Hands-on Machine Learning with Python - Module 1

Hands-on webinar

Katrien Antonio & Jonas Crevecoeur & Roel Henckaerts

hands-on-machine-learning-Python-module-1 | March, 2023

Prologue

Introduction

Course

https://github.com/katrienantonio/hands-on-machine-learning-Python-module-1

The course repo on GitHub, where you can find the data sets, lecture sheets, Google Colab links and Python notebooks.

Us

https://katrienantonio.github.io/ & LinkedIn profile Jonas & LinkedIn profile Roel

katrien.antonio@kuleuven.be & jonas.crevecoeur@kuleuven.be & roel.henckaerts@kuleuven.be

(Katrien) Professor in insurance data science

(Jonas) PhD in insurance data science, now data science consultant at UHasselt and KULeuven

(Roel) PhD in insurance data science, now senior data analyst at Prophecy Labs

Why this course?

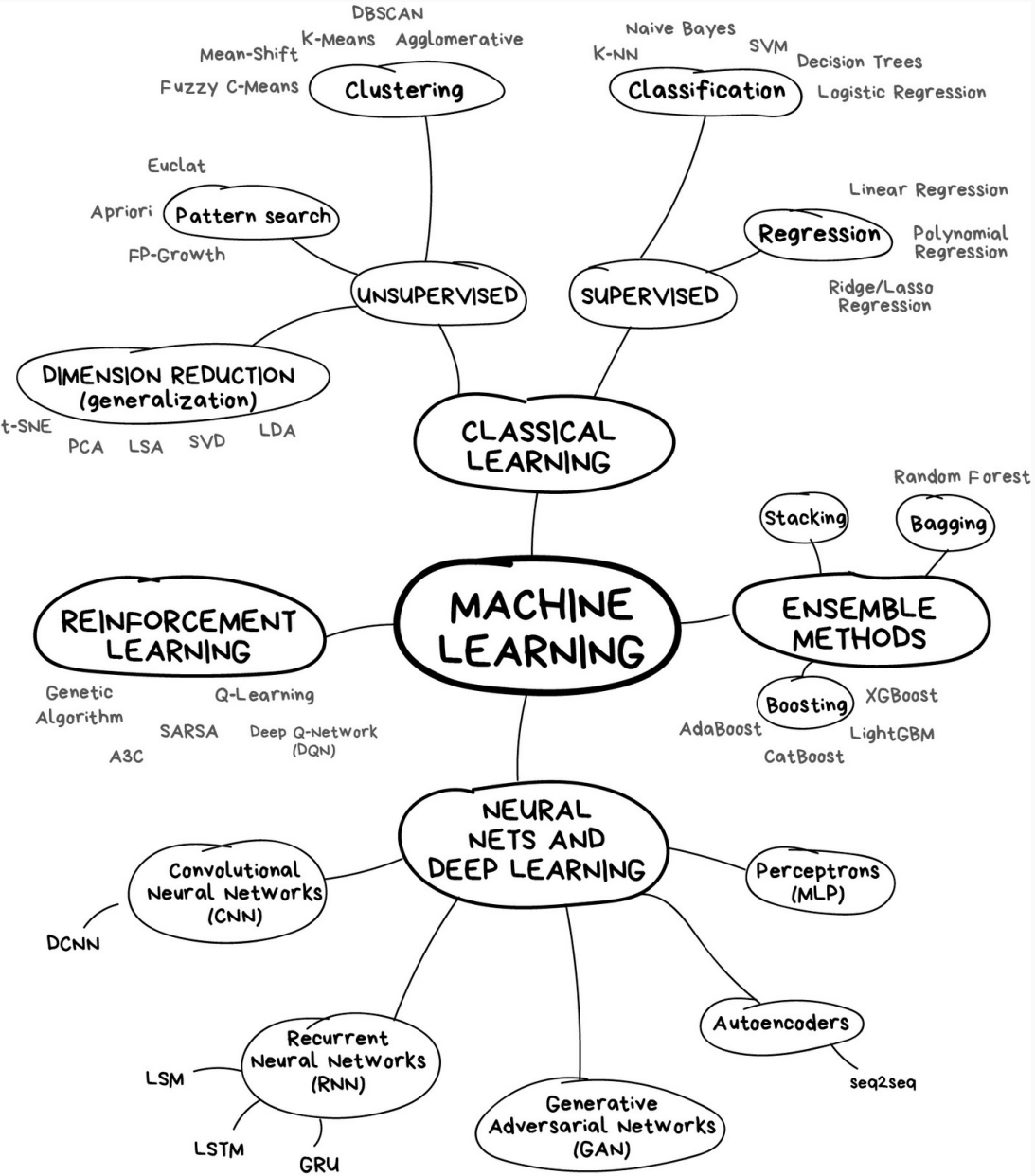
The goals of this course 🚀

- develop practical **machine learning (ML) foundations in Python**
- **fill in the gaps** left by traditional training in actuarial science or econometrics
- focus on the use of ML methods for the **analysis of frequency + severity data**, but also **non-standard data** such as images
- **explore** a substantial range of **methods (and data types)** (from GLMs to deep learning), but - most importantly - **build foundation** so that you can explore other methods (and data types) yourself.

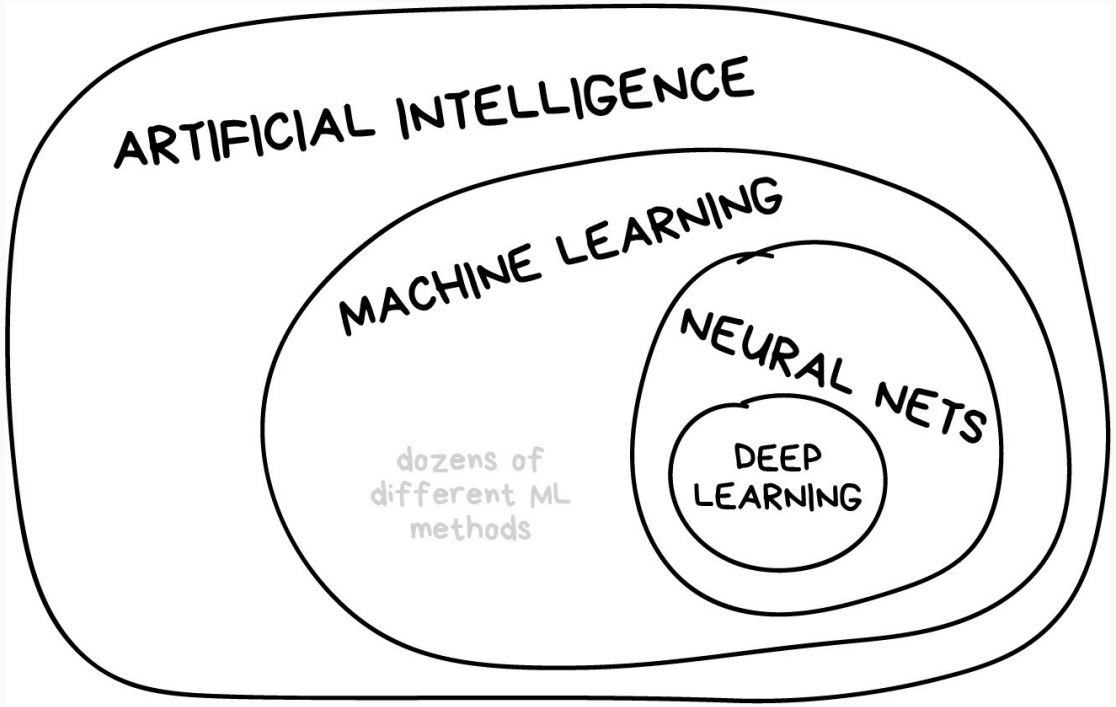
> *"In short, we will cover things that we wish someone had taught us in our undergraduate programs."*
>
> This quote is from the Data science for economists course by Grant McDermott.

Module 1's outline

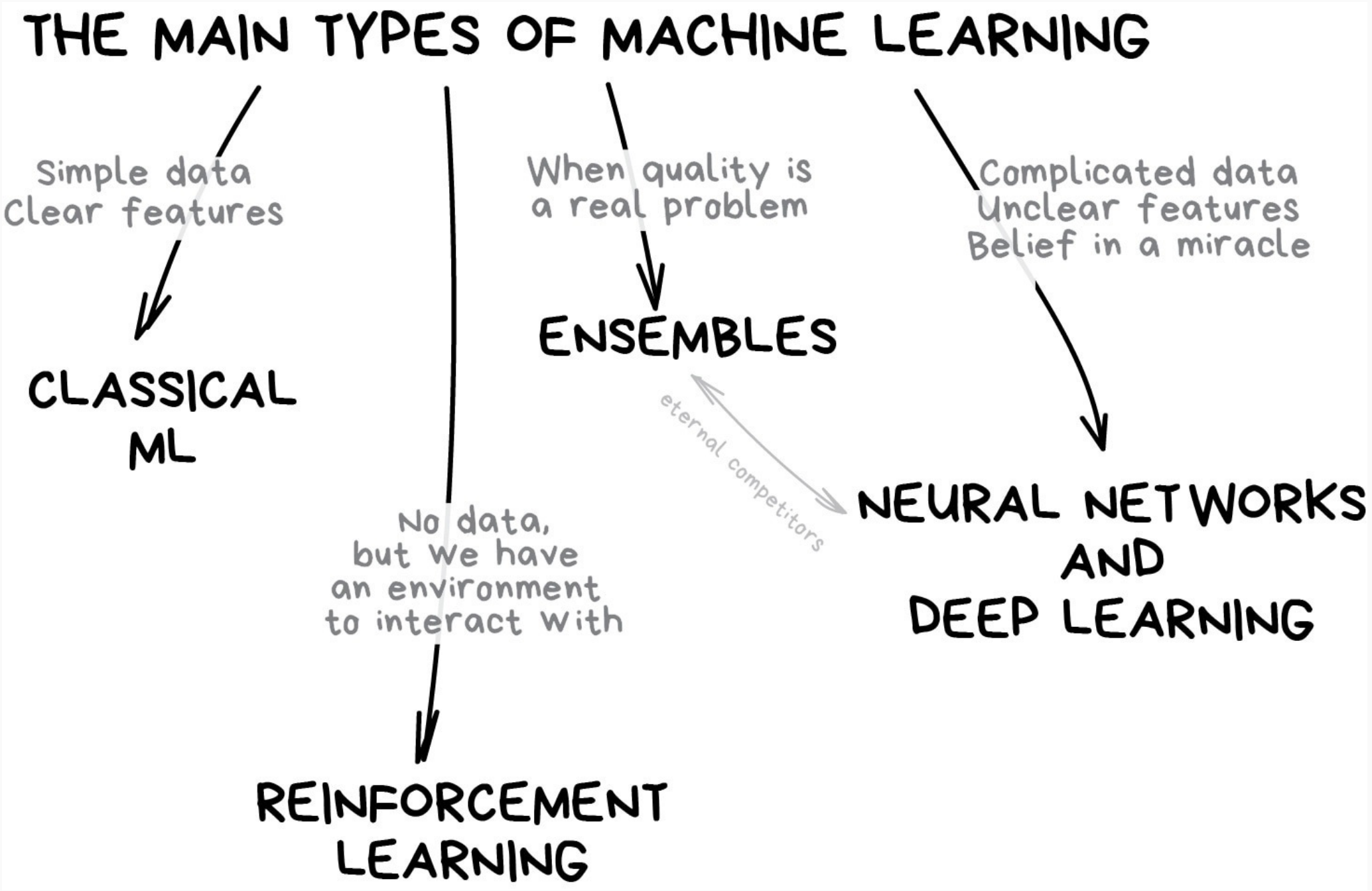
- Prologue
- Knowing me, knowing you:
  statistical and machine learning
  - Supervised and unsupervised learning
  - Regression and classification
  - Statistical modeling: the two cultures
- Model accuracy and loss functions
- Overfitting and bias-variance tradeoff
- Data splitting, Resampling methods
- Parameter tuning
  - with `scikit-Learn`
- Target and feature engineering
  - Data leakage
  - Pre-processing steps
  - Specifying blue-prints with `scikit-Learn`
  - Putting it all together: tuning and preprocessing via the pipeline module
- Regression models
  - Creating models in Python
  - GLMs with `statsmodels`
  - GAMs with `statsmodels`
  - Regularized (G)LMs with `scikit-learn` and `statsmodels`.



Some roadmaps to explore the ML landscape...



Source: Machine Learning for Everyone In simple words. With real-world examples. Yes, again.


