1. A Framework for Prediction

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Data Analysis 3: Prediction

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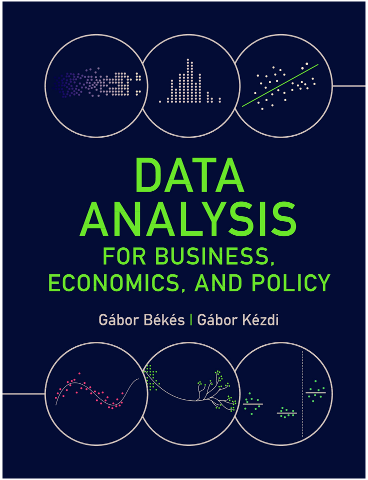
Slideshow for the Békés-Kézdi Data Analysis textbook



- Cambridge University Press, 2021 April
- Available in paperback, hardcover and e-book
- **gabors-data-analysis.com**
  - Download all data and code `https://gabors-data-analysis.com/data-and-code/`
- This slideshow is for **Chapter 13**
  - Slideshow be used and modified for educational purposes only

Prediction setup

- Original data (what we have) –> to build a model
- Live data (data we do not have yet)

- Target variable Y (=dependent variable, response, outcome)
- Predictor variables X (= inputs, covariates, features, independent variables)

- Need to predict value of Y for target observation j in live data
  - Actual value for Y_j unknown
  - Value for X_j known
  - May be more than one target observation
    - Need predicted value of Y for each

Price cars (Case study 1)

The situation

- You want to sell your car through online advertising
- Target is continuous (in dollars)
- Features are continuous or categorical

- The business question
  - What price should you put into the ad?

Price apartments (Case study 2)

The situation

- You are planning to run an AirBnB business
  - Maybe several rooms
- Target is continuous (in dollars)
- Features are varied from text to binary

- The business question
  - How should you price apartments/houses?

Predict company's exit from business (Case study 3)

- Consulting company
- Predict which firms will go out of business (exit) from a pool of partners
- Target is binary: exit / stay
- Features of financial and management info
- Business decision
  - Which firms to give loan to?

Predictive Analysis: what is new?

- DA2 focused on the relationship between X and Y
  - What is the relationship like
  - Is it a robust relationship – true in the population /general pattern?
- Now, we use $x_1, x_2, \ldots$ to predict y

$$\hat{y}_j = \hat{f}(x_j)$$

- How is this different?
- We care less about
  - Individual coefficient values, multicollinearity
  - We still care about the stability of our results.
  - Should we care about causality?

Prediction setup

- Y is quantitative (e.g price)
- Quantitative prediction
  - „Regression" problem

- Y is binary (e.g. Default ot nor)
- Probability prediction
- Classification problem
  - Broadly: Y takes values in a finite set of (unordered) classes (survived/died, sold/not sold, car model)

- Time series prediction (Forecasting)

Our focus in DA3

- Feature engineering (variable selection)
  - choose variables,
  - coding, functional form
- Model building and prediction
  - Estimate models
  - Regressions with a variety of interactions, non-linear functional forms
    - Remember splines, polynomials
  - Machine learning methods
    - Automated model selection under some conditions
- Model evaluation and selection
  - Compare models based on some measure of fit

- Key idea in prediction: systematically combine estimation and model selection

Regression and prediction

- Linear regression produces a predicted value for the dependent variable.
  - Predictions: regressions tell the expected value of y if we know x.
- Linear regression with y, x_1, x_2, etc., is a model for the conditional expected value of y, and it has coefficients β.
- We need estimated coefficients ($\hat{\beta}$) and actual x values (x_j) to predict an actual value $\hat{y}$

$$y^E = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ...$$
$$\hat{y}_j = \hat{\beta}_0 + \hat{\beta}_1 x_{1j} + \hat{\beta}_2 x_{2j} + ...$$

The Prediction Error

- Predicted value $\hat{y}_j$
  - for target observation j
- Actual value $_j$
  - for target observation j
  - Unknown when we make the prediction
- Prediction error

$$e_j = \hat{y}_j - y_j$$

  - Error = predicted value – actual value

Prediction Error

- The ideal prediction error, is zero: our predicted value is right on target. The prediction error is defined by direction of miss and size.
- Direction of miss
  - Positive if we overpredict the value: we predict a higher value than actual value.
  - Negative if we underpredict the value: our prediction is too low.
  - Whether positive versus negative errors matter more, or they are equally bad, depends on the decision problem.
- Size
  - Larger in absolute value the further away our prediction is from the actual value.
  - It is smaller the closer we are.
  - It is always better to have a prediction with as small an error as possible.

