Instituto de Computação

UNIVERSIDADE ESTADUAL DE CAMPINAS

Capacitação profissional em tecnologias de Inteligência Artificial

Machine Learning Overview

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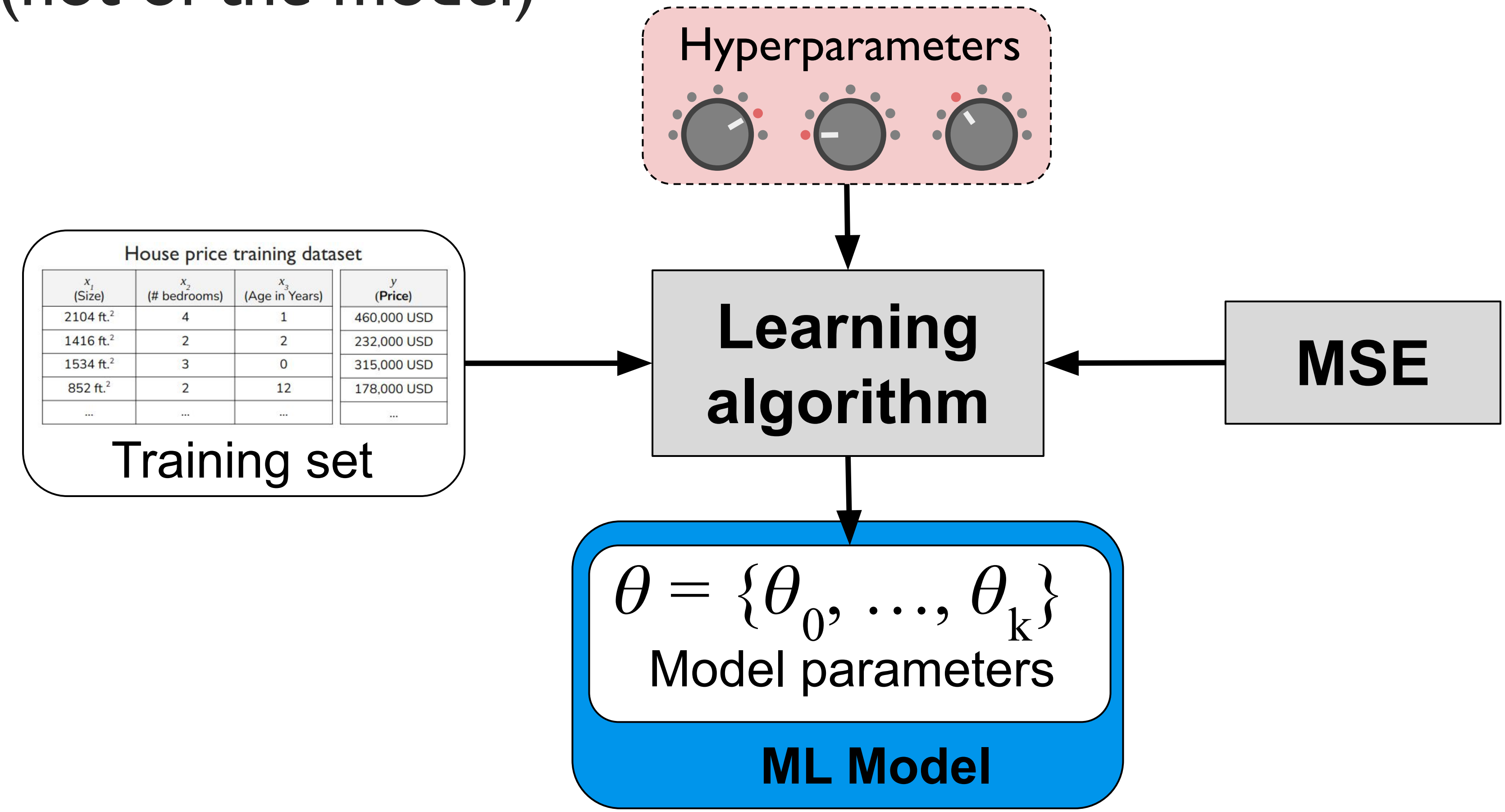
Institute of Computing - UNICAMP

