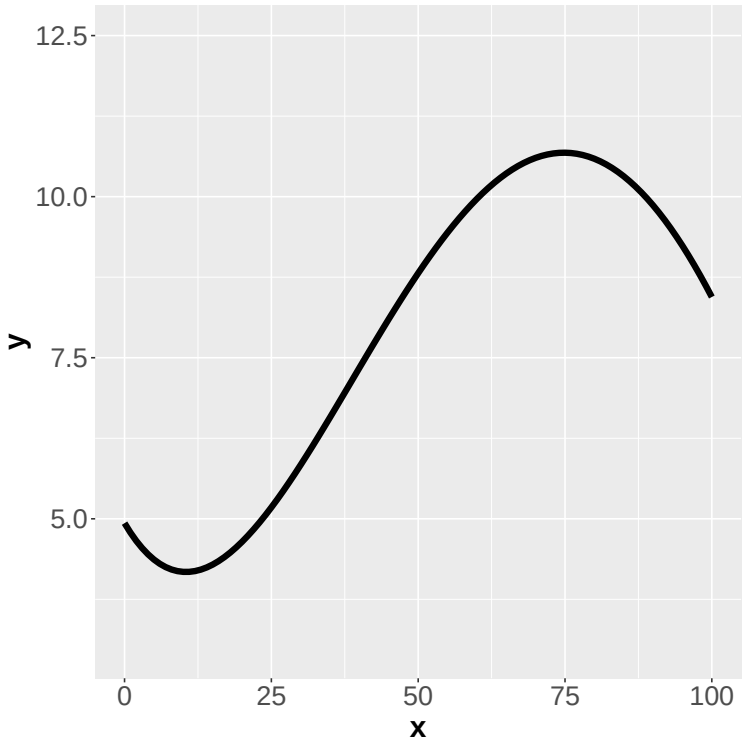
Prediction error

There are two common problems with prediction errors:

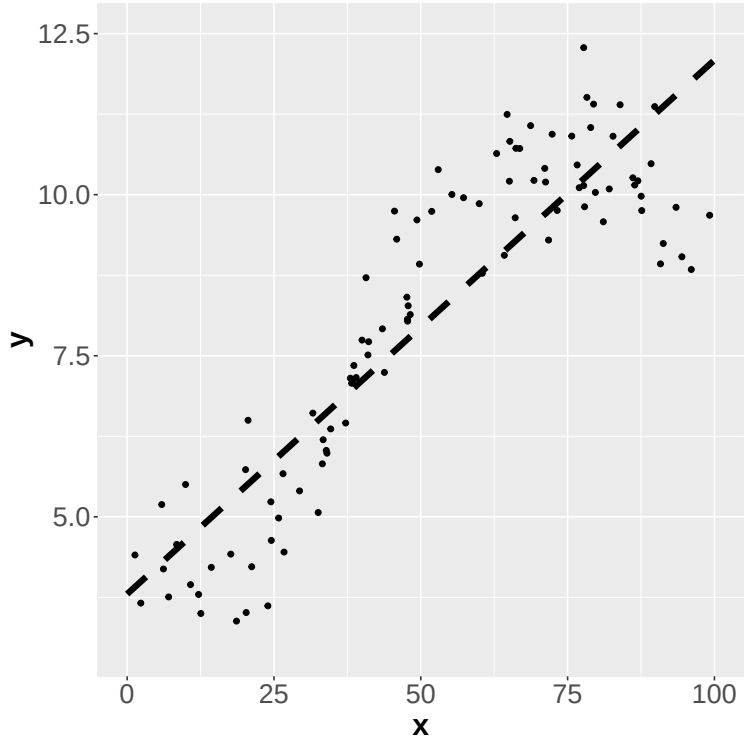
1. A high prediction error could mean underfitting.
    - e.g. You could have the wrong functional form
2. A low prediction error could mean overfitting.
    - e.g. You made your model too flexible

Underfitting

1. A high prediction error could mean underfitting.



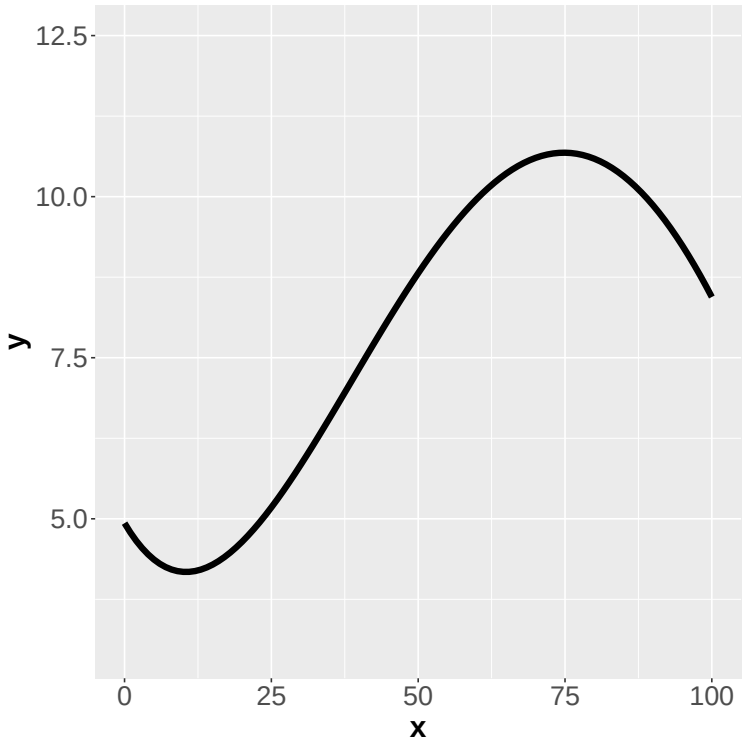
True function f_0.



