

Basic Machine Learning Concepts

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An aside: about the structure of these slides

- This slide deck was created using the R package **xaringan** (/ʃæ.'riŋ.gæn/) and **Rmarkdown**.
- Some slides include hidden comments. To view them, press **p** on your keyboard

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Replicating this presentation

R packages used to produce this presentation

```
library(tidyverse) # for data wrangling and plotting
library(svglight) # for better looking plots
library(kableExtra) # for better looking tables
library(RefManageR) # for referencing
library(truncnorm) # for drawing from a truncated normal distribution
library(tidymodels) # for modelling
library(knitr) # for presenting tables
library(mlbench) # for the Boston Housing data
library(ggdag) # for plotting DAGs
```

If you are missing a package, run the following command

```
install.packages("package_name")
```

Alternatively, you can just use the **pacman** package that loads and installs packages:

```
if (!require("pacman")) install.packages("pacman")

pacman::p_load(tidyvers, svglight, kableExtra, RefManageR,
               truncnorm, tidymodels, knitr, mlbench, ggdag)
```

First things first: "Big Data"

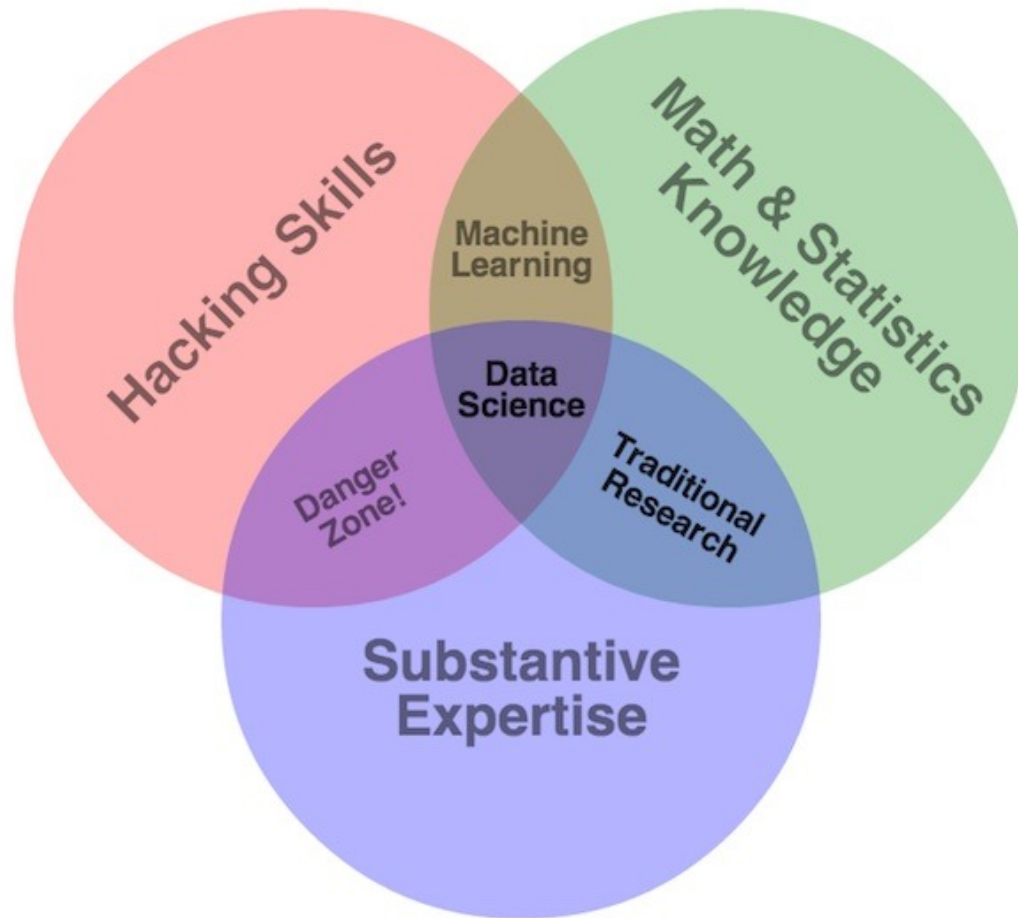
"A billion years ago modern homo sapiens emerged. A billion minutes ago, Christianity began. A billion seconds ago, the IBM PC was released. A billion Google searches ago ... was this morning."

Hal Varian (2013)

The 4 Vs of big data:

- Volume - Scale of data.
- Velocity - Analysis of streaming data.
- Variety - Different forms of data.
- Veracity - Uncertainty of data.

"Data Science"



[*] Hacking coding

Outline

1. What is ML?
2. The problem of overfitting
3. Too complex? Regularize!
4. Putting it All Together
5. What's in it for economists?

What is ML?

So, what is ML?

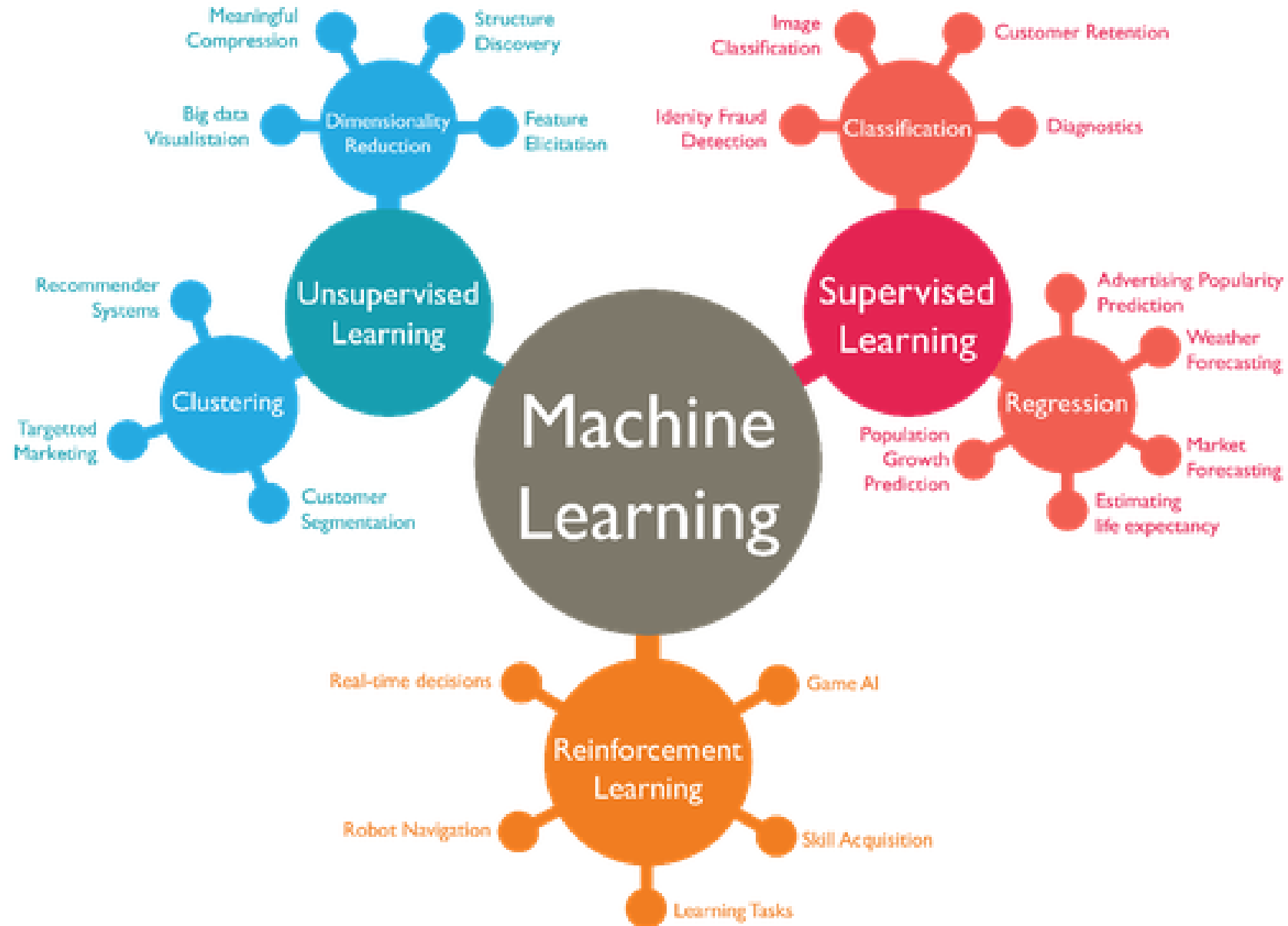
A concise definition by [Athey \(2018\)](#):

"...[M]achine learning is a field that develops algorithms designed to be applied to datasets, with the main areas of focus being prediction (regression), classification, and clustering or grouping tasks."