THE MAIN TYPES OF MACHINE LEARNING
Simple data
Clear features
CLASSICAL ML
No data,
but we have
an environment
to interact with
REINFORCEMENT LEARNING
When quality is
a real problem
ENSEMBLES
eternal competitors
Complicated data
Unclear features
Belief in a miracle
NEURAL NETWORKS AND DEEP LEARNING

Knowing me, knowing you: statistical and machine learning

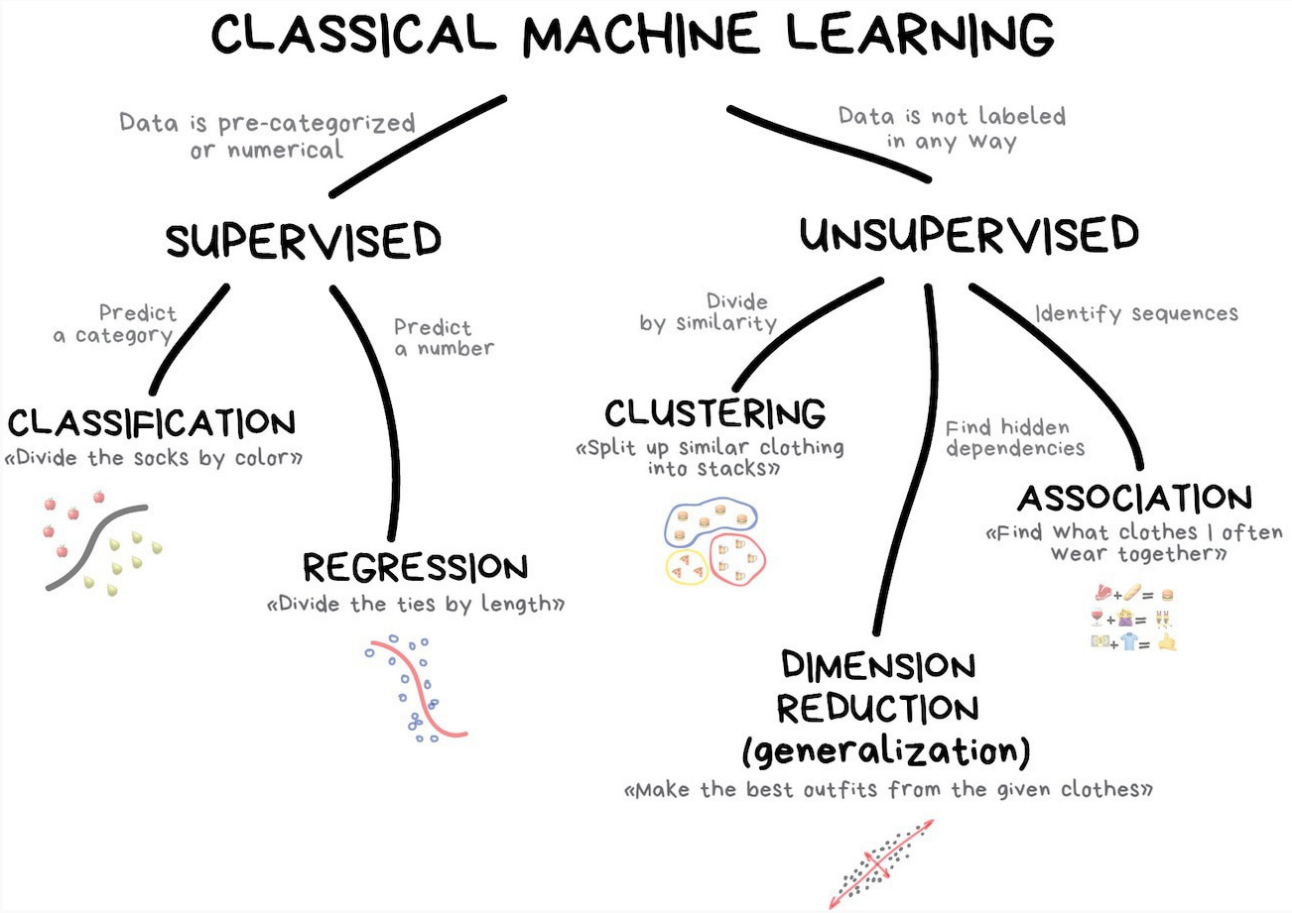
Supervised learning

Supervised learning builds ("learns") a model f (*the Signal*) such that the outcome or target Y can be written as

$$Y = f(x_1, \ldots, x_p) + \epsilon$$

with features $x_1, \ldots, x_p$ and error term ϵ (*the Noise*).

Supervised learners construct **predictive models**.



Picture taken from Machine Learning for Everyone. In simple words. With real-world examples. Yes, again

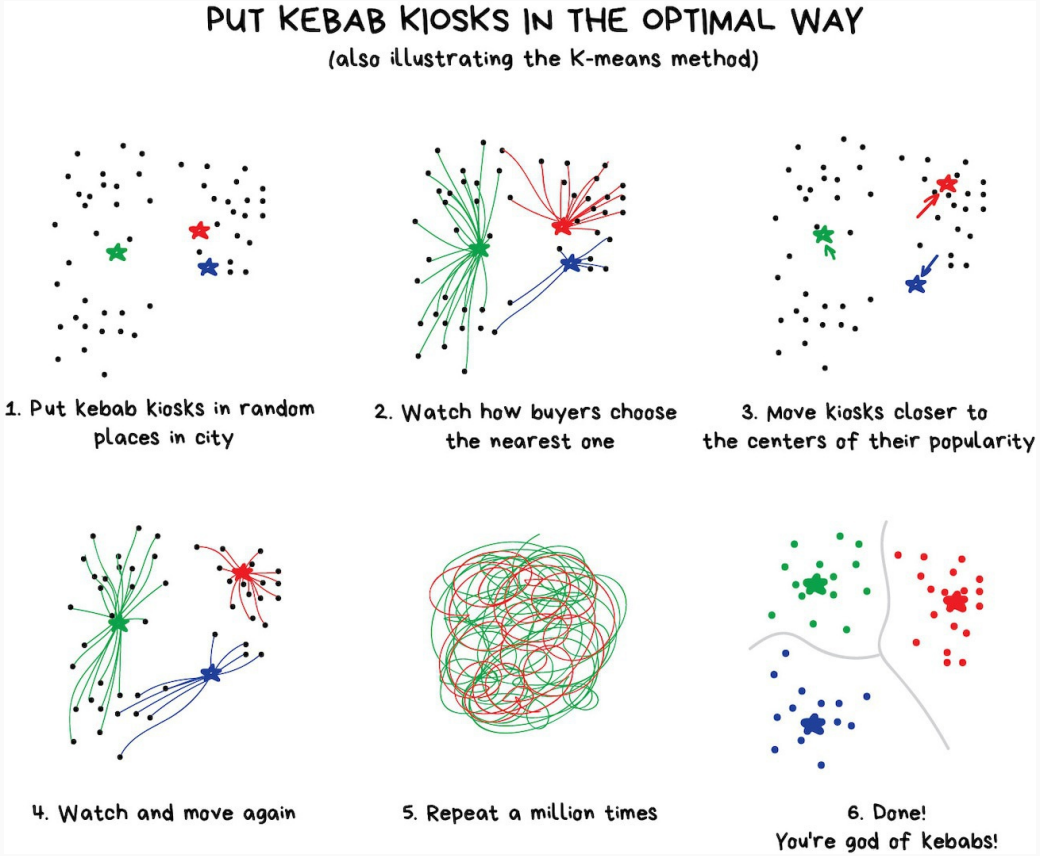
Unsupervised learning

With unsupervised learning there is NO outcome or target Y, only the feature vector $x = (x_1, \ldots, x_p)$.

Let n denote the sample size and p the number of features.

Then, X is the $n \times p$ matrix of features, with $x_{i,j}$ observation i on variable or feature j.

Unsupervised learners construct descriptive models, without any *supervising* output, letting the data "speak for itself".



Picture taken from Machine Learning for Everyone. In simple words. With real-world examples. Yes, again

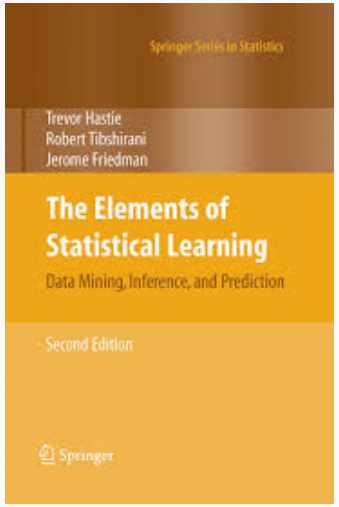
What's in a name?

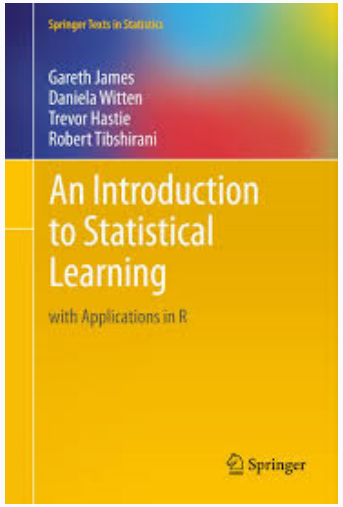
Machine learning constructs algorithms that learn from data.

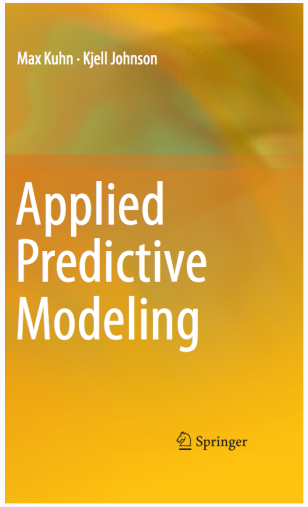
Statistical learning emphasizes statistical models and the assessment of uncertainty.

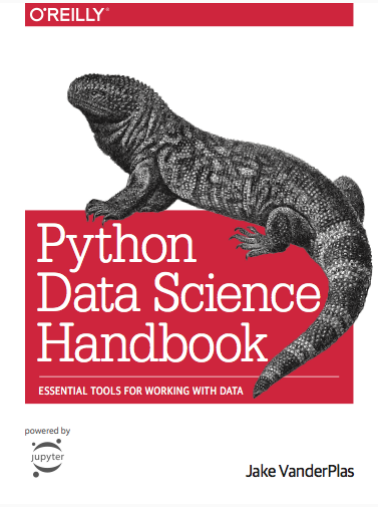
Data science applies mathematics, statistics, machine learning, engineering, etc. to extract knowledge form data.

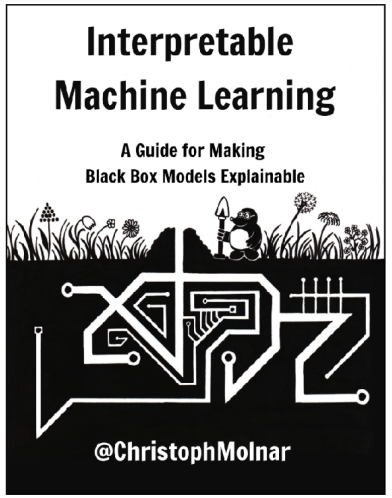
> *"Data Science is statistics on a Mac . "*







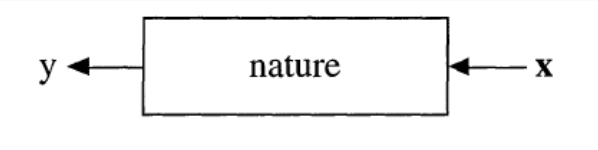




Source: Brandon M. Greenwell on Introduction to Machine Learning in .

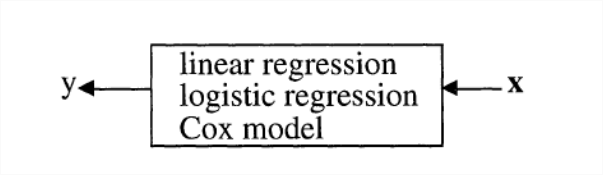
Statistical modeling: the two cultures

Consider a vector of input variables x, being transformed into some vector of response variables y via a black box algorithm.



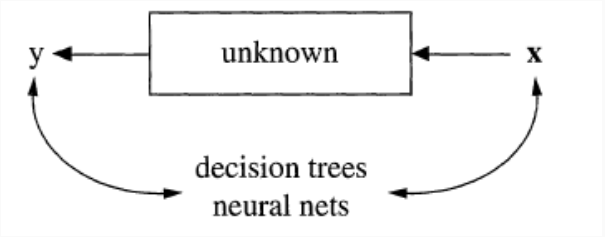
Statistical learning or data modeling culture

- assume statistical model, estimate parameter values
- validate with goodness-of-fit tests and residual inspection



Machine learning or algo modeling culture

- inside of the box is complex and unknown
- find algorithm $f(x)$ to predict y
- measure performance by predictive accuracy



Source: Breiman (2001, Statistical Science) on *Statistical modeling: the two cultures.*

Newspeak from the two cultures

	Statistical learning	Machine learning
origin	statistics	computer science
$f(x)$	model	algorithm
emphasis	interpretability, precision and uncertainty	large scale applicability, prediction accuracy
jargon	parameters, estimation	weights, learning
CI	uncertainty of parameters	no notion of uncertainty
assumptions	explicit a priori assumption	no prior assumption, learn from the data

Source: read the blog Why a mathematician, statistician and machine learner solve the same problem differently

Your turn

As discussed in the lecture, many problems in ML can be approached as a regression, classification or clustering problem.

Q: consider the following **three problem settings** and **label them** as regression, classification or clustering.

1. In disability insurance: how do disability rates depend on the state of the economy (e.g. GDP)?
2. In MTPL insurance: predict whether a claim is attritional or large, *in casu* a claim that exceeds the threshold of 100 000 EUR?
3. How can we group customers based on the insurance products they bought from the company?

Exploring the Google Colab environment

We will now visit the Google Colab for the first time and explore the packages and data sets that will be used in today's session.

We will use the Ames Iowa housing data. There are 2,930 properties in the data set.

The `Sale_Price` (target or response) was recorded along with 80 predictors, including:

- location (e.g. neighborhood) and lot information
- house components (garage, fireplace, pool, porch, etc.)
- general assessments such as overall quality and condition
- number of bedrooms, baths, and so on.

More details in De Cock (2011, Journal of Statistics Education).

The raw data are at `https://vincentarelbundock.github.io/Rdatasets`.

Model accuracy and loss functions

Predictive modeling

How to use the observed data to learn or to estimate the unknown $f(.)$?

$$y = f(x_1, x_2, \ldots, x_p) + \epsilon.$$

How do I **estimate** $f(.)$ - one way to phrase *all questions* that underly statistical & machine learning.

Take-aways - main reasons we want to **learn about** $f(.)$

prediction

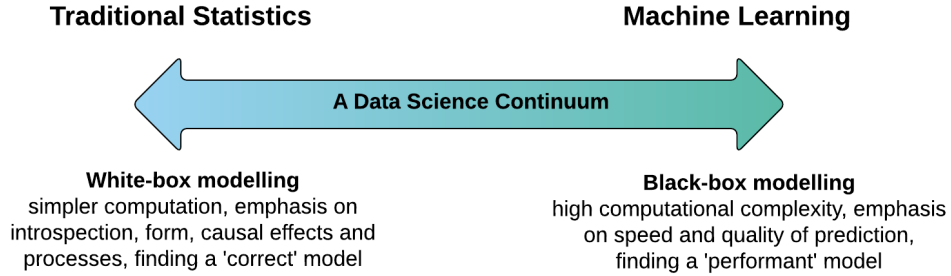
predict the target y as $\hat{f}(x)$

- as black box setting?

inference

how does target y depend on features x?

- as white box setting?