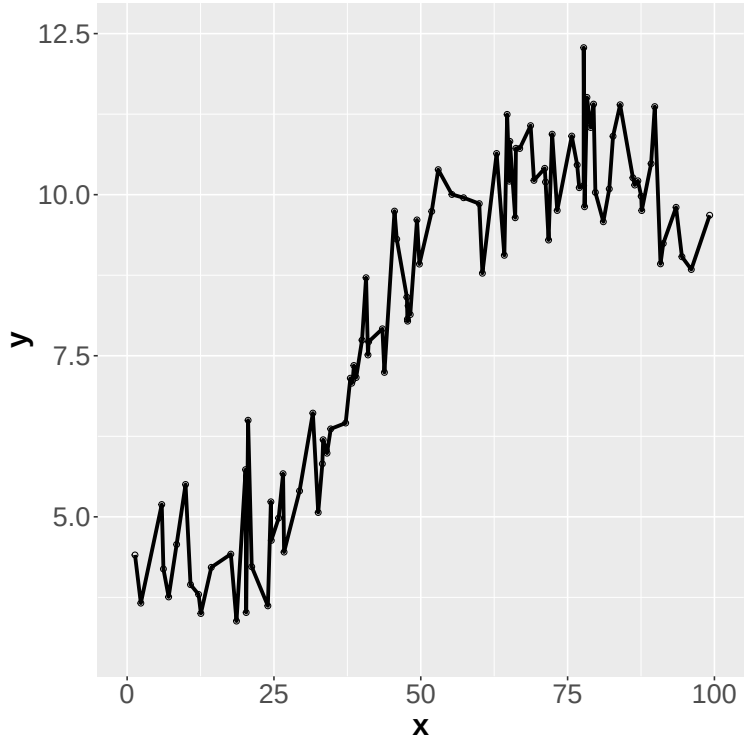
Observed data and estimated function $\hat{f}_n$.

Overfitting

2. A low prediction error could mean overfitting.



True function, f_0.



Observed data and estimated function $\hat{f}_n$.

Prediction error

How to tell if we've under/overfit:

- Evaluate on data not used in training (i.e. from your test set).

Given our test data $(x_i', y_i') : i = 1, 2, ..., m$, we can calculate a more accurate prediction error, e.g.:

$$\widehat{MSE}(\hat{f}_n) = \mathbb{E}_n^{test}[y_i' - \hat{f}_n(x_i')]^2 \quad (10)$$