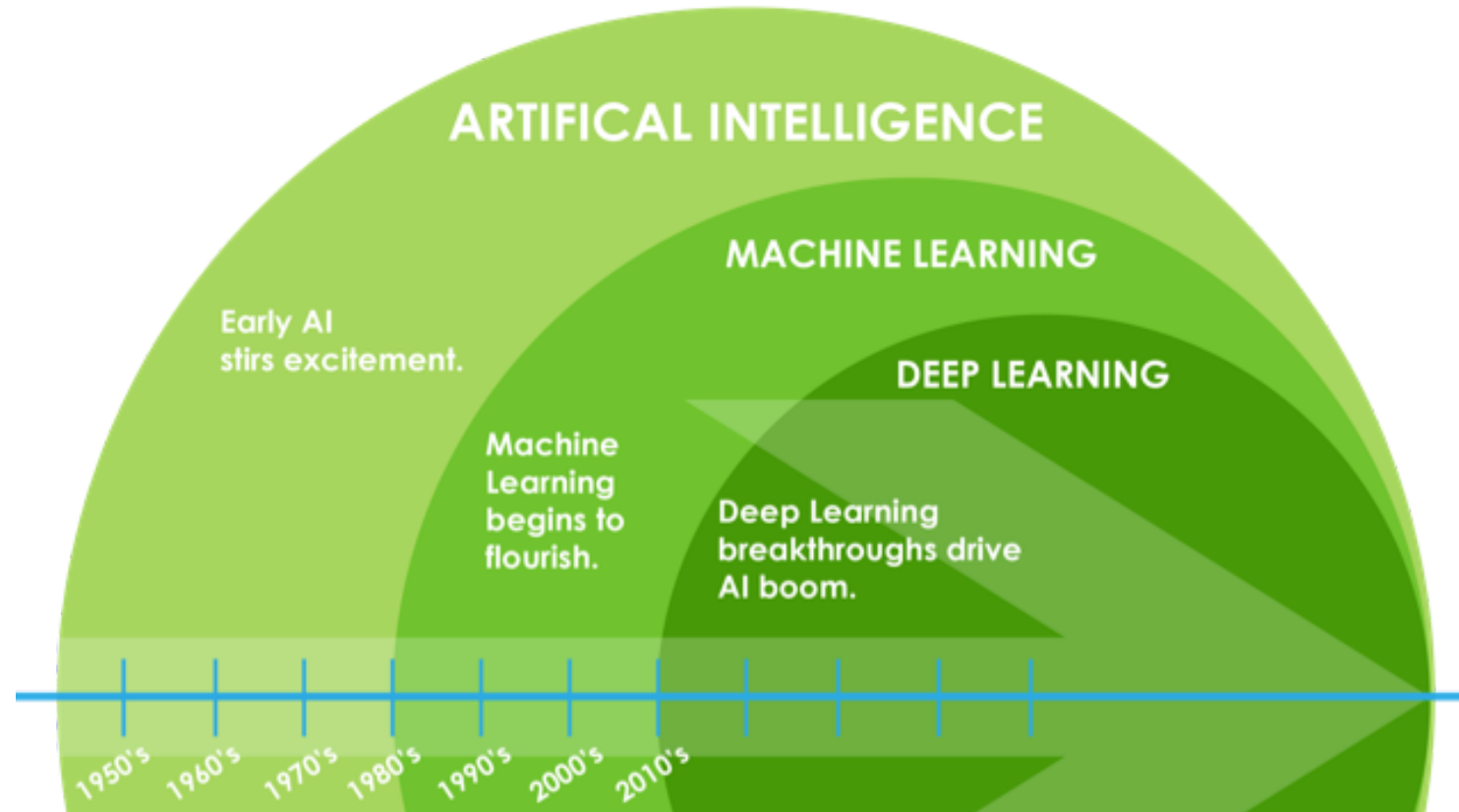
Specifically, there are three broad classifications of ML problems:

- supervised learning.
- unsupervised learning.
- reinforcement learning.

Most of the hype you hear about in recent years relates to supervised learning, and in particular, deep learning.



An aside: ML and artificial intelligence (AI)



Unsupervised learning

In *unsupervised* learning, the goal is to divide high-dimensional data into clusters that are **similar** in their set of features .

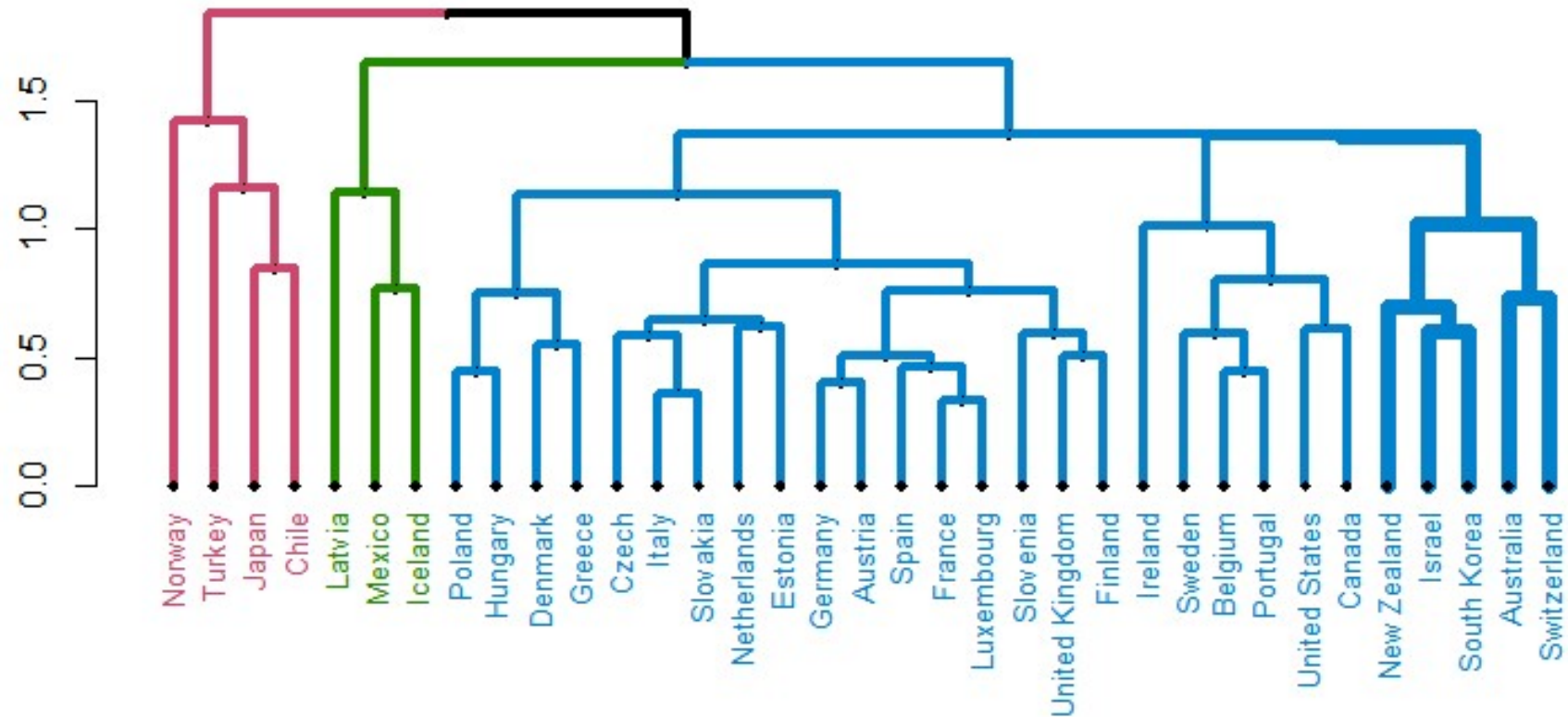
Examples of algorithms:

- principal component analysis
- -means clustering
- Latent Dirichlet Allocation model

Applications:

- image recognition
- cluster analysis
- topic modelling

Example: Clustering OECD Inflation Rates



Source: Baudot-Trajtenberg and Caspi (2018).

Reinforcement learning (RL)

A definition by [Sutton and Barto \(2018\)](#):

"Reinforcement learning is learning what to do—how to map situations to actions—so as to maximize a numerical reward signal. The learner is not told which actions to take, but instead must discover which actions yield the most reward by trying them."

Prominent examples:

- Games (e.g., Chess, AlphaGo).
- Self driving cars.

Supervised learning

Consider the following data generating process (DGP):

where y is the outcome variable, \mathbf{x} is a vector of "features", and ϵ is the irreducible error.

- **Training set** ("in-sample"):
- **Test set** ("out-of-sample"):



Typical assumptions: (1) independent observations; (2) stable DGP across training *and* test sets.

The goal of supervised learning

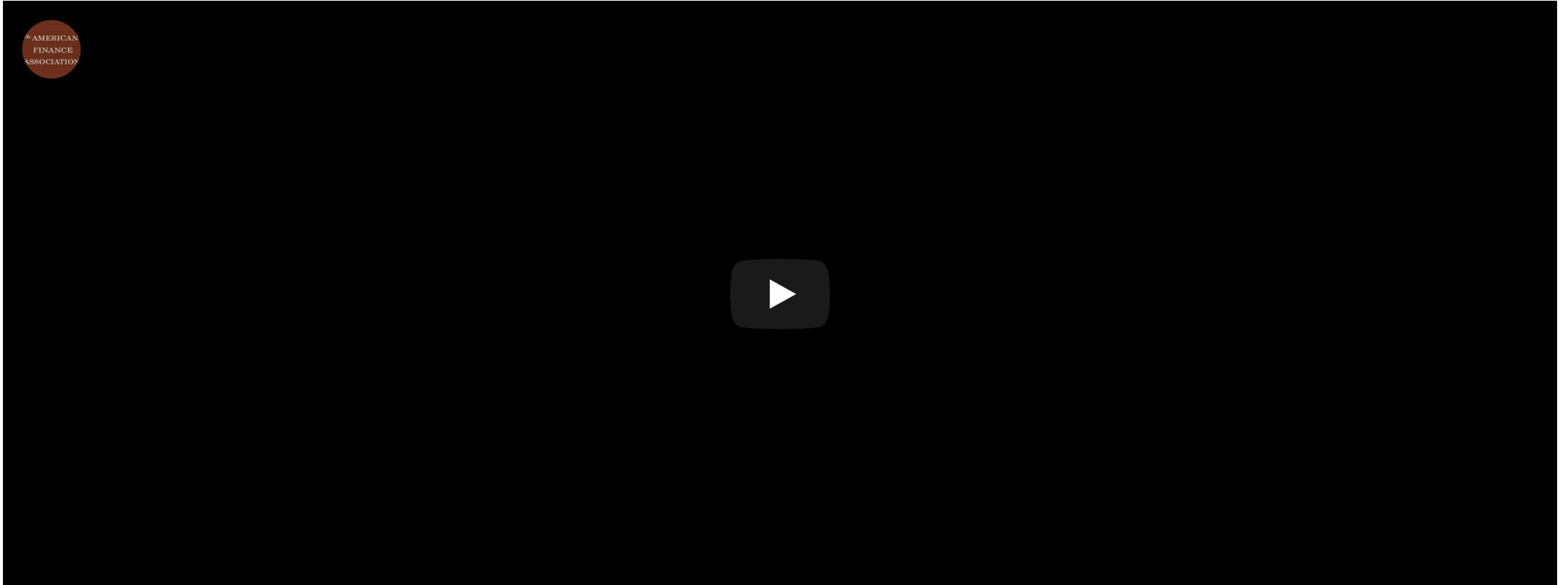
Use a labelled test set (X_{test} and y_{test} are known) to construct f such that it *generalizes* to unseen test set (only X_{test} is known).