Prediction errors

Why we're stuck with **irreducible error**

assume $\hat{f}$ and x given, then

$$
\begin{aligned}
E\left[\{y - \hat{y}\}^2\right] &= E\left[\left\{f(x) + \epsilon - \hat{f}\,(x)\right\}^2\right] \\
&= \underbrace{\left[f(x) - \hat{f}\,(x)\right]^2}_{\text{Reducible}} + \underbrace{\text{Var}(\epsilon)}_{\text{Irreducible}}
\end{aligned}
$$

In **less math**:

- if ϵ exists, then x cannot perfectly explain y
- so even if $\hat{f} = f$, we still have irreducible error.

Thus, to form our **best predictors**, we will **minimize reducible error**.

Model accuracy

We assess **model** or **predictive accuracy** by evaluating how well predictions actually match observed data.

Use **loss functions**, i.e. metrics that compare predicted values to actual values.

Regression, use e.g. the **Mean Squared Error (MSE)**

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

Recall: $y_i - \hat{y}_i = y_i - \hat{f}(x_i)$ is the prediction error.

Objective ◎ : minimize!

Classification, use e.g. the **cross-entropy** or **log loss**

$$-\frac{1}{n}\sum_{i=1}^{n}\left(y_i \cdot \log(p_i) + (1 - y_i) \cdot \log(1 - p_i)\right).$$

Objective ◎ : minimize!

Many other useful loss functions (e.g. deviance in regression, Gini index in classification).

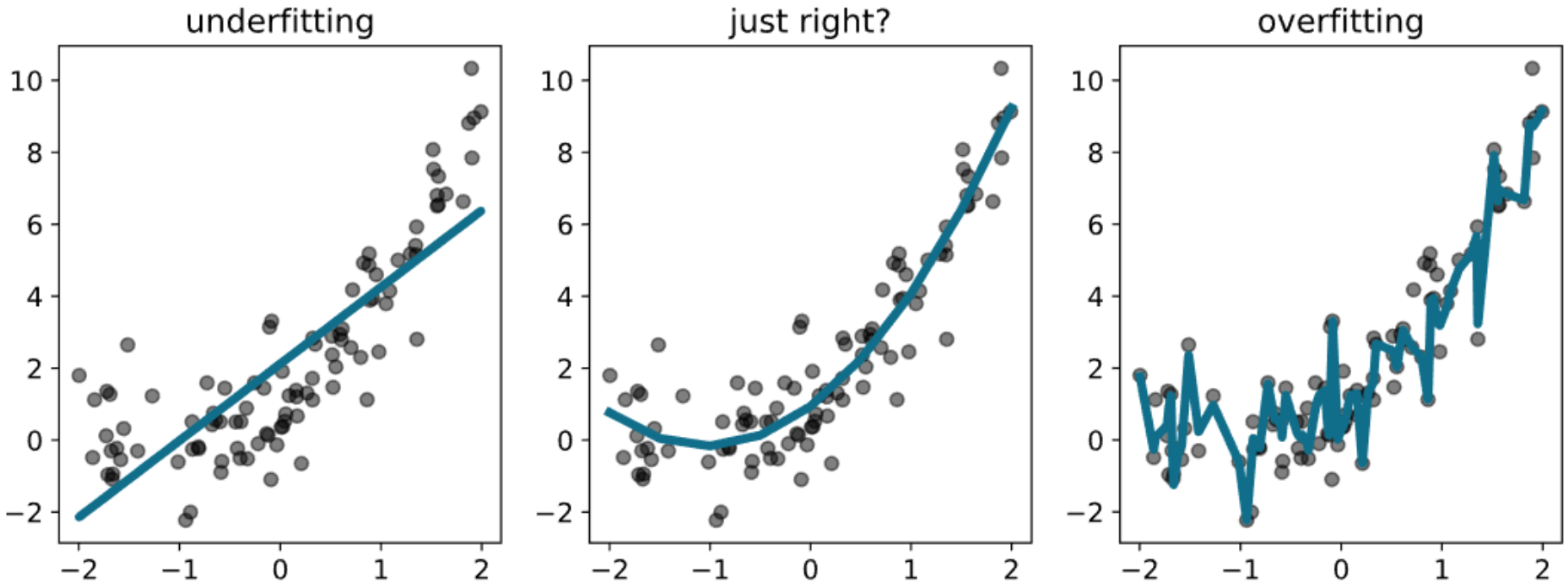
Take-away 📣 - a loss function emphasizes certain types of errors over others ➞ pick a meaningful one!

Overfitting and bias-variance trade off

Overfitting

The Signal and the Noise discussion!

Which of the following three models (in green-blue-ish) will best generalize to new data?



Inspired by Brandon Greenwell's Introduction to Machine Learning in R.

Overfitting (cont.)

With a small training error, but large test error, the model is overfitting or working too hard!

The expected value of the **test MSE**:

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

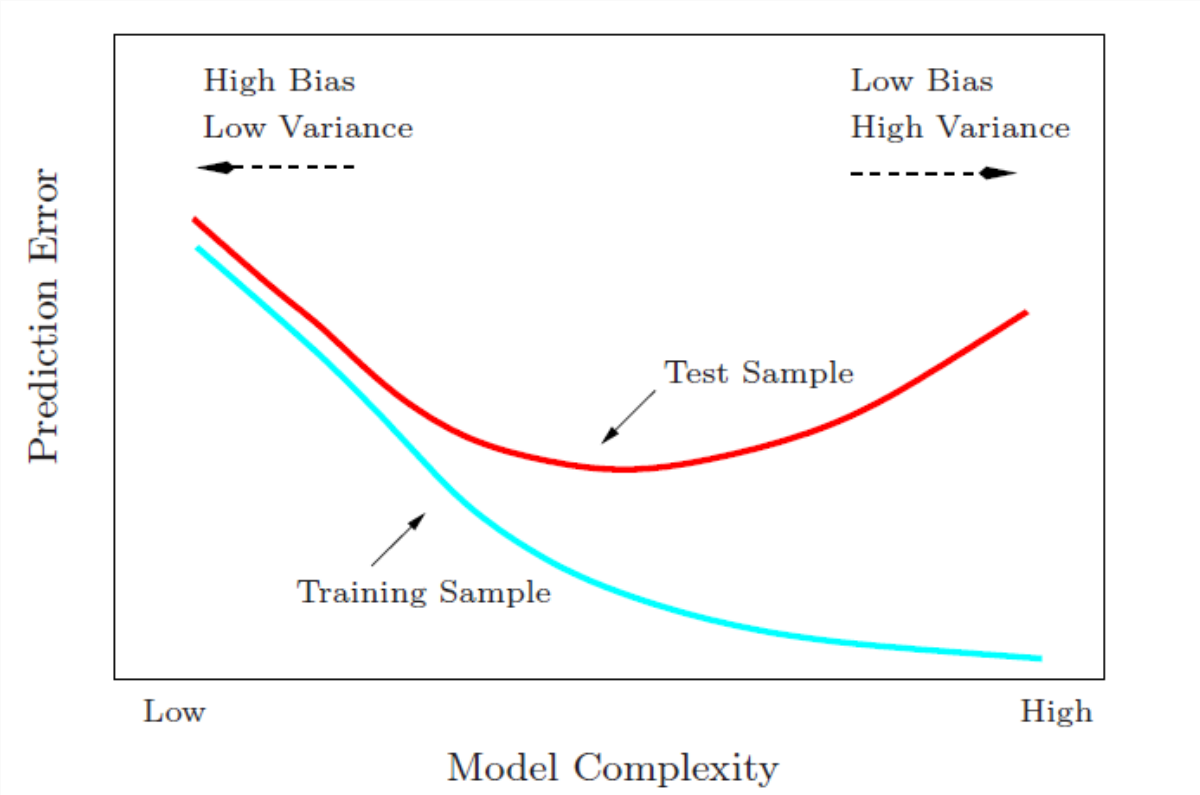
In general - with more flexible methods

- variance ⬆ and bias ⬇
- their relative rate of change determines whether the test error increases or decreases

Take-aways 📣

- U-shape curves of **test MSE** w.r.t model flexibility
- the **bias-variance tradeoff** is central to quality prediction.

Bias-variance trade off

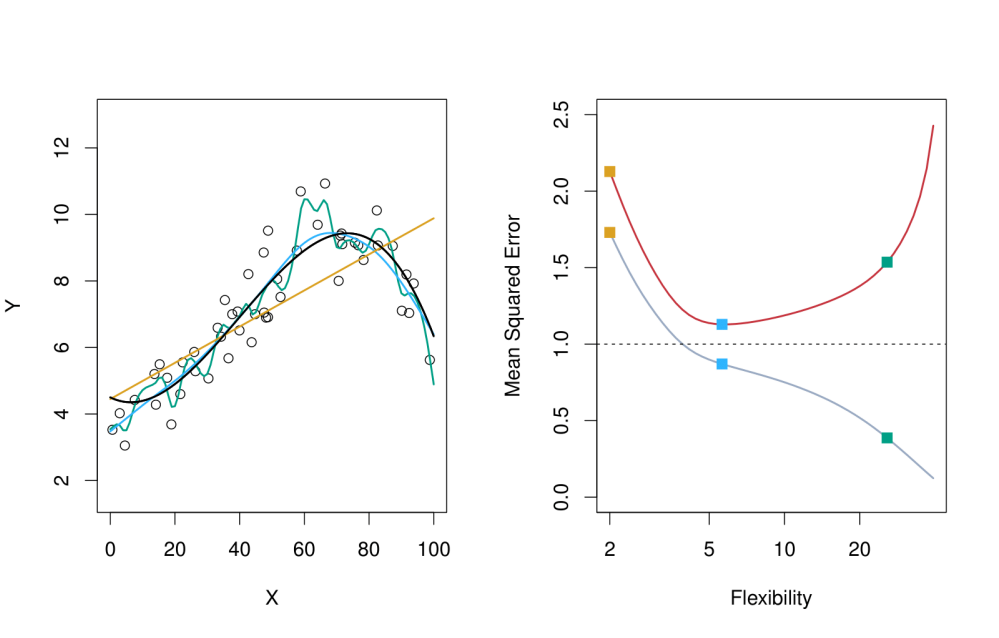


Source: James et al. (2013) on http://faculty.marshall.usc.edu/gareth-james/ISL/.

Your turn

Data are generated from: $y = f(x) + \epsilon$, with the black curve as the true f. The orange (linear regression), blue (smoothing splines) and green (smoothing splines) curves are three estimates for f, with increasing level of complexity.

Q: which model do you prefer (orange, blue, green) for each of the following examples? Why?



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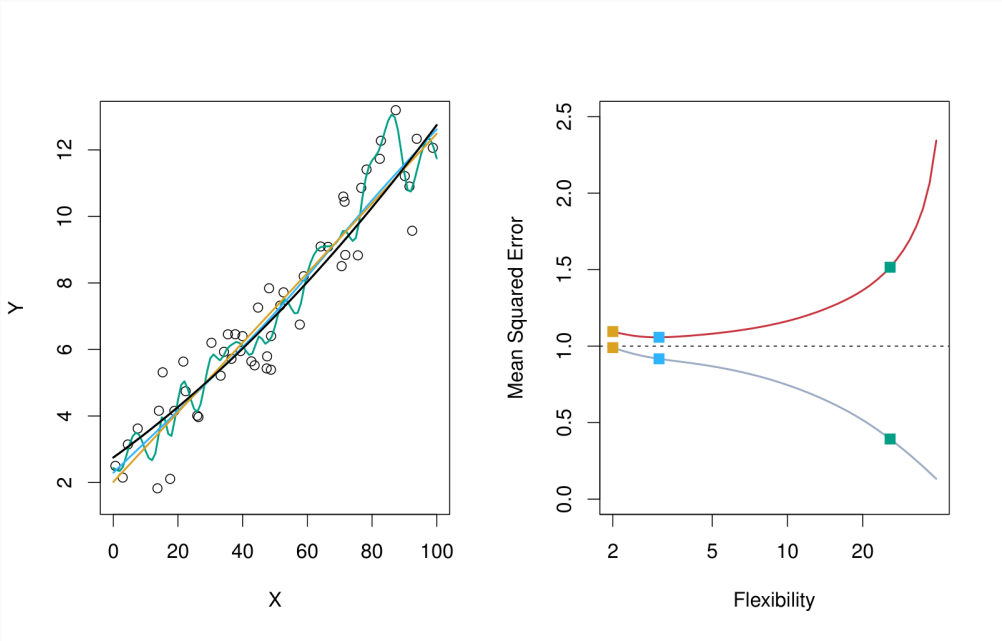

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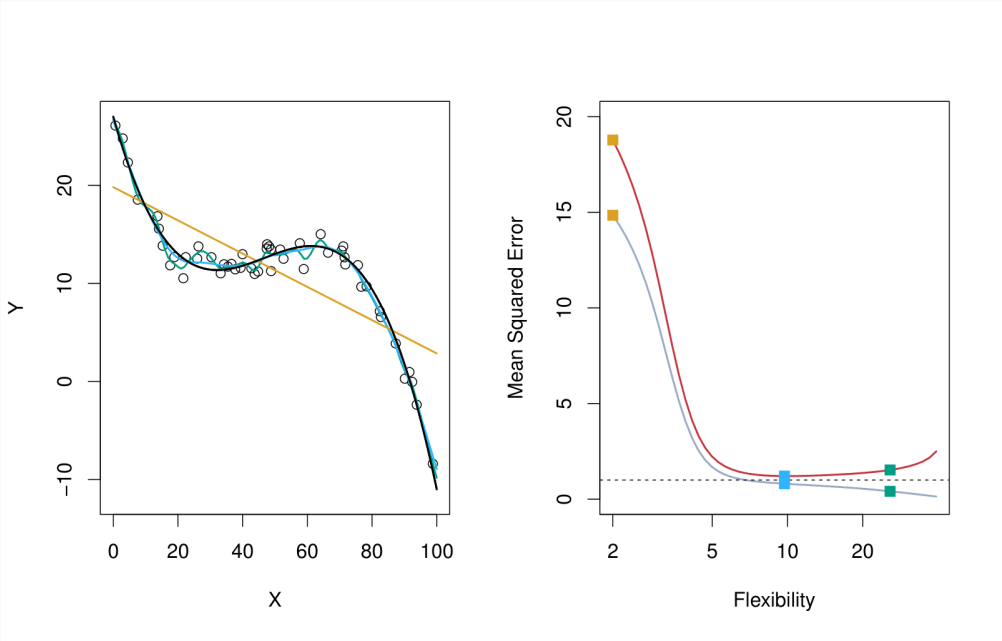