$$= \frac{1}{m}\sum_{i=1}^{m}(y_i' - \hat{f}_n(x_i'))^2 \quad (11)$$

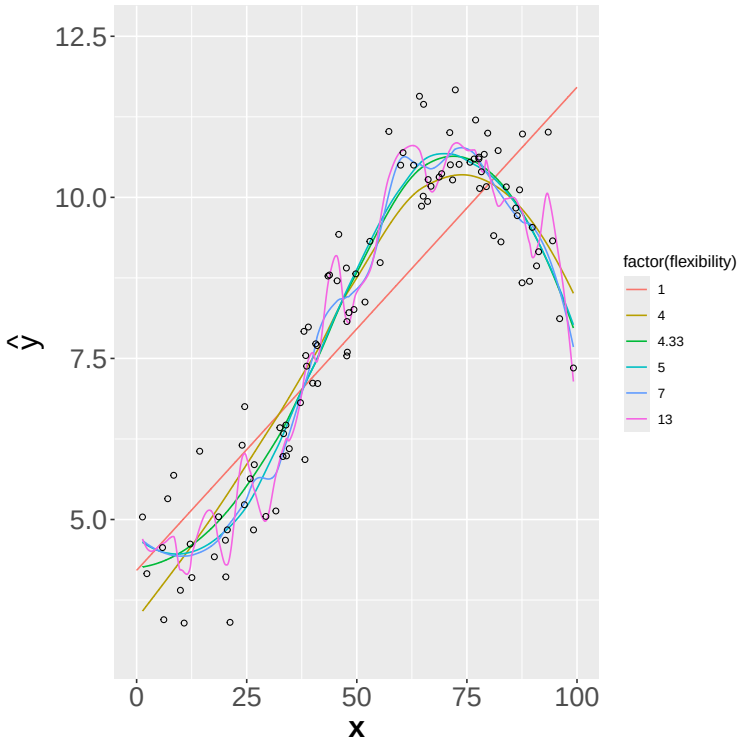
Prediction error

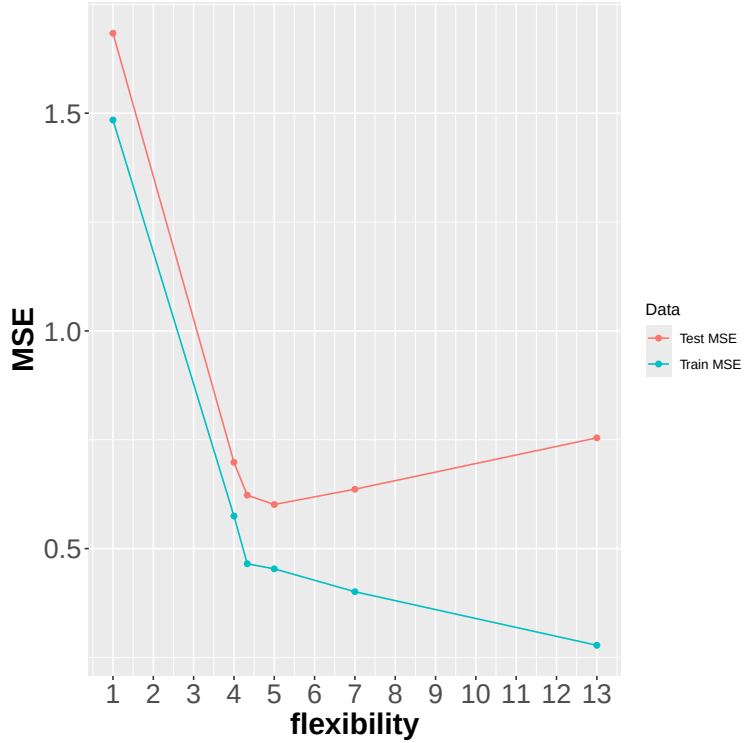
How to tell if we've under/overfit:

- So, now we have two prediction error estimates, e.g.:
  1. $\widehat{MSE}^{train}(\hat{f}_n)$ from our training data
  2. $\widehat{MSE}^{test}(\hat{f}_n)$ from our test data

If $\widehat{MSE}^{train}(\hat{f}_n) << \widehat{MSE}^{test}(\hat{f}_n)$, then we've likely overfit on our training data.

How to tell if we've under/overfit:

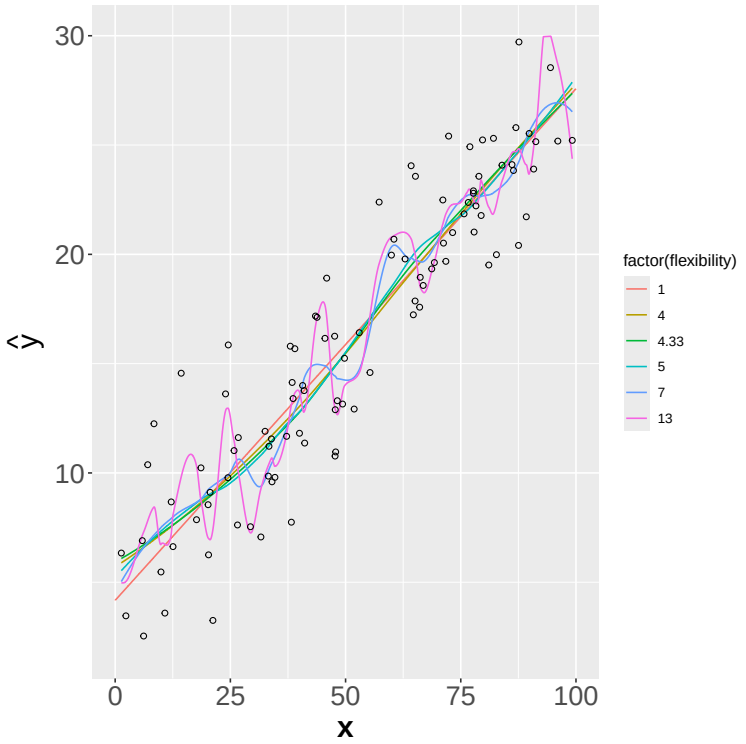


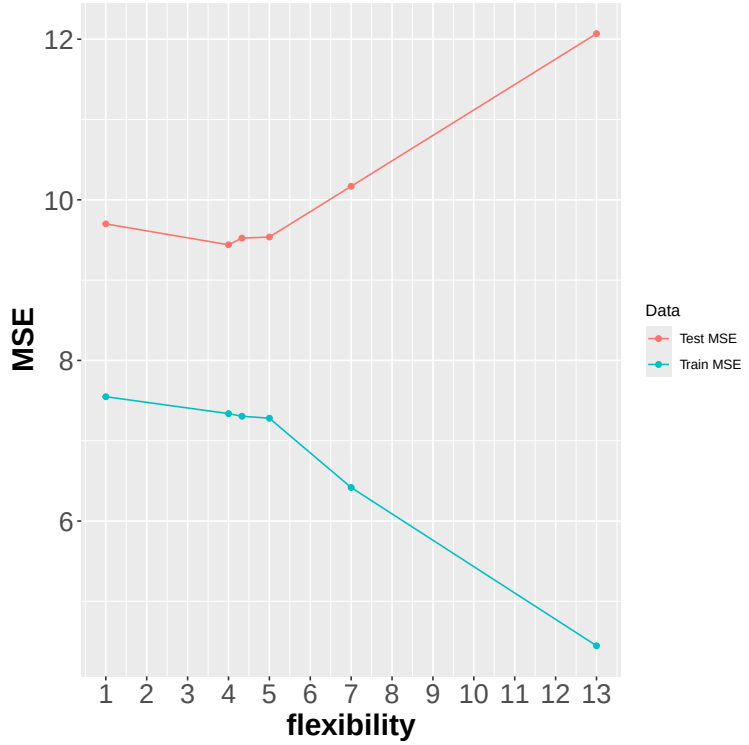


Estimates $\hat{f}_n$ of f_0.