EXAMPLE: Consider the task of spam detection:

ham	Go until jurong point, crazy.. Available only in bugis n great world la e buffet... Cine there got amore wat...
ham	Ok lar... Joking wif u oni...
spam	Free entry in 2 a wkly comp to win FA Cup final tkts 21st May 2005. Text FA to 87121 to receive entry question(std txt rate)T&C's apply 08452810075over18's
ham	U dun say so early hor... U c already then say...
ham	Nah I don't think he goes to usf, he lives around here though
spam	FreeMsg Hey there darling it's been 3 week's now and no word back! I'd like some fun you up for it still? Tb ok! XxX std chgs to send, å£1.50 to rcv
ham	Even my brother is not like to speak with me. They treat me like aids patent.
ham	As per your request 'Melle Melle (Oru Minnaminunginte Nurungu Vettam)' has been set as your callertune for all Callers. Press *9 to copy your friends Callertune
spam	WINNER!! As a valued network customer you have been selected to receive a å£900 prize reward! To claim call 09061701461. Claim code KL341. Valid 12 hours only.
spam	Had your mobile 11 months or more? U R entitled to Update to the latest colour mobiles with camera for Free! Call The Mobile Update Co FREE on 08002986030

In this case, X_{train} , y_{train} , and X_{test} is the email text.

Traditional vs. modern approach to supervised learning



Traditional vs. modern approach to supervised learning

- Traditional: rules based, e.g., define dictionaries of "good" and "bad", and use it to classify text.
- Modern: learn from data, e.g., label text as "good" or "bad" and let the model estimate rules from (training) data.

More real world applications of ML

task	outcome	features
credit score	probability of default	loan history, payment record...
fraud detection	fraud / no fraud	transaction history, timing, amount...
voice recognition	word	recordings
sentiment analysis	good / bad review	text
image classification	cat / not cat	image
overdraft prediction	yes / no	bank-account history
customer churn prediction	churn / no churn	customer features

A rather mind blowing example: Amazon's **"Anticipatory Package Shipping"** patent (December 2013): Imagine Amazon's algorithms reaching such levels of accuracy, casing it to change its business model from shopping-then-shipping to shipping-then-shopping!

Supervised learning algorithms

ML comes with a rich set of parametric and non-parametric prediction algorithms (approximate year of discovery in parenthesis):

- Linear and logistic regression (1805, 1958).
- Decision and regression trees (1984).
- K-Nearest neighbors (1967).
- Support vector machines (1990s).
- Neural networks (1940s, 1970s, 1980s, 1990s).
- Simulation methods (Random forests (2001), bagging (2001), boosting (1990)).
- etc.

So, why now?

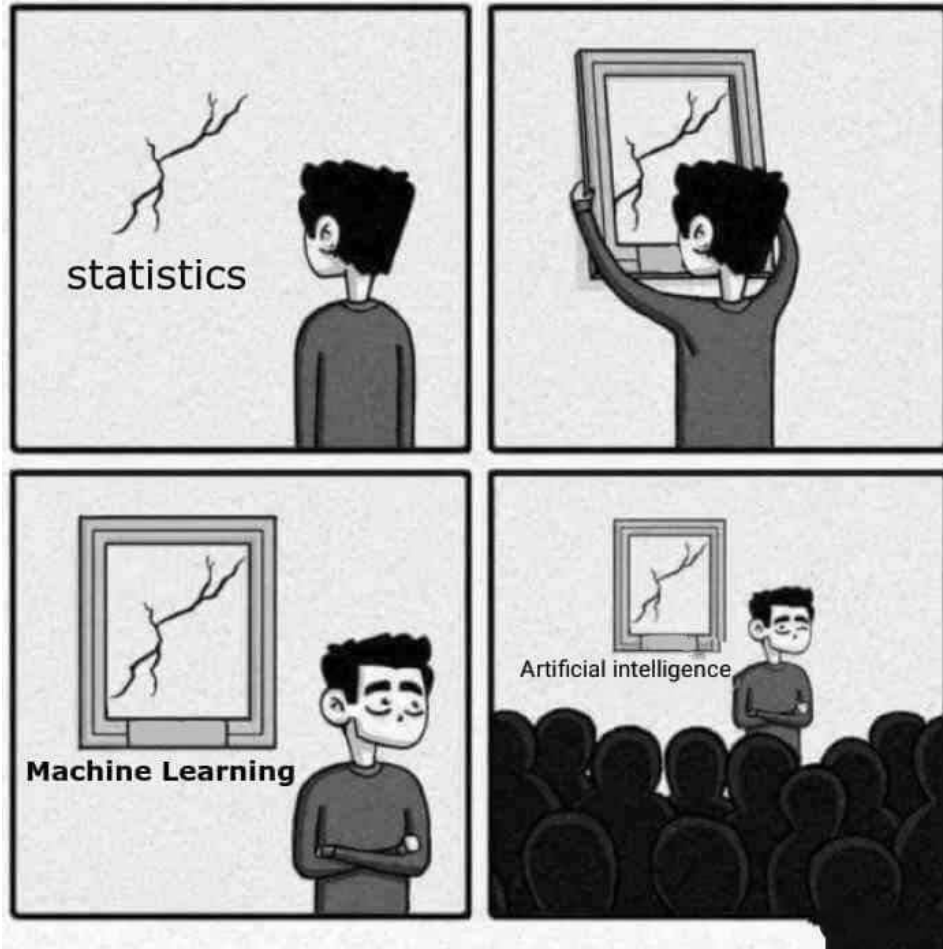
- ML methods are data-hungry and computationally expensive. Hence,
- Nevertheless,

"[S]upervised learning [...] may involve high dimensions, non-linearities, binary variables, etc., but at the end of the day it's still just regression."

— Francis X. Diebold



Wait, is ML just glorified statistics?



The "two cultures" ([Breiman, 2001](#)):

- Statisticians assume a data generating process and try to learn about it using data (parameters, confidence intervals, assumptions.)
- Computer scientists treat the data mechanism as unknown and try to predict or classify with the most accuracy.

Overfitting

Prediction accuracy

Before we define overfitting, we need to be more explicit about what we mean by "good prediction."

- Let \mathbf{x} denote a single realization from the (unseen) test set.
- Define a **loss function** $L(\hat{y}, y)$ in terms of predictions \hat{y} and the "ground truth" y , where y is estimated using the *training* set.
- Examples
 - squared error (SE): $L(\hat{y}, y) = (\hat{y} - y)^2$
 - absolute error (AE): $L(\hat{y}, y) = |\hat{y} - y|$
- There are other possible forms of loss function (e.g., in classification, as the probability of misclassifying a case, or in terms of economic costs.)

The bias-variance decomposition

Under a **squared error loss function**, an optimal predictive model is one that minimizes the *expected* squared prediction error.

It can be shown that if the true model is f^* , then

where the expectation is over the training set *and* \mathbf{x} .

Intuition behind the bias variance trade-off

Imagine you are a teaching assistant grading exams. You grade the first exam. What is your best prediction of the next exam's grade?

- the first test score is an unbiased estimator of the mean grade.
- but it is extremely variable.
- any solution?

Lets simulate it!