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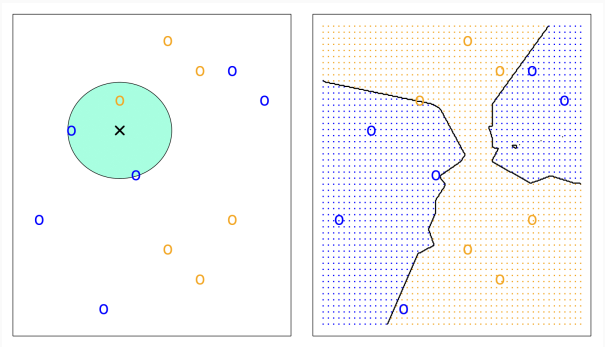
Your turn

The *K*-nearest neighbors (KNN) classifier

- take the *K* observations in the training data set that are 'closest' to test observation x_0, calculate

$$\Pr(Y = j | X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} \mathbb{I}(y_i = j).$$

- KNN then assigns the test observation x_0 to the class j with the highest probability, e.g. with *K*=3 (from James et al., 2013)

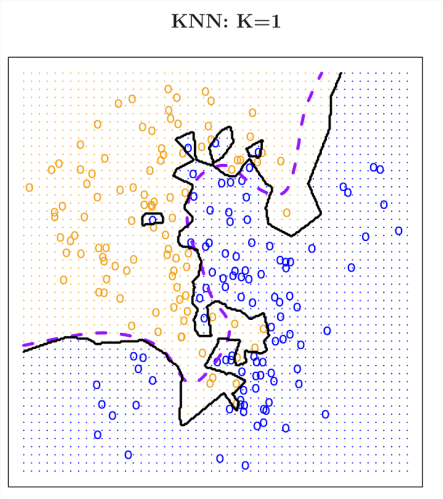


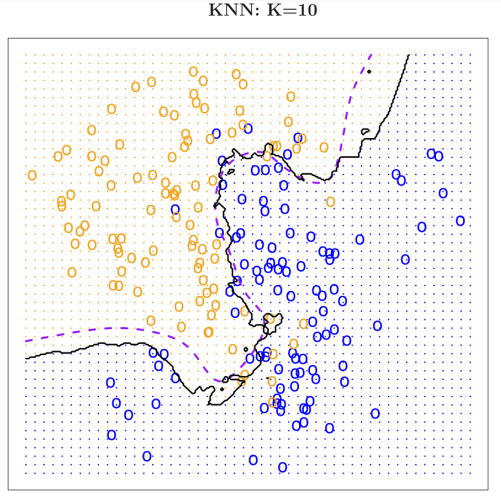
Q: is KNN a supervised learning or unsupervised learning method? Discuss.

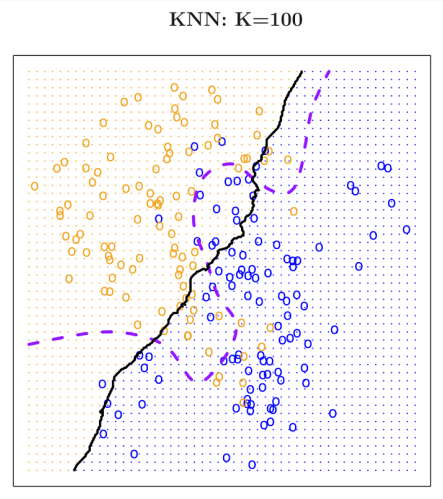
Your turn

The *K*-nearest neighbors (KNN) classifier (cont.)

Now compare KNN with *K* equals 1, 10 and 100.







Q: which classifier do you prefer? Which of these classifiers is under-fitting, which one is over-fitting?

Data splitting and resampling methods with scikit learn

Data splitting

We fit our model on past data $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$ and get $\hat{f}$.

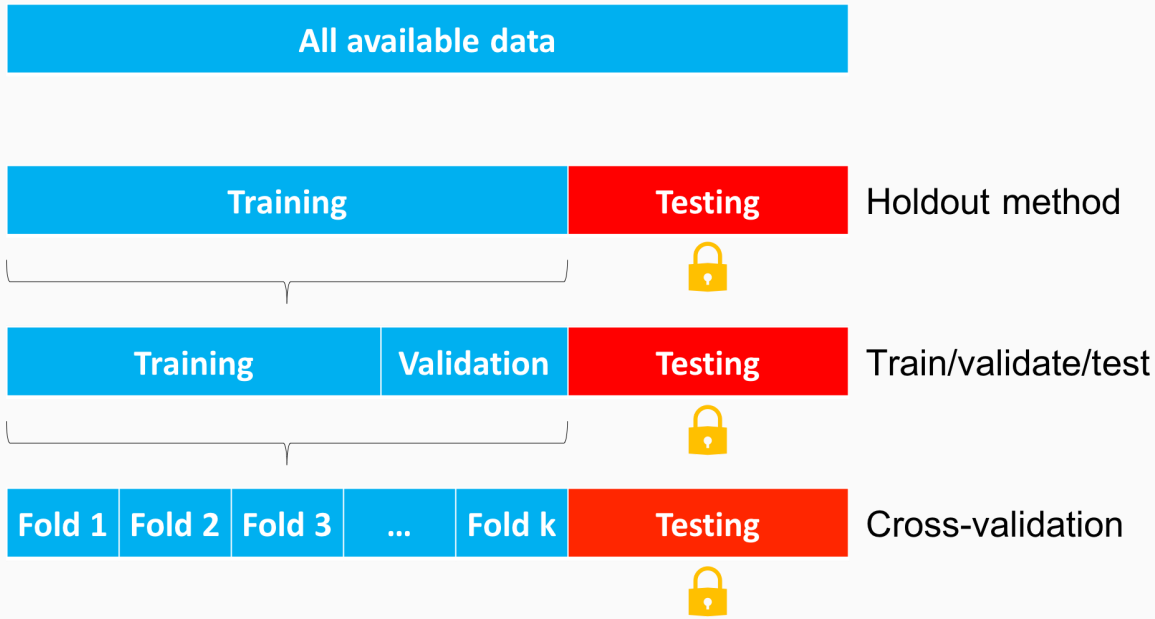
What we want: how does our model **generalize** to new, unseen data (x_0, y_0), or: is $\hat{f}(x_0)$ close to y_0?

Training set

- to develop, to train, to tune, to compare different settings, ...

Test set

- to obtain unbiased estimate of final model's performance.



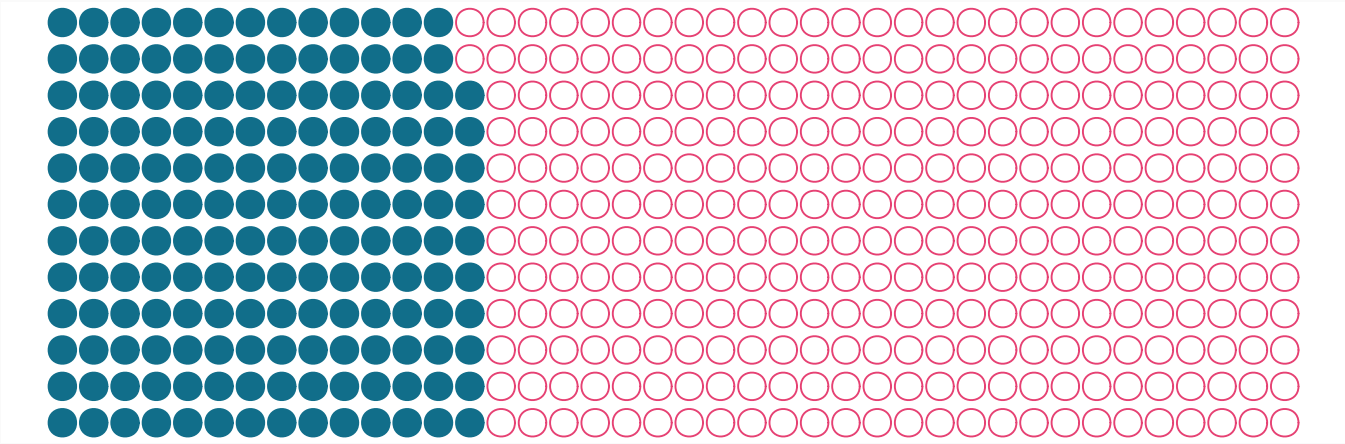
Picture taken from Introduction to Machine Learning in R.

Resampling methods

In Data splitting, we discussed *training* and *test* set. Let's now dive deeper into *resampling* methods.

Validation set (visual inspired by Ed Rubin's course)

- we hold out a subset of the training data (e.g. 30%) and then evaluate the model on this held out validation set
- calculate the loss function on this validation set, as approximation of the true test error
- 👎 high variability + inefficient use of data
- e.g., a **validation set (30%)** and **training set (70%)**.

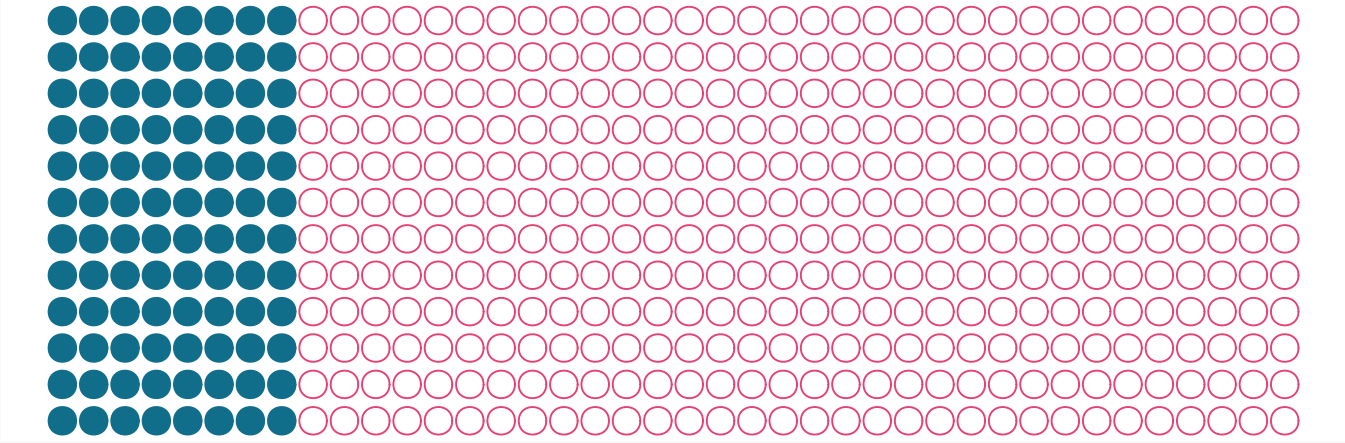


Resampling methods (cont.)

In Data splitting, we discussed *training* and *test* set. Let's now dive deeper into *resampling* methods.

***k* fold cross validation** (visual inspired by Ed Rubin's course)

- divide training data into *k* equally sized groups (e.g. **group 1** on the picture)
- iterate over the *k* groups, treating each as validation set once (and train model on the other *k-1* groups) (e.g. get $\textbf{MSE}_1$ corresponding to fold 1)
- average the folds' loss to estimate the true test error
- 👍 greater accuracy (compared to validation set).



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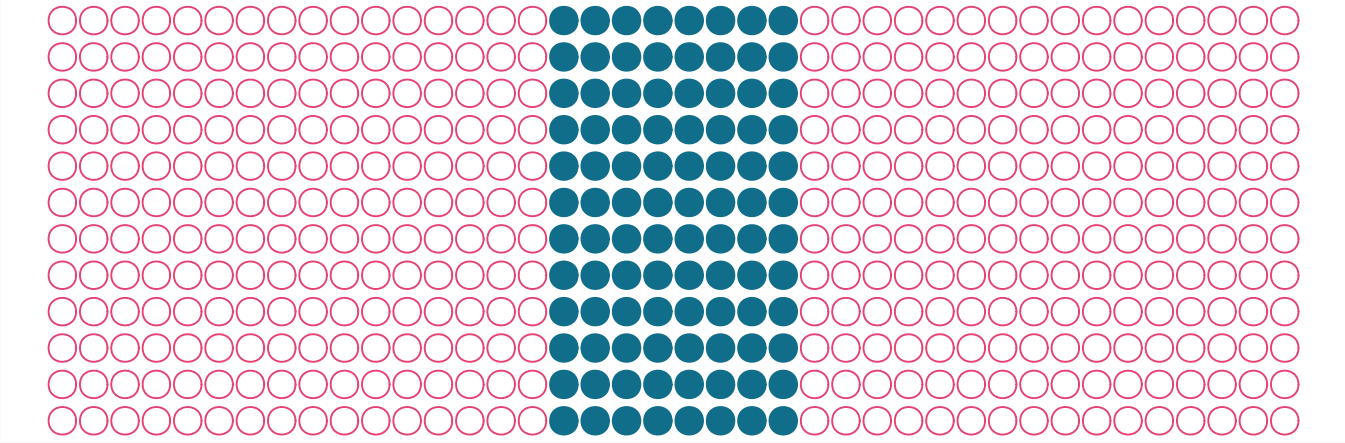