$\widehat{MSE}$ for each $\hat{f}_n$.

How to tell if we've under/overfit (with an almost linear f_0):



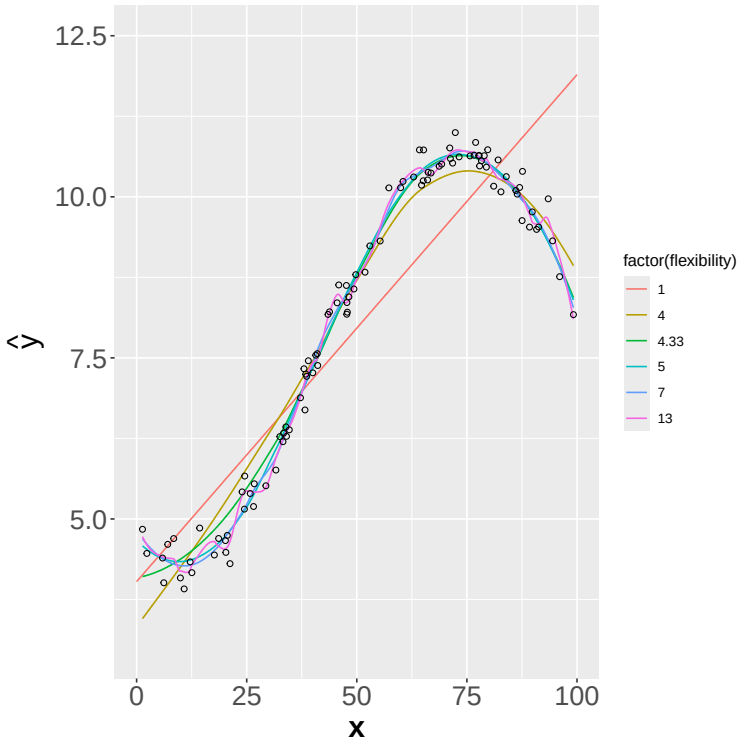


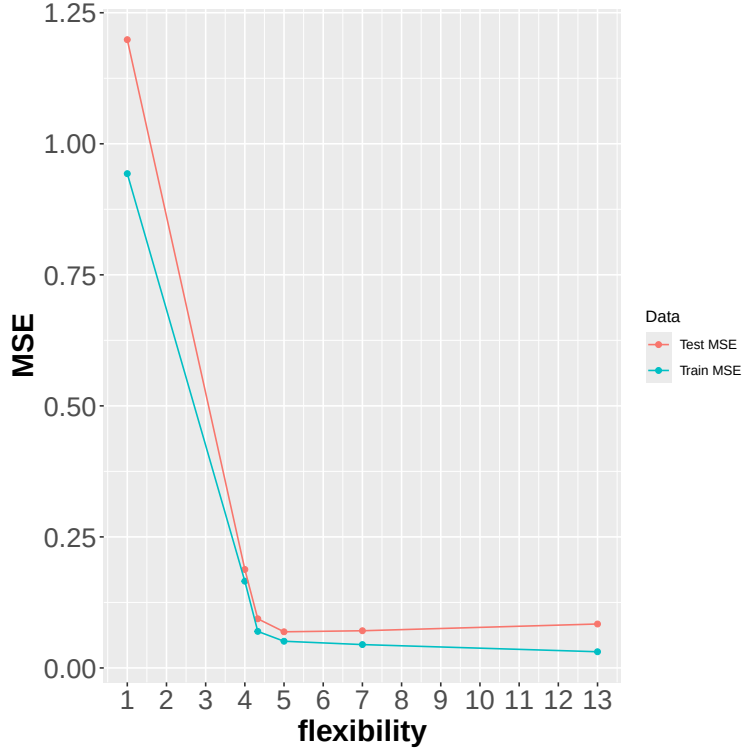
Estimates $\hat{f}_n$ of f_0.

$\widehat{MSE}$ for each $\hat{f}_n$.

Low flexibility models work well.

How to tell if we've under/overfit (with low noise):





Estimates $\hat{f}_n$ of f_0.

$\widehat{MSE}$ for each $\hat{f}_n$.

High flexibility models work well.

Bias variance decomposition

Let x_0 be a fixed point, $y_0 = f_0(x_0) + \epsilon$, and $\hat{f}_n$ be an estimate of f_0 from $(x_i, y_i) : i = 1, 2, ..., n$.