Exam grade prediction simulation

Let's Draw 1000 grade duplets from the following truncated normal distribution

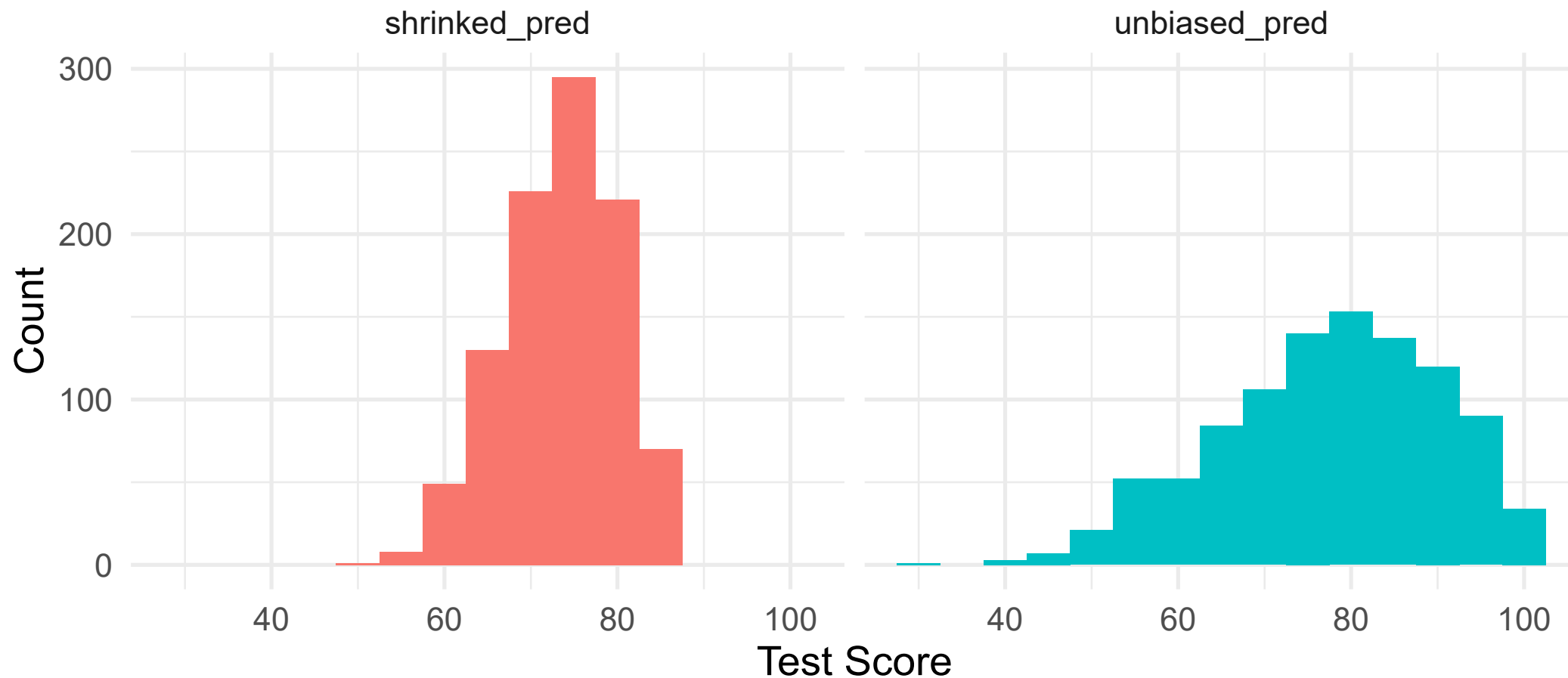
Next, calculate two types of predictions

- unbiased_pred is the first exam's grade.
- shrunked_pred is an average of the previous grade and a *prior* mean grade of 70.

Here a small sample from our simulated table:

attempt	grade1	grade2	unbiased_pred	shrunked_pred
124	87	80	87	78.5
446	59	84	59	64.5
685	47	73	47	58.5
969	44	76	44	57.0
413	83	68	83	76.5

The distribution of predictions



The MSE of grade predictions

unbiased_MSE	shrunked_MSE
324.192	217.9963

Hence, the shrunked prediction turns out to be better (in the sense of MSE) than the unbiased one!

QUESTION: Is this a general result? Why?

Regressions and the bias-variance trade-off

```
set.seed(1505) # for replicating the simulation

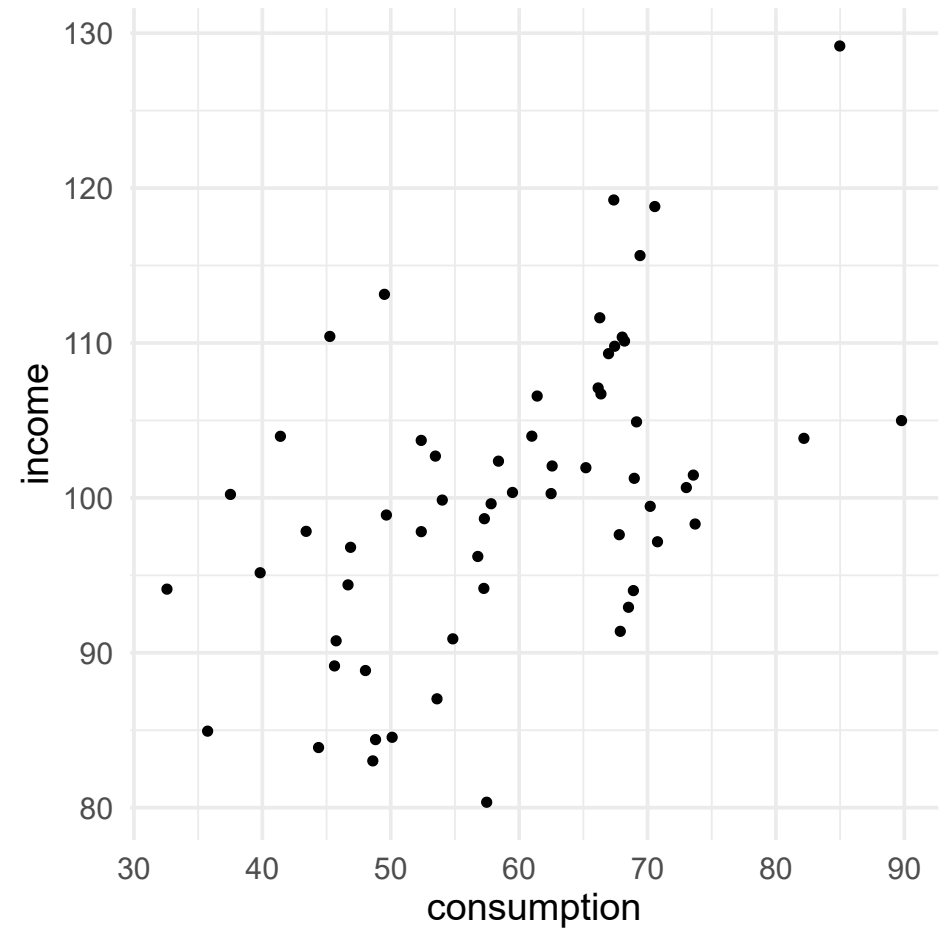
df <- crossing(economist = c("A", "B", "C"),
              obs = 1:20) %>%
  mutate(economist = as.factor(economist)) %>%
  mutate(income = rnorm(n(), mean = 100, sd = 10)) %>%
  mutate(consumption = 10 + 0.5 * income + rnorm(n(), sd = 10))

knitr::kable(sample_n(df,6), format = "html")
```

economist	obs	income	consumption
A	4	98.89330	49.65828
C	14	84.94055	35.73597
C	3	97.83834	43.40877
A	10	102.69686	53.47575
C	8	109.78834	67.43844
A	12	103.71018	52.37188

Scatterplot of the data

```
df %>%  
  ggplot(aes(x = consumption,  
             y = income)) +  
  geom_point()
```

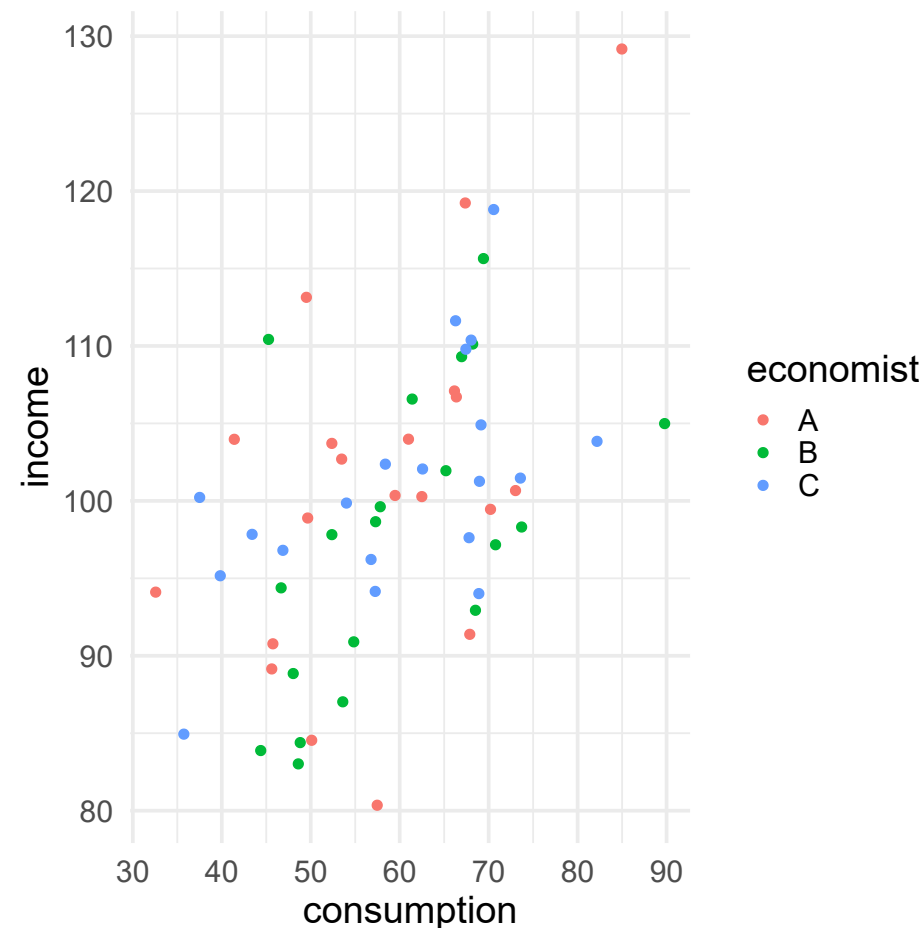


Split the sample between 3 economists

```
df %>%  
  ggplot(aes(x = consumption,  
             y = income,  
             color = economist)) +  
  geom_point()
```

```
knitr::kable(sample_n(df,6), format = "html")
```