Decomposing the prediction error

- The prediction error is the difference between the predicted value of the target variable and its actual (yet unknown) value for the target observation:

$$e_j = \hat{y}_j - y_j$$

- The prediction error can be decomposed into three parts:
  1. **estimation error**: the difference between the estimated value from the model and the true value from the model
  2. **model error**: the difference between the true value from the model and the best predictor value; ie we may not have the best model
  3. **genuine error** (idiosyncratic or irreducible error): error due to not being able to perfectly estimate all predicted values even if estimation error is zero, and we have the best possible model.

Interval prediction for quantitative target variables

- One advantage of regressions - easy quantify uncertainty of prediction
- Interval predictions produce ranges to capture the uncertainty of predicted values
- Interval predictions quantify two out of the three sources of prediction uncertainty: estimation error and genuine (or irreducible) error.
- They do not include the third source, model uncertainty!
- The 95% prediction interval (PI) tells where to expect the actual value for the target observation.
  - The PI for linear regression requires homoskedasticity.

Reminder, prediction interval

- Remember from DA2...
  - Software will do it, don't worry about formulae

$$95\% PI(\hat{y}_j) = \hat{y} + -2SPE(\hat{y}_j)$$

The simple formula for the $SPE(\hat{y}_j)$ is

$$SPE(\hat{y}_j) = Std[e]\sqrt{1 + \frac{1}{n} + \frac{(x_j - \bar{x})^2}{nVar[x]}}$$

Loss Functions

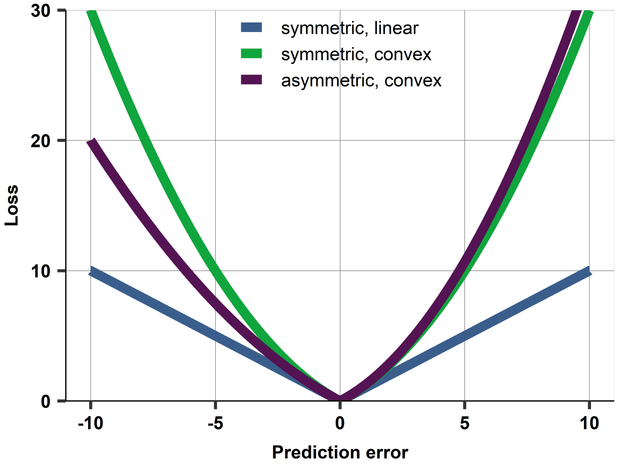
- Value attached to the prediction error
  - Specifying how bad it is
- Loss function determines best predictor
- Ideally derived from decision problem
  - Consequence of error is bad decision
  - Loss due to bad decision
- Difficult to quantify exact value of loss in practice
- But this could be super important in some business cases
  - Even if hard to adjust modelling

Loss Functions

- Think about qualitative characteristics of loss function
- The most important qualitative characteristics of loss functions:

- Symmetry
  - If losses due to errors in opposing direction are similar
- Convexity
  - If twice as large errors generate more than twice as large losses

Loss Functions of Various Shapes



Examples 1 – used cars

- The loss function for predicting the value of our used car depends on how we value money and how we value how much time it takes to sell our car.
- A too low prediction may lead to selling our car cheap but fast;
- A too high prediction may make us wait a long time and, possibly, revising the sales price downwards before selling our car.

- What kind of loss function would make sense?

Examples 2 - creditors

- Creditors decide whether to issue a loan only to potential debtors that are predicted to pay it back with high likelihood.
- Two kinds of errors are possible:
  - debtors that would pay back their loan don't get a loan
  - debtors that would not pay back their loan get one nevertheless.
- The costs of the first error are due to missed business opportunity; the costs of the second error are due to direct loss of money.
- These losses may be quantified in relatively straightforward ways.
- What kind of loss function would make sense?

Squared Loss

- $L(e_j) = e_j^2 = (\hat{y}_j - y_j)^2$
- The most widely used loss function
  - Symmetric: Losses due to errors in opposing direction are same
  - Convex: Twice as large errors generate more than twice as large losses
- Business sense ?