The MSE at x_0 can be decomposed as

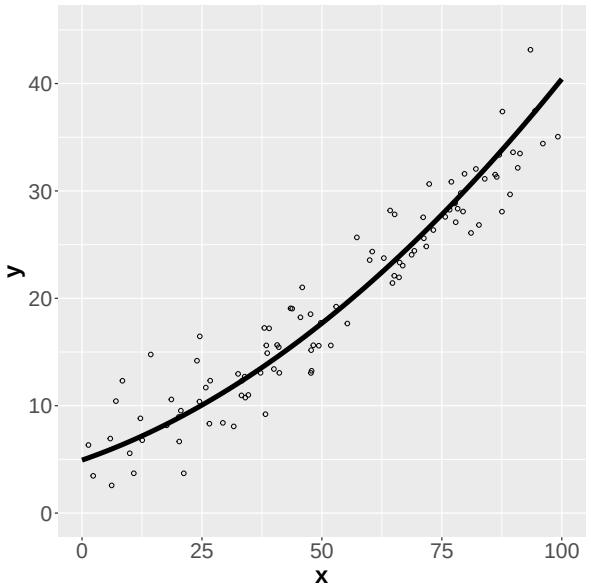
$$\begin{aligned} MSE(x_0) &= \mathbb{E}_0[y_0 - \hat{f}_n(x_0)]^2 && (12) \\ &= \text{Var}(\hat{f}_n(x_0)) + \text{Bias}(\hat{f}_n(x_0))^2 + \text{Var}(\epsilon_0) && (13) \end{aligned}$$

Bias variance decomposition

$$MSE(x_0) = \text{Var}(\hat{f}_n(x_0)) + \text{Bias}(\hat{f}_n(x_0))^2 + \text{Var}(\epsilon_0)$$

$\text{Var}(\epsilon_0)$

Noise from the data distribution, i.e. irreducible error.



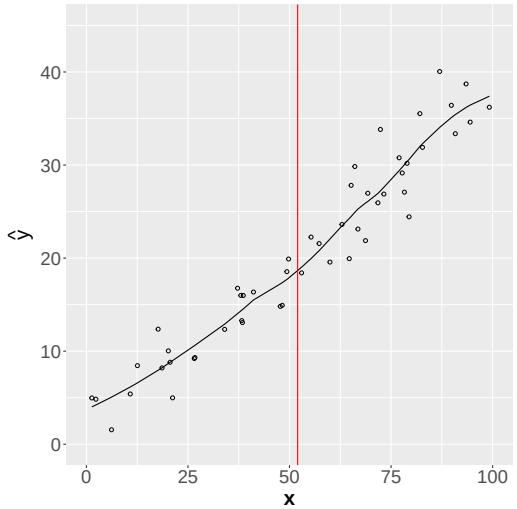
True function, f_0 and observed data.

Bias variance decomposition

$$MSE(x_0) = \text{Var}(\hat{f}_n(x_0)) + \text{Bias}(\hat{f}_n(x_0))^2 + \text{Var}(\epsilon_0)$$

$\text{Var}(\hat{f}_n(x_0))$

The variance of $\hat{f}_n(x_0)$ (i.e. the estimate of y).
How much the estimate $\hat{f}_n$ at x_0 changes with new data.



Observed data and estimate $\hat{f}_n$.

Bias variance decomposition

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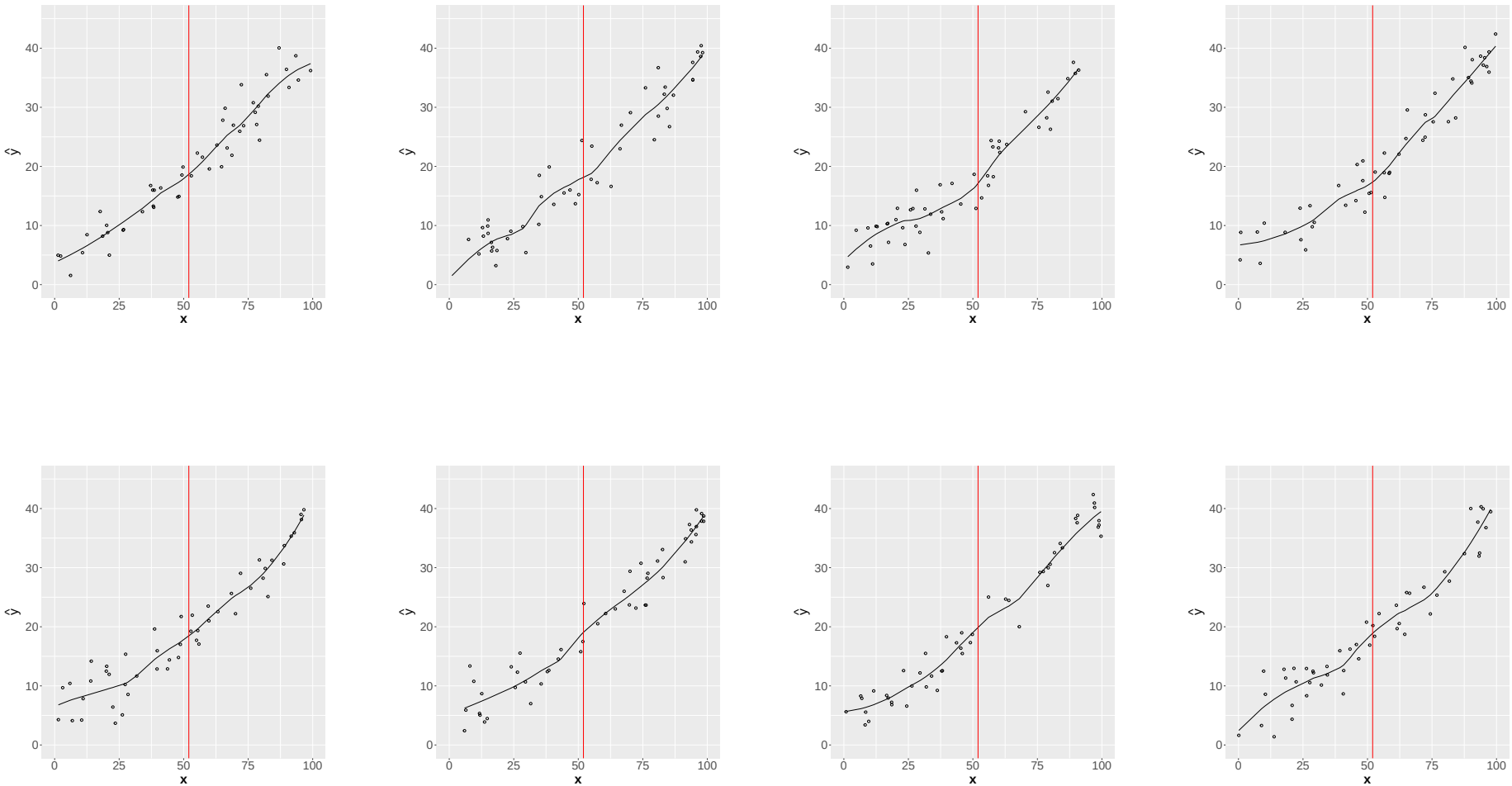