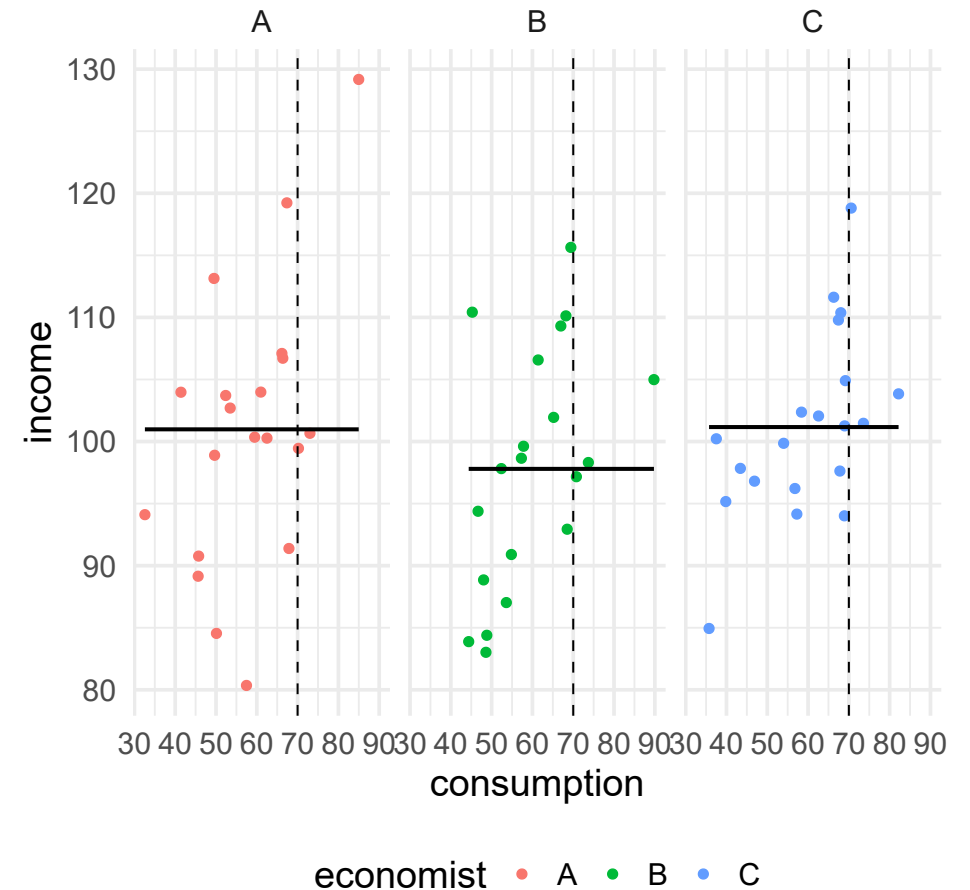
economist	obs	income	consumption
C	10	101.46972	73.56694
B	14	83.02060	48.60142
B	7	87.02760	53.60143
B	17	98.31148	73.70551
A	13	91.38508	67.87680
A	2	119.22994	67.37099



Underfitting: high bias, low variance

The model: unconditional mean

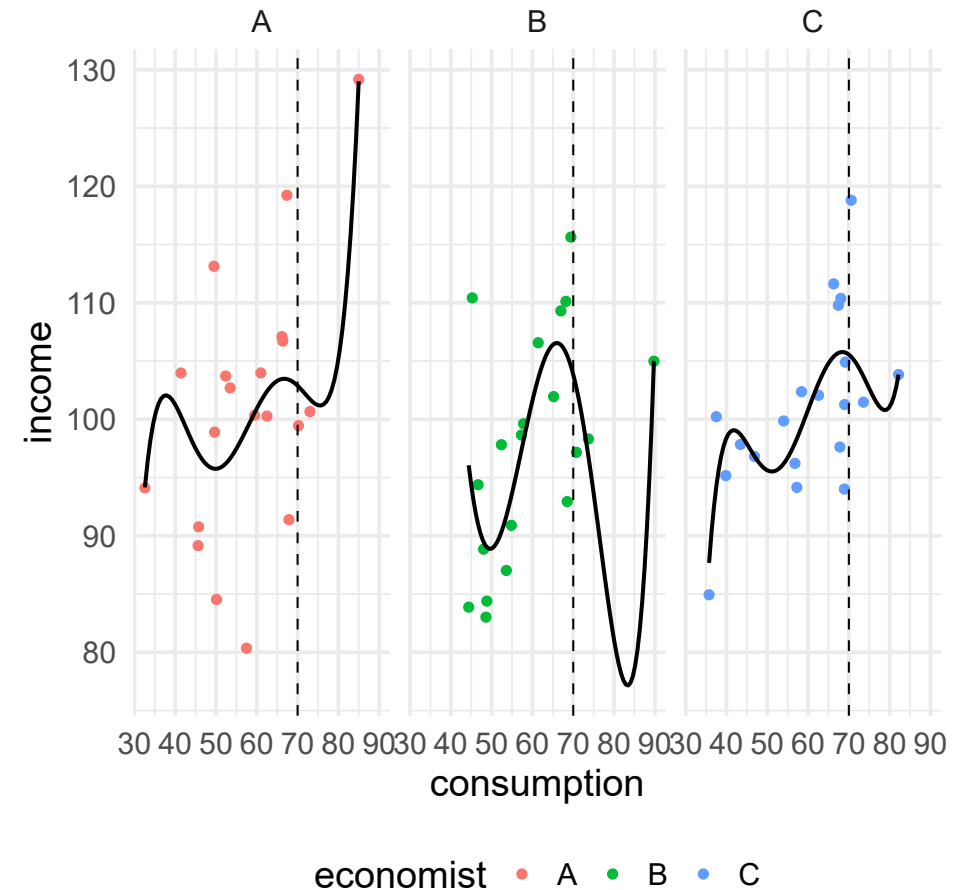
```
df %>%  
  ggplot(aes(x = consumption,  
             y = income,  
             color = economist)) +  
  geom_point() +  
  geom_smooth(method = lm,  
             formula = y ~ 1,  
             se = FALSE,  
             color = "black") +  
  facet_wrap(~ economist) +  
  geom_vline(xintercept = 70, linetype = "dashed") +  
  theme(legend.position = "bottom")
```



Overfitting: low Bias, high variance

The model: high-degree polynomial

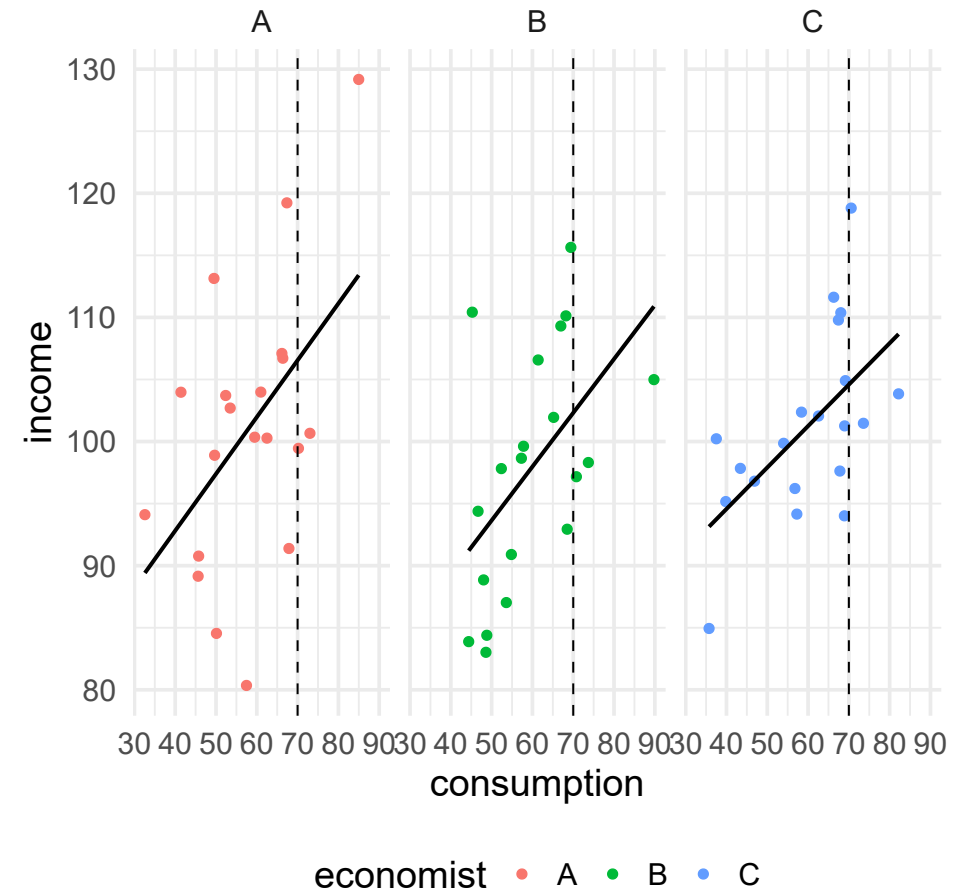
```
df %>%  
  ggplot(aes(x = consumption,  
             y = income,  
             color = economist)) +  
  geom_point() +  
  geom_smooth(method = lm,  
             formula = y ~ poly(x,5),  
             se = FALSE,  
             color = "black") +  
  facet_wrap(~ economist) +  
  geom_vline(xintercept = 70, linetype = "dashed") +  
  theme(legend.position = "bottom")
```



