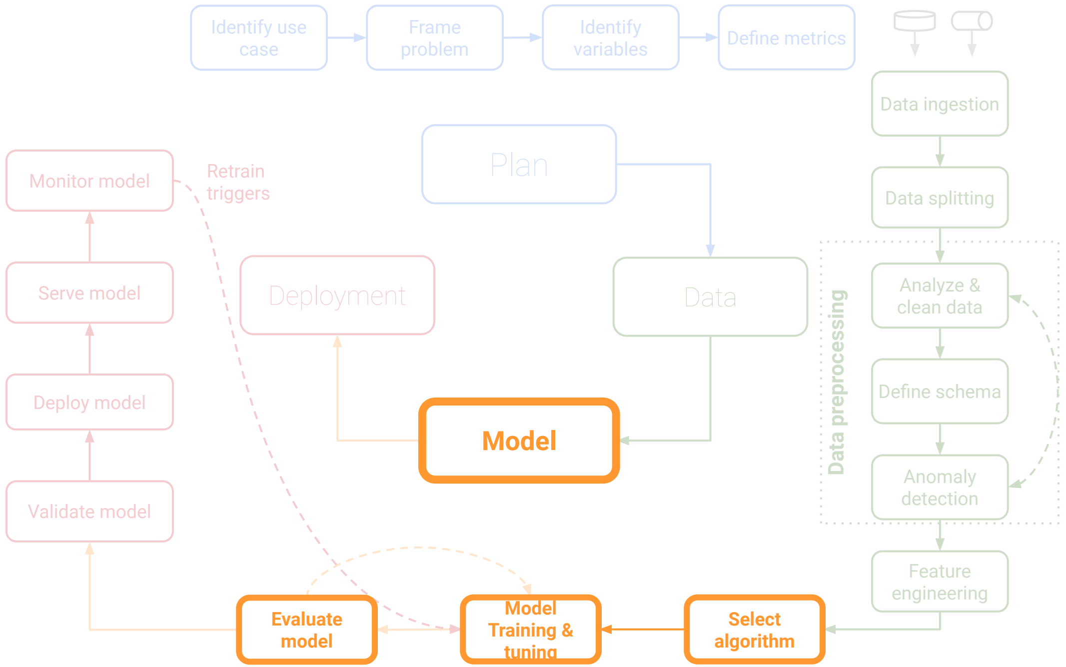
Models

Fundamentals

Prof. Dr. Jan Kirenz
HdM Stuttgart

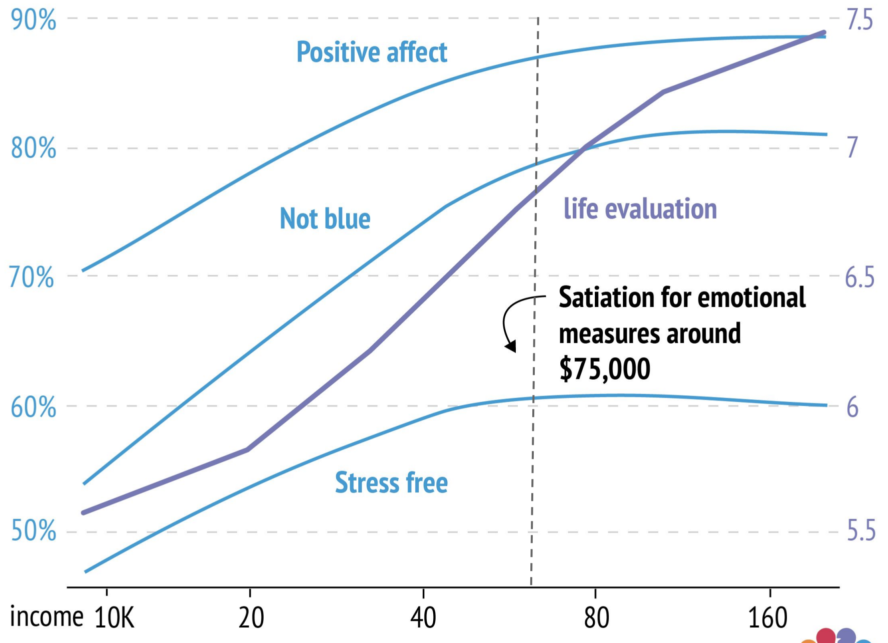
Data Science Lifecycle

Plan | Data | **Model** | Deployment



How do we select, train, tune (optimize) and evaluate models?

Data: Money & Happiness



Note: X axis scale is not linear.
Source: Kahneman and Deaton (2010)

*Widely regarded as one of the world's most influential living psychologist, **Daniel Kahneman** won the Nobel in Economics for his pioneering work in behavioral economics:*

„Below an income of … $60,000 a year, people are unhappy, and they get progressively unhappier the poorer they get. Above that, we get an absolutely flat line. … Money does not buy you experiential happiness, but lack of money certainly buys you misery."

Watch TED-talk: TED

Money can buy happiness, but only to a point

Does money make people happier?

- Get the data at GitHub:

GitHub

- Get the code at GitHub:

GitHub

Country	GDP per capita	Life satisfaction
Hungary	12239.894	4.9
Korea	27195.197	5.8
France	37675.006	6.5
Australia	50961.865	7.3
United States	55805.204	7.2

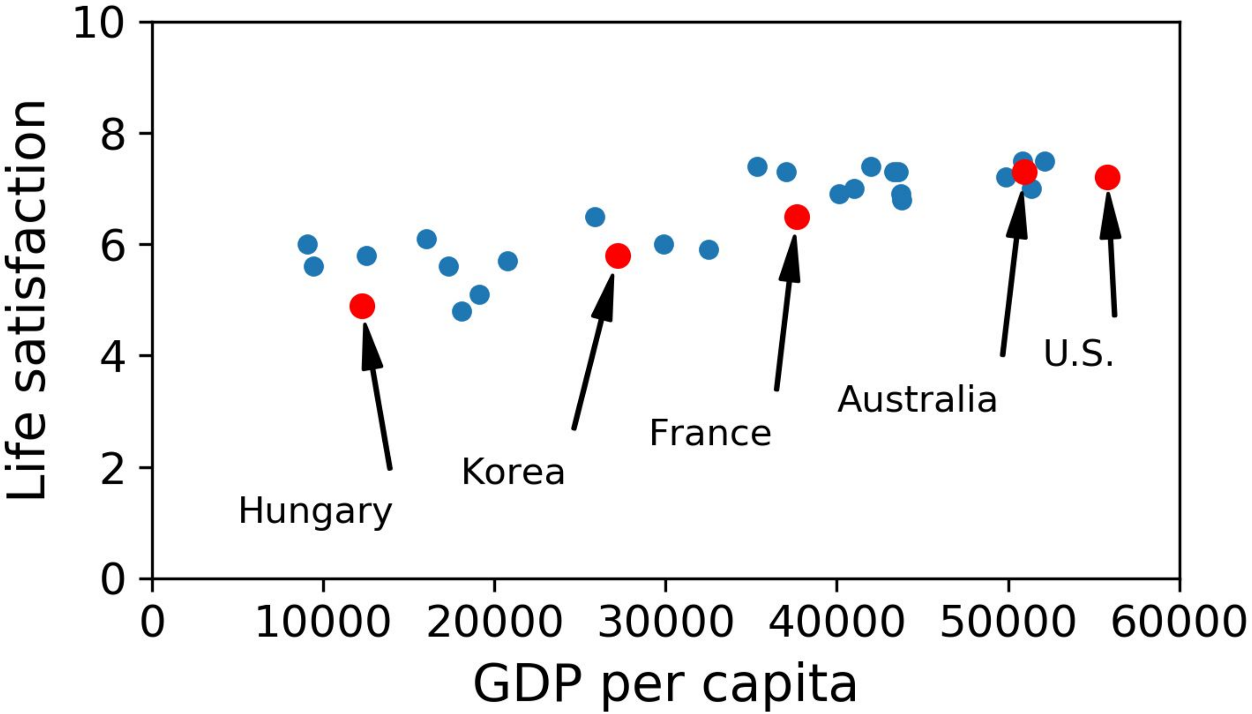
Raw data:

OECD Better Life Index data: **Life satisfaction**

ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT OECD.Stat

IMF: **Gross domestic product per capita**

Exploratory data analysis (EDA)



Do you see a trend?

1. Data exploration gives indication for a trend that is:
    a. Positive or negative?
    b. Linear or non-linear?

… but be careful, the data is noisy (i.e., partly random)

2. Model (type) selection:
    a. Regression or classification?
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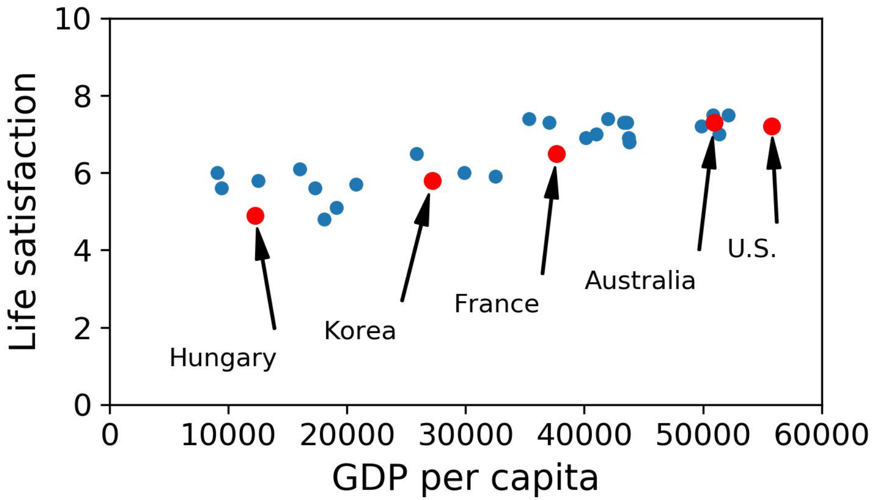

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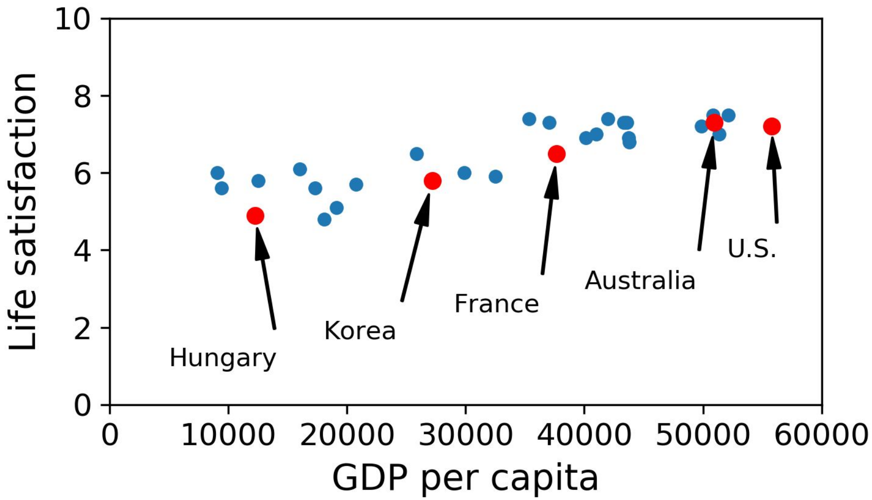

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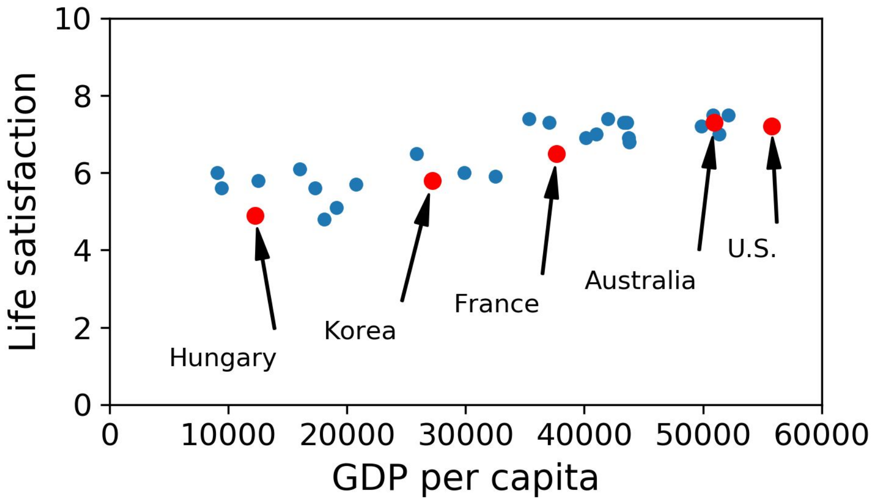

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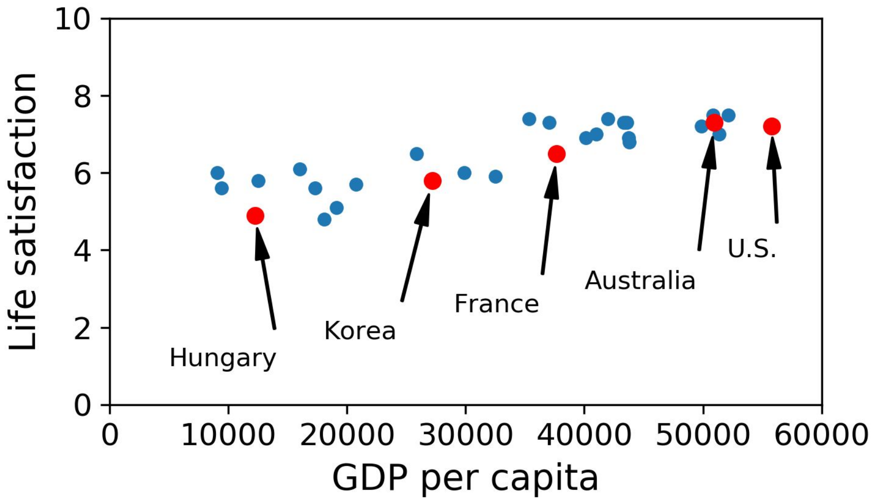

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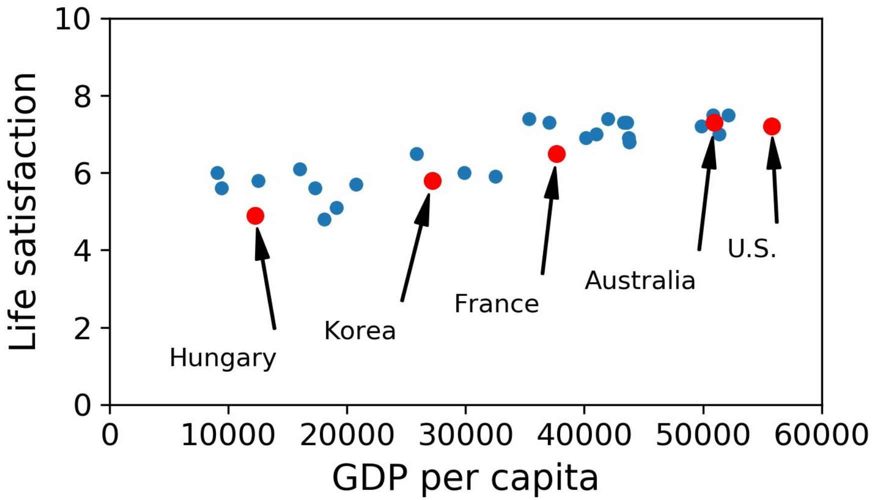

A simple linear regression model

$\hat{y}_i = \theta_0 + \theta_1 \times x_1$

- $\hat{y}_i$ is the predicted output (life satisfaction).
- θ_0 is the bias (the y-intercept).
- θ_1 is the slope of our feature 1 (in machine learning often called weight of the feature)
- x_1 is our feature GDP (a known input).