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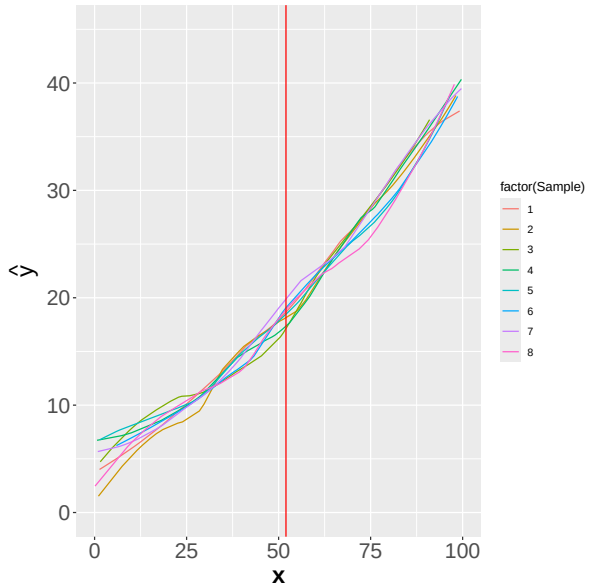
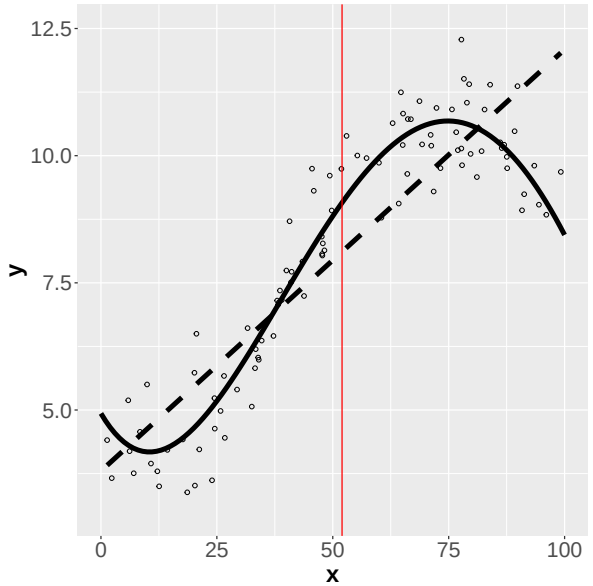


Bias variance decomposition

$$MSE(x_0) = \text{Var}(\hat{f}_n(x_0)) + \text{Bias}(\hat{f}_n(x_0))^2 + \text{Var}(\epsilon_0)$$

$\text{Bias}(\hat{f}_n(x_0))^2$

The square of the expected difference, $\mathbb{E}^2[\hat{f}_n(x_0) - f_0(x_0)]$. How far the average prediction $\hat{f}_n$ is from f_0 at x_0.



Bias variance decomposition

$$MSE(x_0) \quad = \quad \text{Var}(\hat{f}_n(x_0)) + \text{Bias}(\hat{f}_n(x_0))^2 + \text{Var}(\epsilon_0)$$

Implications:

- The MSE is always non-negative.
- Each element on the right side is always non-negative.
- Consequently, lowering one element (beyond some point) typically increases another.