"Justfitting": bias and Variance are just right

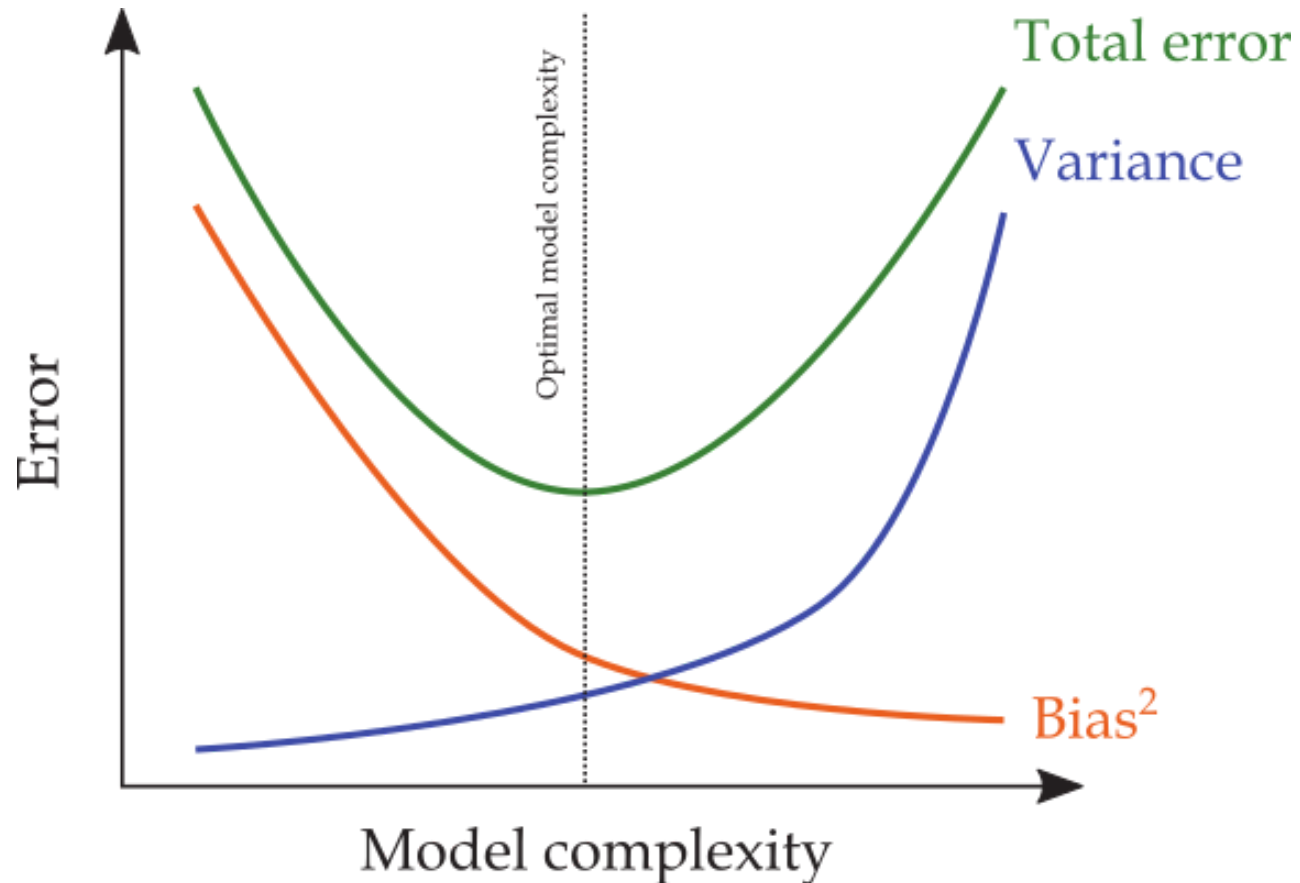
The model: linear regression

```
df %>%  
  ggplot(aes(x = consumption,  
             y = income,  
             color = economist)) +  
  geom_point() +  
  geom_smooth(method = lm,  
             formula = y ~ x,  
             se = FALSE,  
             color = "black") +  
  facet_wrap(~ economist) +  
  geom_vline(xintercept = 70, linetype = "dashed") +  
  theme(legend.position = "bottom")
```



The typical bias-variance trade-off in ML

Typically, ML models strive to find levels of bias and variance that are "just right":



When is the Bias-Variance Trade-off Important?

In low-dimensional settings ()

- overfitting is highly **unlikely**
- training MSE closely approximates test MSE
- conventional tools (e.g., OLS) will perform well on a test set

INTUITION: As , insignificant terms will converge to their true value (zero).

In high-dimensional settings ()

- overfitting is highly **likely**
- training MSE poorly approximates test MSE
- conventional tools tend to overfit

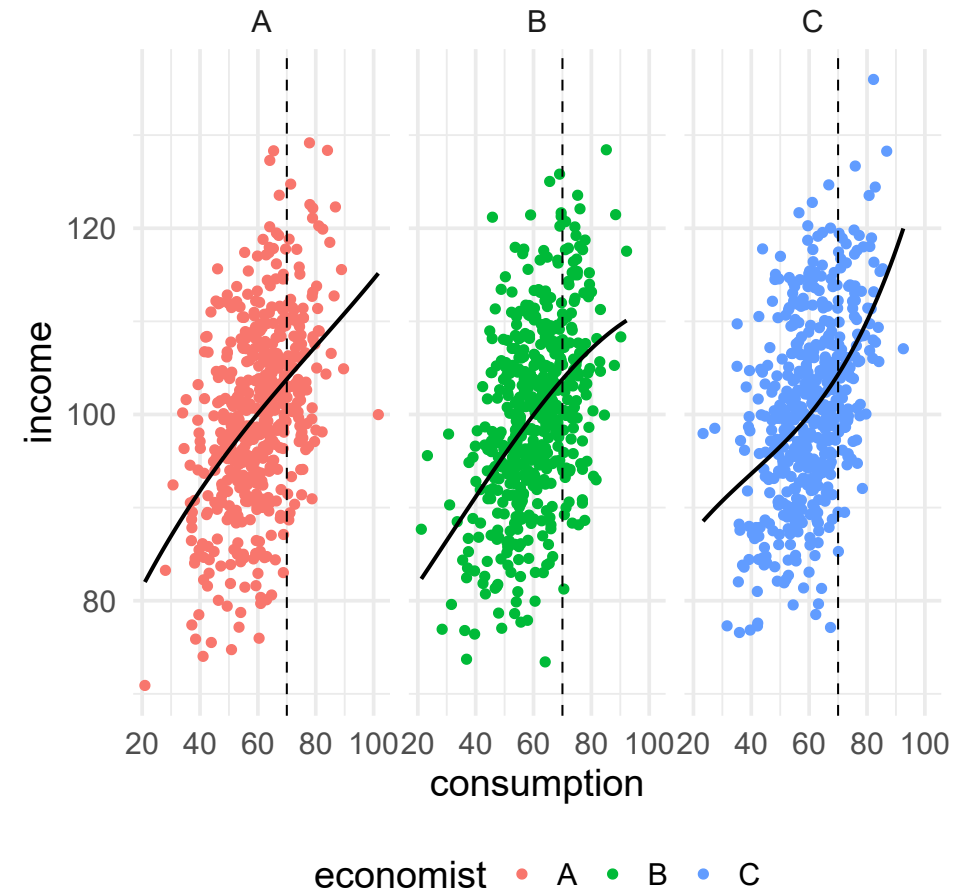
is prevalent in big-data

Bias-variance trade-off in low-dimensional settings

The model is a 3rd degree polynomial

only now, the sample size for each economist increases to $n = 100$.

INTUITION: as n increases, the estimates of the parameters $\beta_0, \beta_1, \beta_2, \beta_3$ converge to their true value, zero.



Regularization

Regularization

- As the *complexity* of our model goes up, it will tend to overfit.
- **Regularization** is the act of penalizing models for their complexity level.

Regularization typically results in simpler and more accurate (though “wrong”) models.

How to penalize overfit?

The test set MSE is *unobservable*. How can we tell if a model overfits?

- Main idea in machine learning: use *less* data!
- Key point: fit the model to a subset of the training set, and **validate** the model using the subset that was *not* used to fit the model.
- How can this "magic" work? Recall the stable DGP assumption.

Validation

Split the sample to three folds: a training set, a validation set and a test set:



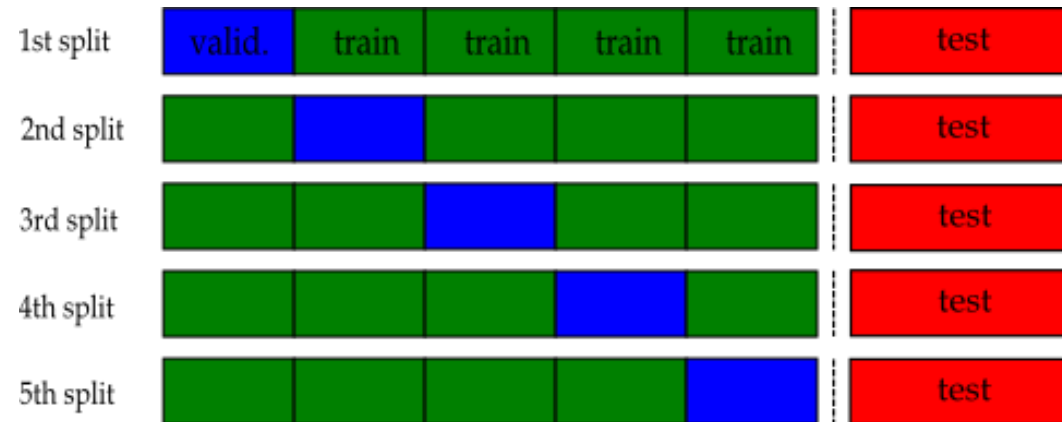
The algorithm:

1. Fit a model to the training set.
2. Use the model to predict outcomes from the validation set.
3. Use the mean of the squared prediction errors to approximate the test-MSE.

CONCERNS: (1) the algorithm might be sensitive to the choice of training and validation set; (2) the algorithm does not use all of the available information.

k-fold cross-validation

Split the training set into roughly equal-sized parts (in this example):



Approximate the test-MSE using the mean of split-MSEs

—

Which model to choose?

- Recall that the test-MSE is unobservable.
- CV-MSE is our best guess.
- CV-MSE is also a function of model complexity.
- Hence, model selection amounts to choosing the complexity level that minimizes CV-MSE.

Sounds familiar?

- In a way, you probably already know this:
 - Adjusted R^2 .
 - AIC, BIC (time series models).

The above two measures indirectly take into account the overfitting that may occur due to the complexity of the model (i.e., adding too many covariates or lags).