All the same, just different notations:

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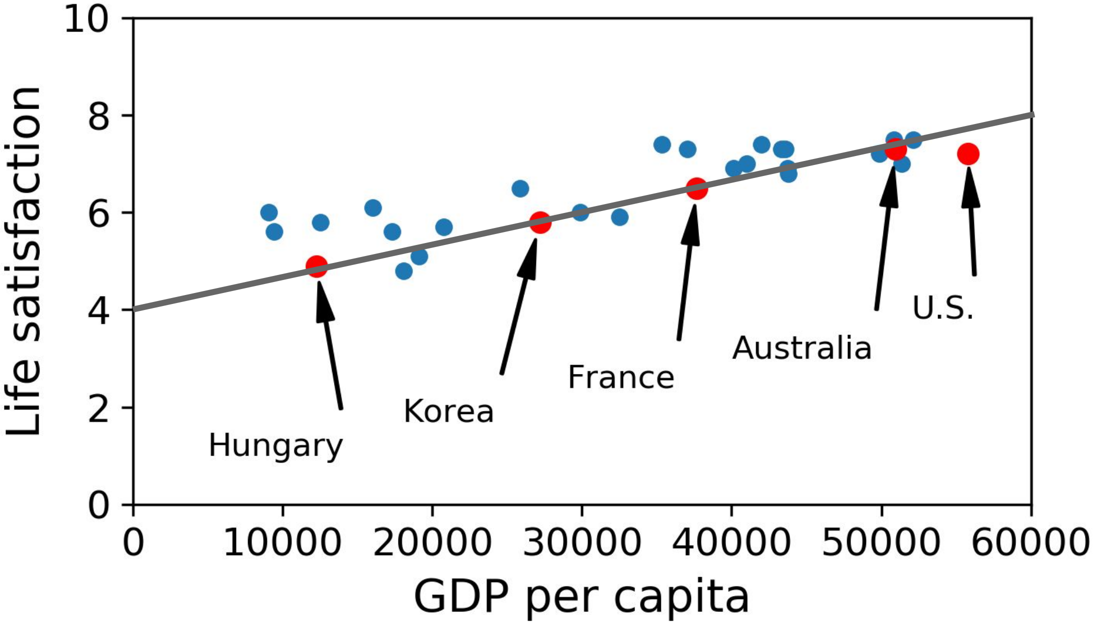

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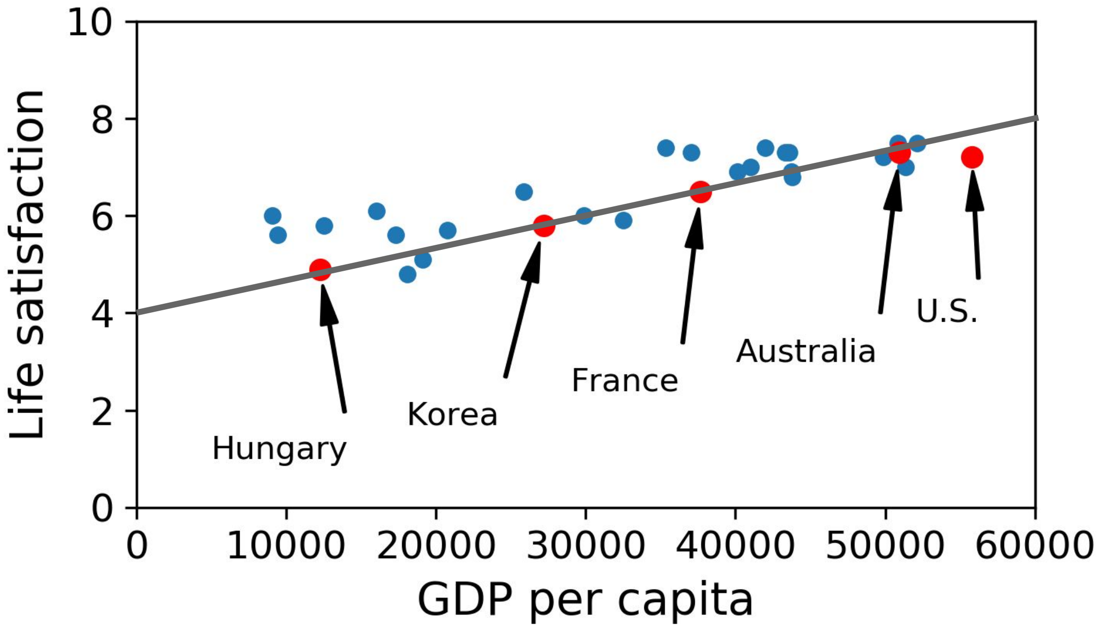

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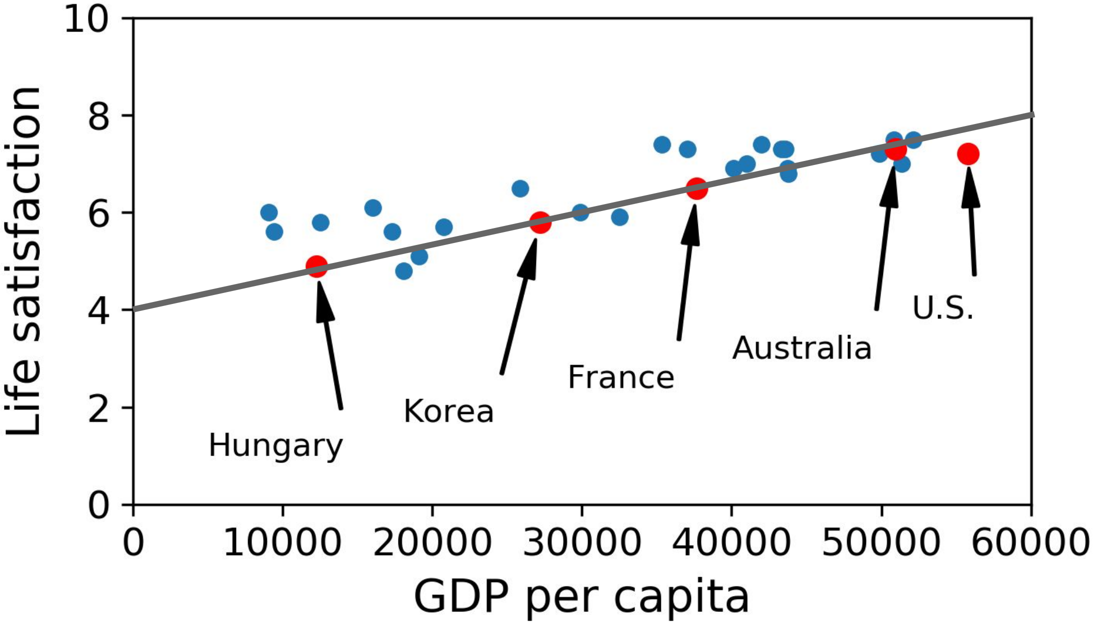

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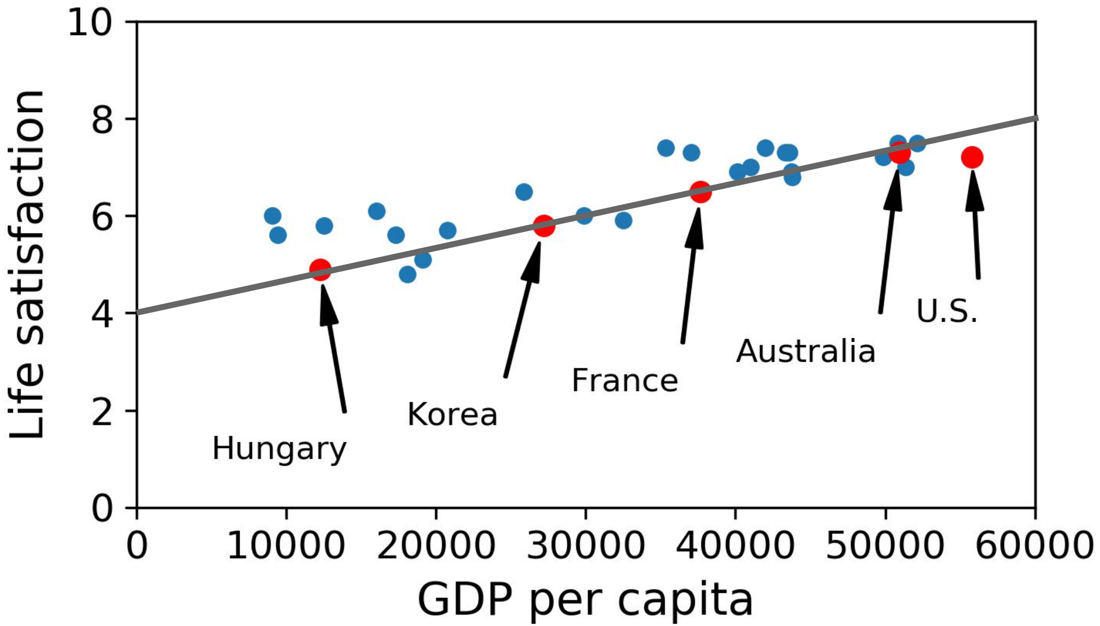

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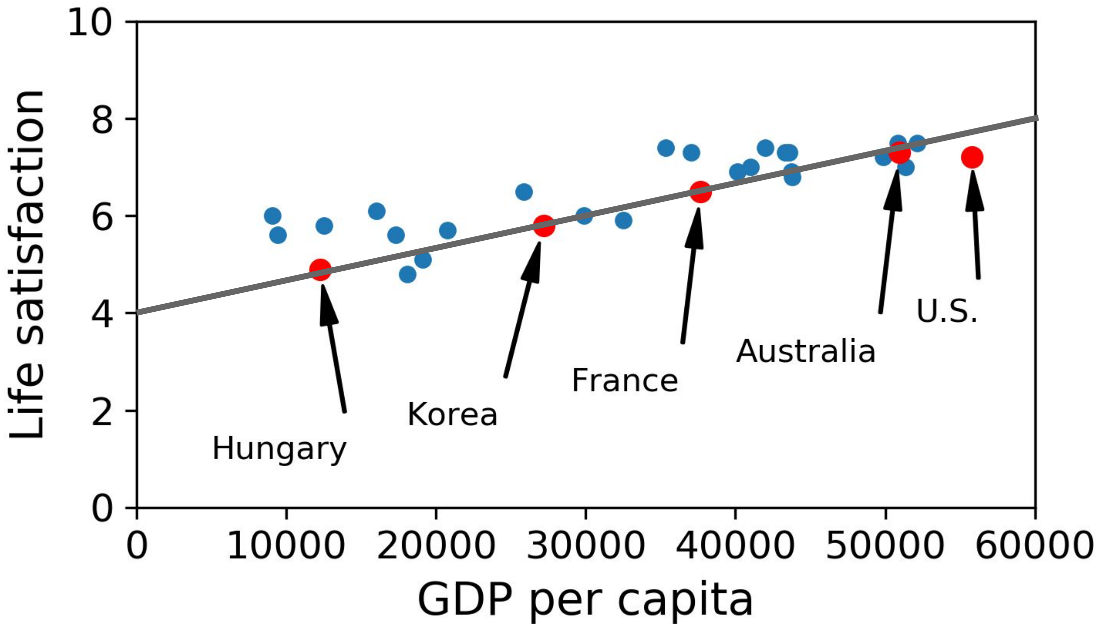

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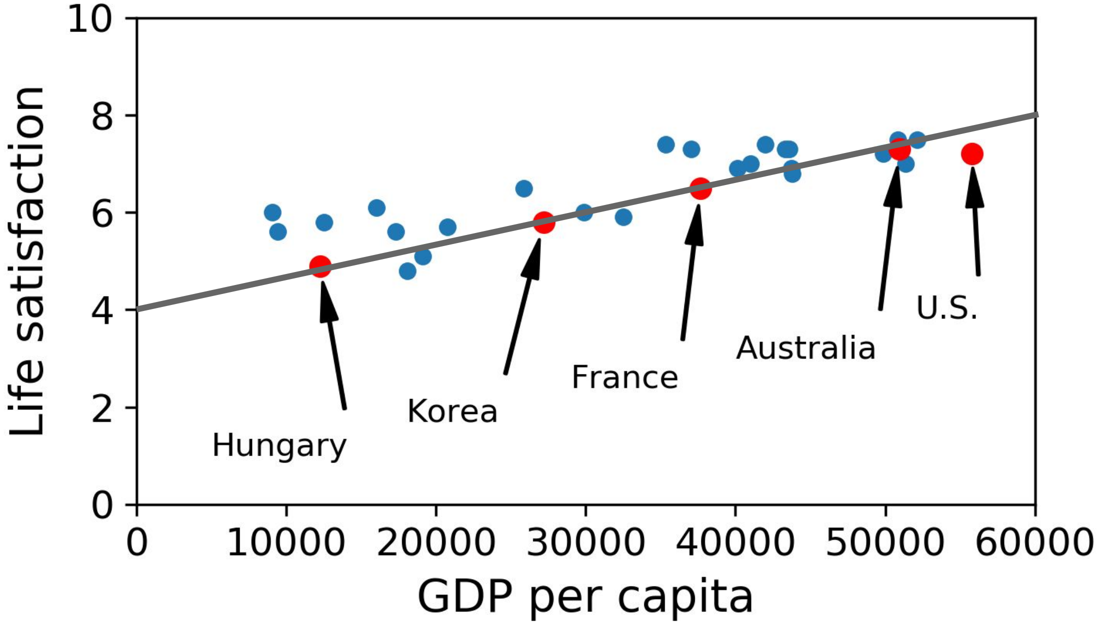

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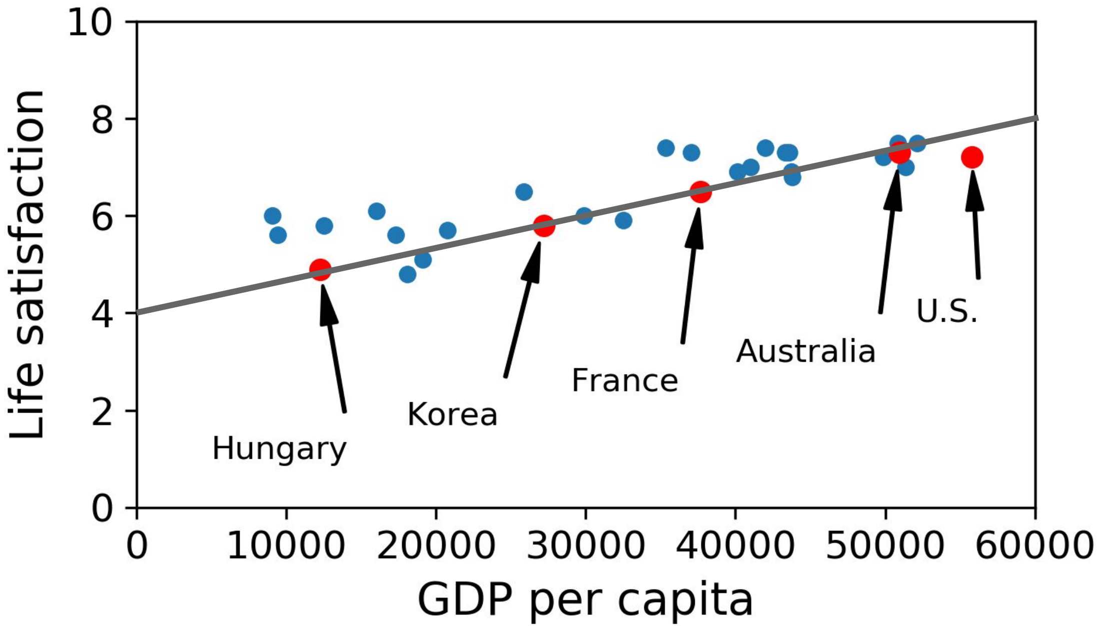
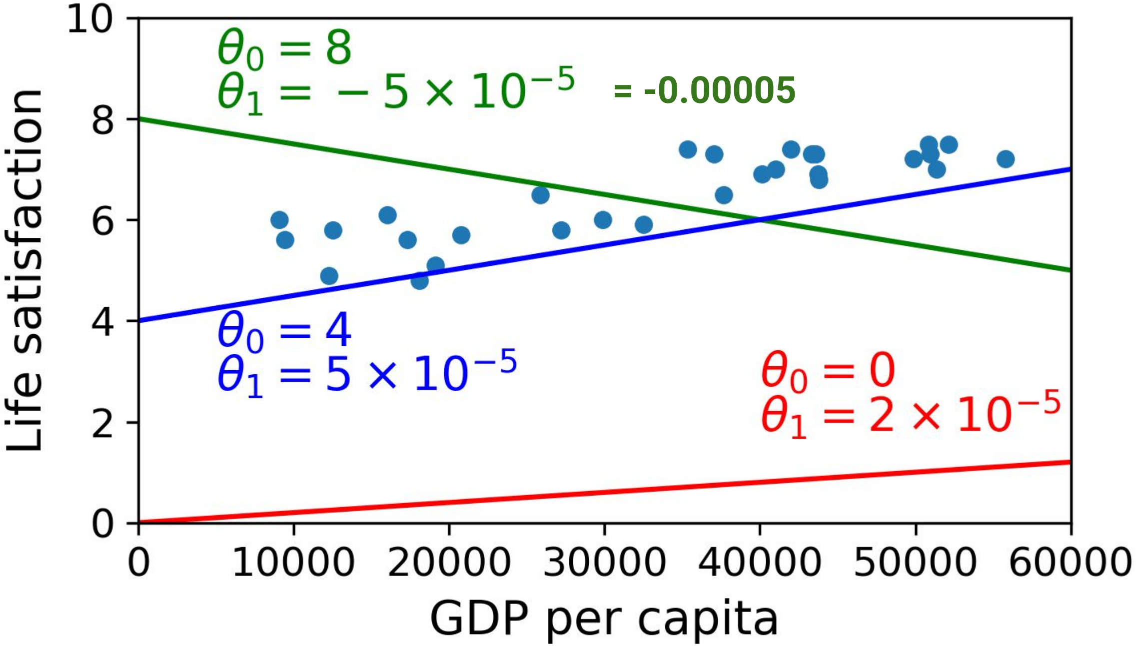


A few possible linear models with different parameters (θ)

$10^{-5} = 0.00001$



Model can refer to a

1. Type of model (we usually call this “algorithm”)
   - e.g., Linear Regression
2. Fully specified model architecture
   - e.g., Linear Regression with one input and one output.
3. Final trained model
   - e.g. Linear Regression with one input and one output, using $\theta_0 = 4.85$ $\theta_1 = 4.91 \times 10^{-5}$

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How to select the **best fitting model**?