Hyperparameters tuning

ML Process - Hyperparameters tuning

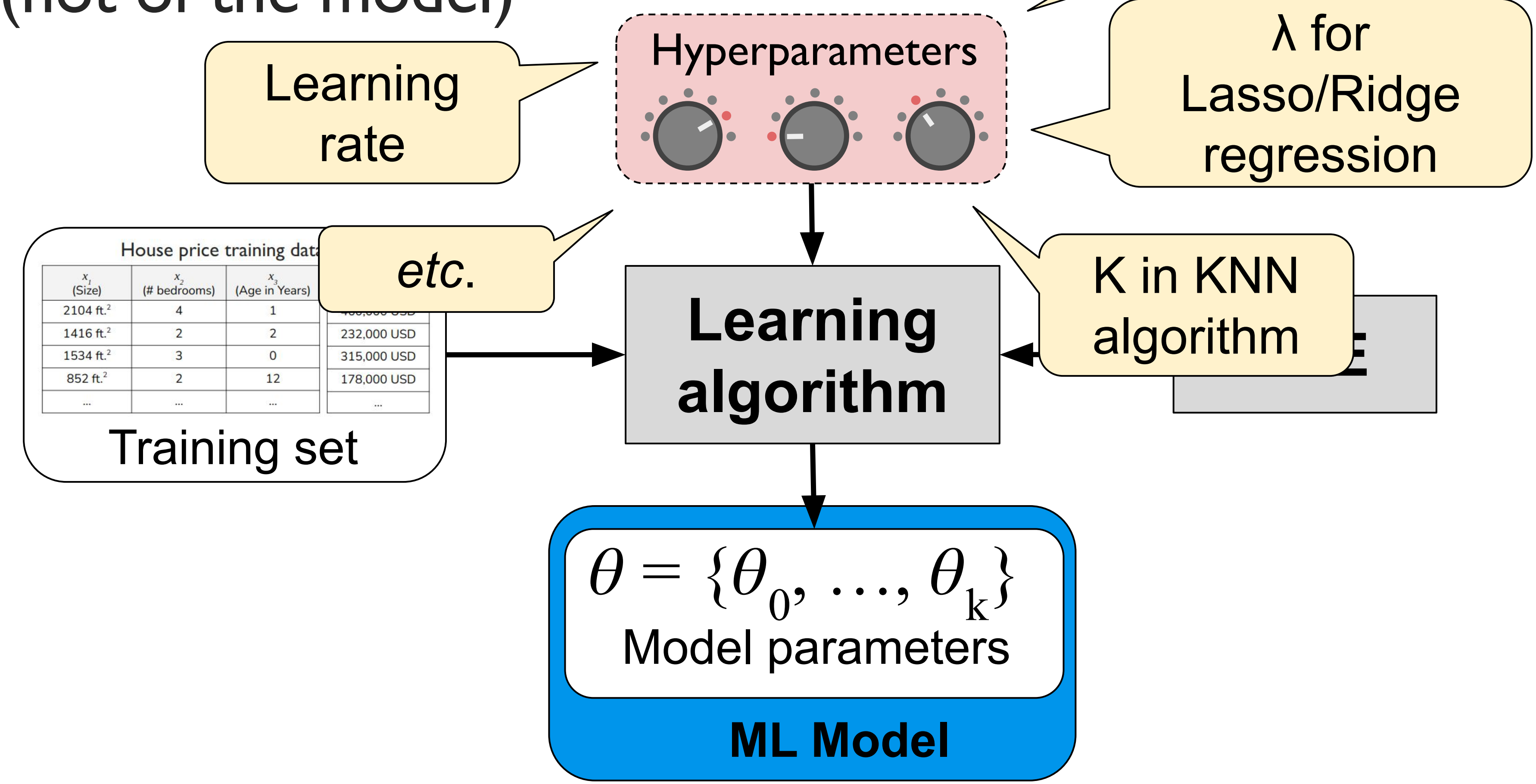
Hyperparameters: parameters of the learning process (not of the model)



x_1 (Size)	x_2 (# bedrooms)	x_3 (Age in Years)	y (Price)
2104 ft.^{2}	4	1	460,000 USD
1416 ft.^{2}	2	2	232,000 USD
1534 ft.^{2}	3	0	315,000 USD
852 ft.^{2}	2	12	178,000 USD
...	...	...	...