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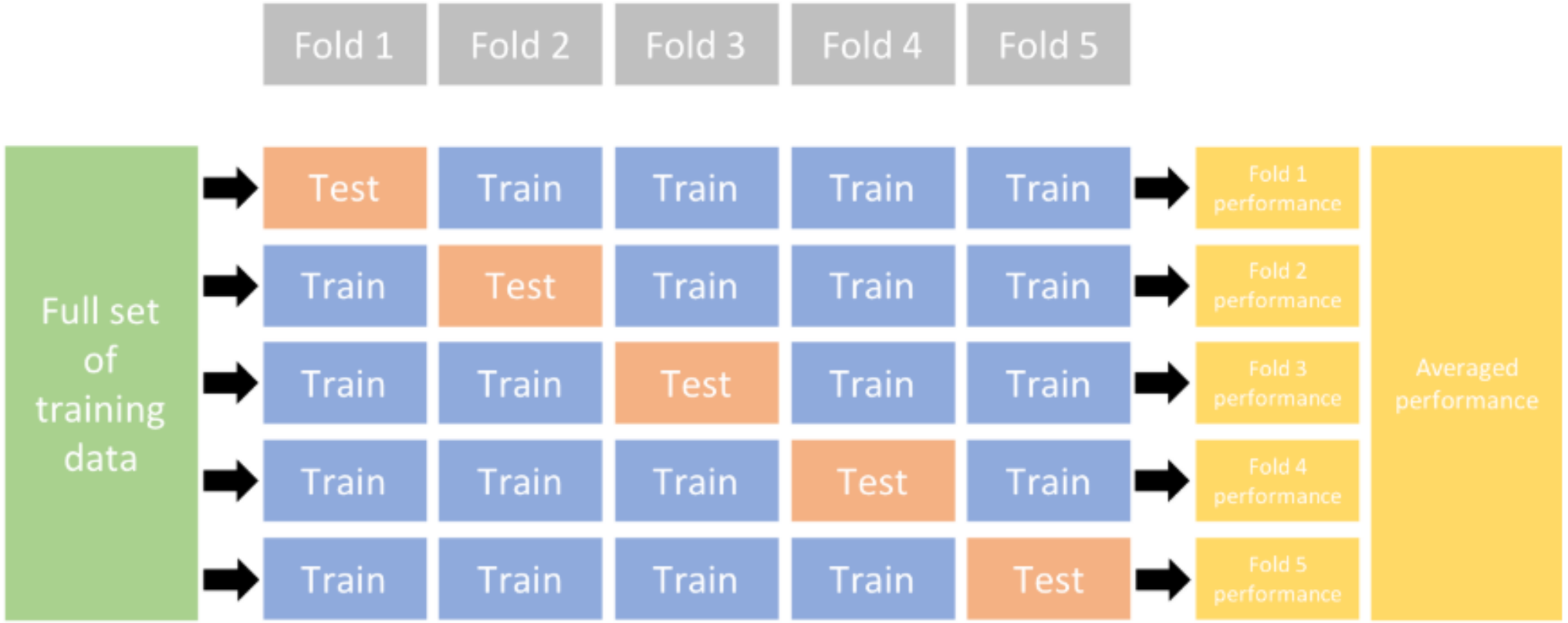

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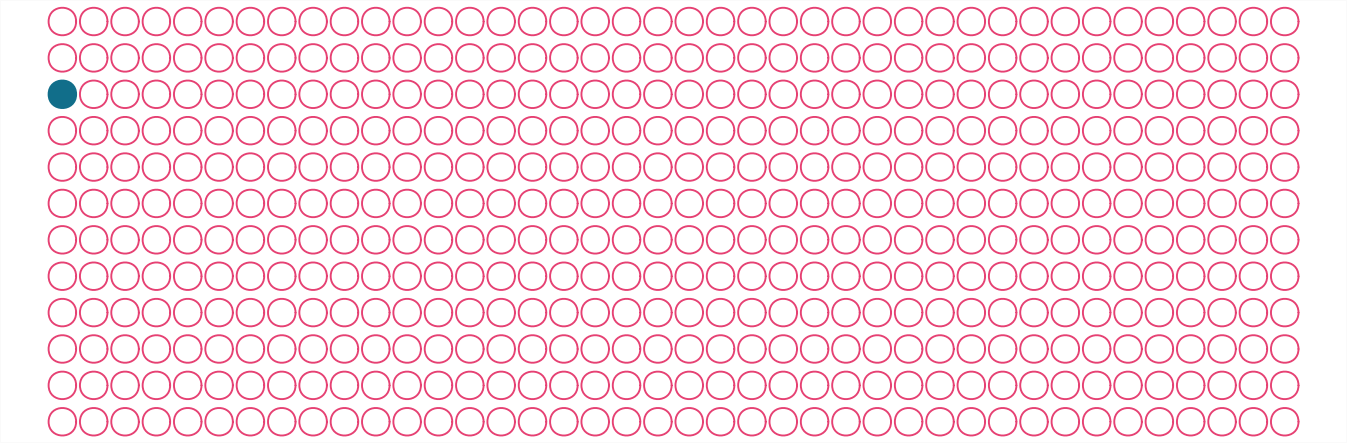
In Data splitting, we discussed *training* and *test* set. Let's now dive deeper into *resampling* methods.

Leave-one-out cross validation (visual inspired by Ed Rubin's course)

- each observation takes a turn as the validation set (e.g. get $\mathbf{MSE_3}$)
- other *n-1* observations are the training set
- average the folds' loss to estimate the true test error
- 👎 very computationally demanding.



Working with pandas and scikit-learn

We will now explore basic instructions to:

- explore the structure of the data set with instructions from `{pandas}`
- visualize the data using `matplotlib` and `seaborn`
- split a data set into a training and test set with instructions from `{numpy}` and `{scikit learn}`.

Here:

- `{pandas}` is a package for data analysis and the manipulation of tabular data; the name is derived from the term **pan**el **da**ta
- `{numpy}` is a package for scientific computation
- `{scikit-learn}` is for machine learning in Python, with functions for a.o. preprocessing, model selection, regression and classification.

scikit-learn

Machine Learning in Python

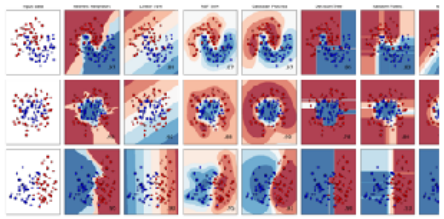
Getting Started | Release Highlights for 1.2 | GitHub

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying which category an object belongs to.

Applications: Spam detection, image recognition.
Algorithms: SVM, nearest neighbors, random forest, and more...

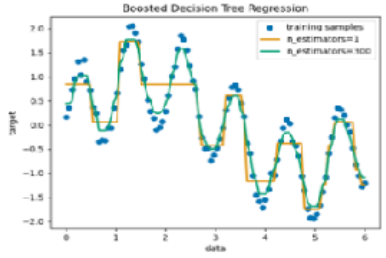


Examples

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: SVR, nearest neighbors, random forest, and more...

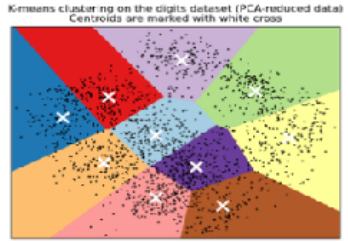


Examples

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, and more...

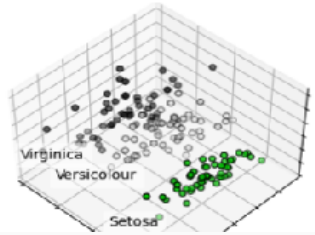


Examples

Dimensionality reduction

Reducing the number of random variables to consider.

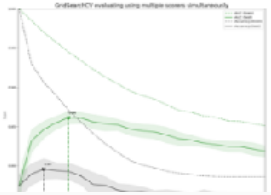
Applications: Visualization, Increased efficiency
Algorithms: PCA, feature selection, non-negative matrix factorization, and more...



Model selection

Comparing, validating and choosing parameters and models.

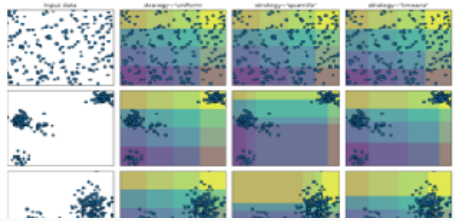
Applications: Improved accuracy via parameter tuning
Algorithms: grid search, cross validation, metrics, and more...

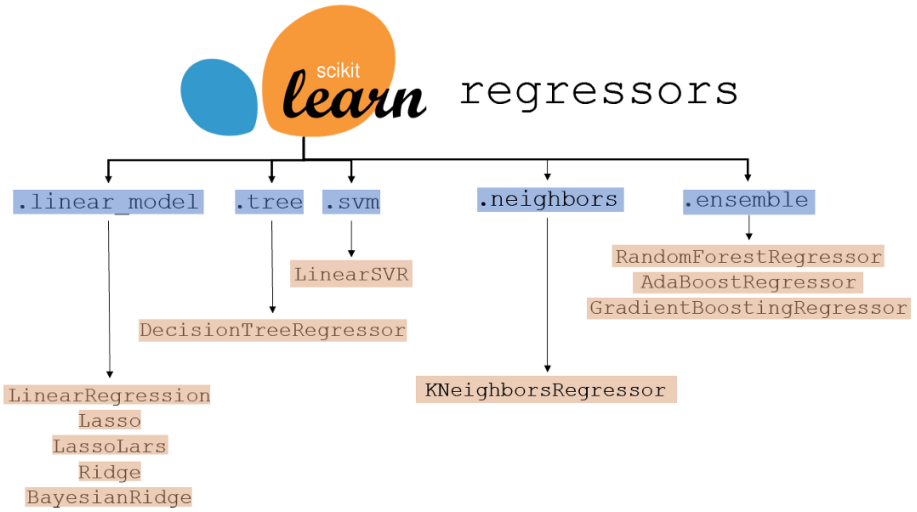


Preprocessing

Feature extraction and normalization.

Applications: Transforming input data such as text for use with machine learning algorithms.
Algorithms: preprocessing, feature extraction, and more...

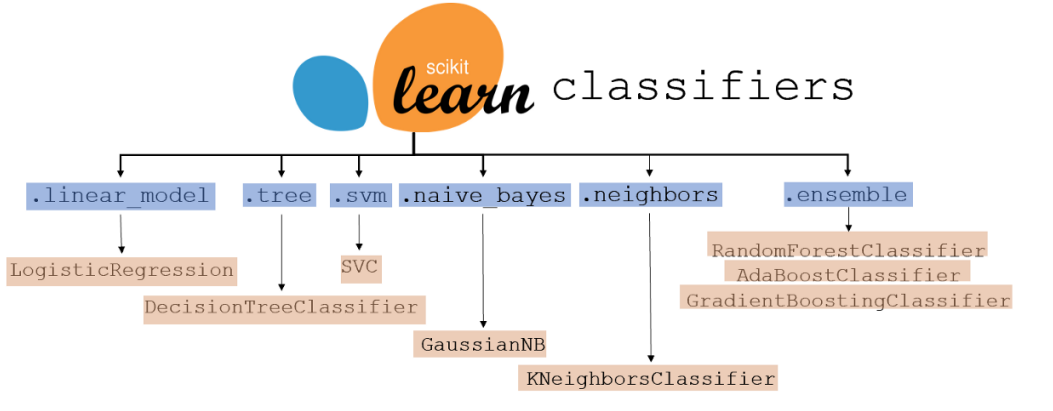





```
#import
from sklearn.branch import model_name

#create instance
model = model_name()

#fit model
model.fit(X_train, y_train)
```




```
#import
from sklearn.metrics import metric_name

#create instance
metric_name(y_test, model.predict(X_test))
```

real target predicted target

Pictures taken from KD Nuggets ultimate scikit-learn ML cheatsheet.

Resampling methods in scikit-learn

We return to the Google Colab and set up 5-fold cross validation using the `scikit-learn` library.

Parameter tuning with scikit-learn

Tuning parameters

Finding the optimal level of flexibility highlights the bias-variance tradeoff.

Bias : the error that comes from inaccurately estimating f.

Variance : the amount $\hat{f}$ would change with a different training sample.

Take-aways : high variance models more prone to overfitting

- use **resampling methods** to reduce this risk
- hyperparameters (or *tuning parameters*) control complexity, and thus the bias-variance trade-off
- identify their optimal setting, e.g. with a *grid search*
- no analytic expression for these hyperparameters.

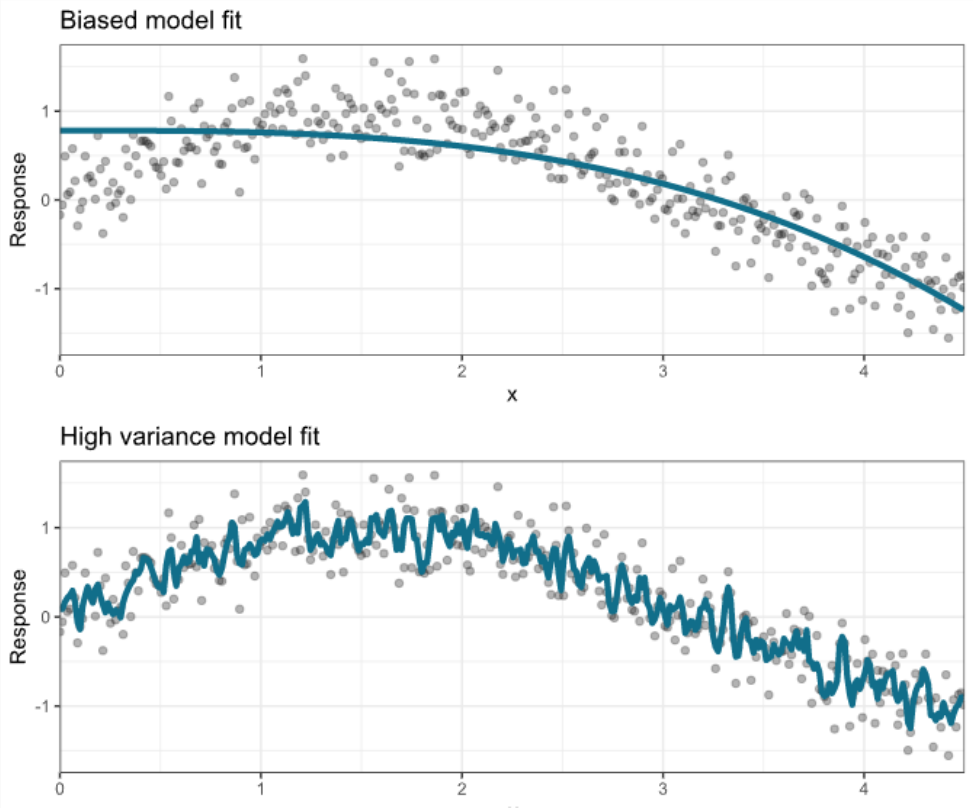
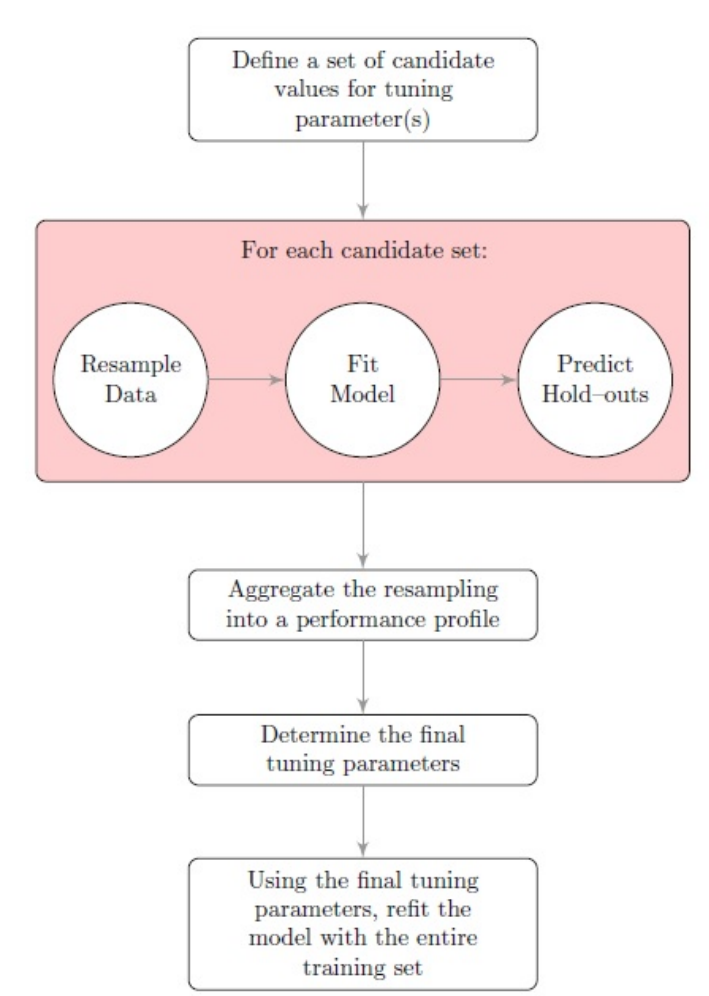