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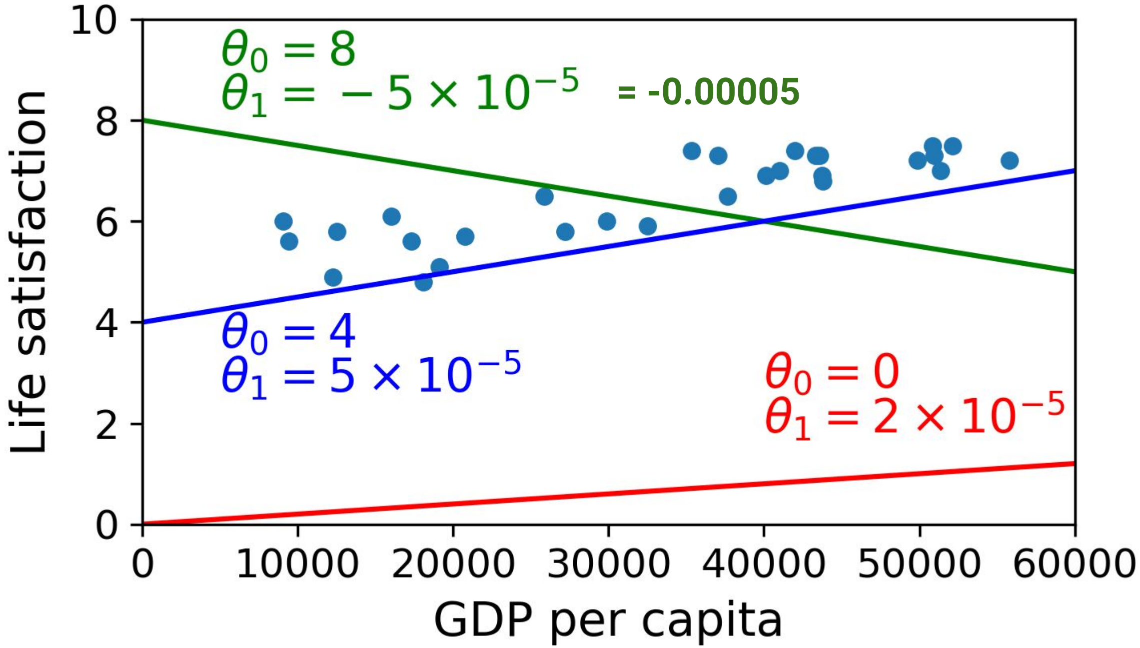

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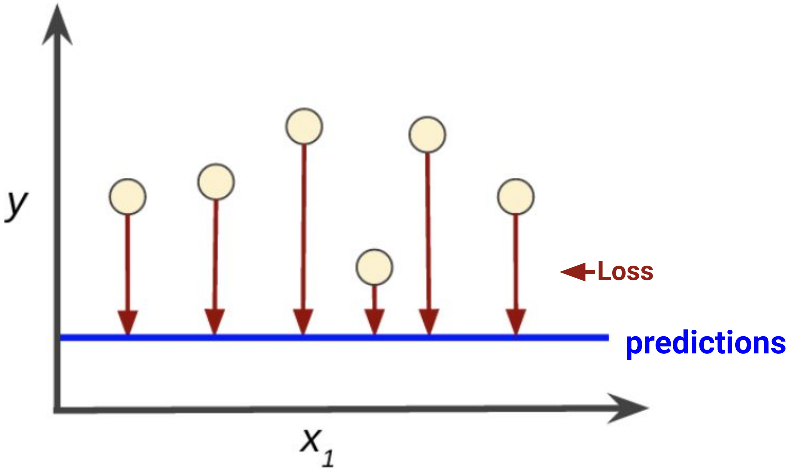

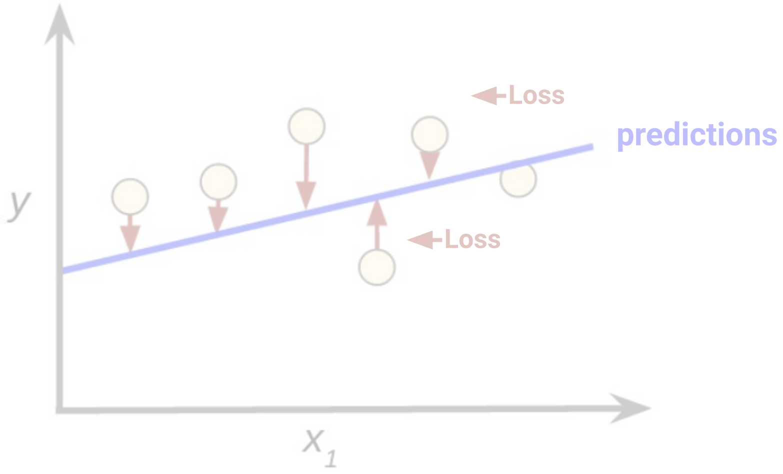

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- The **blue lines** represent predictions.

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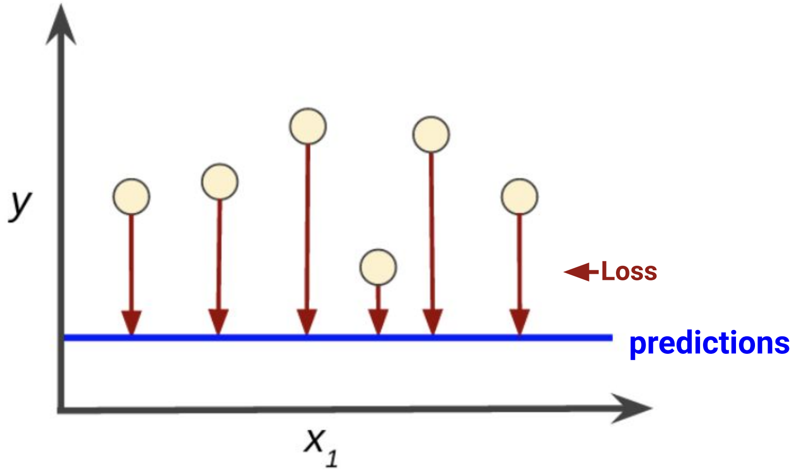

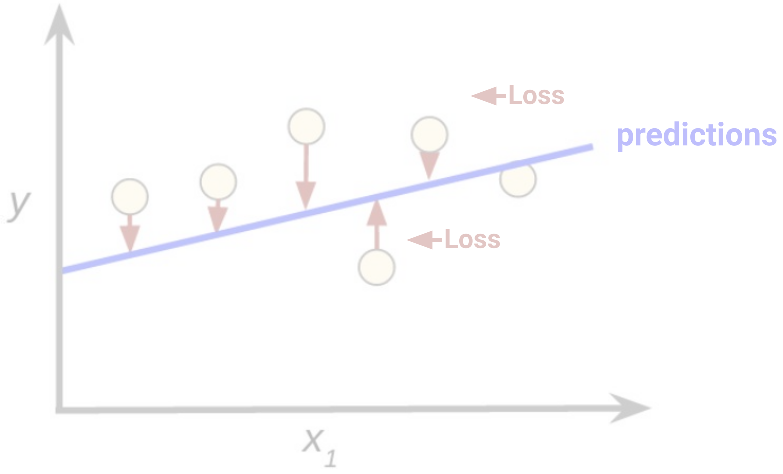

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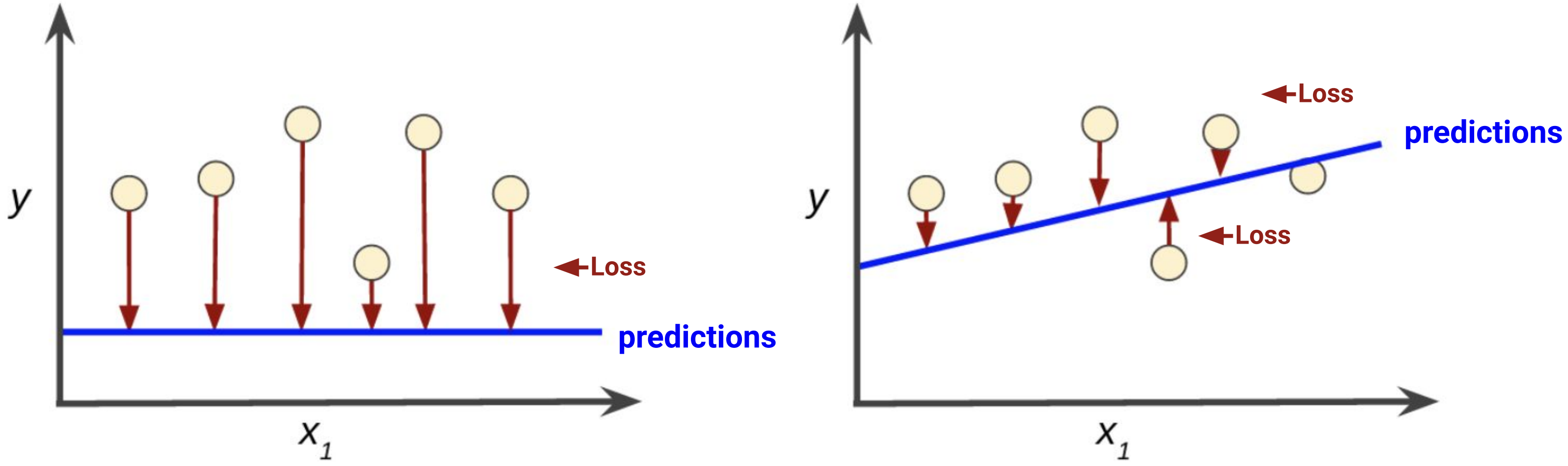

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We calculate the **squared loss**

The squared loss for a **single observation** (example) is as follows

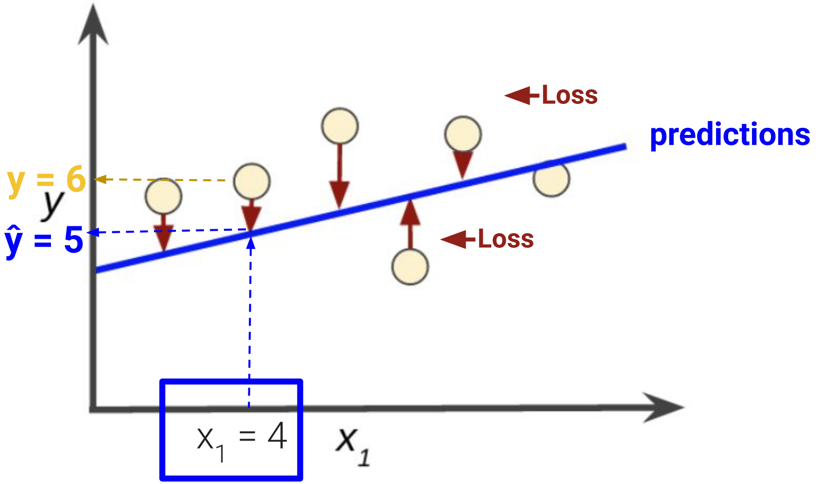
= the square of the difference between the **true outcome (label)** and the **prediction**

= (**observation** - **prediction**(x))^2

= (**y** - **ŷ**)^2

= (**6** - **5**)^2

= 1



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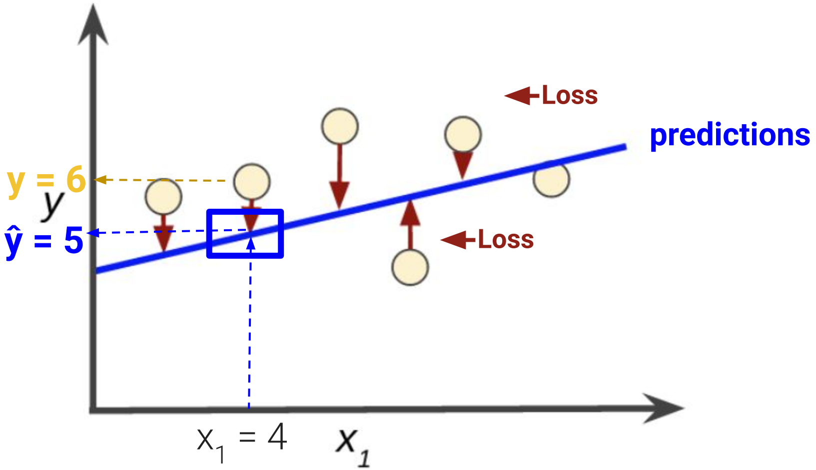

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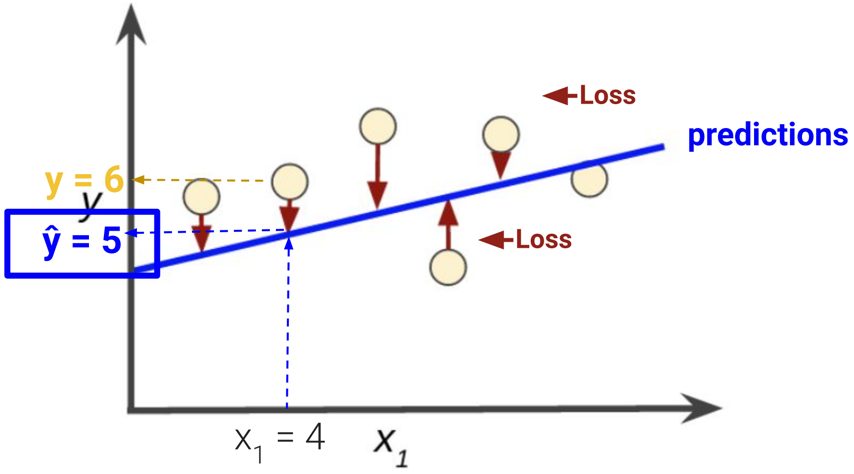

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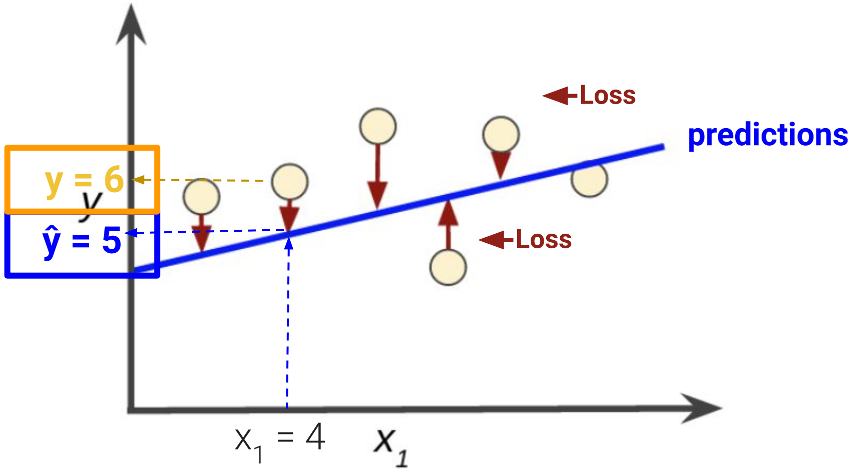

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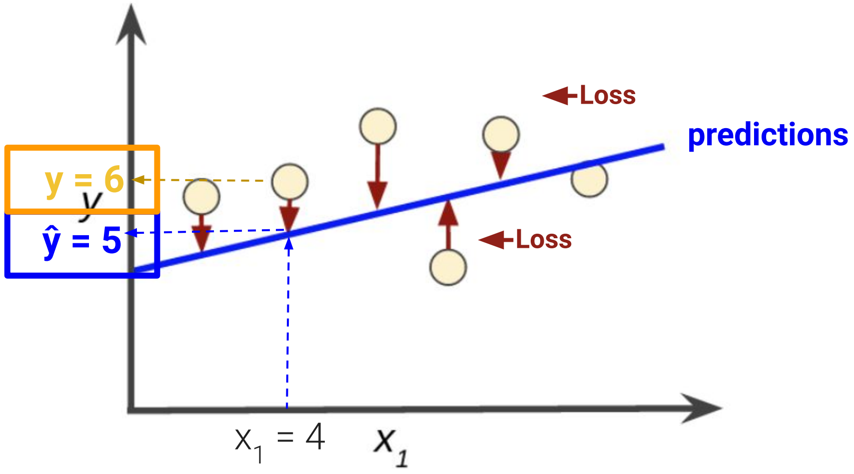

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= (6 - 5)^2

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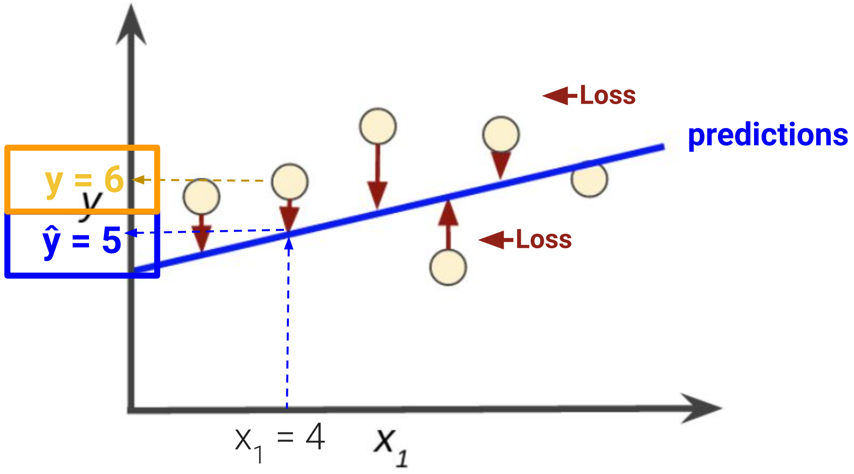

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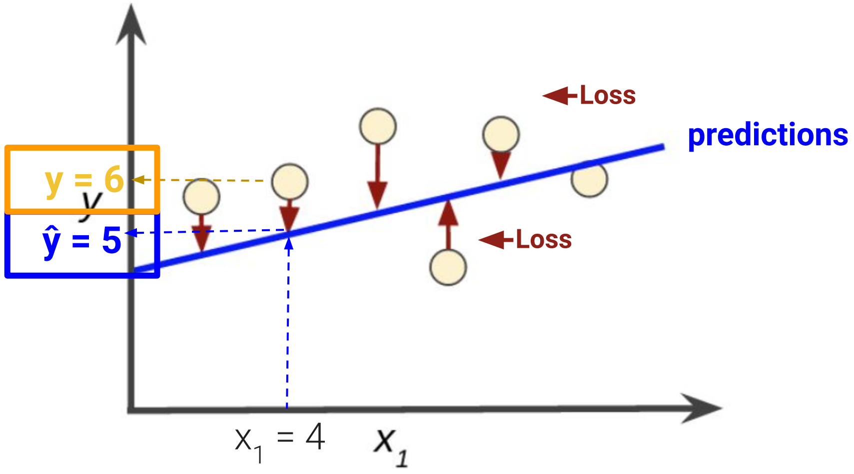

