workday

ML WITH A LARGE SET OF VARIABLES: FEATURE SELECTION FOR REGRESSION

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workday

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Data Scientist

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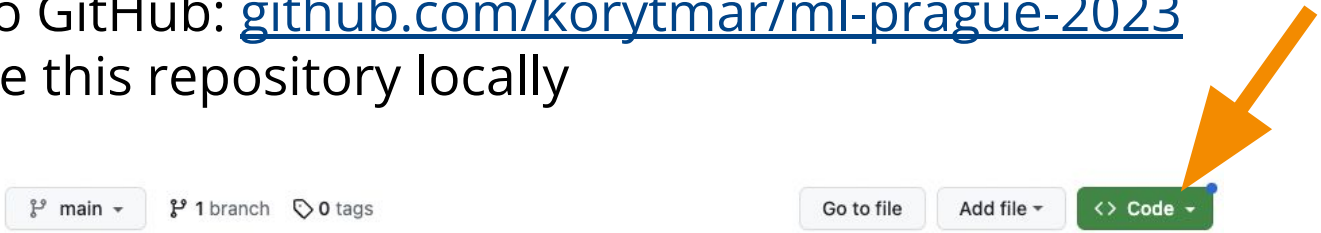
AGENDA

Set-up

A. Go to GitHub: github.com/korytmar/ml-prague-2023
B. Clone this repository locally



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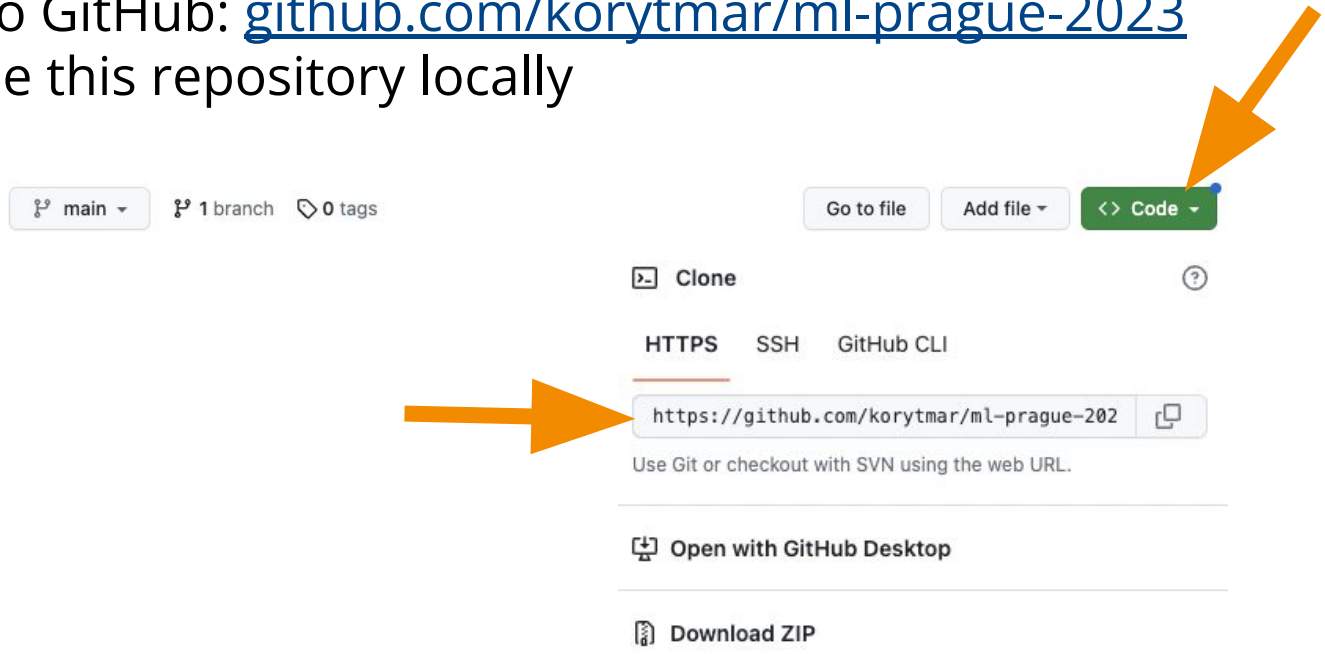

Know the audience

https://t.ly/x9-V

DATA WITH MANY VARIABLES: INTRODUCTION

Dataset with too many variables

Example 1: HR data about employees

```
worker_data.head()
```

	compa_ratio	high_performer	high_potential	is_leader	is_manager	length_of_service	total_compensation	age	compa_ratio_range -> Above Compa-Ratio	compa_ratio_range -> At Compa-Ratio	...
0	1.088	False	False	False	False	1.573	4788.30	24.0	1	0	...
1	0.826	False	False	False	False	4.129	1238.43	28.0	0	0	...
2	0.998	False	False	False	False	7.463	2395.47	29.0	0	1	...
3	0.918	False	False	False	False	0.129	4133.05	22.0	0	0	...
4	1.343	True	False	False	False	1.307	1745.30	39.0	1	0	...

Anka

Goal: Predicting salaries using employee data such as experience, position, etc.

Dataset with too many variables

Example 1: HR data about employees

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1000 rows x 404 columns

Dataset with too many variables

Example 1: HR data about employees

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Angry boyfriend

1000 rows x 404 columns

Manual feature selection time: 2 days

Dataset with too many variables

Example 2: Biology experiment with genetics data

	Gene 1	Gene 2	Gene 3	Gene 4	Gene 5
Batch 1	0.405	0.326	0.234	0.348	0.748
Batch 2	0.089	0.293	0.192	0.123	0.385
Batch 3	0.459	0.125	0.543	0.334	0.218
Batch 4	0.123	0.389	0.238	0.651	0.972

Goal: Predicting protein production of a cell using gene expressions data

Taha

Dataset with too many variables

Example 2: Biology experiment with genetics data

	Gene 1	Gene 2	Gene 3	Gene 4	Gene 5
1	0.405	0.326	0.234	0.348	0.748
2	0.089	0.293	0.192	0.123	0.385
3	0.459	0.125	0.543	0.334	0.218
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~200 rows x 10 000+ columns

Dataset with too many variables

Example 2: Biology experiment with genetics data

	Gene 1	Gene 2	Gene 3	Gene 4	Gene 5
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4	0.123	0.389	0.238	0.651	0.972

~200 rows x 10 000+ columns

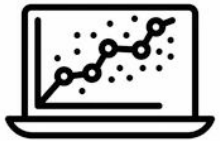
Manual feature selection time: 2 years → Very angry wife

Dataset with too many variables:
So what can we do?

Go home and cry	Do the manual selection anyway	Use all features	Use feature selection algorithm
Option 1	Option 2	Option 3	Option 4

Using all the features → not the best idea

A) Interpretability



B) Correlation among features

C) Inefficiency

D) Overfitting

A) Interpretability

100 features	I can't
1 000 features	I cannot
10 000 features	I am unable to can

B) Correlated features

Too many features → likely many are highly correlated.

Some models such as those based on linear regression (Ridge, Lasso, OMP) have an **assumption of no multicollinearity**
→ if high correlation is present, we get **biased coefficient estimates.**

C) Efficiency

Less data → algorithms are trained faster.

Feature selection is especially useful for algorithms that are trained repeatedly.

D) Overfitting

"Garbage in, garbage out."