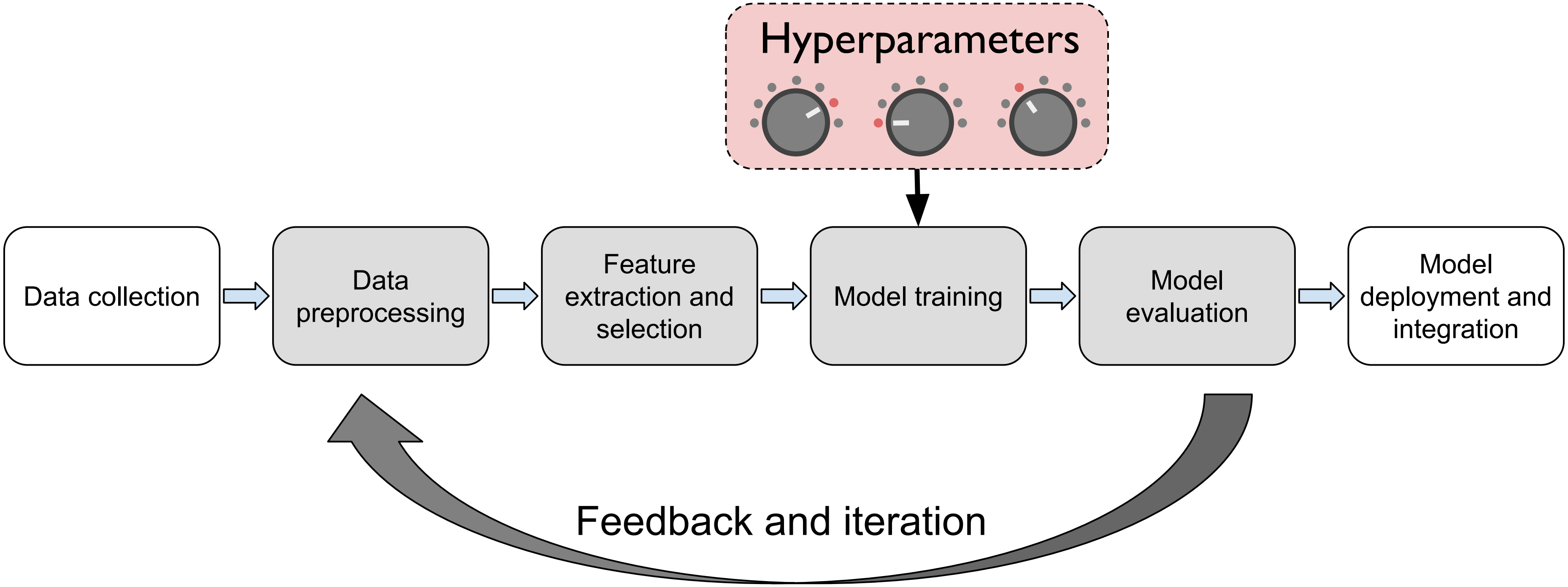
ML Process - Hyperparameters tuning

<u>Hyperparameters</u>: parameters of the le ess (not of the model)



ML Process - Hyperparameters tuning

<u>Hyperparameter tuning</u>: finding the best combination of hyperparameters that causes the learning process to produce the best model!



ML Process - Hyperparameters tuning

Hyperparameter tuning: finding the best combination of hyperparameters that causes the learning process to produce the best model!

- Example: scikit learn SVC models with RBF kernel
  - C: regularization parameter
  - γ: Kernel coefficient
  - Some hyperparameters combinations:
    - $(C, \gamma) \in \{ (10, 0.1), (10, 0.2), (100, 0.1), (100, 1.0)\}$

ML Process - Hyperparameters tuning

Search approach: strategy to evaluate the combinations of hyperparameters

- Several approaches
    - Grid search
    - Random search
    - Bayesian optimization
    - …