Illustration and code from Boehmke & Greenwell (2019, Chapter 2) on Hands-on machine learning with R.

Tuning parameters via grid search



Model training & validation phase

- define a set of candidate values (a *grid*)
- assess model utility across the candidates (use clever *resampling*)
- choose the optimal settings (optimize *loss*)
- refit the model on entire training data with final tuning parameters
- evaluate performance of the model on the test data (under 🔒).

Model selection

- repeat the above steps for different models
- compare performance of these models that will generalize to new data (via test data, under 🔒).

Flow chart from Kuhn & Johnson (2013) on Applied predictive modeling.

Putting it all together

During the tuning process we inspect plots like the one on the right.

Take-aways 📢 *Less is more*:

- we prefer simple over more complex
- choose tuning parameters based on the numerically optimal value OR
- choose a simpler model that is within a certain tolerance of the numerically best value
- use the **'one-standard-error' rule**.

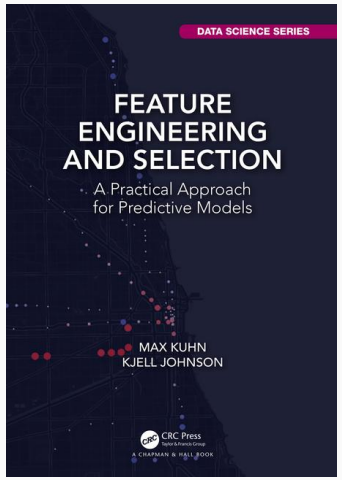
With the selected tuning parameters, we refit the model on the complete training set and use it to predict the test set (under 🔒).

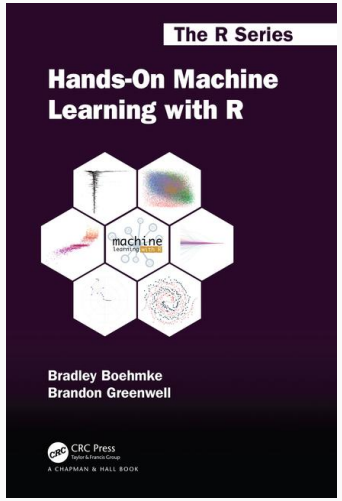
Tuning parameters with scikit-learn

Let's return to our Colab.

Target and feature engineering: data pre-processing steps

What is feature engineering?





Feature engineering:

- applies **pre-processing steps** to predictor (features) variables
- **creates new input features** from your existing ones (e.g. network features derived from a social network in a fraud detection model).

Target engineering:

- transforms the response variable (or target) to improve the performance of a predictive model.

The goal is to make models more effective.

See Kuhn & Johnson (2019) on Feature Engineering and Selection: A Practical Approach for Predictive Models for a detailed discussion.

Take-aways 📢: *different models* have *different sensitivities* to the type of target and feature values in the model.

Table A.1: A summary of models and some of their characteristics

Model	Allows $n < p$	Pre-processing	Interpretable	Automatic feature selection	# Tuning parameters	Robust to predictor noise	Computation time
Linear regression†	×	CS, NZV, Corr	✓	×	0	×	✓
Partial least squares	✓	CS	✓	○	1	×	✓
Ridge regression	×	CS, NZV	✓	×	1	×	✓
Elastic net/lasso	×	CS, NZV	✓	✓	1–2	×	✓
Neural networks	✓	CS, NZV, Corr	×	×	2	×	×
Support vector machines	✓	CS	×	×	1–3	×	×
MARS/FDA	✓		○	✓	1–2	○	○
K-nearest neighbors	✓	CS, NZV	×	×	1	○	✓
Single trees	✓		○	✓	1	✓	✓
Model trees/rules†	✓		○	✓	1–2	✓	✓
Bagged trees	✓		×	✓	0	✓	○
Random forest	✓		×	○	0–1	✓	×
Boosted trees	✓		×	✓	3	✓	×
Cubist†	✓		×	○	2	✓	×
Logistic regression*	×	CS, NZV, Corr	✓	×	0	×	✓
{LQRM}DA*	×	NZV	○	×	0–2	×	✓
Nearest shrunken centroids*	✓	NZV	○	✓	1	×	✓
Naïve Bayes*	✓	NZV	×	×	0–1	○	○
C5.0*	✓		○	✓	0–3	✓	×

†regression only *classification only

Symbols represent affirmative (✓), negative (×), and somewhere in between (○)

Source: Kuhn & Johnson (2013) on Applied predictive modeling.

Feature engineering steps

Examples of common pre-processing steps:

- Some models (e.g. KNN, Lasso, neural networks) require that the predictor variables are on the same scale. **Centering (C)** and **scaling (S)** the predictors can be used for this purpose.
- Other models are very sensitive to correlations between the predictors and filters or PCA signal extraction can improve the model.
- Some models find **(near) zero-variance (NZV)** predictors problematic, and these should be removed before fitting the model.
- In other cases, the data should be **encoded** in a specific way to make sure all predictors are numeric (e.g. one-hot encoding of factor variables in neural networks).
- Many models cannot cope with **missing data** so **imputation strategies** might be necessary.
- Development of new features that represent something important to the outcome.
- (add your own example here!)

This list is inspired by Max Kuhn (2019) on Applied Machine Learning.

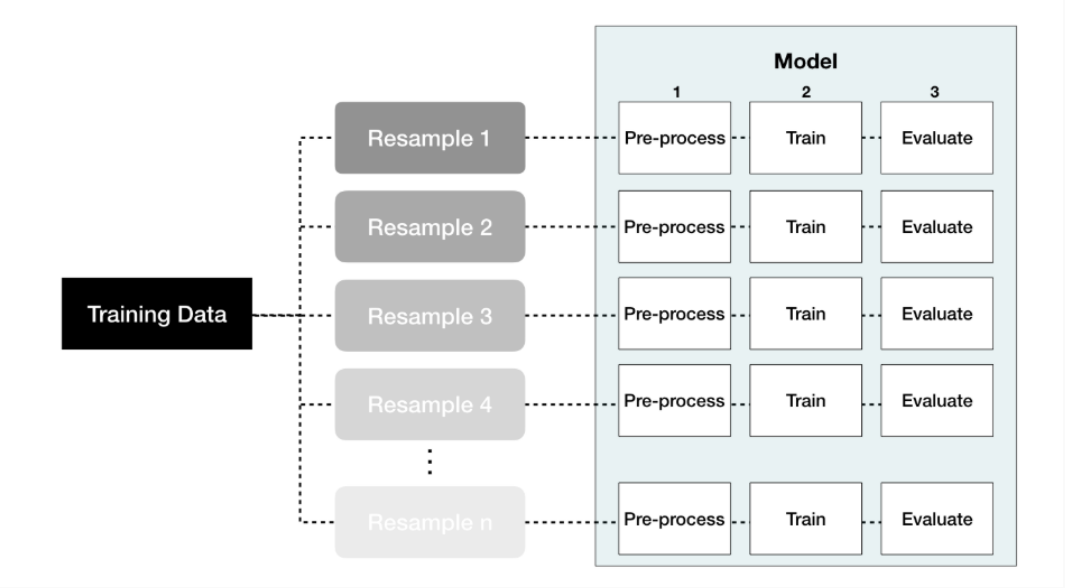
A blueprint for feature engineering

Take-aways 📣 : *a proper implementation*

- draft a **blueprint** of the necessary pre-processing steps, and their order
- Boehme & Greenwell (2019) suggest

1. Filter out zero or near-zero variance features.
2. Perform imputation if required.
3. Normalize to resolve numeric feature skewness.
4. Standardize (center and scale) numeric features.
5. Perform dimension reduction (e.g., PCA) on numeric features.
6. One-hot or dummy encode categorical features.

- avoid **data leakage** in the pre-processing steps when applied to resampled data sets!

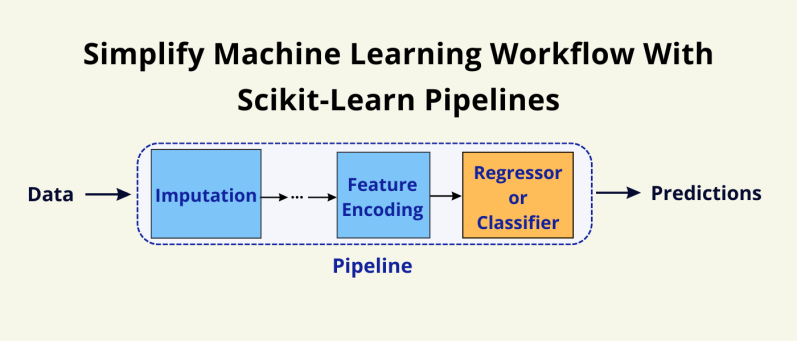


Pipelines

We'll use `pipeline` from the scikit-learn package to build a streamlined blueprint of pre-processing steps.

The main idea is to **preprocess multiple data sets** and to avoid data leakage using a single `pipeline` structure.

Before we start, keep the following fundamentals of `pipeline` in mind!



Creating a `pipeline` takes the following steps:

- build a pre-processing plan by setting up pipelines for distinct groups of variables
- join all the pipelines into one by specifying the family's pipeline and their variables
- add the model to the pipeline, e.g. a linear regression model
- save and load in the pipeline for future use.

Source: Mahmoud Youssef's github

Linear regression models with sklearn and statsmodels

Fitting linear models

`scikit-Learn` and `statsmodels` are used in Python fitting linear models:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \epsilon_i,$$

where the error terms ϵ_i have mean zero and unit variance, and are typically assumed to be normally distributed.

The typical Scikit-learn syntax is as follows:

```
from sklearn.linear_model import LinearRegression

reg1 = LinearRegression()
reg1.fit(X_train.Gr_Liv_Area.values.reshape(-1,1), y_train)
reg1.intercept_
reg1.coef_
```

Here, the data set needs to be in right shape. We therefore apply `reshape` to transform the data set, see the Colab for more discussion.

Fitting linear models

"`statsmodels` provides classes and functions for many different statistical models. Moreover, it supports specifying models using R-style formulas and `pandas` DataFrames." (from the documentation)

```
import statsmodels.api as sm
import statsmodels.formula.api as smf

lin_model = smf.ols('Sale_Price ~ Gr_Liv_Area', data = ames_python).fit()
lin_model.summary()
```

Alternatively, you can also specify models using `numpy` arrays instead of formulas, with syntax of the following type:

```
import statsmodels.api as sm

lin_model = sm.ols(y, X).fit()
lin_model.summary()
```

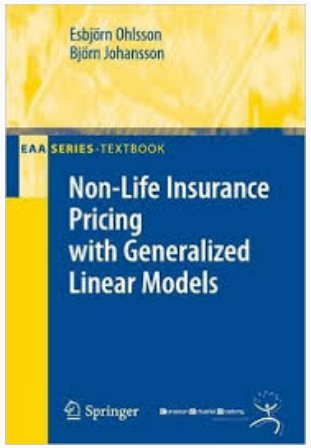
Working with the `statsmodels.api` makes the necessary functions and classes conveniently available, without making the `sm` namespace too crowded, see here.

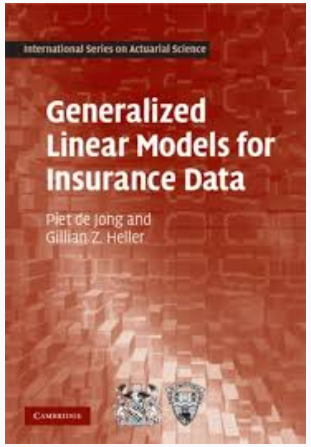
Fitting linear models

Let's return to our Colab.

Generalized Linear Models

Linear and Generalized Linear Models





With **linear regression models** `lm(.)`

- model specification

$$Y = x^{'}\beta + \epsilon.$$

- ϵ is normally distributed with mean 0 and common variance σ^2, thus: Y is normal with mean $x^{'}\beta$ and variance σ^2

With **generalized linear regression models** `glm(.)`

- model specification

$$g(E[Y]) = x^{'}\beta.$$

- $g(.)$ is the link function
- Y follows a distribution from the exponential family.

Motor Third Party Liability data

We will use the Motor Third Party Liability data set. There are 163,231 policyholders in this data set.