→ Model works very well with training data, but does not generalise well with unseen data.

Example: ML Doctor

Training observations

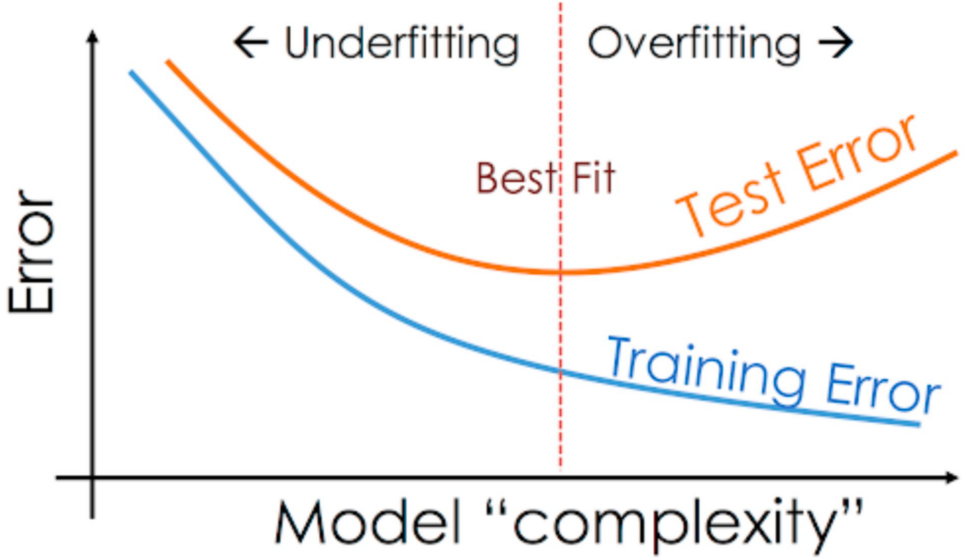
Features: green t-shirt, dark hair, cough → **label**: flu

Testing observation

Features: green t-shirt, dark hair → **label**: flu

D) Overfitting

→ Error on testing dataset is much higher than on training dataset



Using all the features → not the best idea

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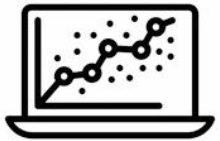

B) Correlation among features

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Dataset with too many variables:
So what can we do?

Go home and cry	Do the manual selection anyway	Use all features	Use feature selection algorithm
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🙃

FEATURE SELECTION ALGORITHMS

Feature selection: how many features are too many?

Rule of thumb: 10 samples to one feature

Research: *Hua, Jianping, et al. (2005)*

- **Uncorrelated features:** optimal number of features is $N-1$ (N = sample size)
- As **feature correlation** increases, optimum is approximately $\sqrt{N}$

Other factors to consider:

- the type of ML problem
- model complexity
- data quality and availability
- performance improvement with more features
- etc.

Feature selection: methods

Feature extraction

= Getting features typically by **transforming them to a new feature space**.

→ **dimensionality reduction**

Example: PCA creates new variables by linearly combining the original ones.

vs.

Feature selection

= Choosing a **subset** of the original features set.

→ Feature selection is a special case of dimensionality reduction.

Feature selection: methods

1. FILTER METHODS

Features are selected based on their **scores in various statistical tests.**

→ Correlation, ANOVA, Chi-Squared, ...

2. WRAPPER METHODS

Many model specifications are tested - based on one model's result, we decide about inclusion/exclusion of a variable in the next model.

→ Boruta, Orthogonal Matching Pursuit, Backward Elimination, ...

3. EMBEDDED METHODS

Algorithms with **built-in methods** for selecting features.

→ Random Forest, Ridge, LASSO, ...

Feature selection: methods

FILTER METHODS

+ Quick and less computationally expensive

- Ignore feature dependencies

WRAPPER METHODS

+ Usually provide better model performance than filter methods

- Can have high computational cost

EMBEDDED METHODS

+ Combine the best characteristics of filtering and wrapping

- Might be also computationally heavy

Feature selection: methods we will cover

1. FILTER METHODS

Features are selected based on their scores in various statistical tests.

→ Correlation, ANOVA, Chi-Square, ...

2. WRAPPER METHODS

According to the conclusions drawn from the previous model, we decide whether to include/exclude certain features.

→ Boruta, Orthogonal Matching Pursuit, Backward Elimination, ...

3. EMBEDDED METHODS

Algorithms with built-in methods for selecting features.

→ Random Forest, Ridge, LASSO, ...

PRACTICAL USE-CASE INTRODUCTION

HR Analytics: Predicting salaries

HR Dataset

- Each row represents individual employee
- Each employee has some attributes:
  - Legal Name
  - Gender
  - Employee ID
  - Job Profile
  - Ethnicity
  - Location
  - **Salary**
  - ...

HR Dataset: Why predicting salaries?

- **Fair Compensation:** based on their skills, qualifications, experience, and contributions to the organization.
- **Transparency:** establishing a transparent and objective system for determining salaries, promoting equality and reducing biases.
- **Employee Retention and Satisfaction:** identifying any discrepancies, such as underpayment or overpayment.

HR Dataset: Example

	compa_ratio	compa_ratio_range	cost_center	country	current_rating	employee_id	ethnicity	gender	generation	high_performer	...	org_level_2
0	1.545	Above Compa-Ratio	AMER - United States of America	United States of America	4 - Exceeds Expectations	1000	Asian	Female	Generation X (1965-1980)	False	...	NaN
1	1.021	At Compa-Ratio	AMER - United States of America	United States of America	3 - Meets Expectations	1001	White	Male	Generation Z (1997 and onwards)	False	...	Board
2	0.981	At Compa-Ratio	Global Support - Asia/Pac	South Korea	5 - Outstanding Performance	1002	Asian	Male	Generation Y/Millenials (1981-1996)	True	...	Board
3	1.342	Above Compa-Ratio	AMER - Canada	Canada	2 - Needs Improvement	1003	Asian	Male	Generation X (1965-1980)	False	...	NaN
4	1.290	Above Compa-Ratio	Global Support - Asia/Pac	South Korea	3 - Meets Expectations	1004	Asian	Female	Generation Y/Millenials (1981-1996)	False	...	Board

DEMO

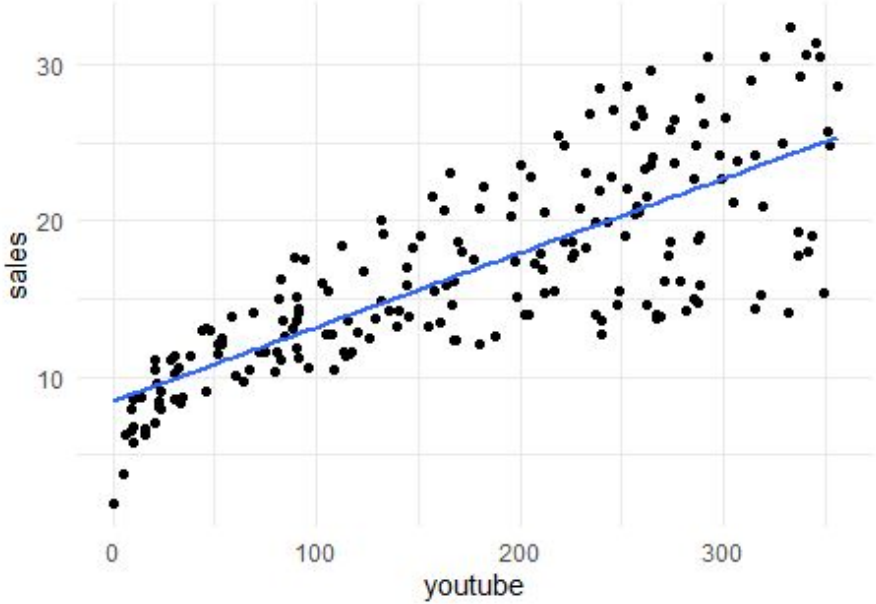
DATA PREPROCESSING PRACTICAL PART

PART I:
LINEAR REGRESSION MODELS

Linear Regression: The simplest example

$$y = \beta_0 + \beta_1 x + \varepsilon$$

youtube	sales
276.12	26.52
53.40	12.48
20.64	11.16
181.80	22.20
216.96	15.48
10.44	8.64
69.00	14.16
144.24	15.84
10.32	5.76
239.76	?
79.32	?
257.64	?