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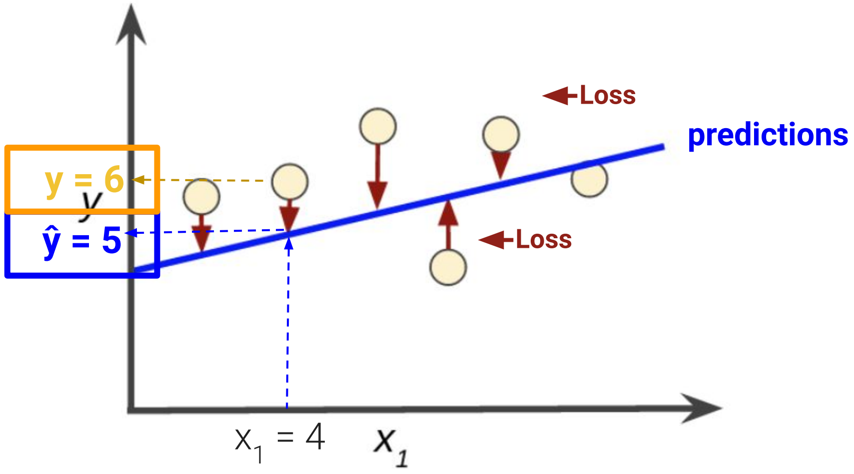

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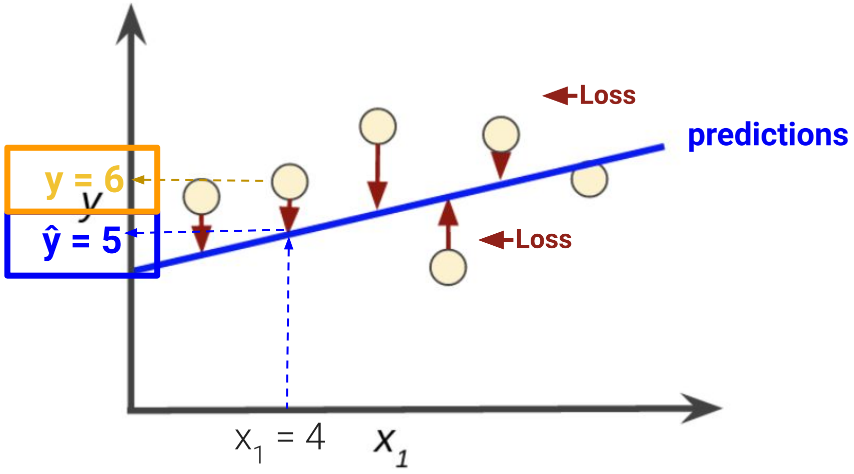

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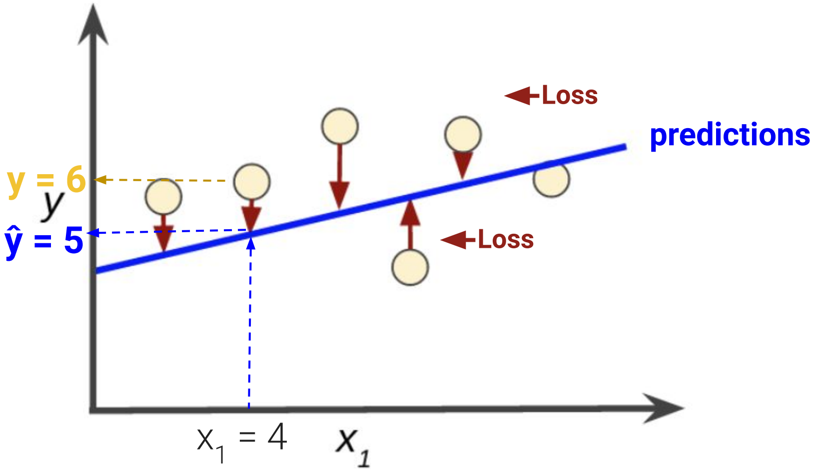
$$(y_i - \hat{y}_i)^2$$

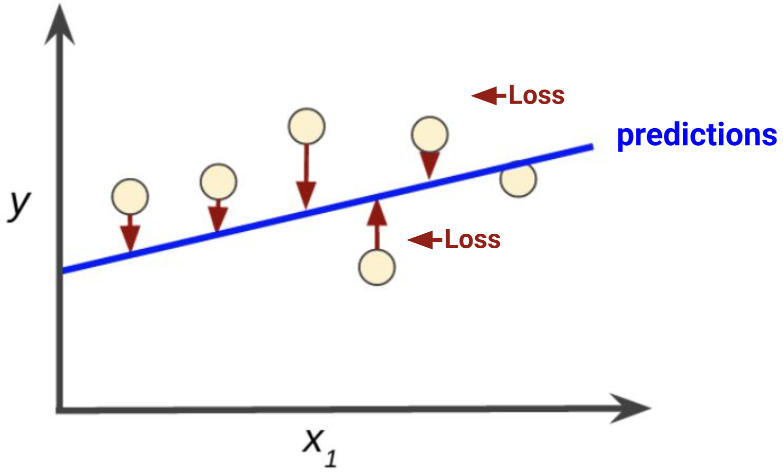


Mean squared error (squared loss; L_2 loss)

Mean square error (MSE) is the **average squared loss per example** over the whole dataset.

To calculate MSE, sum up all the squared losses for individual examples and then divide by the number of examples:

$$MSE = \frac{1}{n}\sum_{i=1}^{n} \boxed{(y_i - \hat{y}_i)^2}$$



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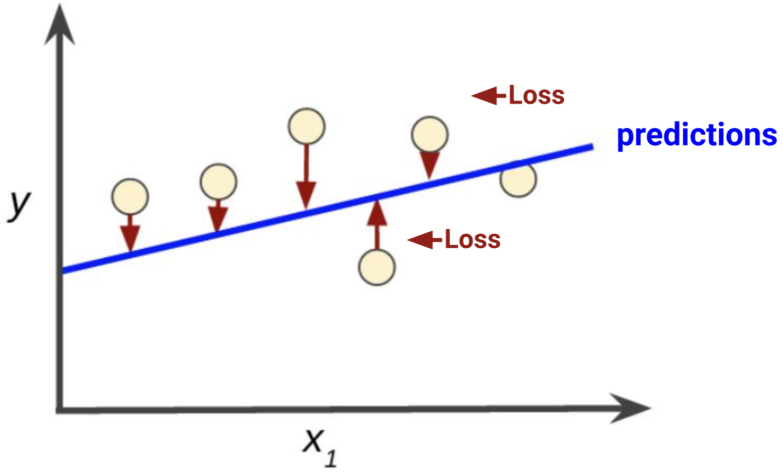

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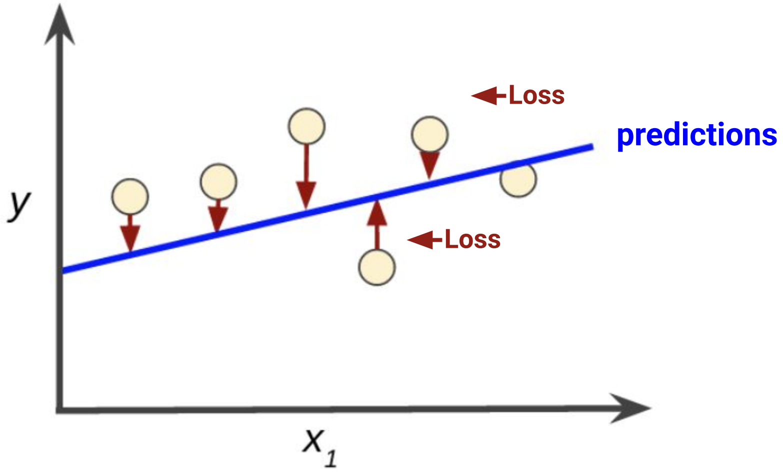

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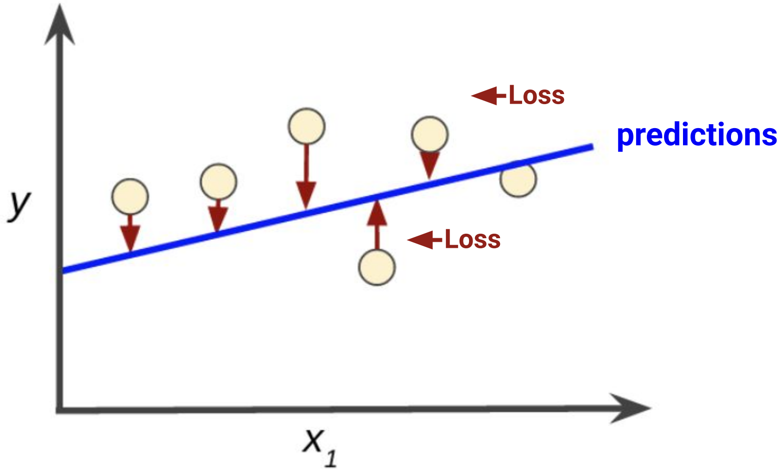
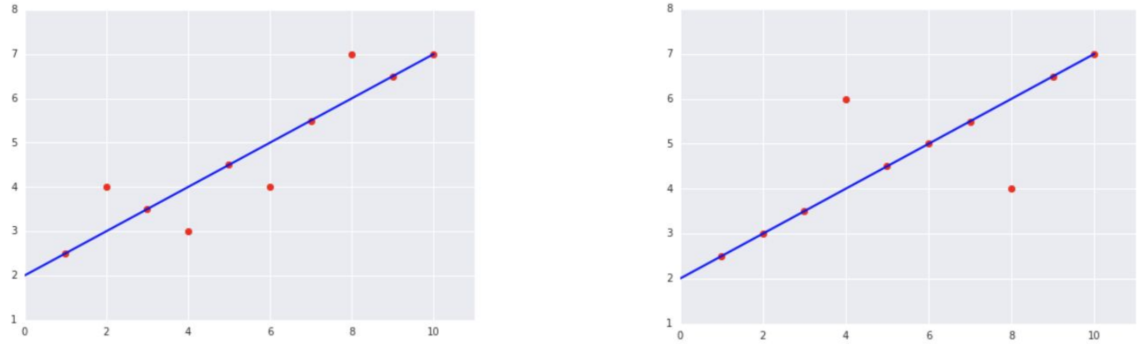


Mean Squared Error

Consider the following two plots:



Explore the options below.

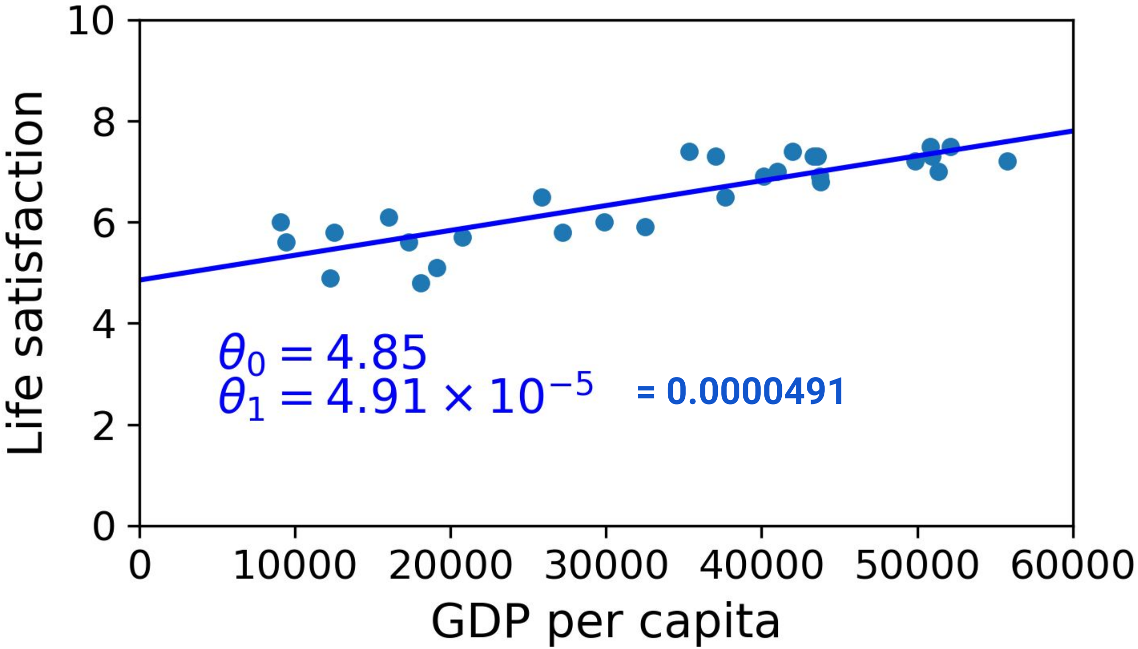
Which of the two data sets shown in the preceding plots has the higher Mean Squared Error (MSE)?

The dataset on the right.

The dataset on the left.

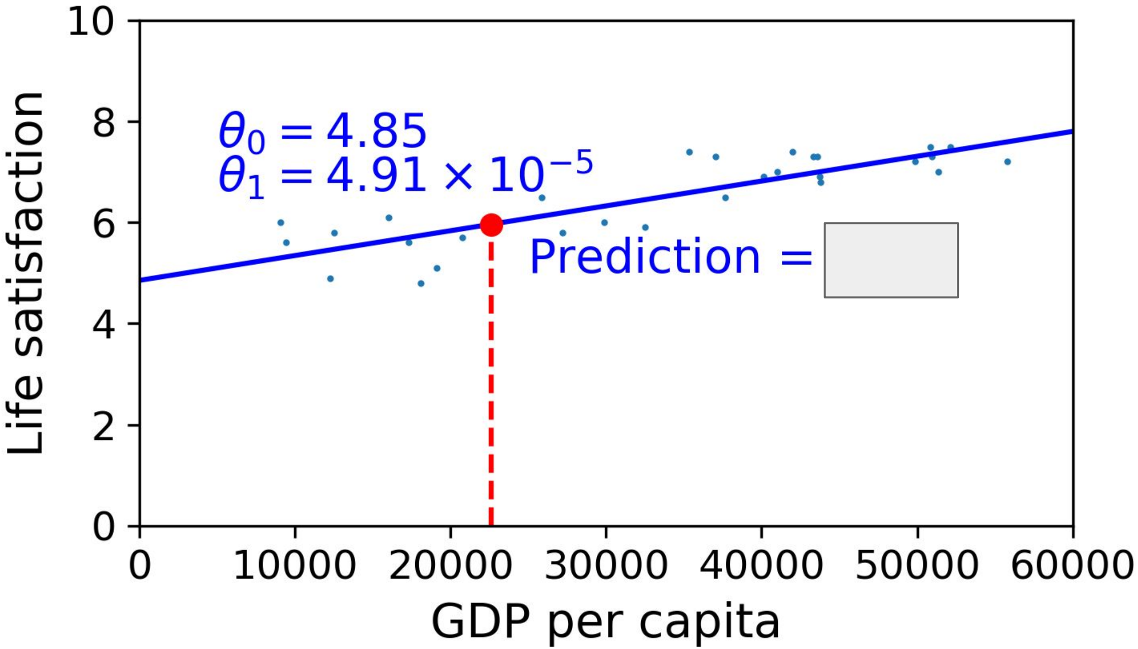
Our **best fitting model**

We used the **mean squared error** to select the best model.

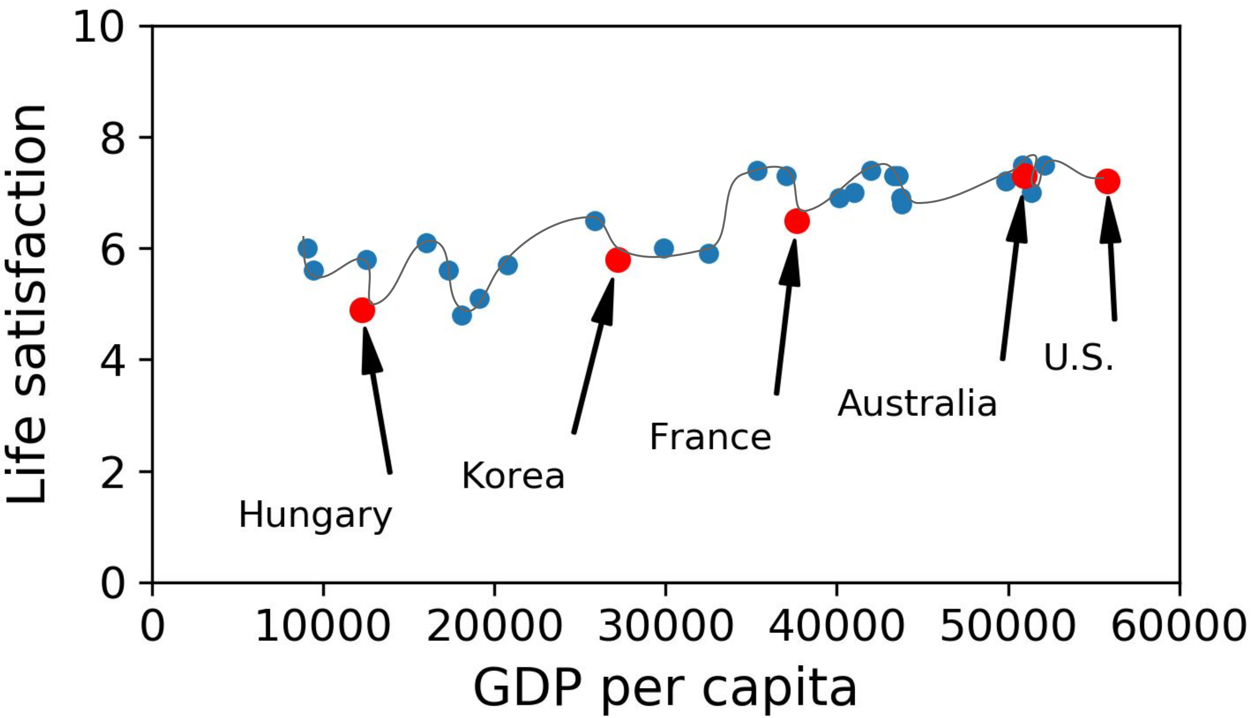


Use your best fitting model to **predict** the life satisfaction of new data (Cypriots).