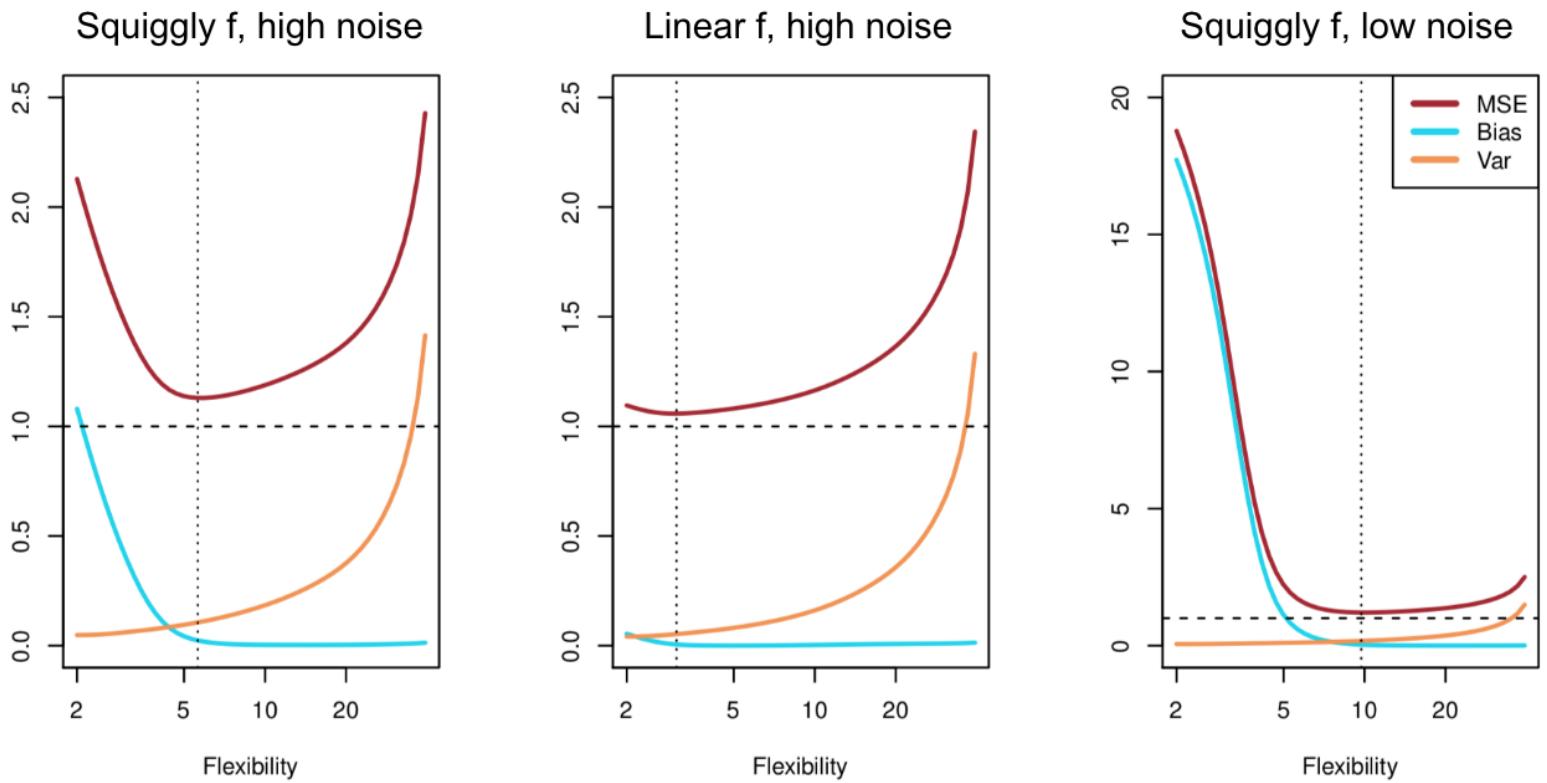
Bias variance trade-off

More flexibility $\iff$ Higher variance $\iff$ Lower bias

Bias variance decomposition

Bias variance trade-off

More flexibility $\iff$ Higher variance $\iff$ Lower bias



Classification

In classification, the output takes values in a discrete set (c.f. continuous values in regression).

Example

If we're trying to predict the brand of a car (based on input features), the function f_0 outputs the (conditional) probabilities of each car brand (e.g. Ford, Toyota, Mercedes, etc.), e.g.

$$\mathbb{P}_0[Y = y|X_1, X_2, ..., X_p] : y \in \{Ford, Toyota, Mercedes, etc.\} \quad (14)$$

Comparisons

Regression: $f_0 = \mathbb{E}_0[Y|X_1, X_2, ..., X_p]$

- A scalar value, i.e. $f_0 \in \mathbb{R}$
- $\hat{f}_n$ therefore gives us estimates of y

Classification: $f_0 = \mathbb{P}_0[Y = y|X_1, X_2, ..., X_p]$

- A vectored value, i.e. $f_0 = [p_1, p_2, ..., p_K] : p_j \in [0, 1], \sum_K p_j = 1$
- n.b. In a binary setting this simplies to a scalar, i.e. $f_0 = p_1 : p_1 = \mathbb{P}_0[Y = 1|X_1, X_2, ..., X_p] \in [0, 1]$
- $\hat{f}_n$ therefore gives us predictions of each class

Bayes classifier

- f_0 gives us a probability of the observation belonging to each class.
- To select a class, we can just pick the element in $f_0 = [p_1, p_2, ..., p_K]$ that's the largest
  - Called the Bayes Classifier
- As a classifier, produces the lowest error rate