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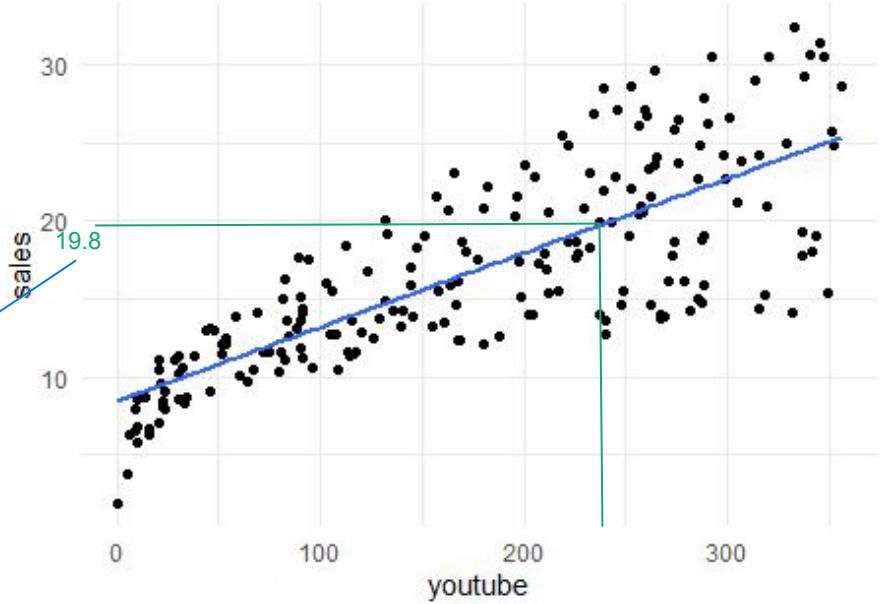


Assumptions

We need to check that model assumptions hold.

- Linear relationship → biased betas
- No multicollinearity → high variance of beta estimates
- Random sample → biased betas
- No omitted variable → biased betas

Impact on values of betas

- Homoskedasticity → invalid inference (use robust errors)
- Normality → invalid inference (large sample desired)

Impact on validity of inference

DEMO

LINEAR REGRESSION PRACTICAL PART

Orthogonal Matching Pursuit (OMP)

- Iterative greedy algorithm for sparse recovery
- OMP uses Linear Regression for estimation of coefficients in each iteration
- Improved version of Matching Pursuit algorithm

Properties

- Convergence guaranteed for any target (signal) that is in the space spanned by the dictionary
- The error decreases monotonically
- At each step, the residuals are orthogonal to the selected features (atoms)

Orthogonal Matching Pursuit (OMP)

Input: X - input dataset, y - target variable
Output: z - selected features, β - weights corresponding to selected Top Drivers

normalize X s.t. L2 norm of each column equals 1 (optional step) and standardize X
residuals <- y
z <- empty set
while y is **not sufficiently explained** do

1. compute a **pseudo correlation score** of residuals for each column in X as a dot product
2. select column from X which has the **highest absolute score** in step 1 and save its index to z
3. form a **new input dataset** consisting of columns in z and name it X'
4. w <- **solve Least square problem** using X' and y
6. **calculate new predictions** for all rows in X using coefficients β
7. **update residuals** as a difference between y and new predictions obtained in step 6

OMP PRACTICAL PART

OMP: Iteration Explained

Inputs

- Feature set (Dictionary) D: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Target (Signal) y: [1.65, -0.25]

Goal

- Estimate coefficients for each vector in dictionary such that signal can be recovered, i.e. $D * x \approx y$

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

Dictionary D consists of 3 atoms (vectors) b_1, b_2 and b_3:

- b_1 = [-0.707, 0.707]
- b_2 = [0.8, 0.6]
- b_3 = [0, -1]

We try to estimate coefficients in vector x using dictionary D and Signal y such that:
$b_1 * x_1 + b_2 * x_2 + b_3 * x_3 = [-0.707, 0.707] * x_1 + [0.8, 0.6] * x_2 + [0, -1] * x_3 \approx y$

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

Let's find the contribution of atoms to Signal y using $b_i^T y$:

- $b_1^T y$ = [-0.707, 0.707] * [1.65, -0.25] = -0.707 * 1.65 - 0.707 * 0.25 = **-1.34**
- $b_2^T y$ = [0.8, 0.6] * [1.65, -0.25] = 1.17
- $b_3^T y$ = [0, -1] * [1.65, -0.25] = 0.25

Atom b_1 has the highest contribution while neglecting the negative value. Furthermore, atom b_1 forms basis A.

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

Next, we calculate the contribution of basis A to signal y. This leads to the Least Square Problem which is formulated as follows:

$$\min \|A * x - y\|_2$$

which can be solved as:

$$A^{+} = (A^{T} * A)^{-1} * A^{T}$$

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

$A^+ = (A^T * A)^{-1} * A^T$

- $x_1 = A^+ * y = [b_1] * y = [[-0.707, 0.707]] * [1.65, -0.25] = -1.34$
- $x_2 = 0$
- $x_3 = 0$

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

- Residuals = Signal - current predictions
- $r = y - A * x = y - b_1 * x_1 = [0.7, 0.7]$

OMP: Iteration Explained

- Dictionary: [
  [-0.707, 0.8, 0],
  [0.707, 0.6, -1]
  ]
- Signal: [1.65, -0.25]

Second iteration and so on:

- b_2 contributes better than b_3
- Coefficients are updated as follows x = [-1.2, 1, 0]
- Residuals are zeros after update, i.e. [0, 0, 0]
- The algorithm **stops** after this iteration as residuals are already vanished

OMP: Summary

$x, r, \Lambda = \text{OMP}(\Phi, y);$

$x^0 \leftarrow 0;$

$r^0 \leftarrow y$; // $r = y - \Phi x$

$\Lambda^0 = \varnothing$; // Index set of chosen atoms

$k \leftarrow 0$; // Iteration counter

repeat

- $h^{k+1} \leftarrow \Phi^T r^k$; // Match
- $\lambda^{k+1} = \arg\max_{j \notin \Lambda^k} |h_j^{k+1}|$; // Identify
- $\Lambda^{k+1} \leftarrow \Lambda^k \cup \{\lambda^{k+1}\}$; // Update support
- $x^{k+1} \leftarrow 0$;
- $x^{k+1}_{\Lambda^{k+1}} \leftarrow \Phi^{\dagger}_{\Lambda^{k+1}} y$; // Update representation LS
- $y^{k+1} = \Phi x^{k+1}$; // Update approximation
- $r^{k+1} \leftarrow y - y^{k+1}$; // Update residual
- $k \leftarrow k + 1$; // Update iteration counter

until *halting criteria is satisfied*;

$x \leftarrow x^k$; $\Lambda \leftarrow \Lambda^k$; $r \leftarrow r^k$;

Quiz

Are these statements true or false?