Cyprus's GDP per capita: $22587.



Can a model be too good? Yes, it can



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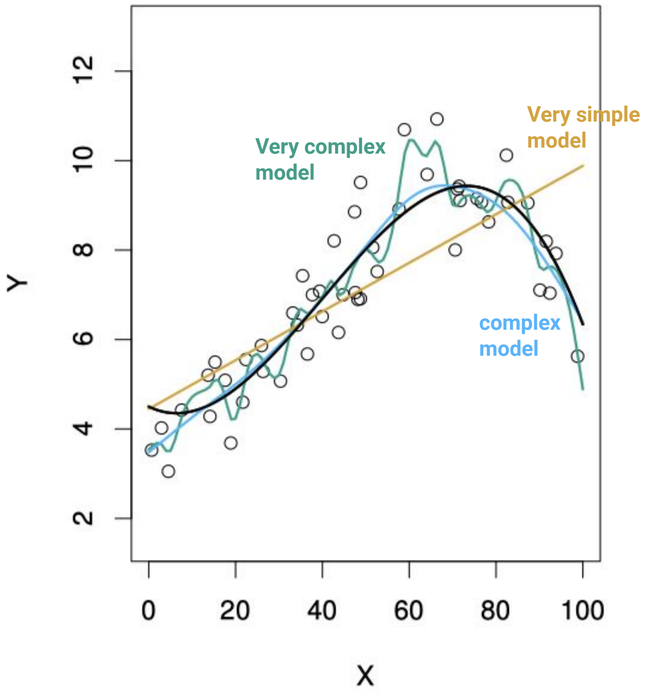


Bias-Variance trade-off

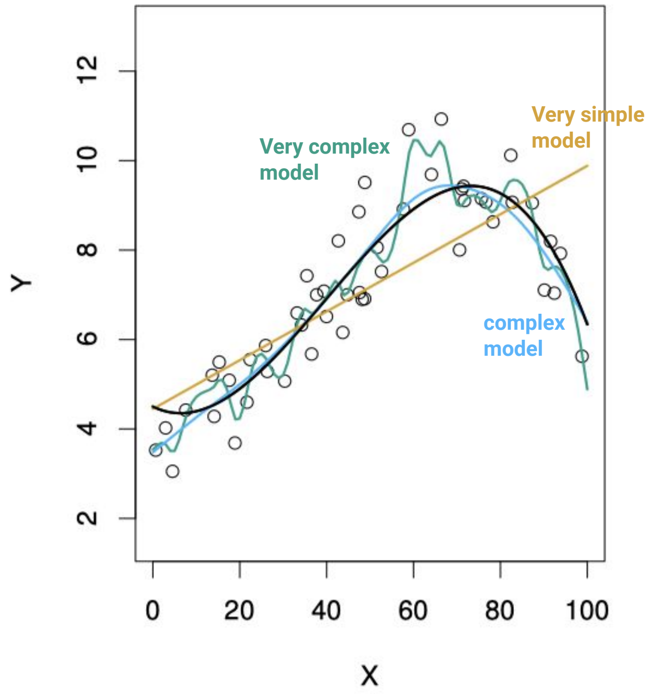
Source: James et. al. (2013)

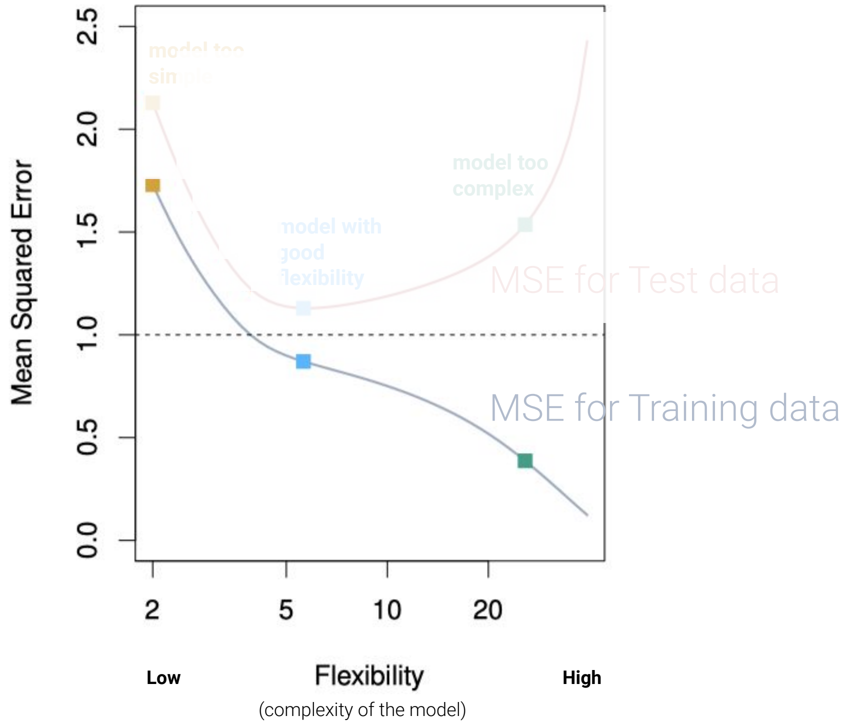
Bias-Variance trade-off

Underfitting ← → Overfitting

High bias
Low variance

Low bias
High variance





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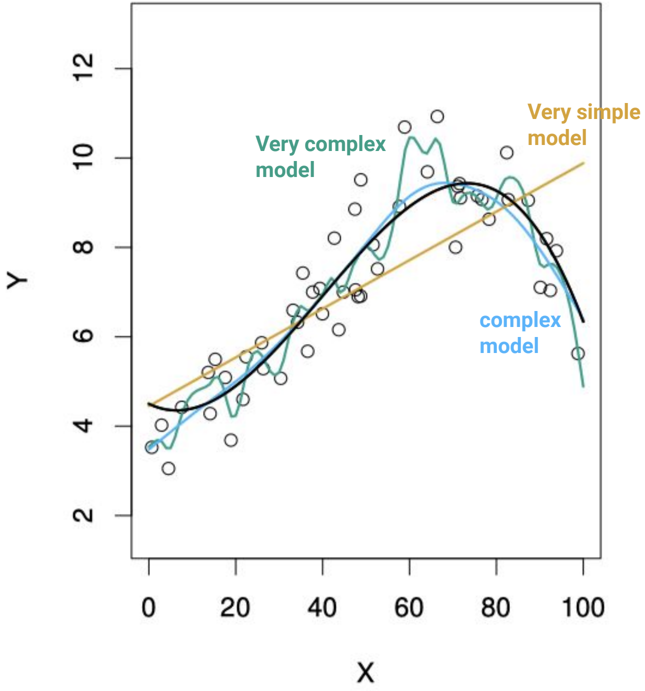

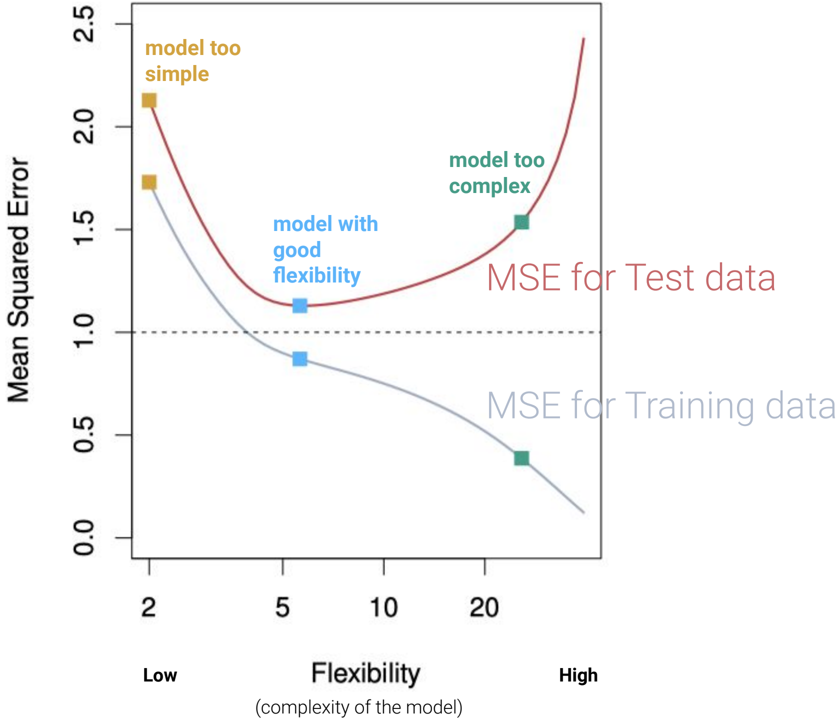

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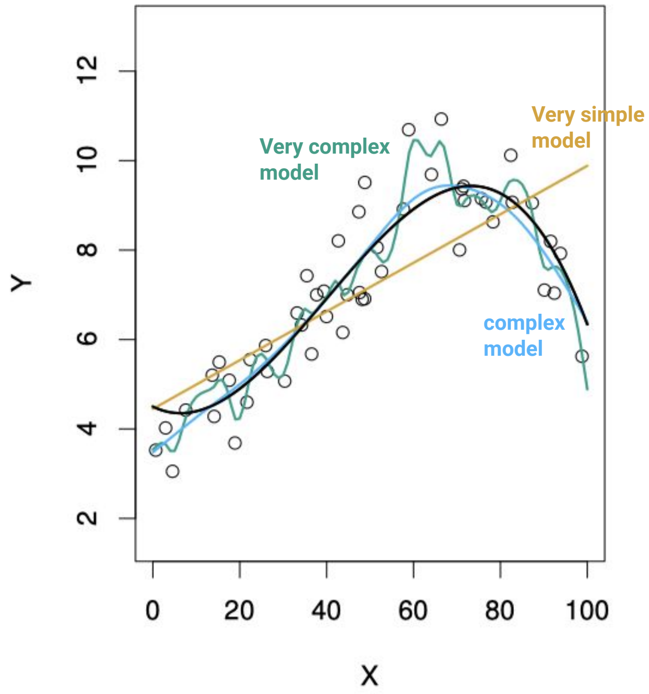

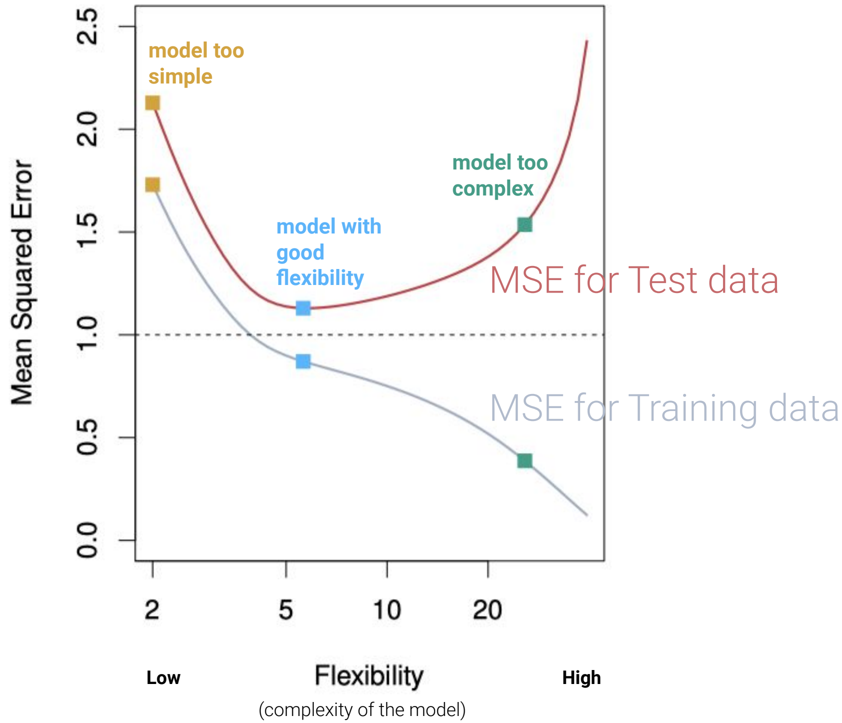

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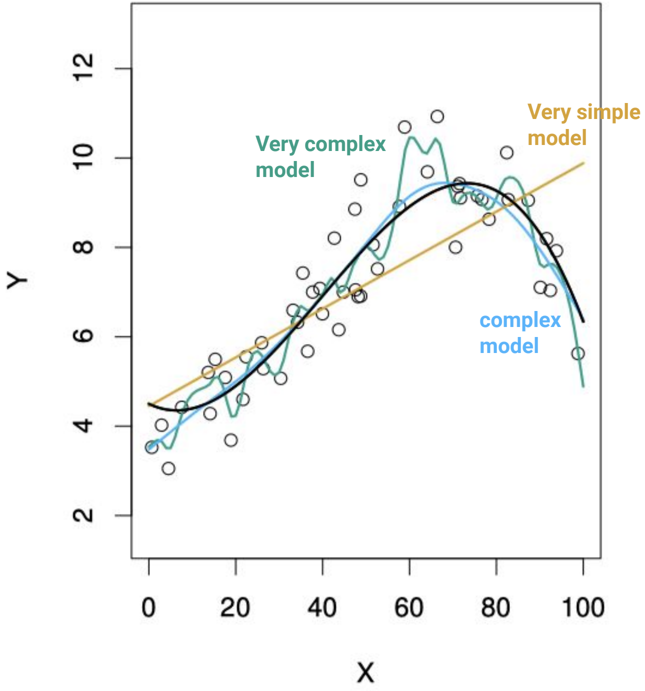
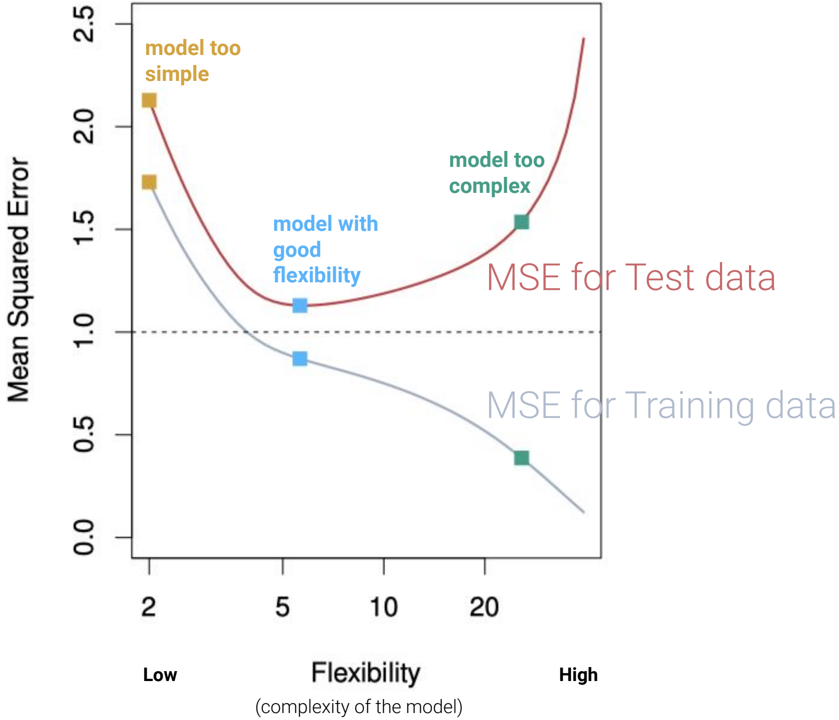
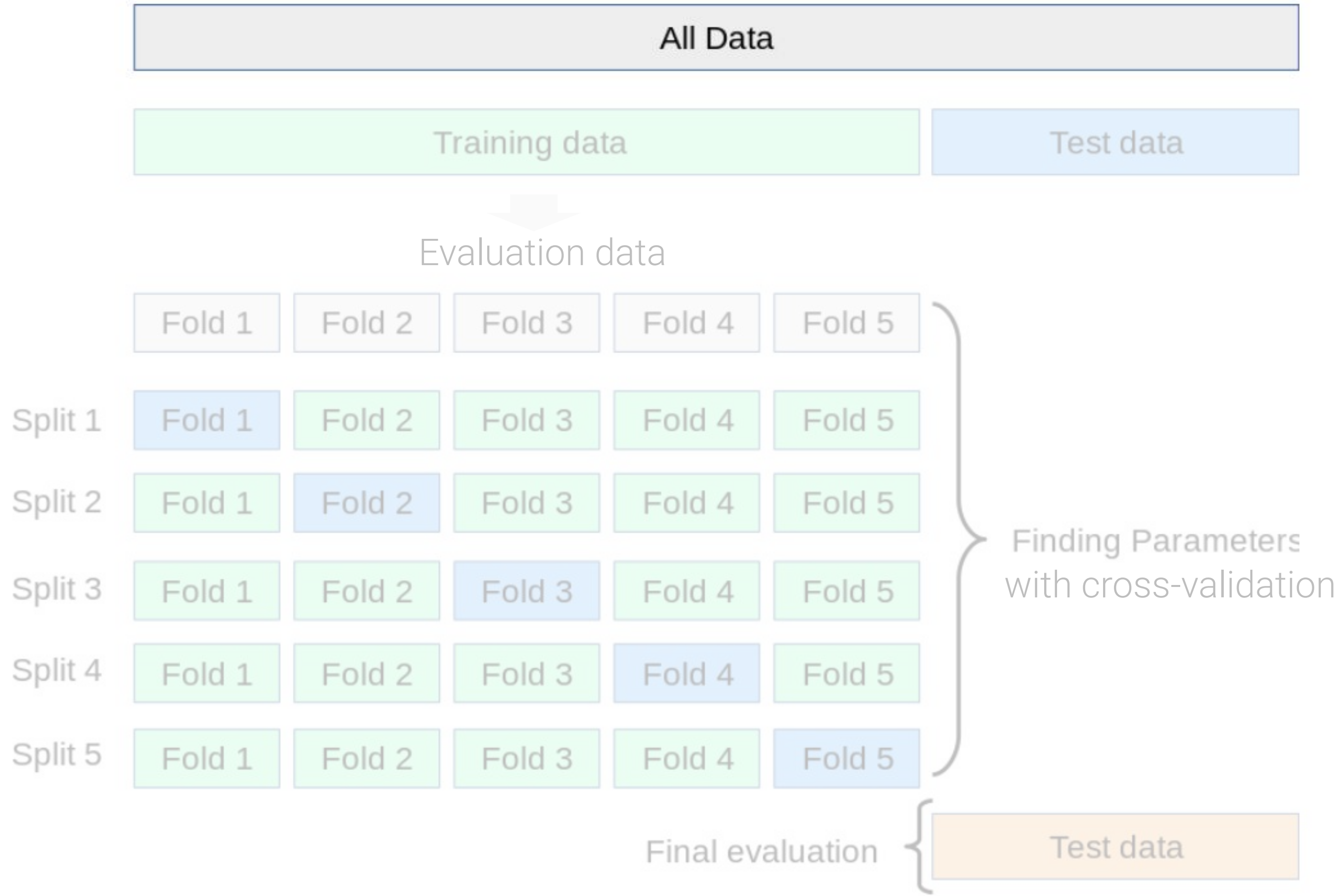