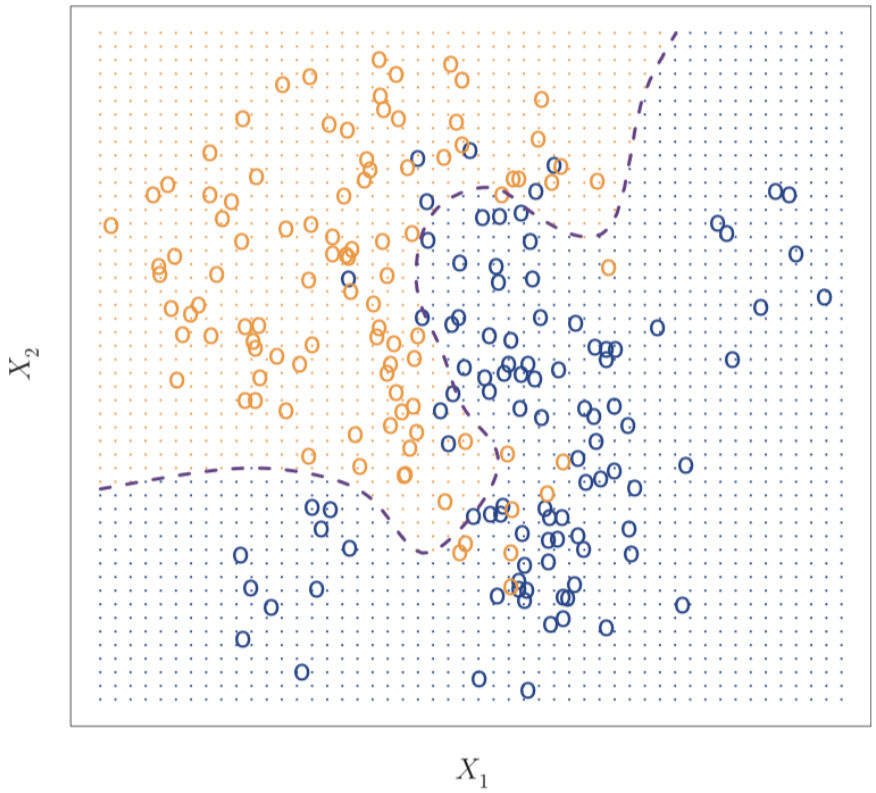
Bayes error rate

$$1 - \mathbb{E}_0 \left[\max_y \mathbb{P}_0[Y = y | X_1, X_2, ..., X_p] \right] \tag{15}$$

Analogous to the irreducible error described previously

Bayes classifier

Example: Classifying in 2 classes with 2 features.

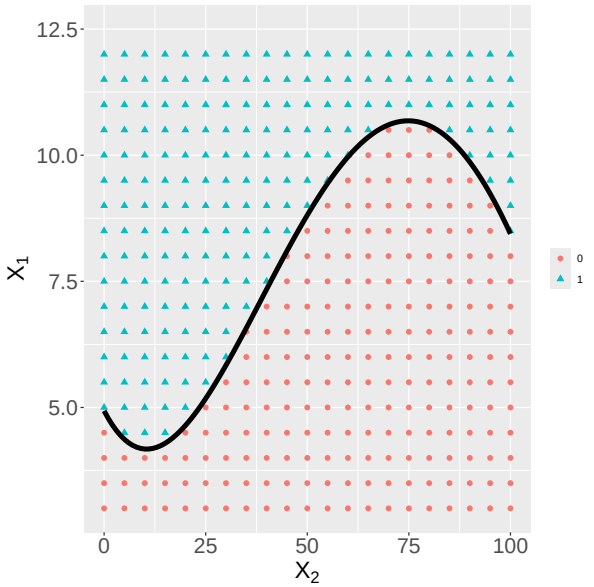


The Bayes error rate is 0.1304.

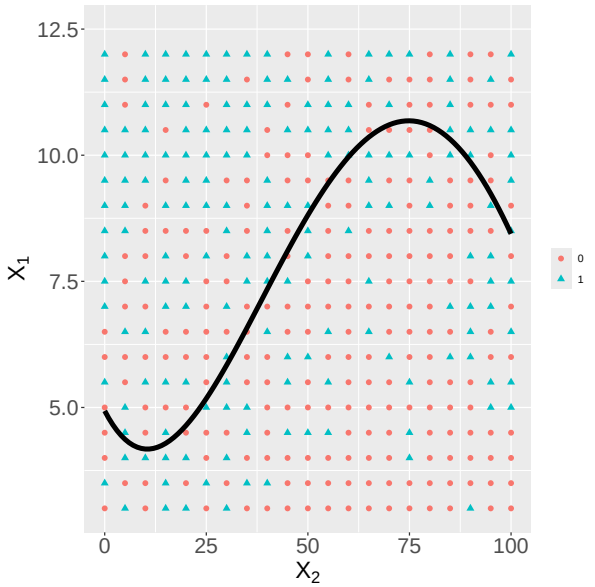
Bayes classifier

Note: $\mathcal{C}(\mathbf{x}) = \arg\max_y f_0(y)$ may seem easier to estimate

- Can still be hard, depending on the distribution f_0, e.g.



Bayes error = 0.0



Bayes error = 0.3

References

[1] ISL. Chapters 1-2.

[2] ESL. Chapters 1-2.