- OMP sequentially selects atoms from the dictionary that best match the residual signal.
- OMP guarantees exact recovery of the sparse signal in a finite number of iterations.
- OMP assumes that the signal can be represented as a linear combination of a few dictionary atoms.

PART II:
TREE-BASED METHODS FOR FEATURE SELECTION

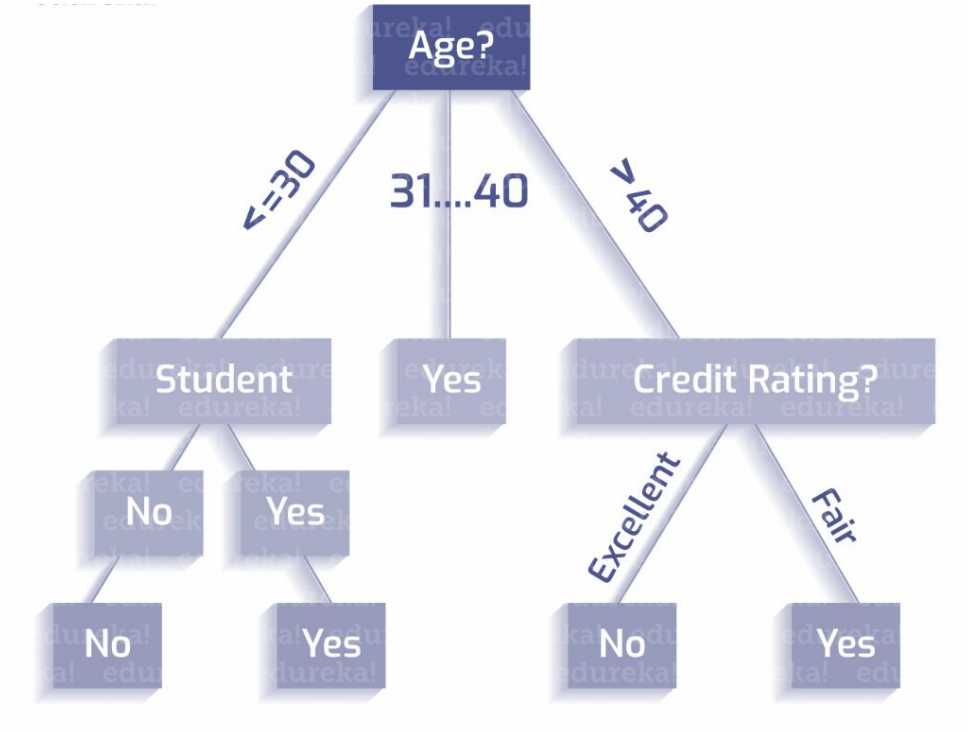
TREE-BASED METHODS

DECISION TREES

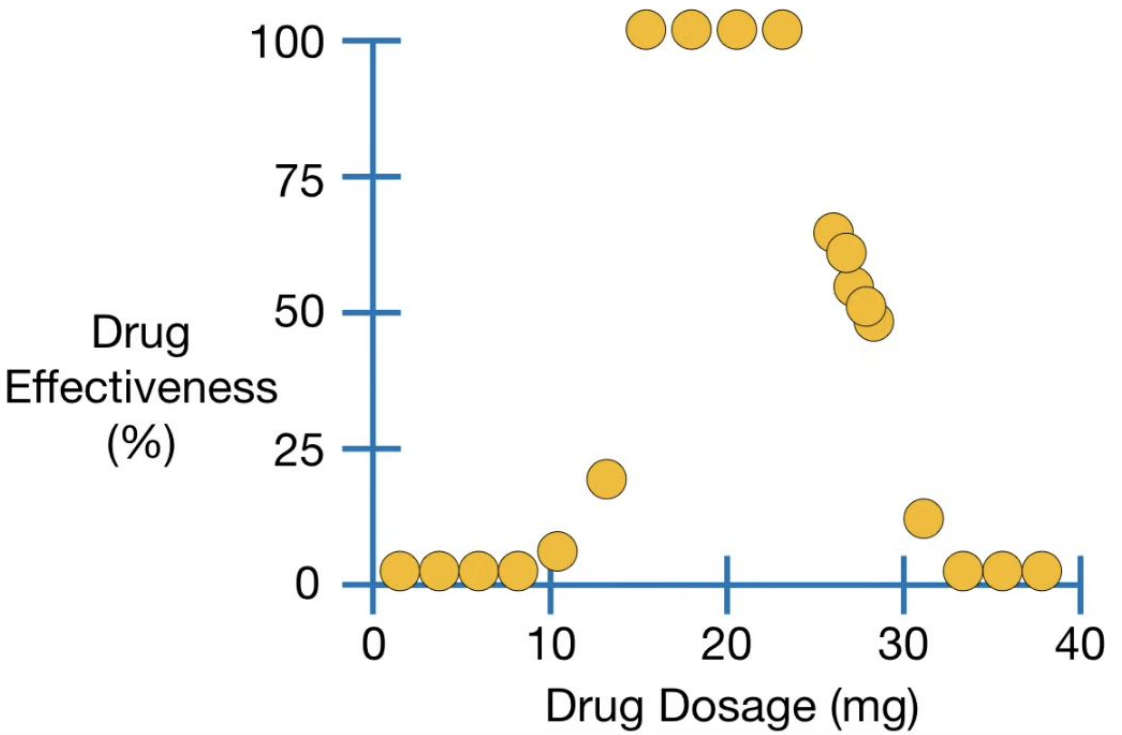
Decision Tree: the starting algorithm

EXAMPLE:

Predicting if a person will buy given product or not



Decision Tree for regression: non-linearity



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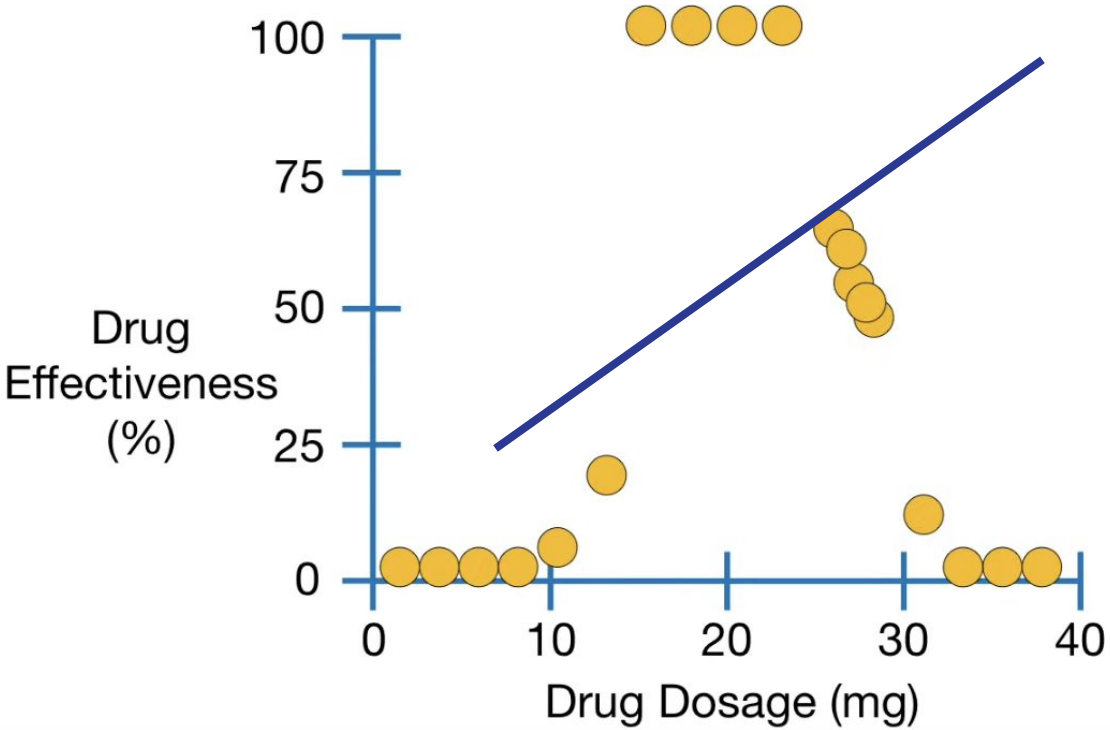
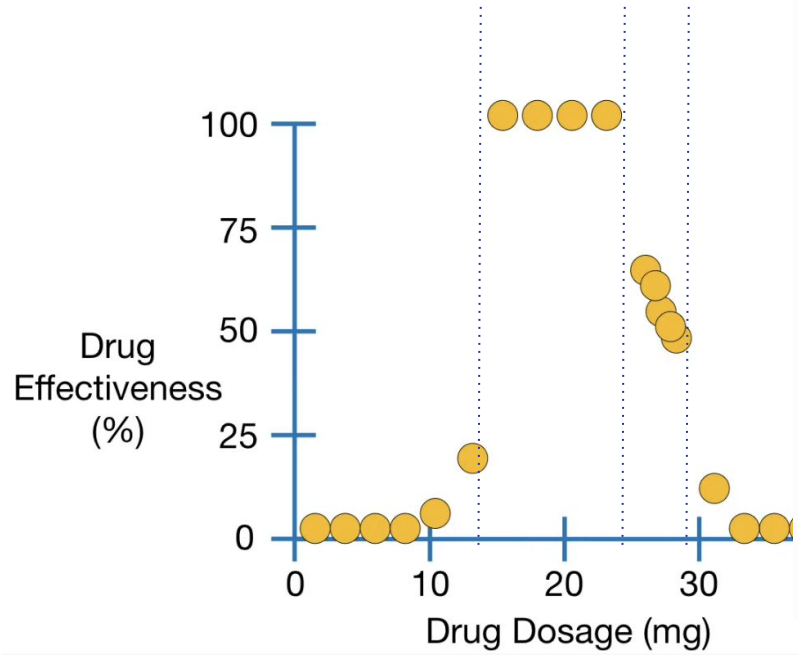
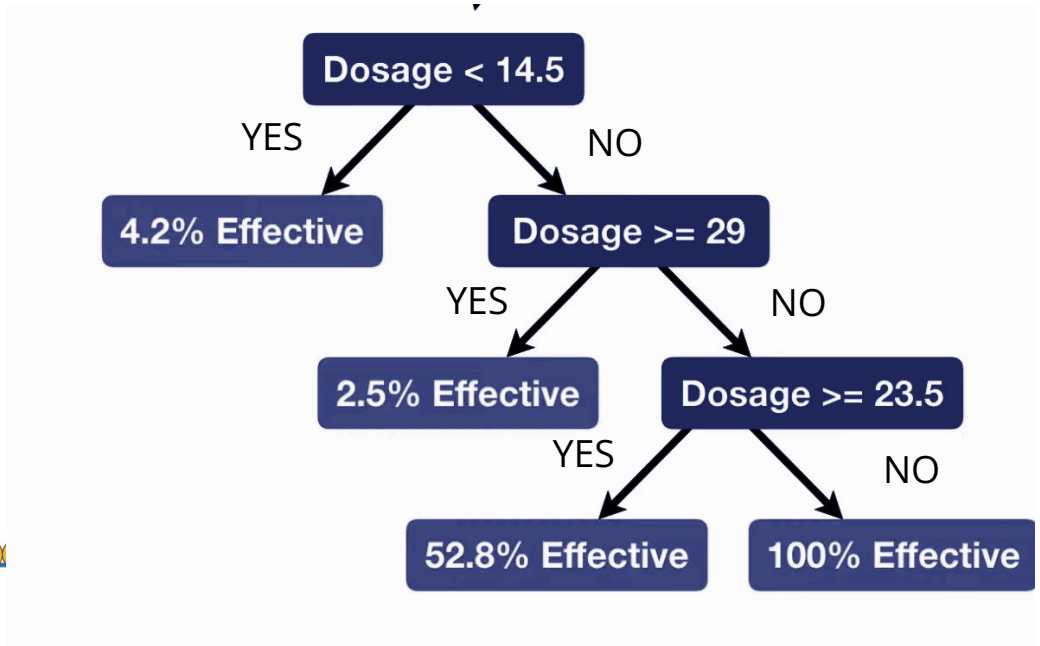
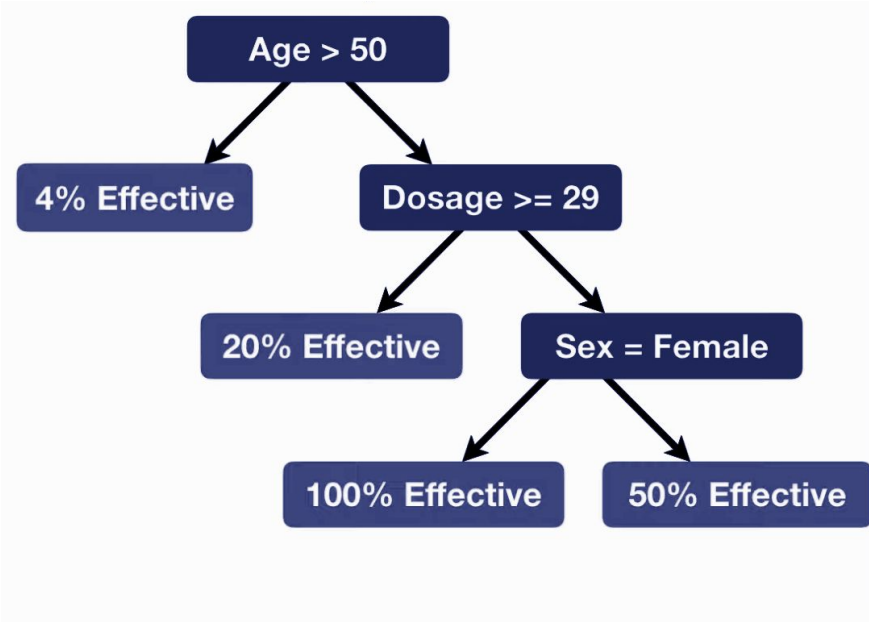