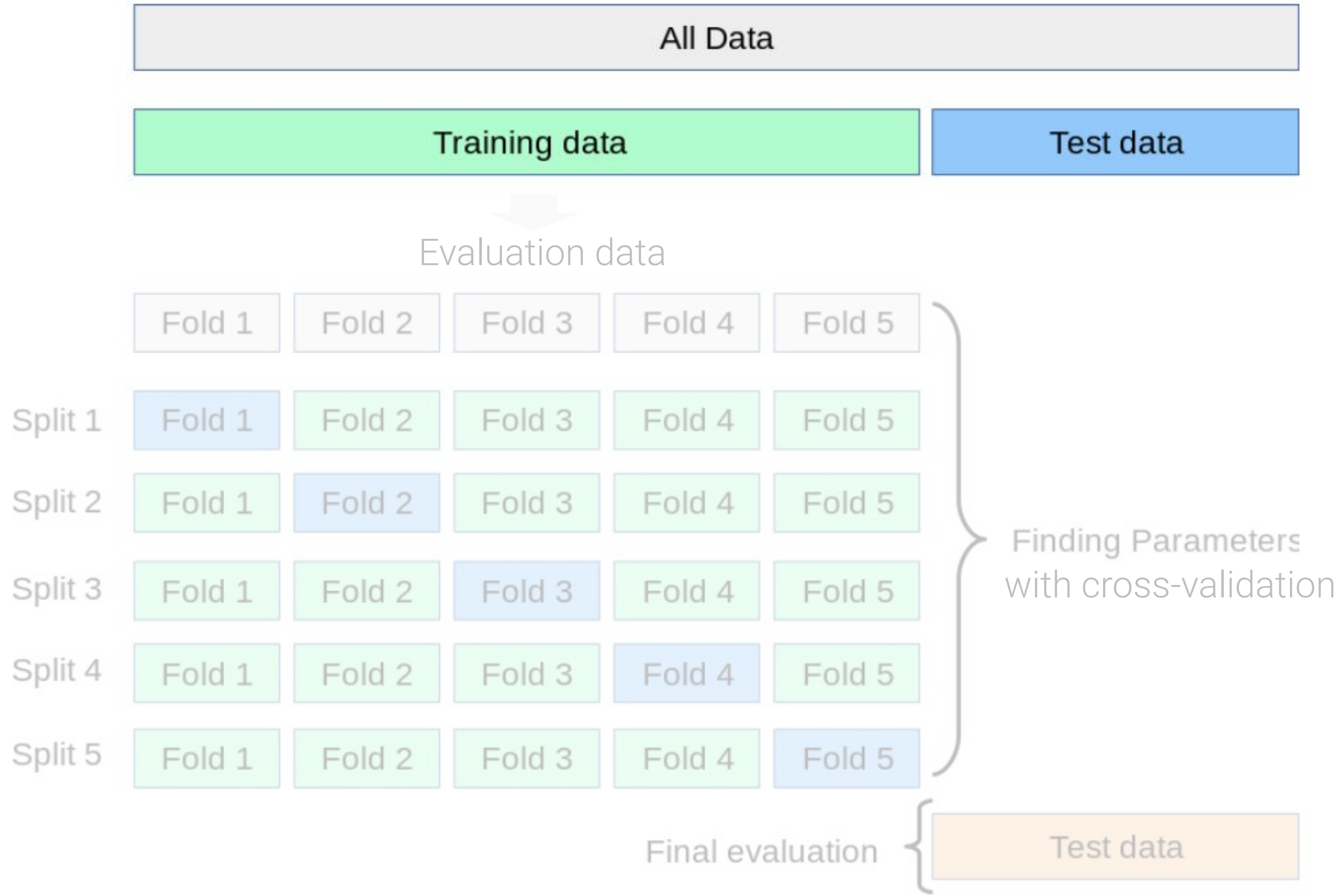


Source: James et. al. (2013)

Training, evaluation and testing data



Source: scikit-learn https://scikit-learn.org/stable/modules/cross_validation.html



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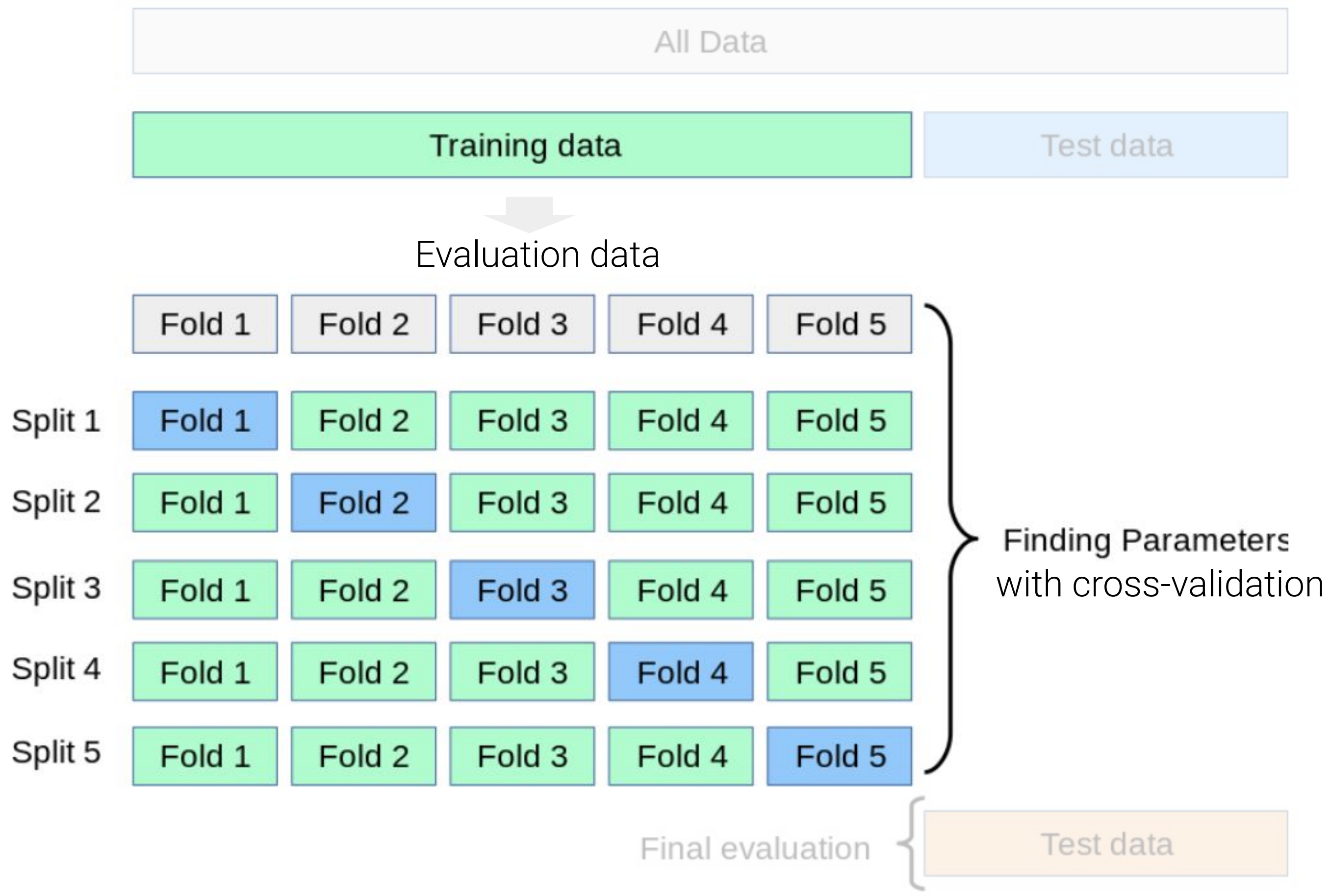

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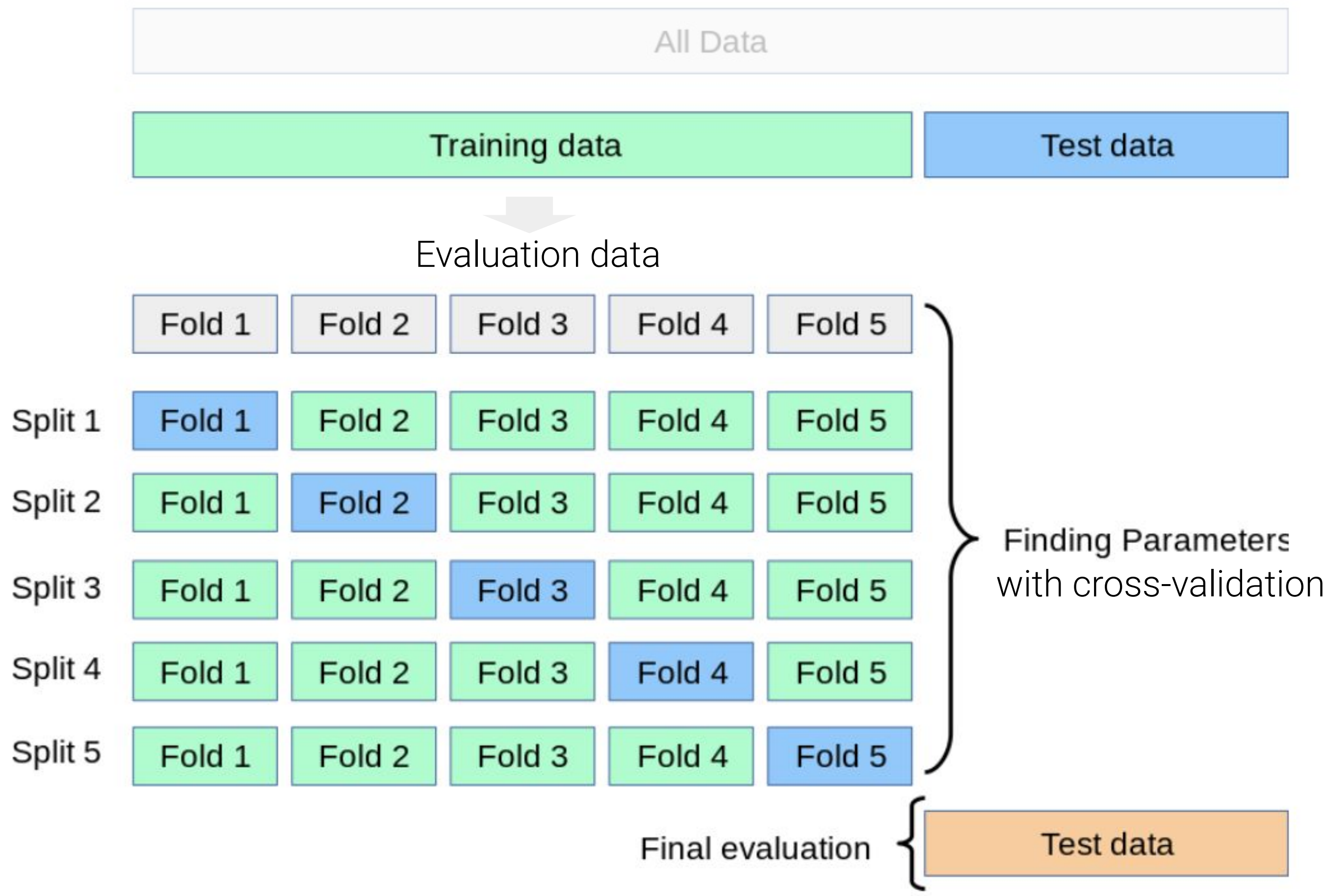

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Training set, **evaluation** set and **test** set

Training set

- Usually 80% of the data, but depends on sample size
- The error rate on training data is called the training error

Evaluation set (holdout set; development set)

- We split the training set into smaller k sets (usually 5 or 10) to be able to find optimal parameters (**hyperparameters**)
- This approach is called **cross-validation**

Test set

- Also called hold out data (usually 20%)
- The error rate on new cases is called the test error or generalization error (out-of-sample error)
- Low training error in combination with a high test error is a sign of overfitting

Source: Géron, A. (2019)

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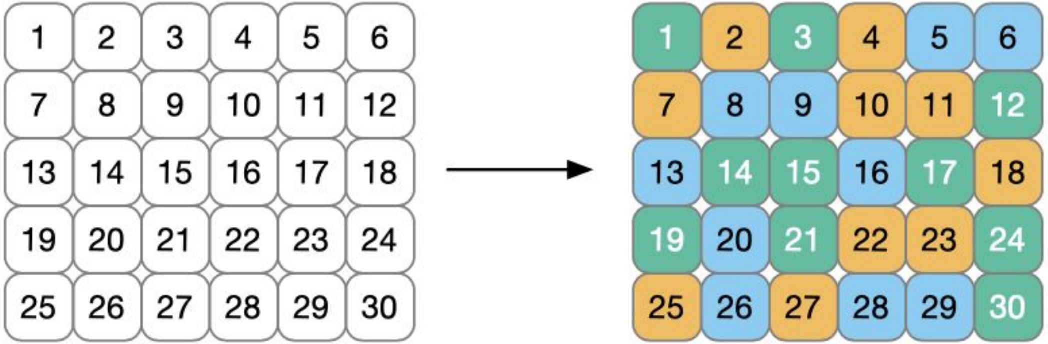
Closer look at **cross-validation (k=3)**

- While there are a number of variations, the most common cross-validation method is k-fold cross-validation
- The data are randomly partitioned into k sets of roughly equal size (called the "**folds**").

Step 1: assign each observation to one of 3 folds



For illustration, k = 3 is shown for a data set of thirty training set points with random fold allocations.

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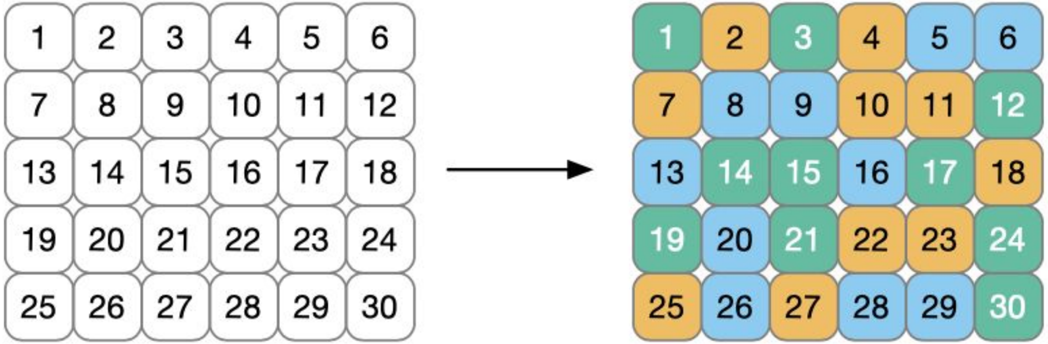

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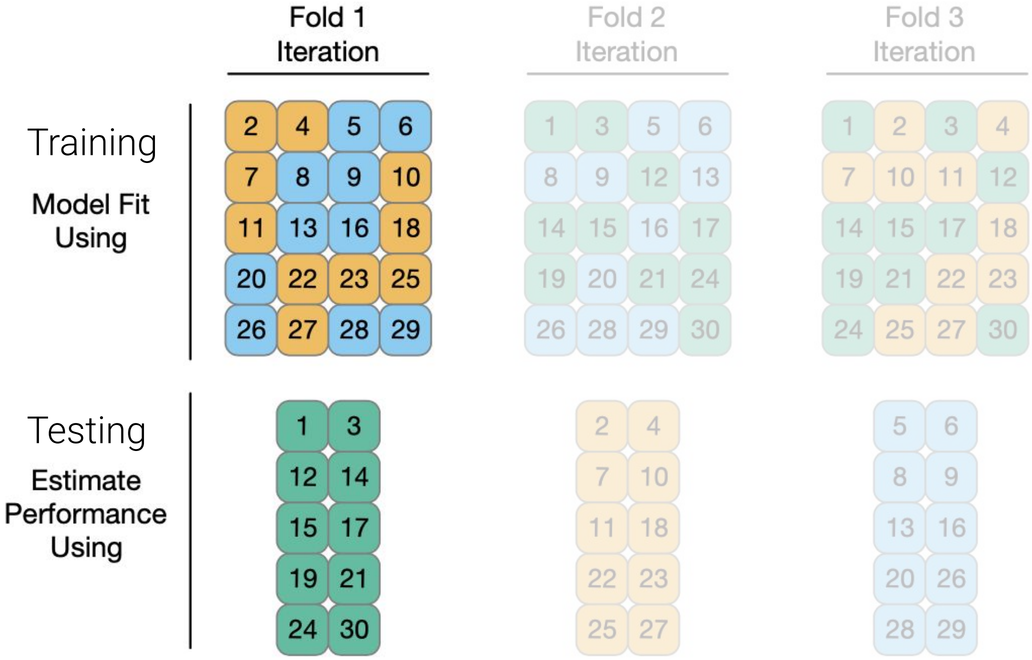
Closer look at **cross-validation (k=3)**

- For each iteration, one fold is held out for assessment statistics and the remaining folds are substrate for the model.
- This process continues for each fold so that three models produce three sets of performance statistics.