Adding up – MSE and MAE

- Many target observations in practice
- Or we can think about many situations with a single target observation
- Squared loss -> Mean Squared Error (MSE)

For $k = 1...K$ observations:

$$MSE = \frac{1}{K}\sum_{k=1}^{K}(\hat{y}_k - y_k)^2$$

(1)

$$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{K}\sum_{k=1}^{K}(\hat{y}_k - y_k)^2} \quad (2)$$

MSE implies expected value

$$MSE = \frac{1}{K}\sum_{k=1}^{K}(\hat{y}_k - y_k)^2$$

- MSE implies mean value for best predictor
  - Linear (least squares) regression
  - Why?
    - Because the solution to least squares minimization problem is the average.
    - Technically: first-order condition of minimization problem
- RMSE = square root of MSE
  - MSE is the numerator of the R-squared!

MSE decomposition : Bias and Variance

May decompose MSE into Bias + Variance

- The bias of a prediction is the average of its prediction error.
  - An unbiased prediction produces zero error on average across multiple predictions.
  - A biased prediction produces nonzero error on average; the bias can be positive or negative
- The variance of a prediction describes how it varies around its average value when multiple predictions are made.
  - It's the variance of the prediction error around its average value.
  - The variance is zero if the prediction error is the same for all predictions.
  - The variance is higher the larger the spread of specific predictions around the average prediction

MSE decomposition : Bias and Variance

- MSE is the sum of squared bias and the prediction variance.
- This decomposition helps appreciate a trade-off.

$$
\begin{aligned}
MSE &= \frac{1}{K}\sum_{k=1}^{K}(\hat{y}_k - y_k)^2 \\
&= (\frac{1}{K}\sum_{k=1}^{K}(\hat{y}_k - \bar{y}))^2 + \frac{1}{K}\sum_{k=1}^{K}(y_k - \bar{y})^2 \\
&= Bias^2 + PredictionVariance
\end{aligned}
$$

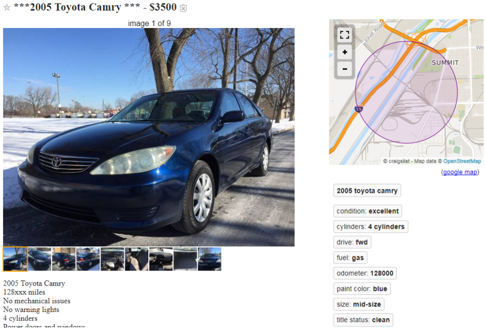
- OLS is unbiased. Some other methods will allow for some bias in return for lower variance.

Case study: used cars data

- Suppose you want to sell your car of a certain make, type, year, miles, condition and other features.
- The prediction analysis helps uncover the average advertised price of cars with these characteristics
  - That helps decide what price you may want to put on your ad.

Case study: used cars data

- Scraped from a website
- Year of make (age), Odometer (miles)
- Tech specifications such as fuel and drive
- Dealer or private seller



Case study: Loss function

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- A too low prediction may lead to selling our car cheap but fast;
- A too high prediction may make us wait a long time and, possibly, revising the sales price downwards before selling our car.

- Symmetric
- Sensitive to big deviations
- RMSE and OLS

Case study - used cars: features

- Odometer, measuring miles the car traveled (**Continuous, linear**)
- More specific type of the car: LE, XLE, SE (missing in about 30% of the observations). (**Factor – set of dummies , incl N/A**)
- Good condition, excellent condition or it is like new (missing for about one third of the ads). (**Factor – set of dummies, incl N/A**)
- Car's engine has 6 cylinders (20% of ads say this; 43% says 4 cylinders, and the rest has no information on this). (**Binary for 6 cylinders**)

Case study: models by hand

- Model 1: age, age squared
- Model 2: age, age squared, odometer, odometer squared
- Model 3: age, age squared, odometer, odometer squared, LE, excellent condition, good condition, dealer
- Model 4: age, age squared, odometer, odometer squared, LE, excellent condition, good condition, dealer, LE, XLE, cylinder
- Model 5: same as Model 4 but with all variables interacted with age (won't show in next table)

Case study: Car price model results

VARIABLES	(1) Model 1	(2) Model 2	(3) Model 3	(4) Model 4
age	-1,530.09	-1,149.22	-873.47	-836.64
agesq	35.05	27.65	18.21	17.63
odometer		-303.84	-779.90	-788.70
odometersq			18.81	19.20
LE			28.11	-20.48
XLE				301.69
SE				1,338.79
cond_likenew				558.67
cond_excellent			176.49	190.40
cond_good			293.36	321.56
cylind6				-370.27
dealer			572.98	822.65
Constant	18,365.45	18,860.20	19,431.89	18,963.35
R-squared	0.847	0.898	0.913	0.919

Note: *Chicago cars. Prices in dollars. N=281. Source:* `used-cars` *dataset.*

Case study: Results

- When doing prediction, coefficients are less important.
- But we shall use them for sanity check: age negative, convex (flattens out)
- SE may not be even displayed. It is helpful for model selection, but only along with other measures

- and values of the predictor variables for our car: age = 10 (years), odometer= 12 (10 thousand miles), type= LE, excellent condition=1.