Regression tree example





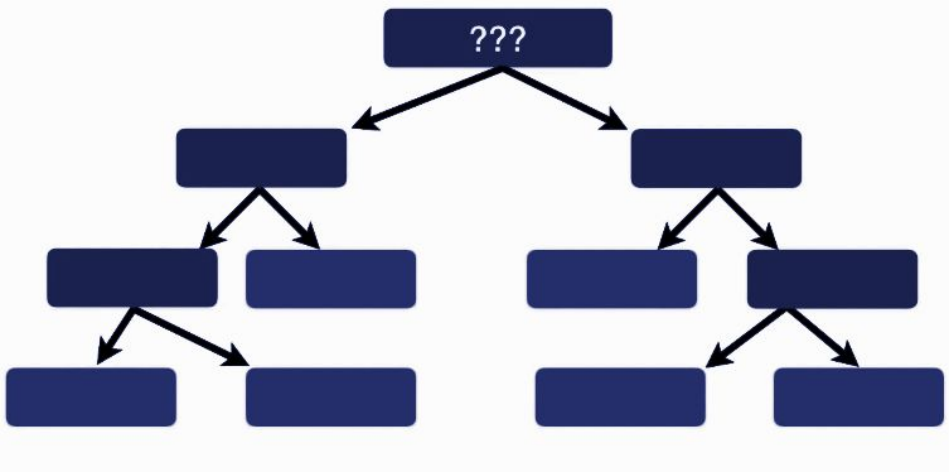
Regression tree example - multiple variables



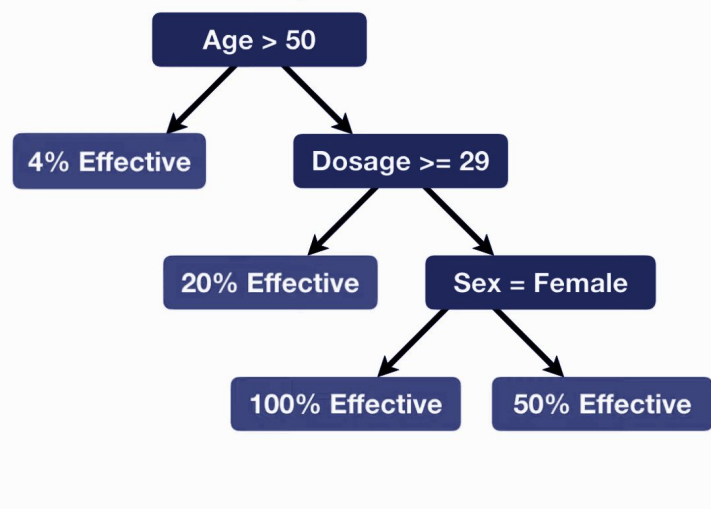
Dosage	Age	Sex	Etc.	Drug Effect.
10	25	Female	…	98
20	73	Male	…	0
35	54	Female	…	100
5	12	Male	…	44
etc…	etc…	etc…	etc…	etc…

Building a tree - predicting effectiveness by dosage

What condition do we start with?



Is this the best tree?



Building a tree - predicting effectiveness by dosage

What condition do we start with?

We try all possible thresholds, and **see which threshold gives us the lowest error.**

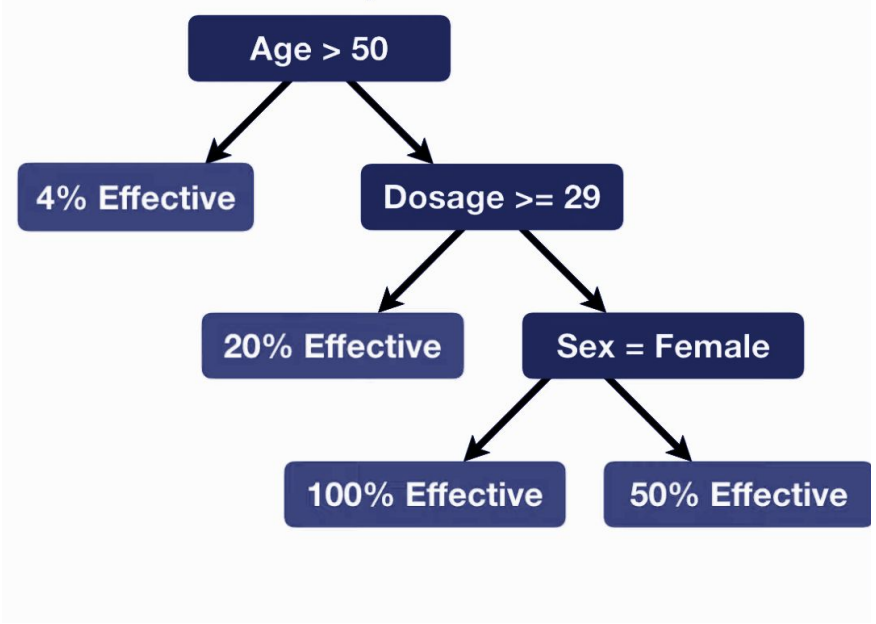
$$\text{Sum of squared residuals} = \sum (\text{Predicted value} - \text{Observed value})^2$$

Patient ID	Gender F	Weight	Diabetes	Effectiveness - observed	Effectiveness - predicted
111	1	55	1	65	67
112	1	68	0	72	74
113	0	80	0	33	32
114	1	59	0	83	79

Predicting effectiveness using multiple variables

We calculate **sum of squared residuals for every threshold of every variable.**

→ We choose the one with the lowest error value.



Decision Tree: Pros and Cons

Advantages

- easy to visualize
- non-linear patterns can be captured easily
- no special data processing needed