Step 2: split the folds into training and test partitions



For 3-fold cross-validation, the three iterations of resampling are illustrated above.

Source: Kuhn & Silge (2020) https://www.tmwr.org/resampling.html

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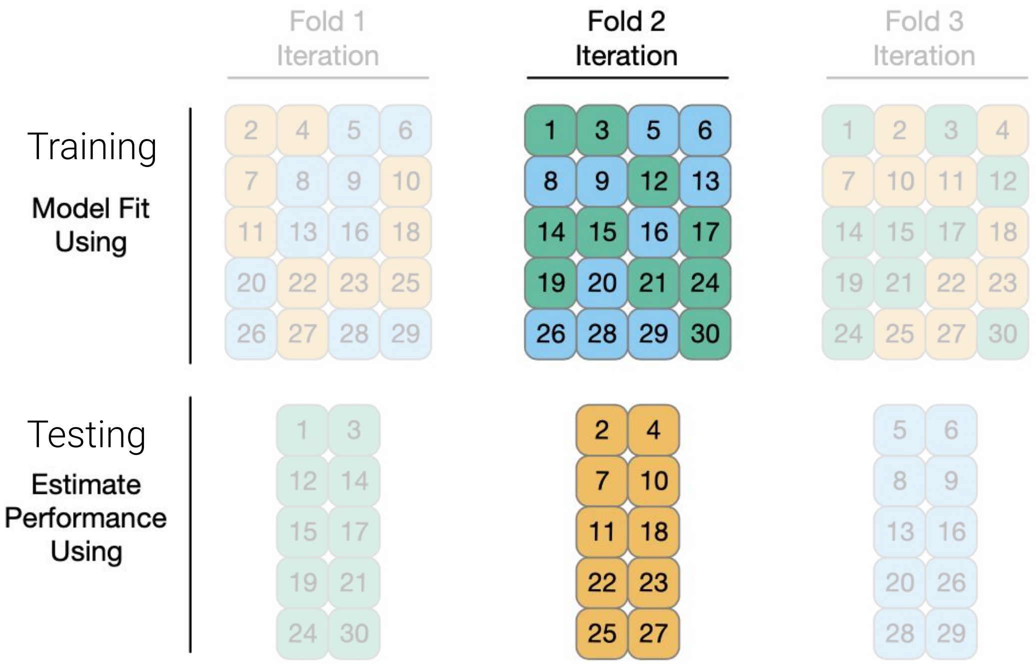

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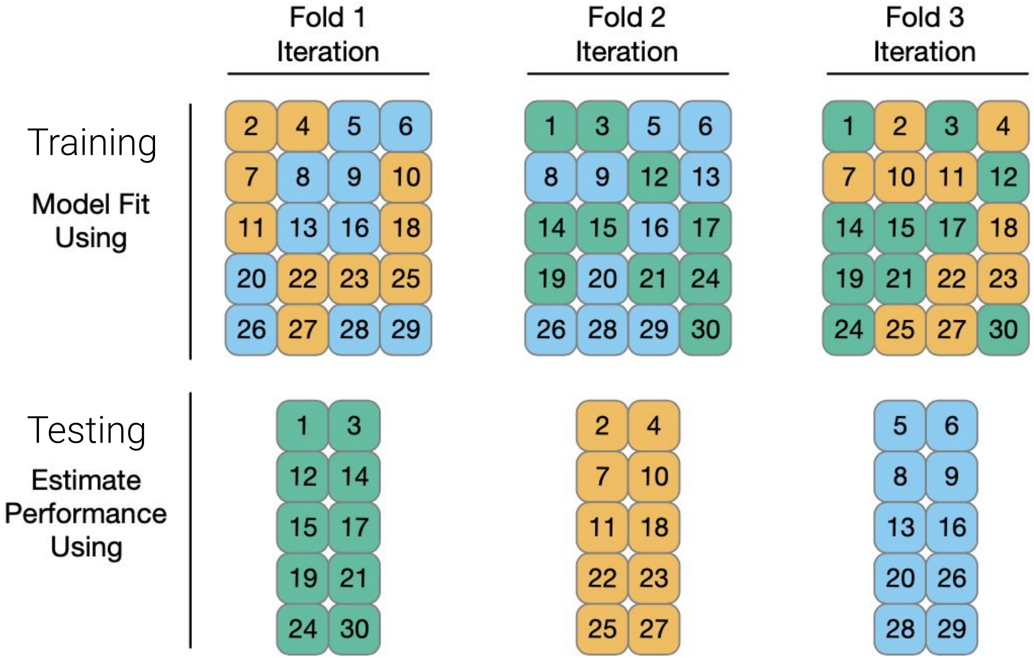

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k-Fold-Cross-Validation

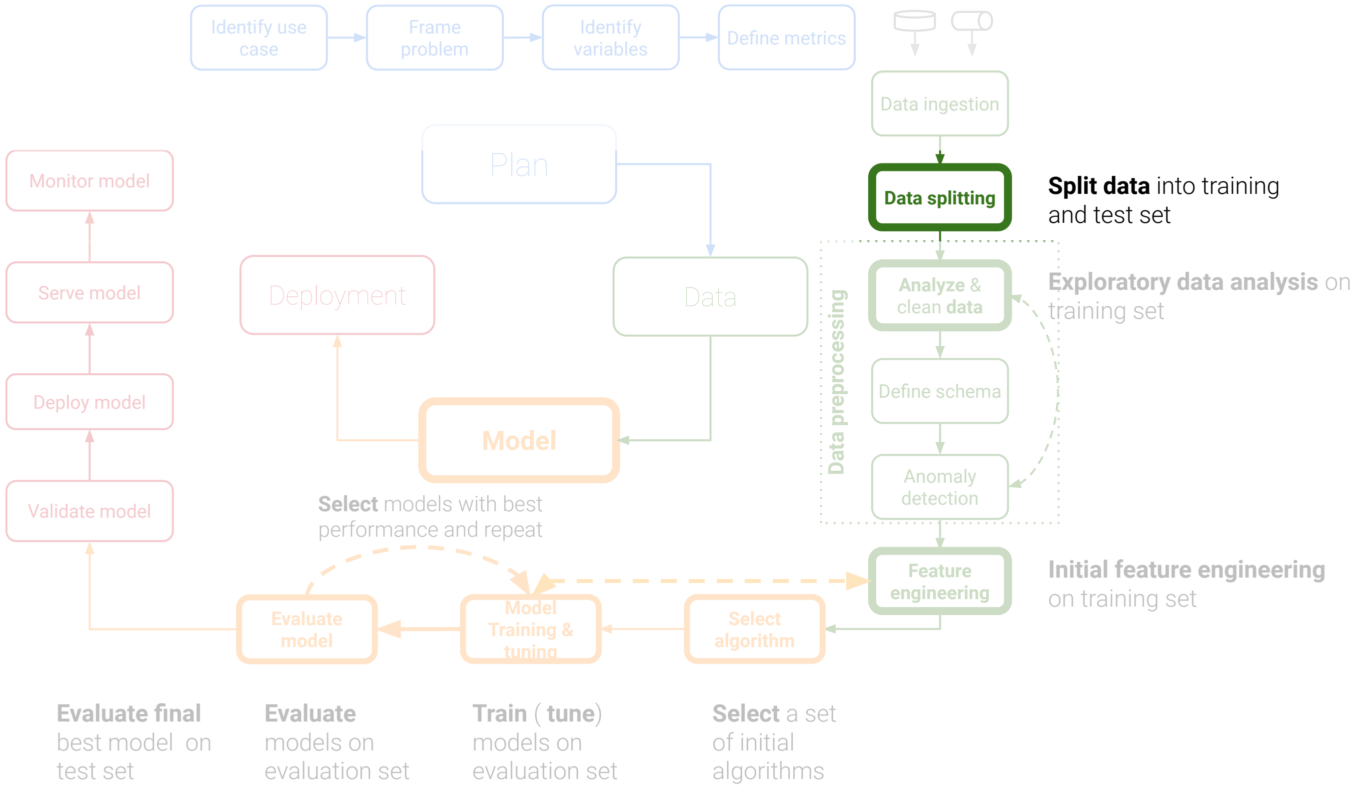
- Using k = 3 is a good choice to illustrate cross-validation but is a poor choice in practice.
- Values of **k** are most often **5** or **10**.
- We generally prefer 10-fold cross-validation as a default.

Source: Kuhn & Silge (2020) https://www.tmwr.org/resampling.html

Procedure

Data Science Lifecycle with focus on **modeling**

Plan | Data | **Model** | Deployment



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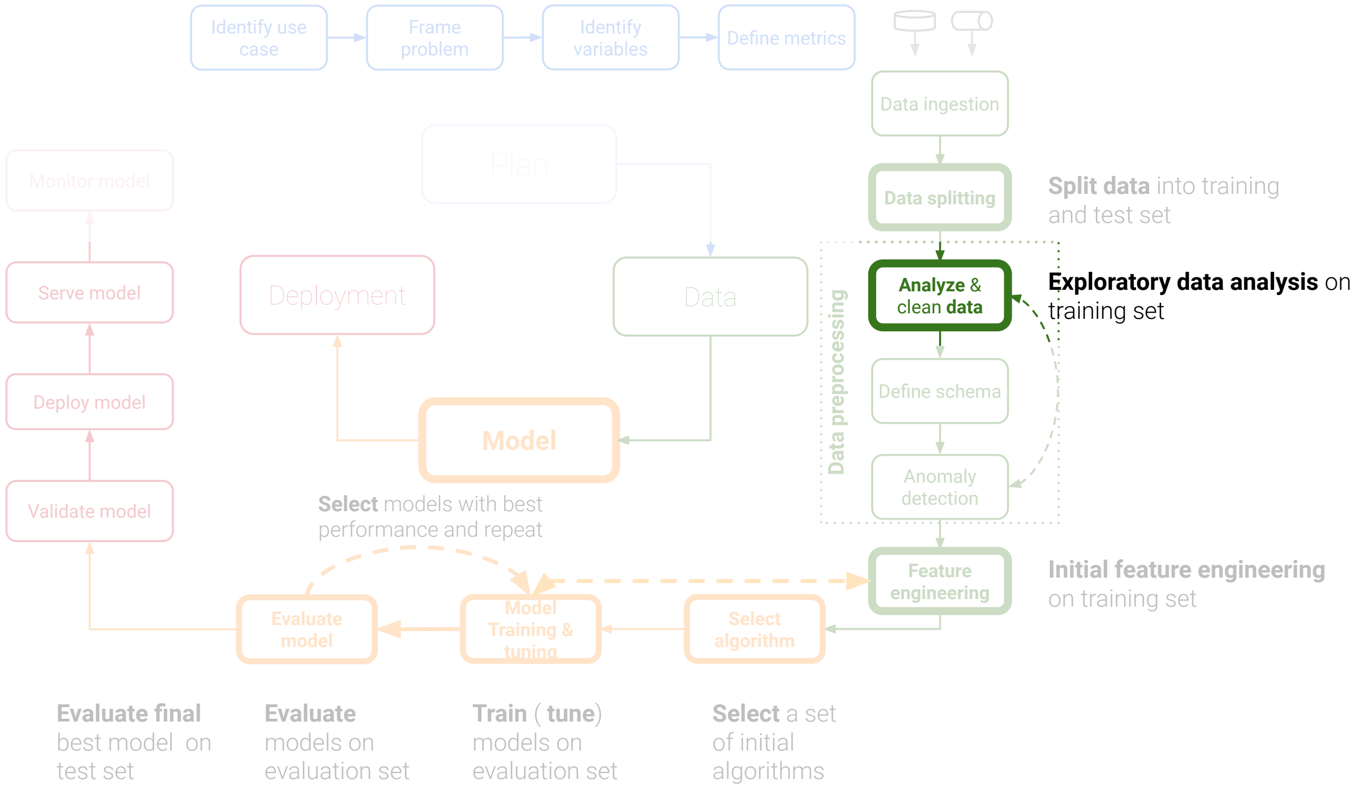

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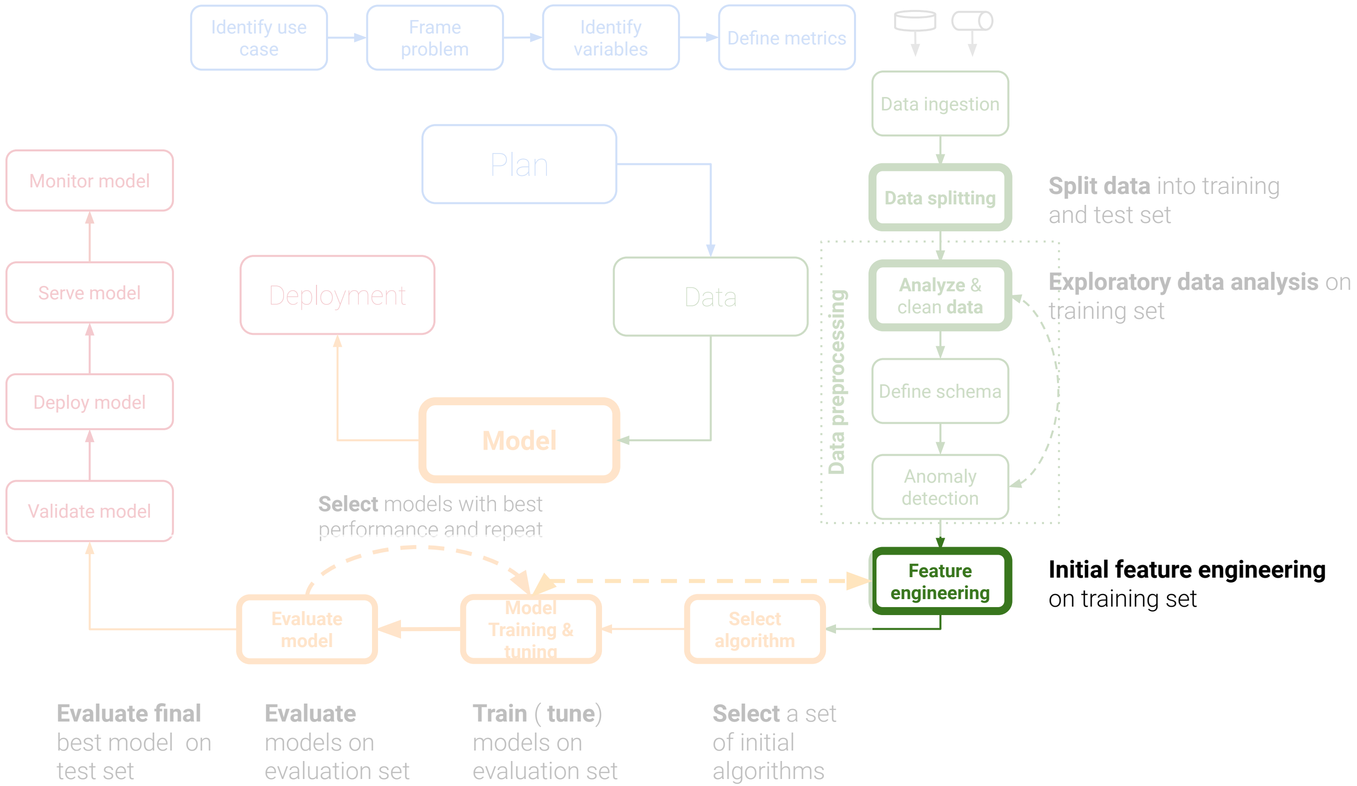