The frequency of claiming (`nclaims`) and corresponding severity (`avg`, the amount paid on average per claim reported by a policyholder) are the **target variables** in this data set.

Predictor variables are:

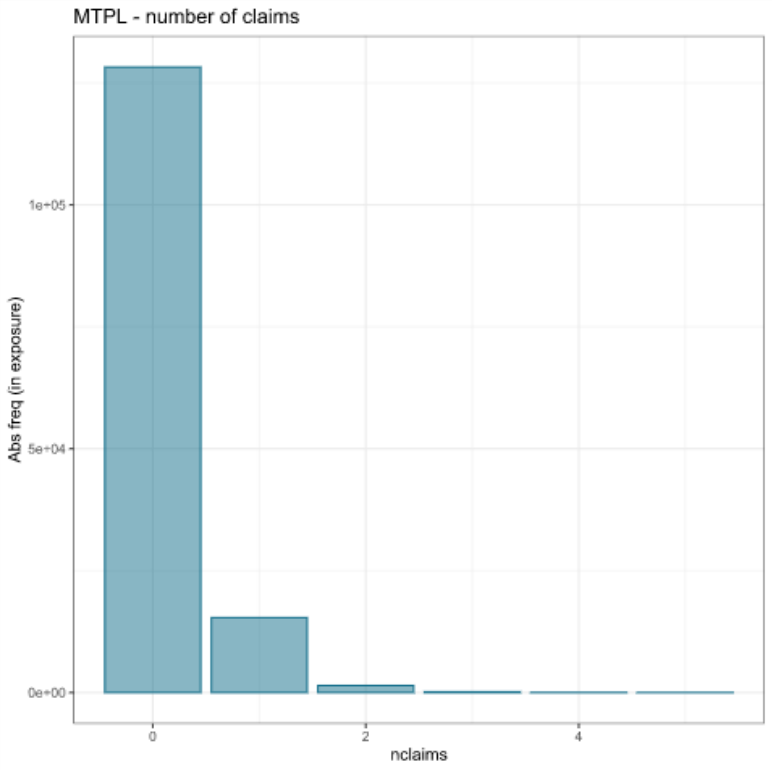
- the exposure-to-risk, the duration of the insurance coverage (max. 1 year)
- factor variables, e.g. gender, coverage, fuel
- continuous, numeric variables, e.g. age of the policyholder, age of the car
- spatial information: postal code (in Belgium) of the municipality where the policyholder resides.

More details in Henckaerts et al. (2018, Scandinavian Actuarial Journal) and Henckaerts et al. (2020, North American Actuarial Journal).

Generalized Linear Models (GLMs)

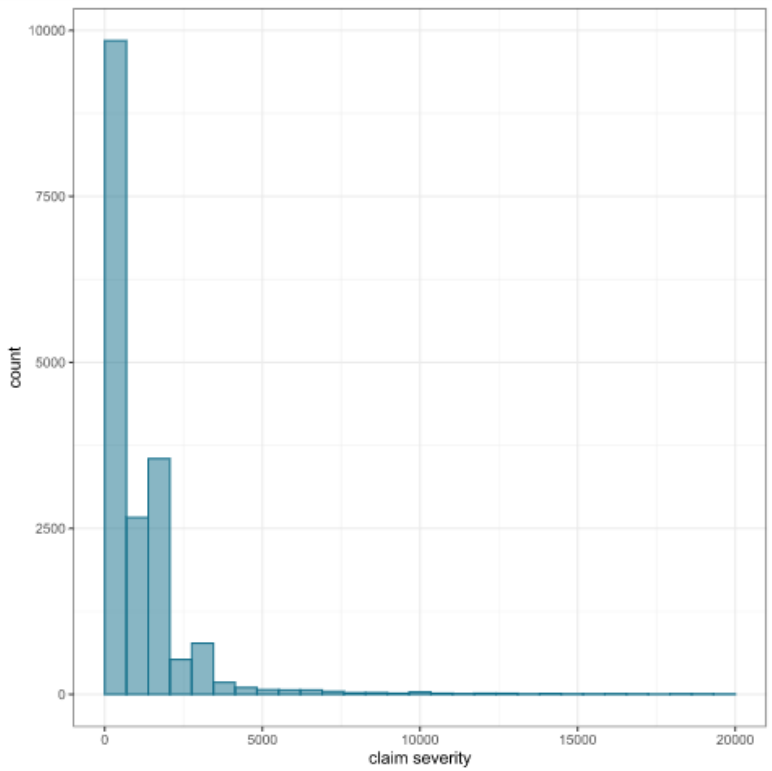
Modeling claim **frequency** and **severity** in the `mtpl` data set.

Target variable `nclaims` (frequency)



Suitable distributions: Poisson, Negative Binomial.

... and `avg` (severity).



Suitable distributions: log-normal, gamma.

A Poisson GLM

```
import statsmodels.api as sm
import statsmodels.formula.api as smf

freq_glm_1 = smf.glm(formula= 'nclaims ~ sex', data = mtpl, exposure = mtpl.expo, family = sm.families.Poisson()).fit
```

Fit a Poisson GLM, with logarithmic link function.

This implies:

Y ~ Poisson, with

$$\log(E[Y]) = x^{'}\beta,$$

or,

$$E[Y] = \exp\left(x^{'}\beta\right).$$

Fit this model on `data = mtpl`.

A Poisson GLM (cont.)

```
freq_glm_1 = smf.glm(formula='nclaims ~ sex', data = mtpl, exposure = mtpl.expo, family = sm.families.Poisson()).fit(
```

Use `nclaims` as Y.

Use `gender` as the only (factor) variable in the linear predictor.

Include `expo` as an exposure term, c.q. `log(expo)` is an offset term in the linear predictor.

Then,

$$x^{'}\beta = \log\left(\mathbf{expo}\right) + \beta_0 + \beta_1 \mathbb{I}(\mathbf{male}).$$

Put otherwise,

$$E[Y] = \mathbf{expo} \cdot \exp\left(\beta_0 + \beta_1 \mathbb{I}(\mathbf{male})\right),$$

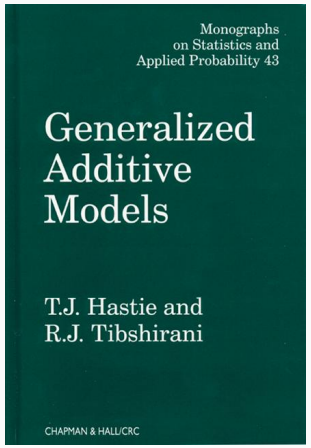
where **expo** refers to `expo` the exposure variable.

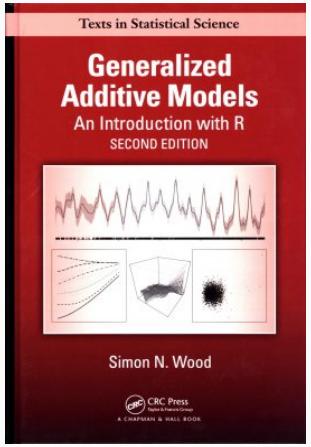
Fitting generalized linear models

Let's return to our Colab.

Generalized Additive Models

Generalized Additive Models (GAMs)





With **GLMs** `glm(.)`

- transformation of the mean modelled with a linear predictor

$$x'\beta$$

- not well suited for continuous risk factors that relate to the response in a non-linear way.

With **Generalized Additive Models (GAMs)**

- the predictor allows for smooth effects of continuous risk factors and spatial covariates, next to the linear terms, e.g.

$$x'\beta + \sum_j f_j(x_j) + f(\texttt{lat}, \texttt{long})$$

- predictor is still additive
- preferred R package is {mgcv} by Simon Wood.

More on GAMs

So, a GAM is a GLM where the linear predictor depends on **smooth functions** of covariates.

Consider a GAM with the following predictor:

$$x^{'}\beta + f_j(x_j).$$

GAMs use **basis functions** to estimate the smooth effect $f_j(.)$

$$f_j(x_j) = \sum_{m=1}^{M} \beta_{jm} b_{jm}(x_j),$$

where the $b_{jm}(x)$ are known basis functions and β_{jm} are coefficients that have to be estimated.

GAMs avoid overfitting by adding a **wiggliness penalty** to the likelihood

$$\int \left(f_j(x)''\right)^2 = \beta_j^t \mathbf{S}_j \beta_j.$$

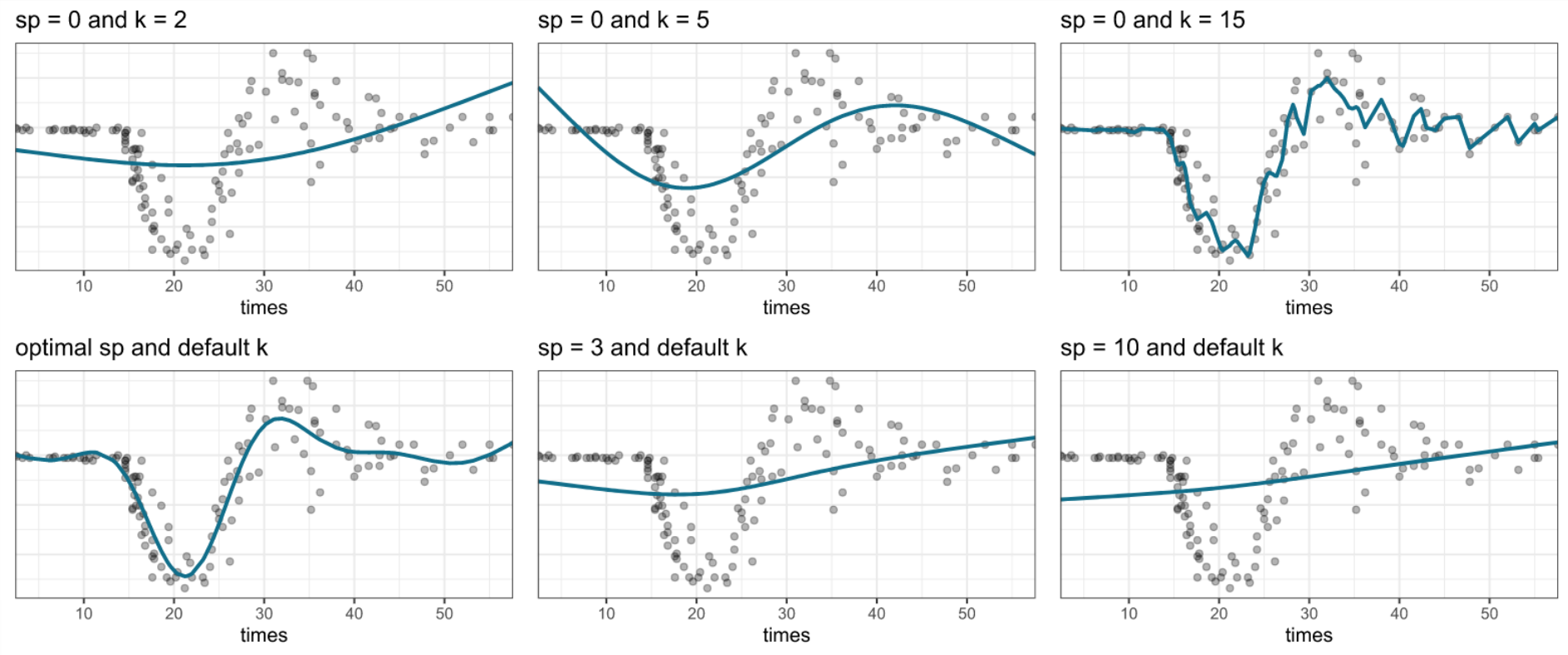
GAMs then balance goodness-of-fit and wiggliness via

$$\log \mathcal{L}(\beta, \beta_j) - \lambda_j \cdot \beta_j^t \mathbf{S}_j \beta_j,$$

with λ_j the **smoothing parameter**.

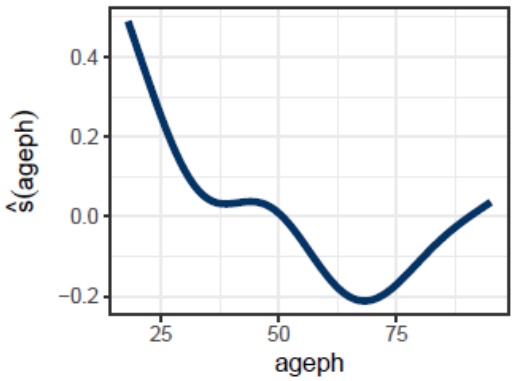
The smoothing parameter λ_j controls the trade-off between fit & smoothness.

Let's run some experiments to illustrate the effect of the smoothing parameter and the number of basis functions. We use the `mcycle` data from {MASS}.

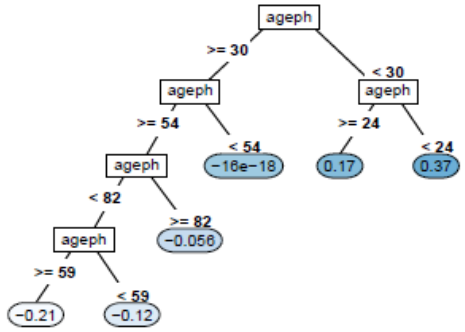


In our opinion the functionalities currently available in `pyGAM` and `statsmodels` are not meeting the R standard of {mgcv} (yet).

