13. Framework for prediction

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Data Analysis 3: Prediction

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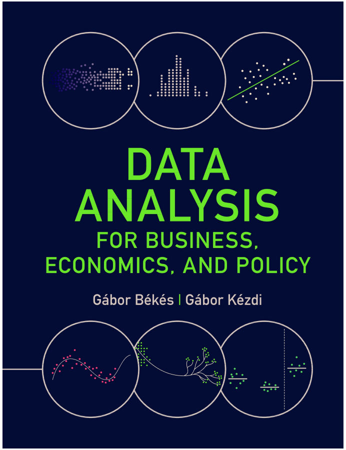
Slideshow for the Békés-Kézdi Data Analysis textbook


DATA ANALYSIS
FOR BUSINESS, ECONOMICS, AND POLICY
Gábor Békés | Gábor Kézdi

- Cambridge University Press, 2021
- **gabors-data-analysis.com**
  - Download all data and code: gabors-data-analysis.com/data-and-code/
- This slideshow is for **Chapter 13**

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?

- Earlier classes 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

- Time series prediction (Forecasting)

- 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 $\hat{y}$

$$y^E = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots$$

$$\hat{y}_j = \hat{\beta}_0 + \hat{\beta}_1 x_{1j} + \hat{\beta}_2 x_{2j} + \ldots$$

The Prediction Error

- Predicted value $\hat{y}_j$ for target observation j
- Actual value y_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

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

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

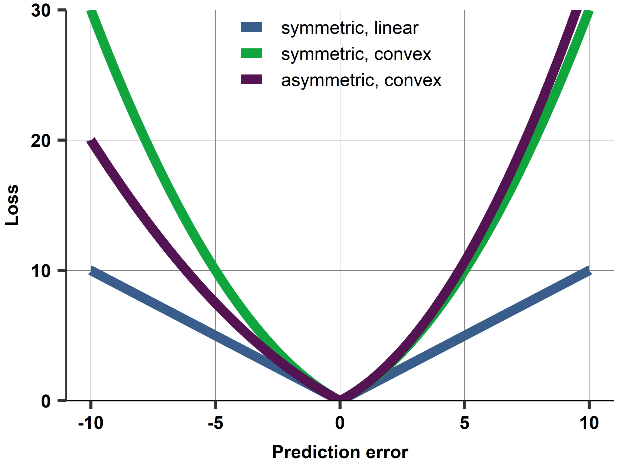
- Value attached to the prediction error
  - Specifying how bad it is
- Loss function determines best predictor
- Ideally derived from decision problem
  - Consequence of error is bad decision
  - Loss due to bad decision
- Difficult to quantify exact value of loss in practice
- But this could be super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



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

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

For $k = 1 \ldots K$ observations:

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

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

MSE decomposition : Bias and Variance

May decompose MSE into Bias + Variance

- The bias of a prediction is the average of its prediction error.
  - 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.
  - 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.

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

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

	(1)	**(2)**	**(3)**	**(4)**
Variables	**Model 1**	**Model 2**	**Model 3**	**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

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

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- 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

- 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?

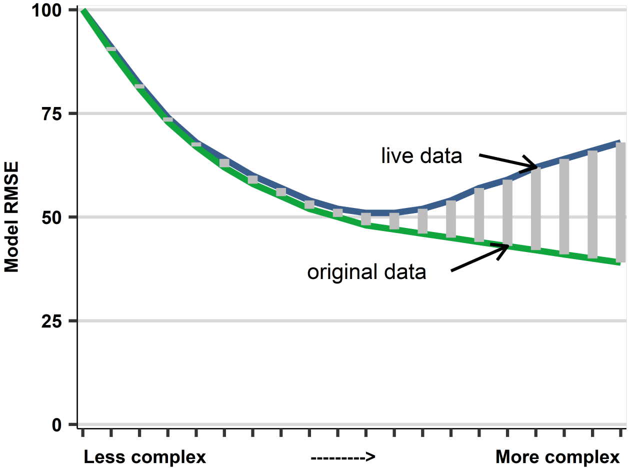
- Pick a model that can predict well....

- 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.
- 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.

Underfitting and overfitting 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.

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,

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

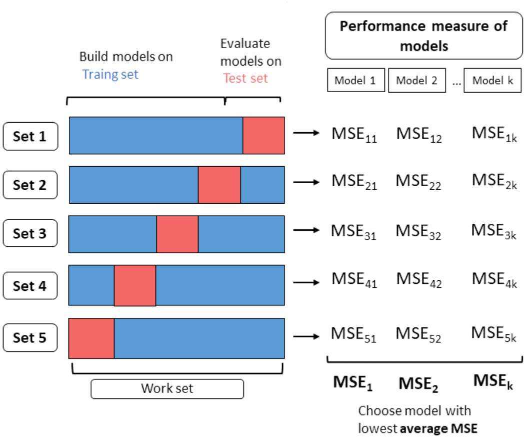
Model fit evaluation

- 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.

5-fold cross-validation


Build models on
Traing set
Evaluate models on
Test set
Performance measure of models
Work set
Choose model with lowest **average MSE**

	Model 1	Model 2	...	Model k
Set 1	MSE_{11}	MSE_{12}		MSE_{1k}
Set 2	MSE_{21}	MSE_{22}		MSE_{2k}
Set 3	MSE_{31}	MSE_{32}		MSE_{3k}
Set 4	MSE_{41}	MSE_{42}		MSE_{4k}
Set 5	MSE_{51}	MSE_{52}		MSE_{5k}
	MSE_1	MSE_2		MSE_k

- 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

Finding the best model by cross-validation

- The training–test split partitions the original data into two sets in a random way. All analysis and estimation takes place using observations in the training set. The evaluation of prediction takes place using observations in the test set
- The training–test split avoids overfitting the training set; however, it may overfit the test set
- k-fold cross-validation improves on the single training–test split by repeating it k times. Each split is called a fold. The prediction of a model is evaluated across the folds, such as the average MSE
- k-fold cross-validation is a good way to find the model that would give the best prediction for the population, or general pattern, represented by the original data

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)?

External validity and stable patterns

- A prediction has high external validity if the best model for the population, or general pattern, behind the original data is also the best model for the population, or general pattern, behind the live data
- High external validity of a prediction requires that the patterns of association between y and x are stable, so that they are very similar in the original data and the live data
- Domain knowledge, thinking, and data from multiple time periods can help assess external validity

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.

Main takeaways

- Prediction uses the original data with y and x to predict the value of y for observations in the live data, in which x is observed but y is not
  - Prediction uses a model that describes the patterns of association between y and x in the original data
  - Cross-validation can help find the best model in the population, or general pattern, represented by the original data
  - Stability of the patterns of association is needed for a prediction with high external validity