Case study: Results

- When doing prediction, coefficients are less important.
- But we shall use them for sanity check: age negative, convex (flattens out)
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- and values of the predictor variables for our car: age = 10 (years), odometer= 12 (10 thousand miles), type= LE, excellent condition=1.
- A point prediction, Model 3: age: -873.47, age squared=18.21, odometer -799.90, odometer sq = 18.81, LE=28.11, cond excellent: 176.49+ C=19.431.89
- Predicted is price is 6073.

Case study: Prediction Interval

- Calculating prediction intervals for the baseline models
- Very wide interval despite high R2
- Prediction is hard!
- Even with a good model, you'll make plenty of errors
- Should be aware
- Let your clients know in advance...

Case study: Prediction Interval

- Based on the third model, we have a point prediction of $6073
- Have a 80% prediction intervals (PI) – Ads for cars just like ours may ask a price ranging from $4,317 to $7,829 with a 80% chance.

Table: Car price model

	Model 1	Model 3
Point prediction	6,569	6,073
Prediction Interval (80%)	[4,296-8,843]	[4,317-7,829]
Prediction Interval (95%)	[3,085-10,053]	[3,382-8,763]

Note: *Chicago cars. Prices in dollars.*
Source: `used-cars` dataset.

Model selection

Model selection is finding the best fit while avoiding overfitting and aiming for high external validity

External validity, avoiding overfitting and model selection

- Have a dataset and a target variable. Compare various models of prediction.
- How to choose a model?

- Pick a model that can predict well....
  - Best prediction - best model that would produce the smallest prediction error.
  - Context of squared loss function –> finding the regression that would produce the smallest RMSE for the target observations.

External validity, avoiding overfitting and model selection

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- How to choose a model?

- Pick a model that can predict well....
  - Best prediction - best model that would produce the smallest prediction error.
  - Context of squared loss function –> finding the regression that would produce the smallest RMSE for the target observations.
- Pick a model that can predict well on the **live data**

Underfit, overfit

- Comparing two models (model 1 and model 2)
- Model 1 can give a worse fit in the live data than model 2 in two ways.
- Model 1 may give a worse fit both in the original data and the **live** data. In this case, we say that model 1 underfits the original data.
  - Simple: we should build a better model.
- Model 1 may actually give a better fit in the original, but a worse fit in the **live** data. In this case, we say that model 1 overfits the original data.

Overfitting

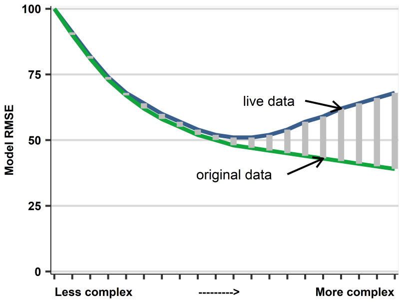
- Overfitting is a key aspect of external validity
  - finding a model that fits the data better than alternative models
  - but makes worse actual prediction.

- Thus, the problem of overfitting the original data is best split into two problems:
- fitting patterns in the original data that are not there in the population, or general pattern, it represents;
- fitting patterns in the world of the original data that will not be there in the world of the live data.

Reason for overfitting

- The typical reason for overfitting is fitting a model that is too complex on the dataset.
  - Complexity: number of estimated coefficients
- Often: fitting a model with too many predictor variables.
  - Including too many variables from the dataset that do not really add to the predictive power of the regression,
    - often because they are strongly correlated with other predictor variables.
- Specifying too many interactions,
- Too detailed nonlinear patterns
  - as piecewise linear splines with many knots
  - polynomials of high degree.