Disadvantages

- overfitting (imprecise predictions on new data) → large variance

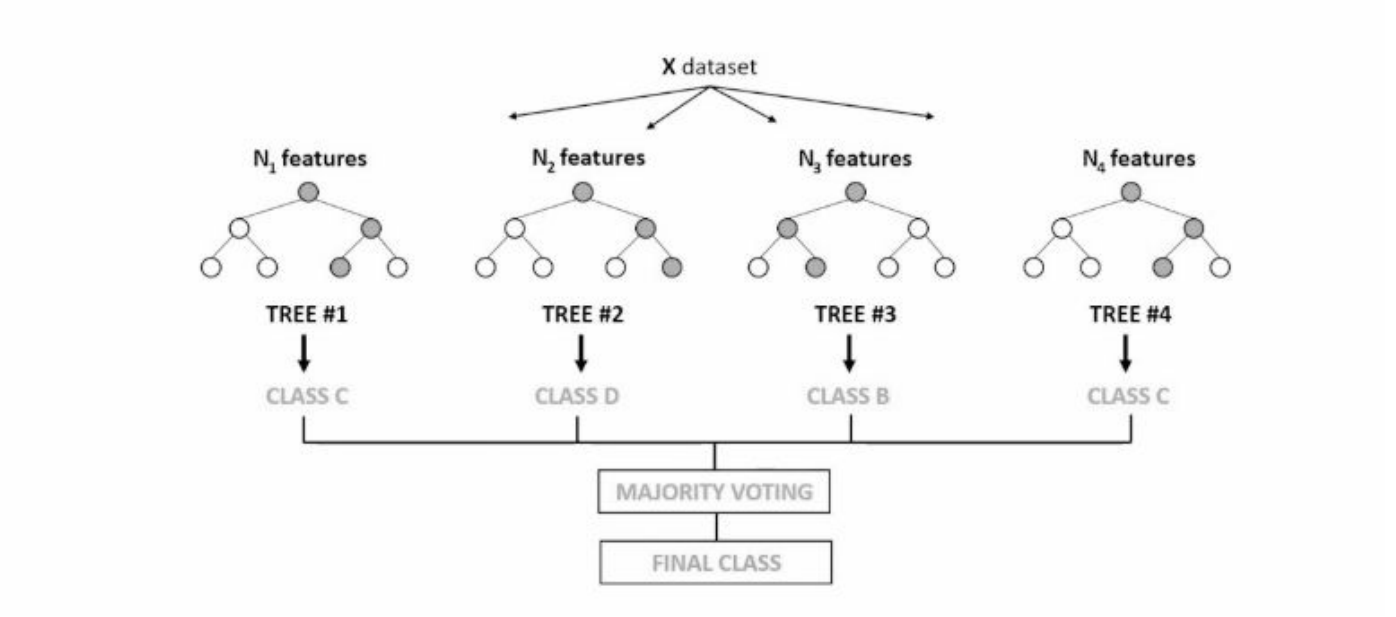
RANDOM FOREST

Random Forest

- **Ensemble method** that builds **multiple decision trees**
- It can have 50, 100, 200, 500, … trees → depends on the data size

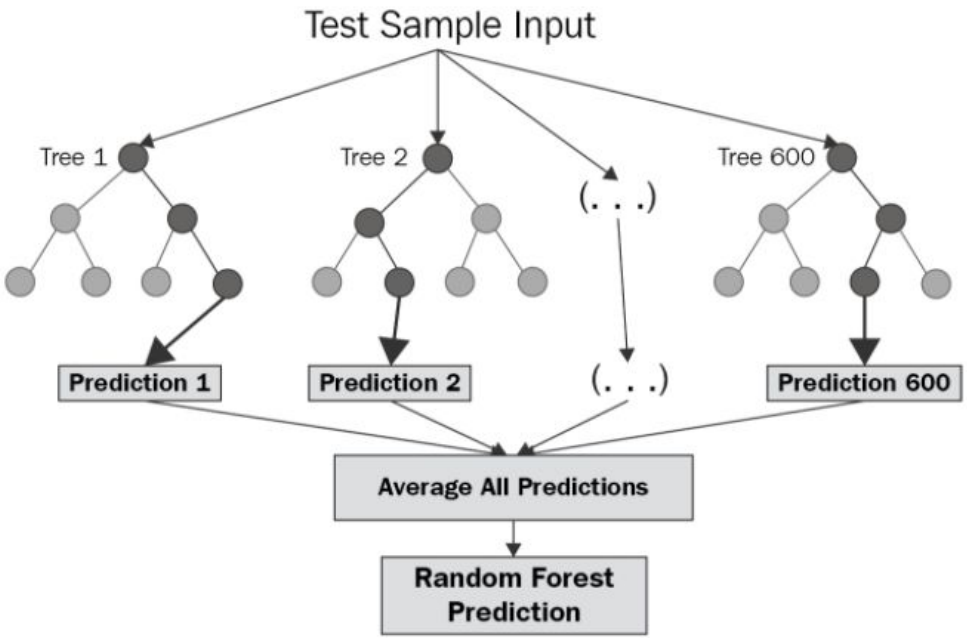
Random Forest

In classification, the prediction is **the majority vote of all decision trees' predictions.**



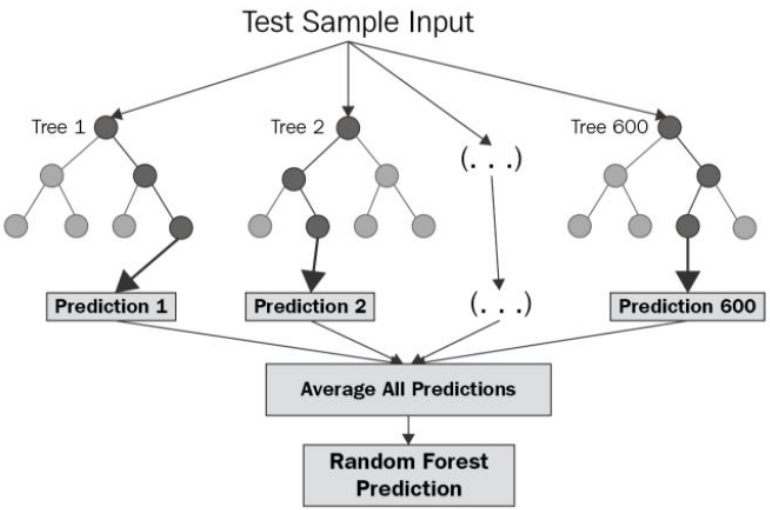
Random Forest

In regression, the prediction is **the average of all decision trees' predictions.**



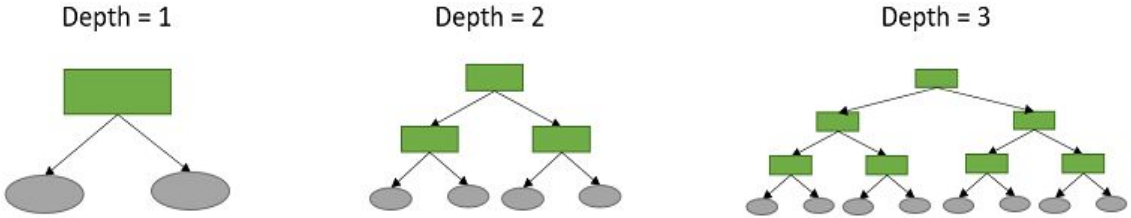
Random Forest: How it works

- Each tree is build based on a **random sample from training data**.
- The algorithm **randomly selects a subset of explanatory variables** for each split in each decision tree.
- We use the **majority vote/average as the final prediction.**



Random Forest: Hyperparameters tuning

a) **Maximum depth** of the trees



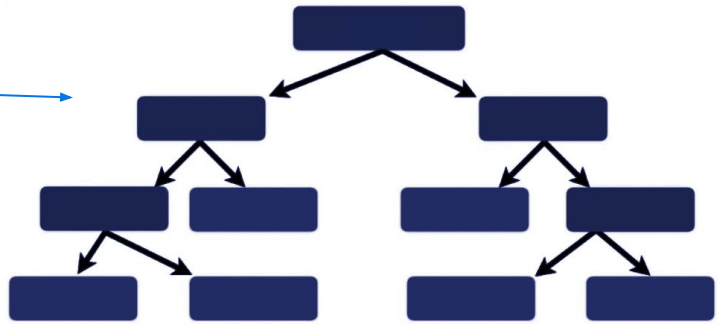
b) **Number of trees** in the forest

c) **Maximum number of features** to be considered at each node split

Random Forest: Hyperparameters tuning

d) Minimum number of samples required to split a node

e) Minimum number of samples in a leaf node



RF feature selection: Variable importance

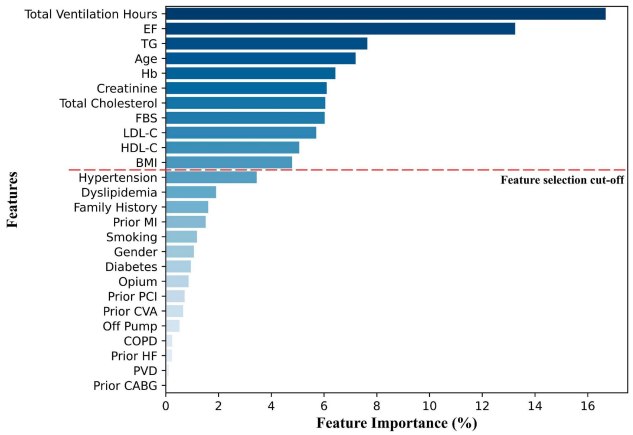
- Measure for **ranking our explanatory variables**
- Not interpreted as betas in linear regression

Variable Importance → increase in node purity: how much the sum of squared errors is reduced whenever a variable is chosen to split.