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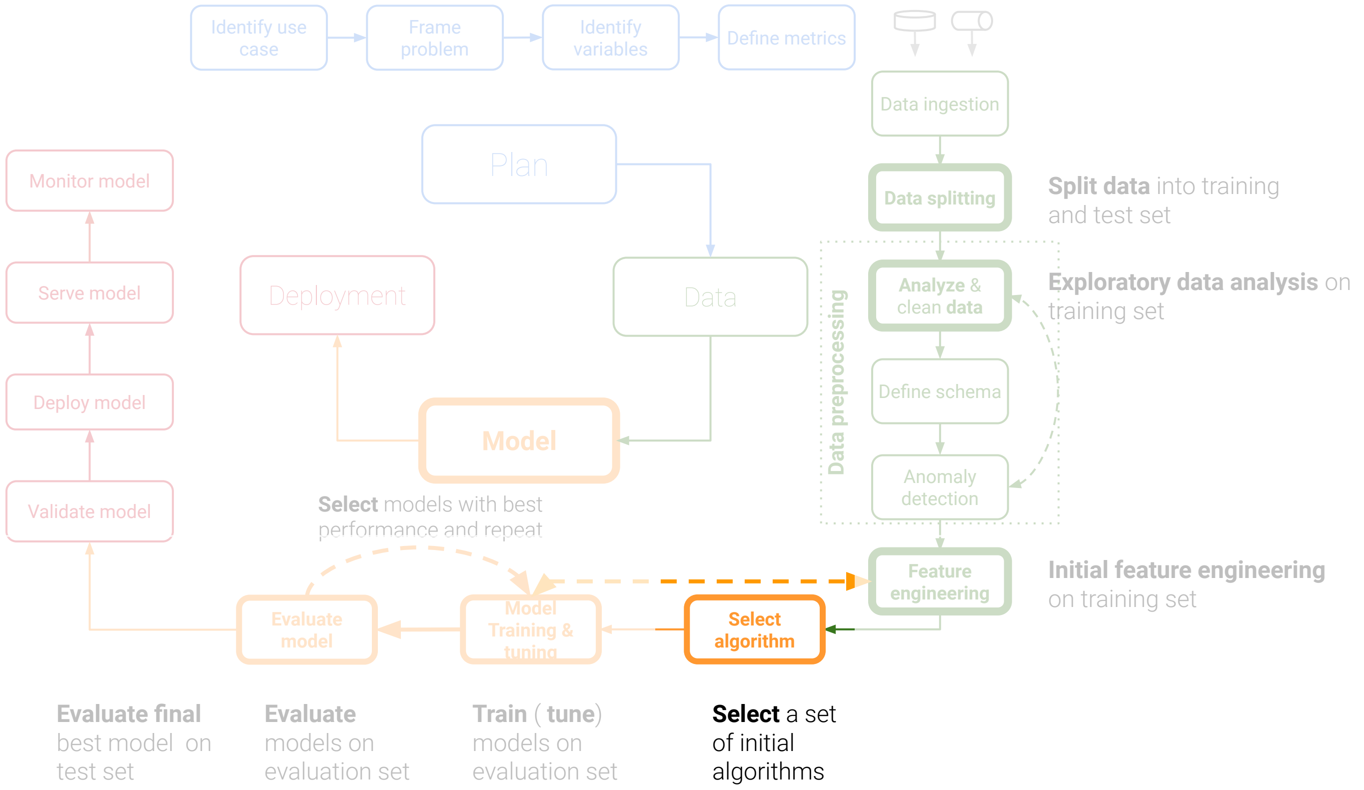

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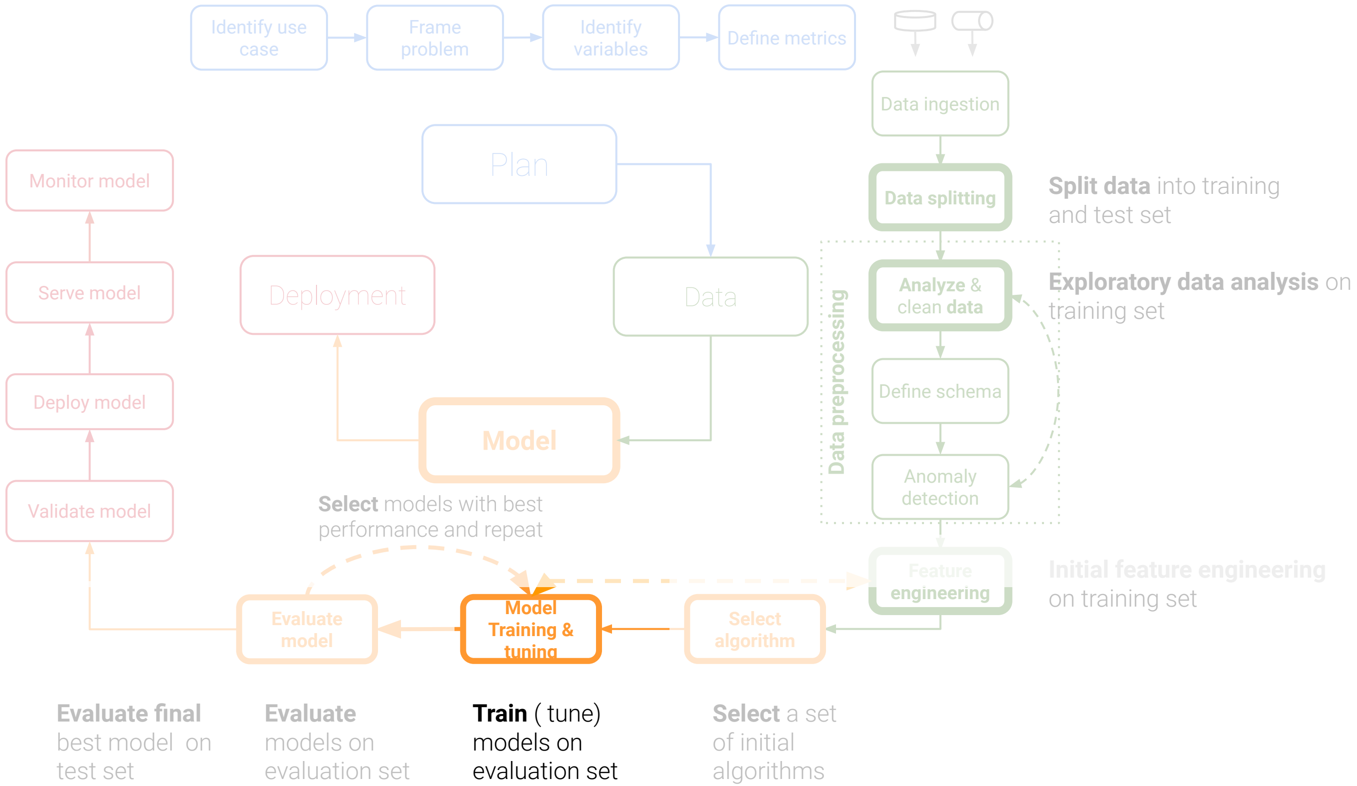

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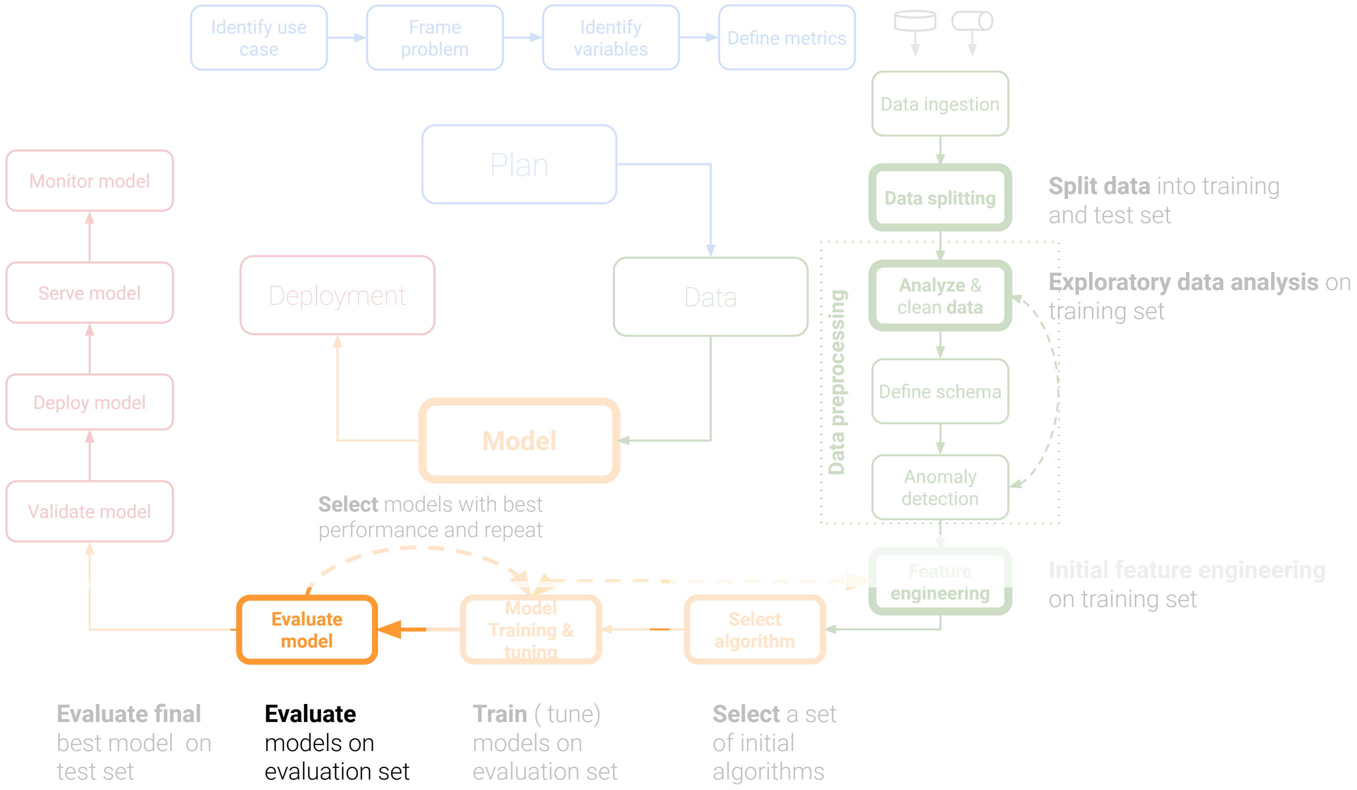

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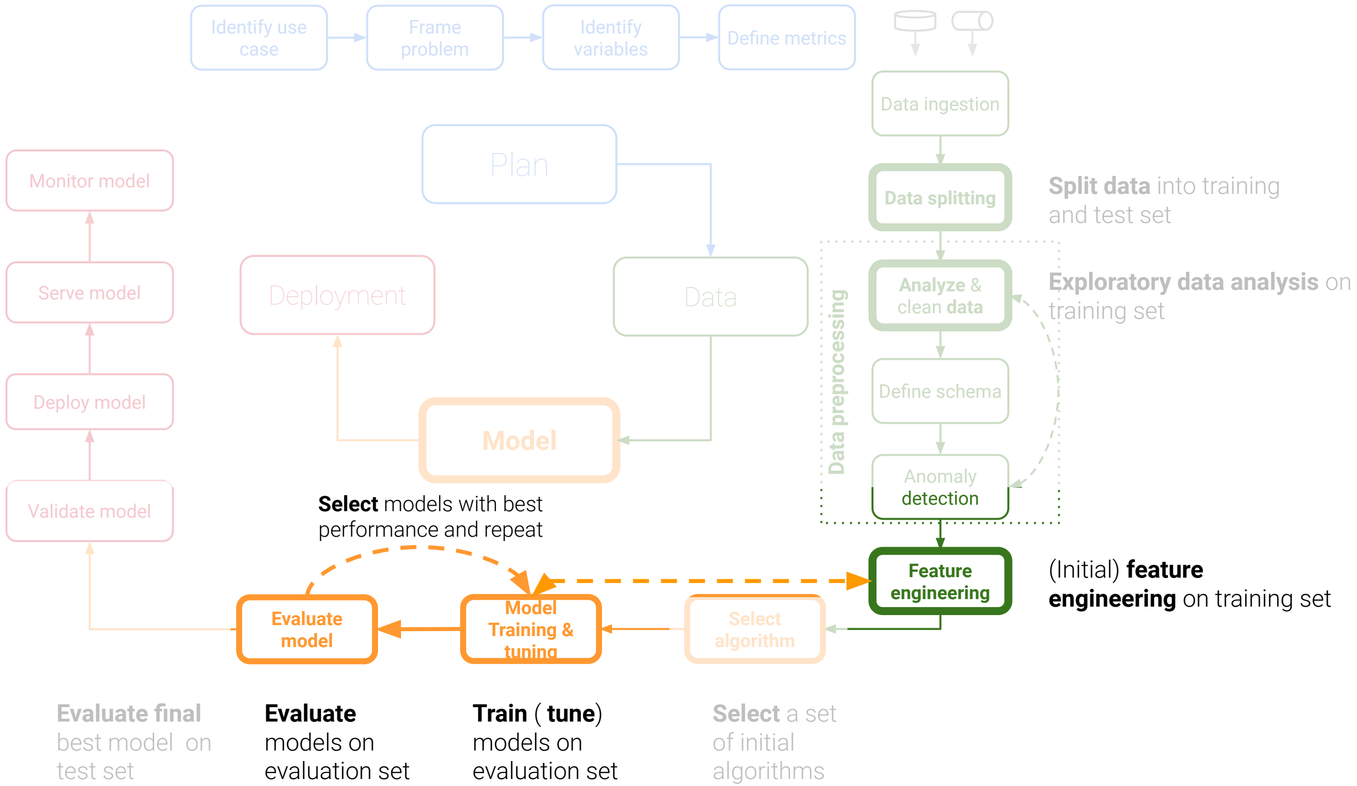

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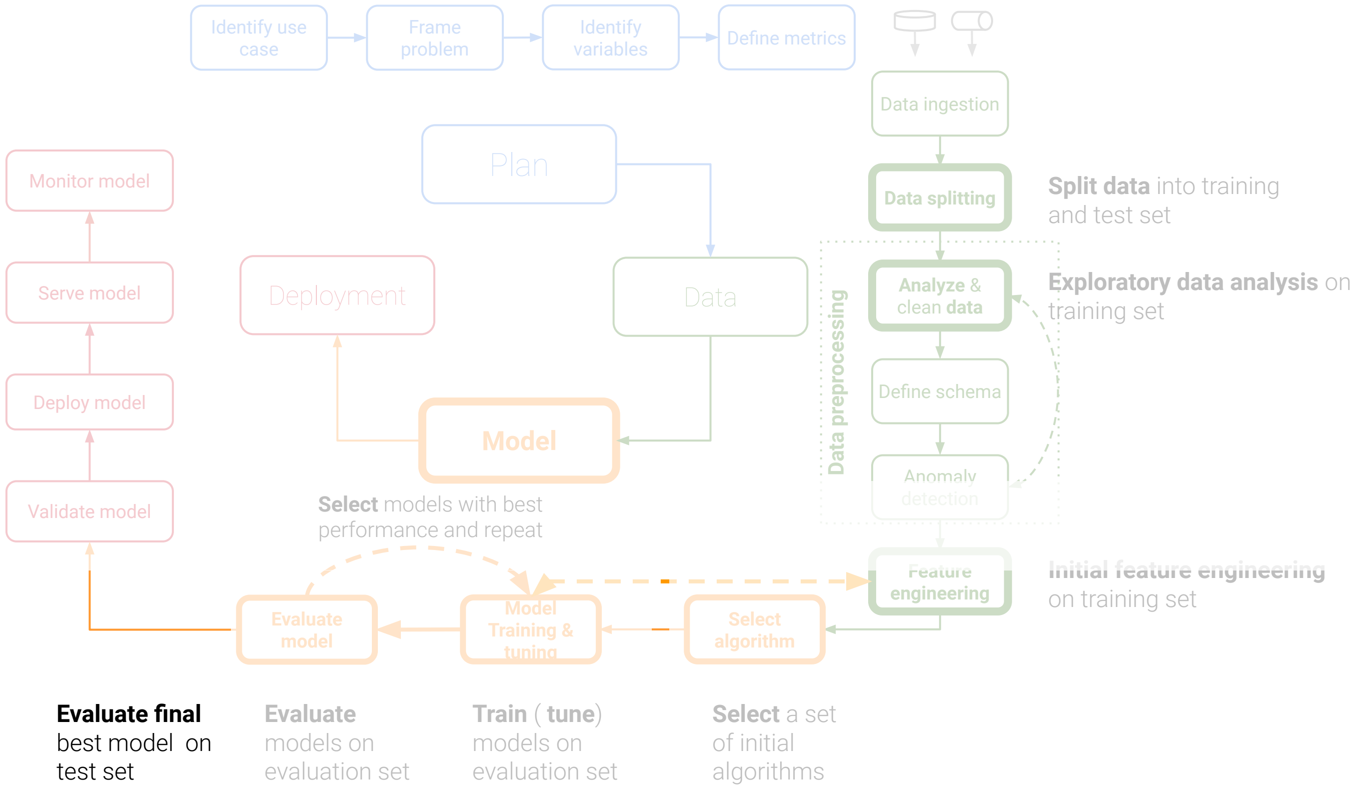

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Modeling procedere in summary

1. **Split data** into training and test set
2. Create **evaluation set** from training data (cross-validation)
3. **Train** a set of initial models using cross-validation (without extensive tuning)
4. **Select** the models with the best performance on the validation set
5. **Optimize** your models (hyperparameter tuning) on the validation set
6. Train the best model one more time on the **full training set**
7. Evaluate the final model on the **test set**
8. Do not further improve the model (this is your final result!)

Source: Géron (2019)

Literature

Géron, A. (2019). *Hands-on machine learning with Scikit-Learn, Keras, and TensorFlow: Concepts, tools, and techniques to build intelligent systems*. O'Reilly Media.

Kuhn, M., & Silge, J. (2020). Tidy Modeling with R.

Training, evaluation and testing data

The only way to know how well a model will **generalize to new cases** is to actually try it out on new cases

Training set

Evaluation set; Holdout validation

Cross-validation

Test set

Training error

Generalization error

Hyperparameter tuning