Increasing model complexity



- As we increase model complexity
- Such as number of features (variables)
  - By adding interactions, etc.
- We will see
  - RMSE within dataset to fall monotonously
  - RMSE for target observations (ie. not in our dataset) to fall and then rise as we overfit
    - example to come in class 2

Finding the best model by best fit and penalty: The BIC

- *Approach 1: Indirectly*
- Estimate it by an adjustment
  - Use a method based on some distributional assumptions
  - Need to pick an evaluation criterion
- =In-sample evaluation with penalty
  - Specify and estimate model using all data
  - Use a measure of fit that helps avoid overfitting
- Such as
  - adjusted R^2
  - BIC = Bayesian Information Criterion, or Schwarz criterion

Indirect evaluation criteria

- Main methods: AIC, BIC and adjusted R^2
  - Advantage: easy to compute
  - Disadvantage: assumptions
- Adjusted R^2 – just add a penalty for having many RHS vars
  - corrects with $(n-1)/(n-p-1)$
- Akaike Information Criterion
  - $\text{AIC} = -2 \times ln(likelihood) + 2 \times k$
- Schwarz – Bayesian Information Criterion
  - $\text{BIC} = -2 \times ln(likelihood) + ln(N) \times k$
    - Both quantities that take the log likelihood and apply a penalty for the number of parameters being estimated.Both are based on information loss theory from the fifties.
    - BIC puts heavier penalty on models with many RHS variables, than AIC.

Model fit evaluation

- Use a good measure of fit to compare models.
- Don't
  - Don't use MSE or R-squared (the two very closely related).
  - They choose best fit in data and don't care about overfitting.
- In practice, use BIC.
  - BIC good approximation of what more sophisticated methods would pick. Or even more conservative...
  - That introduces a "penalty term"
    - More predictor variables leads to worse value
    - Even more so in large samples.

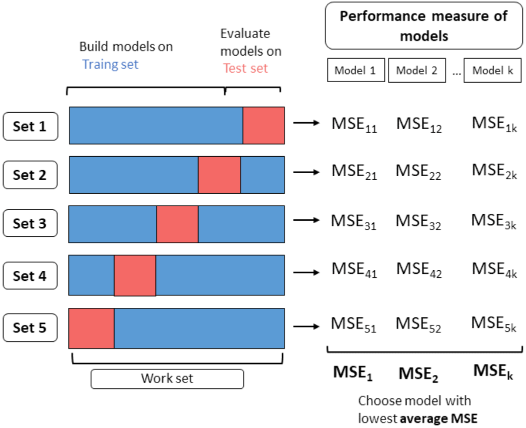
Finding the best model by training and test samples

- *Approach Nr.2: Directly*
- Estimate it using a test (validation) set approach.
  - Needs cutting the dataset into training and test sample
  - No assumption
  - Need to pick evaluation criterion (loss function) = RMSE (root mean squared error)
- Estimate the model in part of the data (say, 80%).
  - *Training sample*
- Evaluate predictive performance on the rest of the data.
  - *Test sample*
- Avoid overfitting in training data by evaluating on test data.

Training and Test Samples

- Creating two sub-samples
  - Randomly! (ie. not 1—80 and 81—100)
- Randomly generate an ID, sort and create two sub-samples.
- Training sample 80%
  - Regressions will be on run on this sample
  - Coefficients estimated
- Test (validation) sample 20%
  - Using estimated coefficients, we predict values for flats in the validation sample
  - Calculate residual, RMSE in the test sample
    - RMSE rather than MSE – smaller numbers....

5-fold cross-validation



- Split sample k=5 times to train and test
- For each folds:
  - Estimate model on training.
  - Get coefficients.
  - Use them to estimate on Test
  - Calculate test MSE
- Average and take Sqrt
- Repeat for models
- Pick model w lowest avg RMSE

BIC vs test RMSE

- In our experience, in practice, BIC is the best indirect criterion – closest to test sample.

- The advantage of BIC is that it needs no sample splitting which may be a problem in small samples.
- The advantage of test MSE is that it makes no assumption.

- BIC is a good first run, quick, is often not very wrong.
- Ultimately, you want to do a test MSE.

Case study: Model selection

- We have the ingredients, we need to pick a model.
- This process involves variable selection and a decision rule of choosing the model based on some loss function.

- BIC on the actual data
- Test-sample RMSE
- Cross-validated (CV) RMSE

- If enough data / computer power, use CV RMSE
- With larger dataset, overfit becomes less of an issue.