RF feature selection: Variable importance

Final set of features:

- best **k** attributes
- best **x %** of attributes
- make **a cutoff at the biggest difference in importance scores**



Random Forest for feature selection

- One of the **most accurate** algorithms available (even with a lot of missing data)
- **Efficient** with large datasets
- Variable importance as a **straightforward metrics**
- However, gives us just **relative ranking, not the magnitude** of feature impact

Quiz

Are these statements true or false?

- Random forest randomly selects a subset of explanatory variables for each split in each decision tree.
- There is no generally applicable variable importance threshold.
- Decision tree maximizes the sum of squared residuals when it selects the decision conditions.

DEMO

RANDOM FOREST PRACTICAL PART

BORUTA

Boruta

- An algorithm that builds up on random forest
- **First, another data frame** is created from original X data by **randomly shuffling each feature**
- The newly created data frame is attached to the original dataframe → now we have **twice as many columns**

Boruta: shadow features

- Variables created by random shuffling of original values are called **shadow features**

	age	height	weight	shadow_age	shadow_height	shadow_weight
0	25	182	75	51	176	75
1	32	176	71	32	182	71
2	47	174	78	47	168	78
3	51	168	72	25	181	72
4	62	181	86	62	174	86

- Random Forest is run with all (old + shadow) features and variable importance is calculated

Boruta: feature selection

Threshold for variable selection: a feature must have importance higher than **the highest feature importance recorded among the shadow features**

→ **The main idea:** a feature is useful only if it's capable of doing better than the best randomized feature.

Boruta: feature selection

→ Based on a high variable importance, we tag some features as **‘important’**

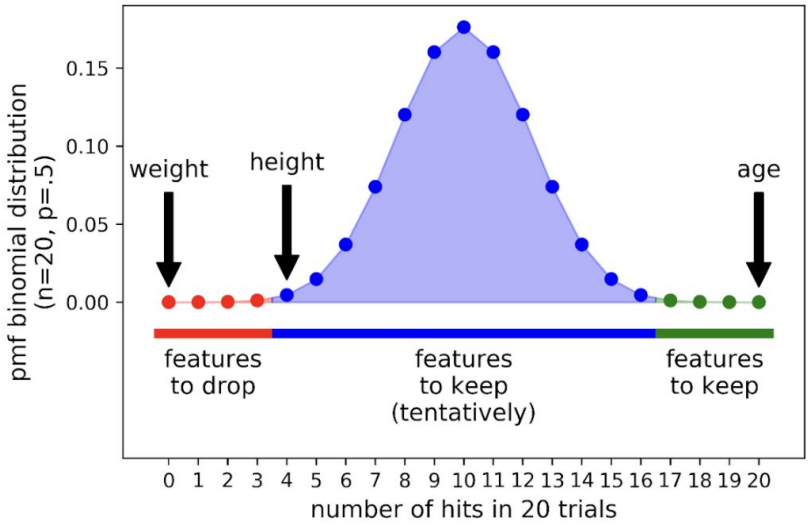
→ If **some features have significantly lower importance** than the best shadow feature, we tag them as ‘unimportant’ and **remove them**

Boruta: multiple randomized runs

We **use multiple boruta runs:**

- a specified number of iterations, or
- until all features are tagged as ‘important’ or ‘unimportant’

A series of *n* trials follows a binomial distribution.



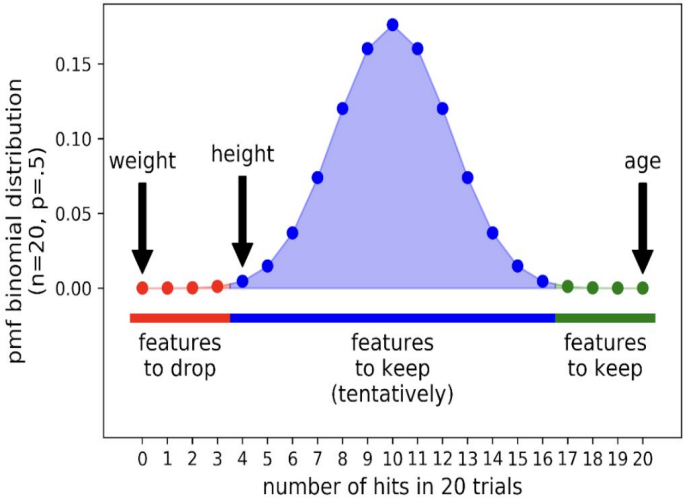
Boruta: final decision for selection

Boruta has three areas:

- **area of refusal** (red): features are dropped

- **area of irresolution** (blue): Boruta is indecisive about these features → up to a data scientist, but these features are typically kept

- **area of acceptance** (green): features are kept



Quiz

Are these statements true or false?

- For each variable, Boruta gives us a definite answer on whether to keep it in the model or not.
- Boruta uses original features and shadow features in one model all at the same time.
- Shadow features are created by randomly shuffling values of the original features.

DEMO

BORUTA PRACTICAL PART

CONCLUSION

How are the selected features similar?

Jaccard similarity:

$$J(A,B) = \frac{|A \cap B|}{|A \cap B|}$$

Selected features by all models:

{'age', 'compa_ratio', 'cost_center -> Global Support - Asia/Pac', 'is_leader', 'job_level -> M5', 'job_level -> M6', 'job_level -> M7', 'job_level -> M8', 'job_level -> P1', 'job_level -> P3', 'job_level -> P5', 'region -> AMER'}

	OMP	**RF**	**Boruta**
OMP	1	0.43	0.48
RF	0.43	1	0.87
Boruta	0.48	0.87	1

How to choose your algorithm?

Multiple metrics which are used for model evaluation on the testing dataset.

Metric	OMP	RF	Boruta
RMSE	24,917	6,821	6,700
MAPE	9.84 %	0.5 %	0.46 %

How to evaluate/compare models?

- Compare **performance metrics** (consider multiple metrics)
- Check results of other models (**consistency** of outputs)
- Consider **model complexity** (architecture, number of parameters or training time – always prefer less complex model)
- Consider **domain-specific knowledge** and interpretability
- External **benchmarks** (SOTA models in the field)
- Consider also models not covered in this workshop such as Lasso, Ridge and Gradient boosted trees

Conclusion

What we learned today:

- Issues when dealing with too many **features:** interpretability, correlation, efficiency, overfitting
- **Algorithms**: linear & tree based methods
- Metrics (RMSE, MAPE) to **evaluate models**
- **Select the best model** based on: performance, consistency, complexity, or domain knowledge

Conclusion

What we learned today:

- Issues when dealing with too many **features:** interpretability, correlation, efficiency, overfitting
- **Algorithms**: linear & tree based methods
- Metrics (RMSE, MAPE) to **evaluate models**
- **Select the best model** based on: performance, consistency, complexity, or domain knowledge

workday.

Thank You

workday.

Questions?

Your feedback is important!

https://t.ly/u9R6

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