- In ML we use the data to tune the level of complexity such that it maximizes prediction accuracy.

Putting it All Together

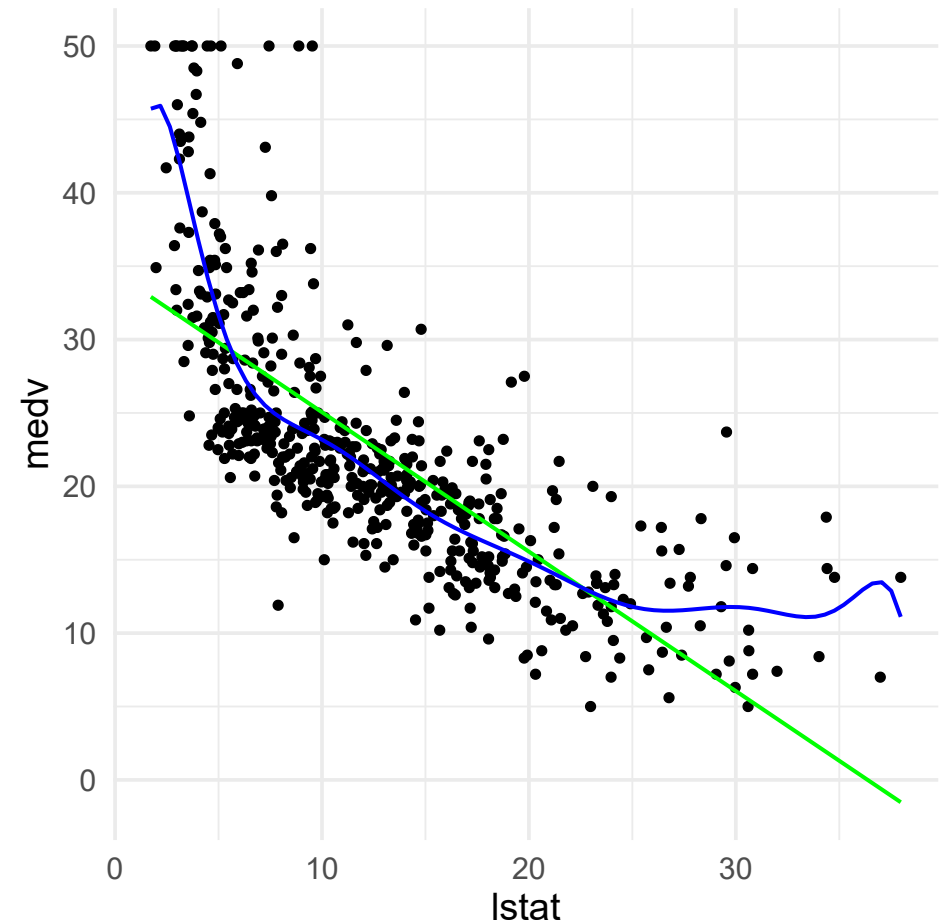
Toy problem: Predicting Boston housing prices

We will use the BostonHousing: housing data for 506 census tracts of Boston from the 1970 census ([Harrison Jr and Rubinfeld, 1978](#))

- medv (outcome): median value of owner-occupied homes in USD 1000's.
- lstat(predictor): percentage of lower status of the population.

OBJECTIVE: Find the best prediction model within the class of polynomial regression.

Examples: in green: linear relation ;
in blue, .



Step 1: The train-test split

We will use the `initial_split()`, `training()` and `testing()` functions from the **rsample** package to perform an initial train-test split

```
set.seed(1203) # for reproducibility

df_split <- initial_split(df, prop = 0.75)
df_split
```

```
## <380/126/506>
```

```
training_df <- training(df_split)
testing_df  <- testing(df_split)

head(training_df, 5)
```

```
## # A tibble: 5 x 2
##   medv lstat
##   <dbl> <dbl>
## 1  21.6   9.14
## 2  34.7   4.03
## 3  36.2   5.33
## 4  28.7   5.21
## 5  22.9  12.4
```

Step 2: Prepare 10 folds for cross-validation

We will use the `vfold_cv()` function from the **rsample** package to split the training set to 10-folds:

```
cv_data <- training_df %>%  
  vfold_cv(v = 10) %>%  
  mutate(train      = map(splits, ~training(.x)),  
         validate   = map(splits, ~testing(.x)))  
cv_data
```

```
## # 10-fold cross-validation  
## # A tibble: 10 x 4  
##   splits      id    train      validate  
## * <list>    <chr> <list>    <list>  
## 1 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>  
## 2 <split [342/38]> Fold02 <tibble [342 x 2]> <tibble [38 x 2]>  
## 3 <split [342/38]> Fold03 <tibble [342 x 2]> <tibble [38 x 2]>  
## 4 <split [342/38]> Fold04 <tibble [342 x 2]> <tibble [38 x 2]>  
## 5 <split [342/38]> Fold05 <tibble [342 x 2]> <tibble [38 x 2]>  
## 6 <split [342/38]> Fold06 <tibble [342 x 2]> <tibble [38 x 2]>  
## 7 <split [342/38]> Fold07 <tibble [342 x 2]> <tibble [38 x 2]>  
## 8 <split [342/38]> Fold08 <tibble [342 x 2]> <tibble [38 x 2]>  
## 9 <split [342/38]> Fold09 <tibble [342 x 2]> <tibble [38 x 2]>  
## 10 <split [342/38]> Fold10 <tibble [342 x 2]> <tibble [38 x 2]>
```


Step 3: Set search range for lambda

We need to vary the polynomial degree parameter when building our models on the train data. In this example, we will set the range between 1 and 10:

```
cv_tune <- cv_data %>%  
  crossing(lambda = 1:10)
```

```
cv_tune
```

```
## # A tibble: 100 x 5
```

```
##   splits      id  train      validate      lambda  
##   <list>    <chr> <list>    <list>    <int>  
## 1 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      1  
## 2 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      2  
## 3 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      3  
## 4 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      4  
## 5 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      5  
## 6 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      6  
## 7 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      7  
## 8 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      8  
## 9 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>      9  
## 10 <split [342/38]> Fold01 <tibble [342 x 2]> <tibble [38 x 2]>     10  
## # ... with 90 more rows
```

Step 4: Estimate CV-MSE

We now estimate the CV-MSE for each value of λ .

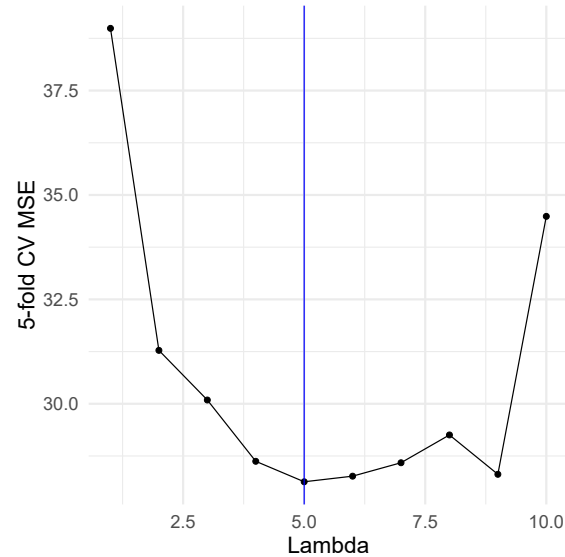
```
cv_mse <- cv_tune %>%  
  mutate(model = map2(lambda, train, ~ lm(medv ~ poly(lstat, .x), data = .y))) %>%  
  mutate(predicted = map2(model, validate, ~ augment(.x, newdata = .y))) %>%  
  unnest(predicted) %>%  
  group_by(lambda) %>%  
  summarise(mse = mean((.fitted - medv)^2))
```

cv_mse

```
## # A tibble: 10 x 2  
##   lambda    mse  
##   <int> <dbl>  
## 1      1  39.0  
## 2      2  31.3  
## 3      3  30.1  
## 4      4  28.6  
## 5      5  28.1  
## 6      6  28.3  
## 7      7  28.6  
## 8      8  29.3  
## 9      9  28.3  
## 10     10  34.5
```

Step 5: Find the best model

Recall that the best performing model minimizes the CV-MSE.



"[I]n reality there is rarely if ever a true underlying model, and even if there was a true underlying model, selecting that model will not necessarily give the best forecasts..."