Case study: Model selection

Table: Car price models -BIC and in-sample RMSE

	Model	N vars	N coeff	R-squared	RMSE	BIC
1	Model 1	1	3	0.85	1,755	5,018
2	Model 2	2	5	0.90	1,433	4,910
3	Model 3	5	9	0.91	1,322	**4,893**
4	Model 4	6	12	0.92	1,273	**4,894**
5	Model 5	6	22	0.92	**1,239**	4,935

Note: *In sample values. Model 1: age, age squared, Model 2= Model 1 +odometer, odometer squared, Model 3= Model2 + SE, excellent condition, good condition, dealer, Model 4= Model 3 + LE, XLE, like new condition, 6cylinder, Model 5 = Model 4 + many interactions.* Source: `used-cars` dataset.

Case study: Model selection

- Cross-validate using 4-fold cross validation.
- Run the regression on 3/4 of the sample, predicting on the remaining 1/4 of the sample, get RMSE on test sample.
- We then average out RMSE values over the 4 test samples

Table: Car price models -CV RMSE

	Fold No.	Model 1	Model 2	Model 3	Model 4	Model 5
1	Fold1	1,734	1,428	1,331	1,395	1,391
2	Fold2	2,010	1,781	1,692	1,638	1,693
3	Fold3	1,465	1,251	1,256	1,253	1,436
4	Fold4	1,823	1,325	1,250	1,246	1,307
5	Average	1,769	1,460	**1,394**	**1,392**	1,464

Source: `used-cars` dataset.

Case study: Model selection

- Model 3 has lowest BIC, lowest average RMSE on test samples. Model 4 is close.
- Interestingly, both approaches suggests that Model 3 is the one that has the best prediction properties
- Small sample, simple model.

External validity and stable patterns

- BIC, Training-test, k-fold cross-validation...
- All very nice
- But, in the end, they all use the information in the data.
- How would things look for the target observation(s)?
- The issue of stationarity – how our data is related to other datasets we may use our model
  - We may have some ideas
  - We may use non-random test samples that may mimic the difference in our data and the target observations
- **In the end we can't know but need to think about it.**
- **Plus be aware, that some difference is likely, so your model fit in an outside data source is likely to be worse...**

External validity and stable patterns

- Most predictions will be on future data
- High external validity requires that the environment is **stationary**.
- Stationarity means that the way variables are distributed remains the same over time.
  - Here that distribution is to be understood in a general way: the joint distribution of predictor variables and target variable are required to remain the same throughout the time covered in the data and the time of the forecast.
- Stationarity ensures that the relationship between predictors and the target variable is the same in the data and the forecasted future.
  - If the relationship breaks down whatever we establish in our data won't be true in the future, leading to wrong forecasts.

External validity and stable patterns

- External validity and stable patterns - Very broad concept
- It's about representativeness of actual data –> to live data
- Often hard to know.
  - Remember hotels (other dates, other cities).
- Domain knowledge can help.
- Study if patterns were stable in the past / other locations were stable can help.

Machine Learning and the Role of Algorithms

- **Predictive analytics** is often used for data analysis whose goal is prediction. But a more popular, and related, term is machine learning.
- **Machine learning** is an umbrella concept for methods that use algorithms to find patterns in data and use them for prediction purposes.
- An **algorithm** is a set of rules and steps that defines how to generate an output (predicted values) using various inputs (variables, observations in the original data).
- A **formula** is an example of an algorithm – one that can be formulated in terms of an equation.
  - OLS formula for estimating the coefficients of a linear regression is an algorithm.

Machine Learning Algorithms

- Machine learning is about algorithms, machines and learning

- Algorithms specify each and every step to follow in a clear way.
- Not all algorithms can be translated into a formula.
  - The bootstrap estimation of a standard error (Chapter 5, Section 5.6) is an example.
  - K-fold cross-validation.

- Heavy use of **machines** = computers. Steps of algorithm translated into computer code and make the computer follow those steps. Fast.
- Learning - learn something from the data with data and an algorithms.
  - Predicted value of y=? If combine x variables using a particular model.
  - learning which model is best for predicting y as well as what that predicted value is.

What is, machine learning?

- Many definitions, discussions.
- Here: Machine learning is an approach to predictive data analysis – achieving the best possible prediction from available data.
- Consequence 1: understanding the patterns of associations between y and x is of secondary importance.
  - We need stable patterns for good prediction in live data, but that is it.
- The machine learning *attitude* - a preference for evaluating methods based on data as opposed to abstract principles.
  - Original data to live data
  - Not a general rule or philosophy

- Machine learning broadly: all prediction models including OLS
- Machine learning narrowly: prediction models with no formula, ie not OLS