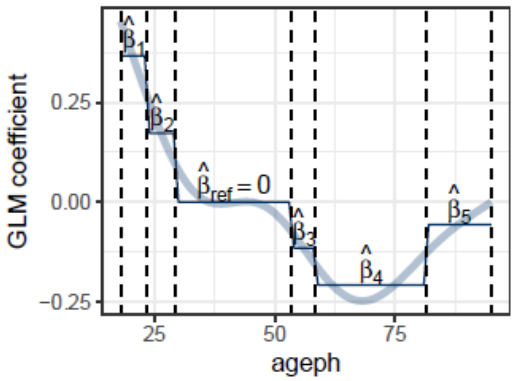
GAMs in insurance pricing analytics



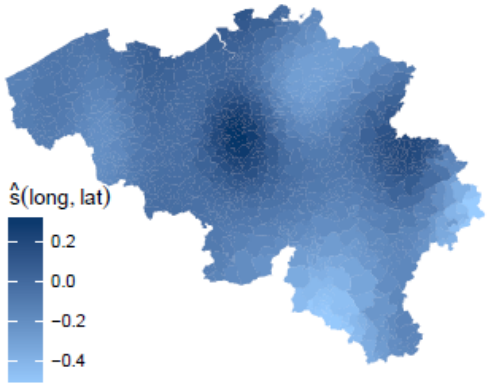
(1a) Smooth continuous effect



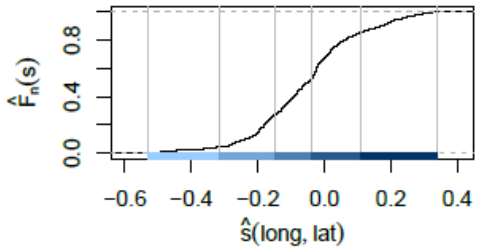
(1b) Supervised decision tree



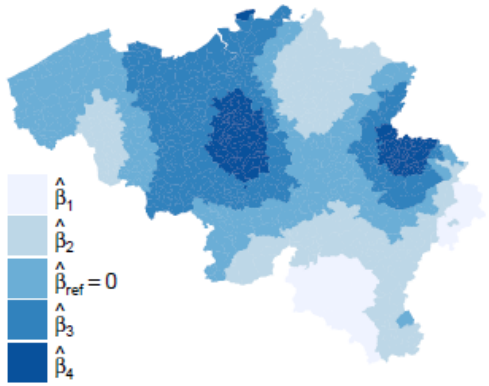
(1c) Binned continuous effect



(2a) Smooth spatial effect



(2b) Unsupervised clustering



(2c) Binned spatial effect

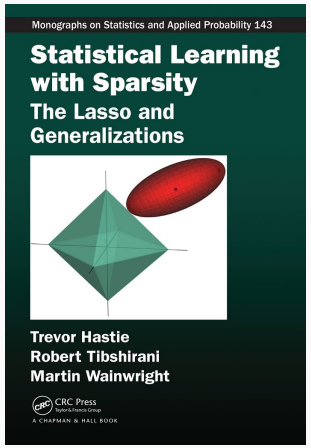
A data driven binning strategy for the construction of insurance tariff classes by Henckaerts, Antonio, Clijsters and Verbelen (2018, Scandinavian Actuarial Journal).

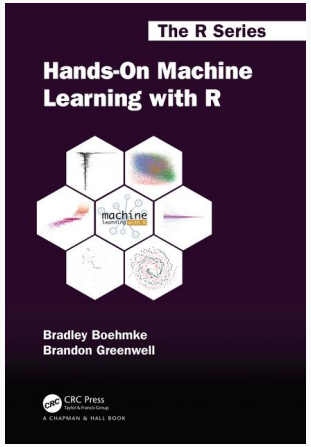
Fitting generalized additive models

Let's return to our Colab.

Regularized (G)LMs

Statistical learning with sparsity





Why?

- Sort through the mass of information and bring it down to **its bare essentials**.
- One form of simplicity is **sparsity**.
- Only a relatively small number of predictors play a role.

How? Automatic feature selection!

- Fit a model with all p predictors, but constrain or **regularize** the coefficient estimates.
- Shrinking the coeffcient estimates can signifcantly reduce their variance.
- Some types of shrinkage put some of the coefficients exactly equal to zero!

Ridge and lasso (least squares) regression

Ridge considers the least-squares optimization problem

$$\min_{\beta_0, \boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 = \min_{\beta_0, \boldsymbol{\beta}} \text{RSS}$$

subject to a **budget constraint**

$$\sum_{j=1}^{p} \beta_j^2 \leq t,$$

i.e. an ℓ_2 penalty.

Shrinks the coefficient estimates (not the intercept) to zero.

Lasso considers the least-squares optimization problem

$$\min_{\beta_0, \boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 = \min_{\beta_0, \boldsymbol{\beta}} \text{RSS}$$

subject to a **budget constraint**

$$\sum_{j=1}^{p} |\beta_j| \leq t,$$

i.e. an ℓ_1 penalty.

Shrinks the coefficient estimates (not the intercept) to zero and does variable selection!

Lasso is for **L**east **a**bsolute **s**hrinkage and **s**election **o**perator.

Ridge and lasso (least squares) regression (cont.)

The dual problem formulation:

- with ridge penalty:

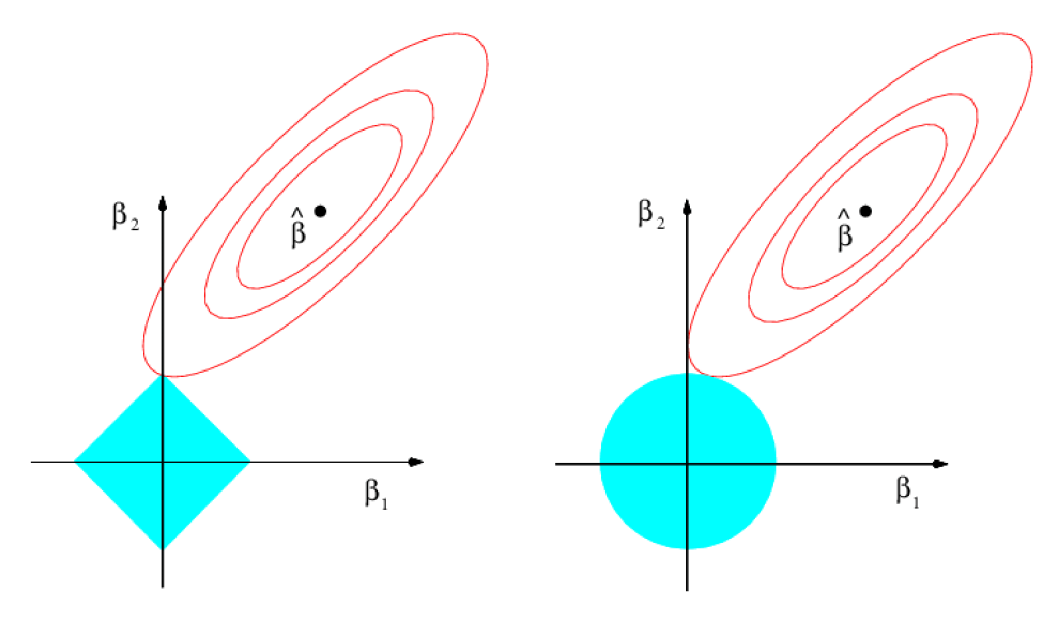
$$\min_{\beta_0, \boldsymbol{\beta}} \text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2$$

- with lasso penalty:

$$\min_{\beta_0, \boldsymbol{\beta}} \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|.$$

λ is a tuning parameter; use resampling methods to pick a value!

Both ridge and lasso require **centering and scaling** of the features.



Ellipses (around least-squares solution) represent regions of constant RSS.

Lasso budget on the left and ridge budget on the right.

Source: James et al. (2013) on An introduction to statistical learning.

Regularized GLMs

We now focus on generalizations of linear models and the lasso.

Minimize

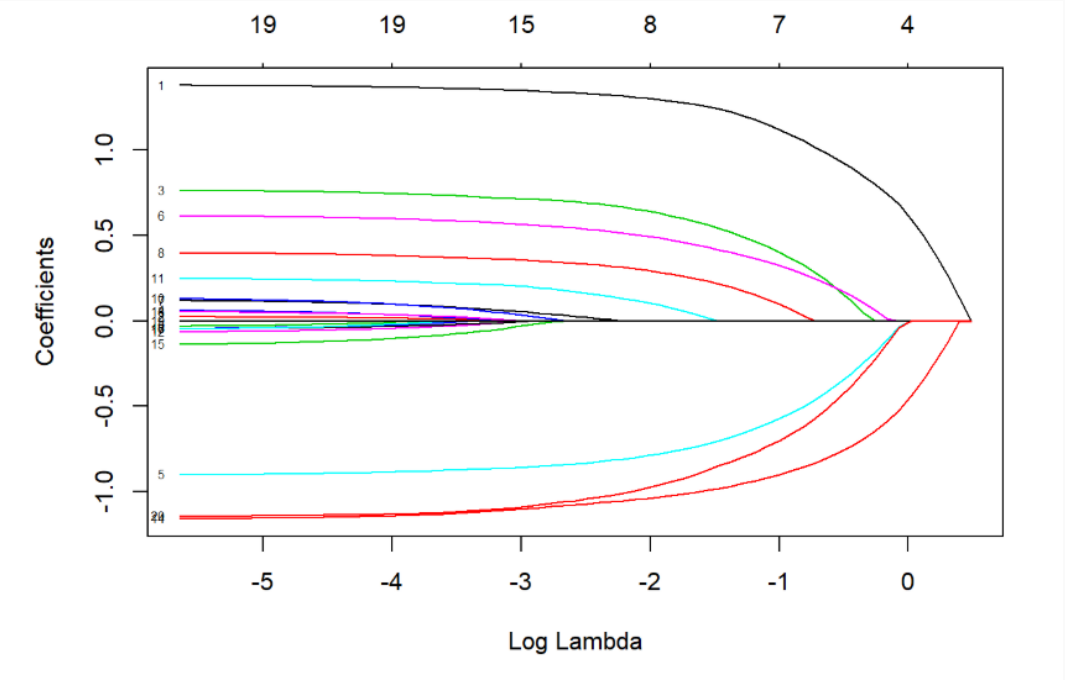
$$\min_{\beta_0,\,\beta} -\frac{1}{n}\mathcal{L}(\beta_0,\ \beta;\ y,\ X) + \lambda\|\boldsymbol{\beta}\|_1.$$

Here:

- $\mathcal{L}$ is the log-likelihood of a GLM.
- n is the sample size
- $\|\boldsymbol{\beta}\|_1 = \sum_{j=1}^{p} |\beta|_j$ the ℓ_1 penalty.

What happens if:

- $\lambda \to 0$?
- $\lambda \to \infty$?

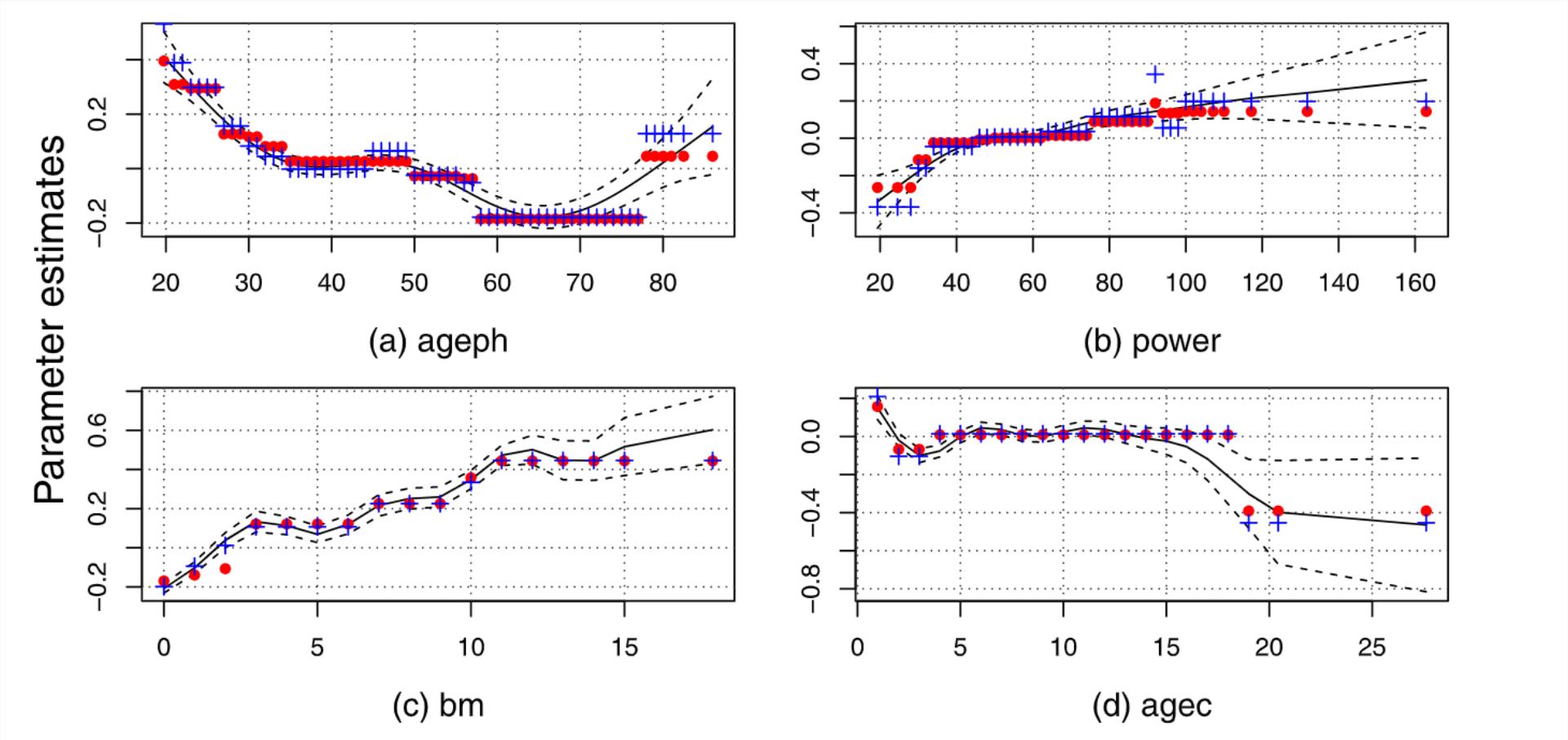


A more general penalty is the so-called **elastic net penalty**:

$$\alpha\left(\lambda|\beta|_1 + \frac{1-\lambda}{2}|\beta|_2^2\right)$$

.

Regularization in insurance pricing analytics



Sparse regression with Multi-type Regularized Feature Modeling by Devriendt, Antonio, Reynkens and Verbelen (2021, Insurance: Mathematics and Economics).

Fitting regularized LMs and GLMs

Let's return to our Colab and fit regularized regression models with `scikit-learn` and `statsmodels`.

Thanks!

Slides created with the R package xaringan.

Course material available via

https://github.com/katrienantonio/hands-on-machine-learning-Python-module-1