Step 6: Use the test set to evaluate the best model

Fit the best model () to the training set, make predictions on the test set, and calculate the test root mean square error (test-RMSE):



```
training_df %>%  
  lm(medv ~ poly(lstat, 5), data = .) %>% # fit model  
  augment(newdata = testing_df) %>%      # predict unseen data  
  rmse(medv, .fitted)                    # evaluate accuracy
```

```
## # A tibble: 1 x 3  
##   .metric .estimator .estimate  
##   <chr>   <chr>      <dbl>  
## 1 rmse    standard      5.11
```

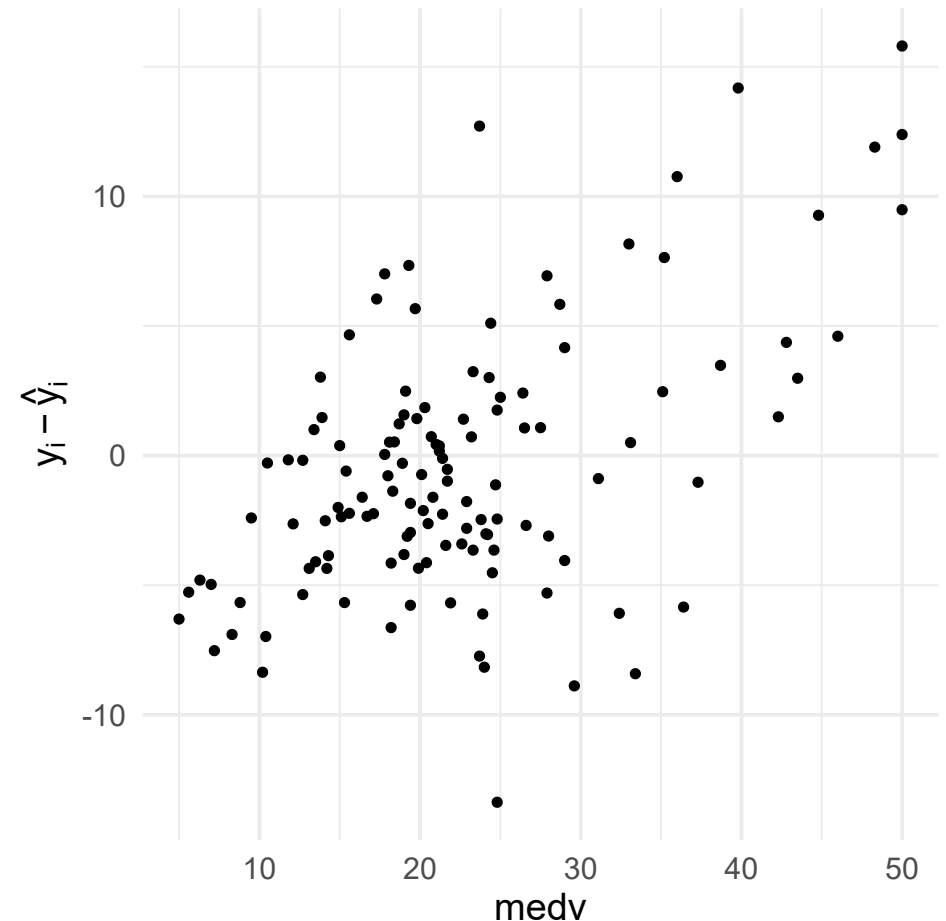
NOTE: the test set RMSE is an estimator of the expected squared prediction error on unseen data *given* the best model.

An aside: plot your residuals

The distribution of the prediction errors are another important sources of information about prediction quality.

```
training_df %>%  
  lm(medv ~ poly(lstat, 5), data = .) %>%  
  augment(newdata = testing_df) %>%  
  mutate(error = medv - .fitted) %>%  
  ggplot(aes(medv, error)) +  
  geom_point() +  
  labs(y = expression(y[i] - hat(y)[i]))
```

For example, see how biased the prediction for high levels of medv are.



ML and econometrics

ML vs. econometrics

Apart from jargon (Training set vs. in-sample, test-set vs. out of sample, learn vs. estimate, etc.) here is a summary of some of the key differences between ML and econometrics:

Machine Learning	Econometrics
prediction	causal inference
minimize prediction error	unbiasedness, consistency, efficiency
---	statistical inference
stable environment	counterfactual analysis
black-box	structural

ML and causal inference

"Data are profoundly dumb about causal relationships."

— Pearl and Mackenzie, *The Book of Why*

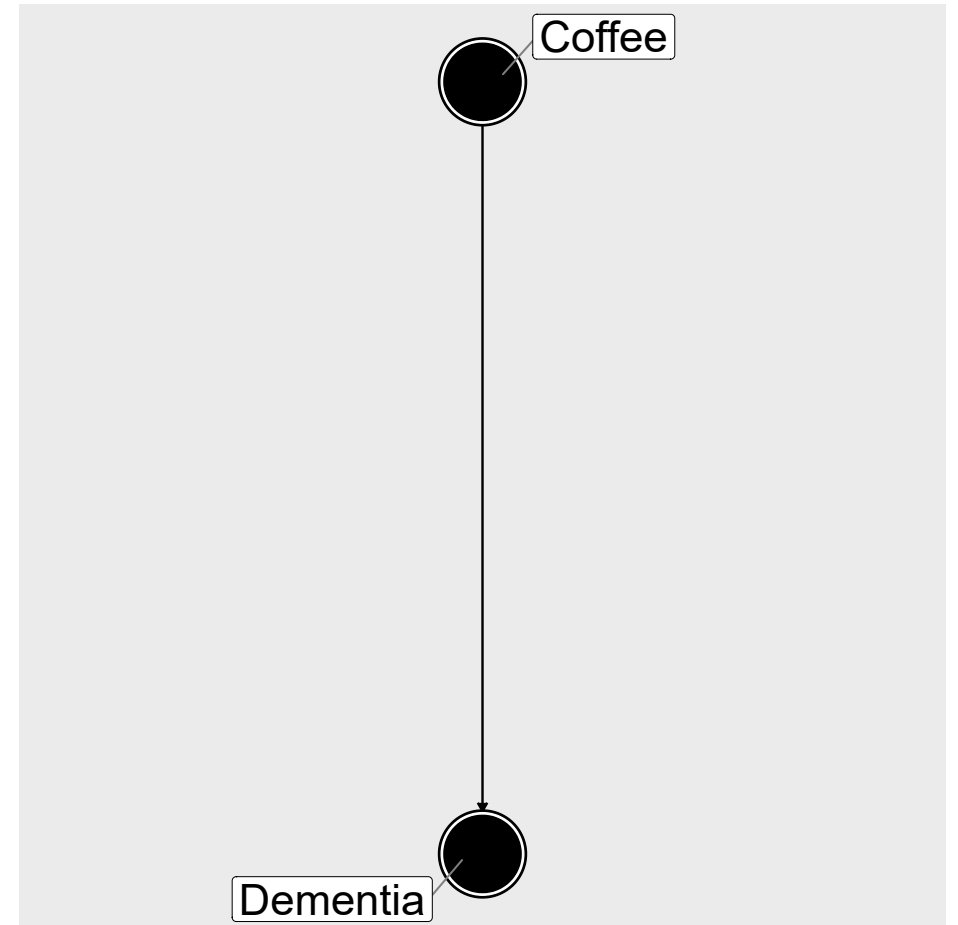
Intervention violates the stable DGP assumption:

where

- $P(Y=y|X=x)$ is the the probability of $Y=y$ given that we *observe* $X=x$.
- $P(Y=y|X=x, Z=z)$ is the the probability of $Y=y$ given that we *intervene* to set $Z=z$.

"A new study shows that..."

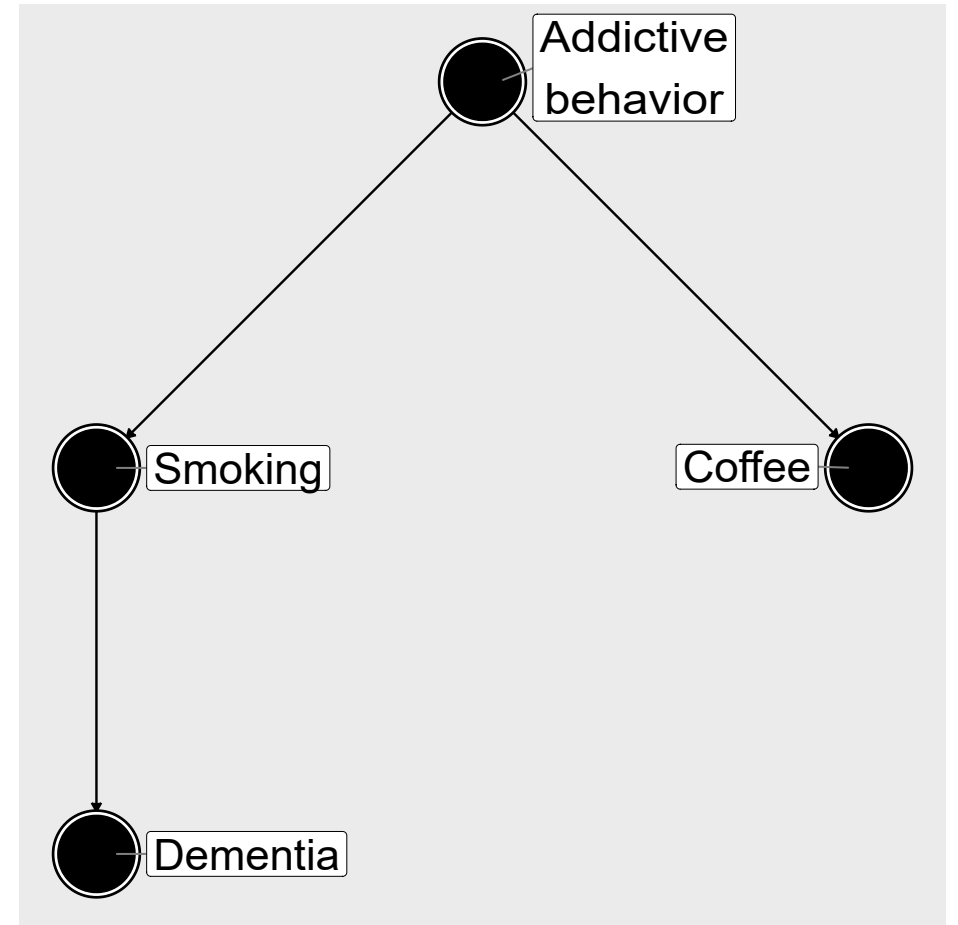
TOY PROBLEM: Say that we find in the data that coffee is a good predictor of dementia. Is avoiding coffee a good idea?



To explain or to predict?

- In this example coffee is a good *predictor* of dementia, despite not having any causal link to it.
- Controlling for smoking will give us the causal effect of coffee on dementia, which is zero.

In general, causal inference always and everywhere depends on *assumptions* about the DGP (i.e., the data never "speaks for itself").



ML in aid of econometrics

Consider the standard "treatment effect regression":

where

- An outcome
- A treatment assignment
- A vector of control variables

Our object of interest is often τ , the average treatment effect (ATE).

```
slides::end()
```

 [Source code](#)

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