Search approach: **Grid Search**

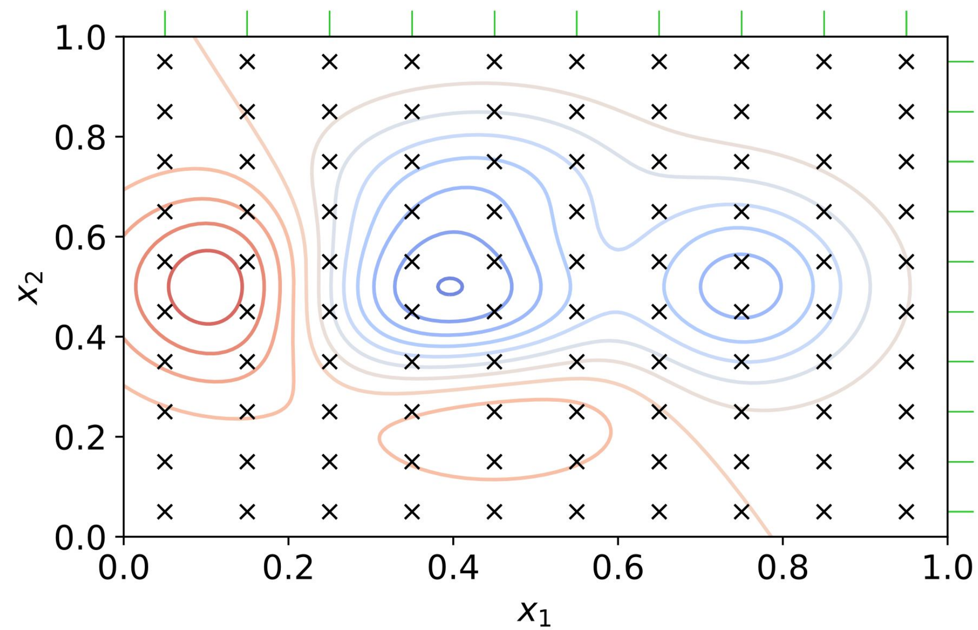
- Grid search (or parameter sweep) consists on a exhaustive search on a grid defined by the cartesian product of all parameters candidate values
- Example 1:
    - For $C \in \{10, 50, 100\}$, γ = {0.1, 0.2, 0.5, 1.0}, defined by the practitioner
    - $C \times \gamma$ = { (10, 0.1), (10, 0.2), (10, 0.5), (10, 1.0),
      (50, 0.1), (50, 0.2), (50, 0.5), (50, 1.0),
      (100, 0.1), (100, 0.2), (100, 0.5), (100, 1.0) }

ML Process - Hyperparameters tuning

Search approach: **Grid Search**

- Grid search (or parameter sweep) consists on a exhaustive search on a grid defined by the cartesian product of all parameters candidate values

- Example:
  - x_1 = np.arange(0.05, 1.0, 0.1)
  - x_2 = np.arange(0.05, 1.0, 0.1)

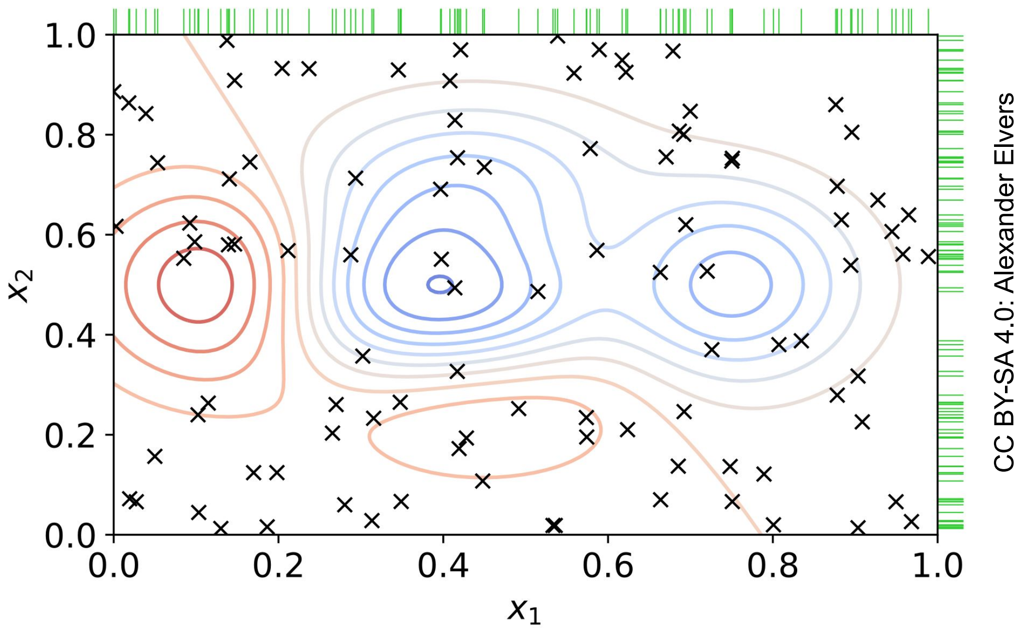


ML Process - Hyperparameters tuning

Search approach: **Random Search**

- Randomly selects values for hyperparameters
  - Bounds (max, min) values are defined by the user

- Example:
  - $x_1 \in = [0.0, 1.0]$
  - $x_2 \in = [0.0, 1.0]$

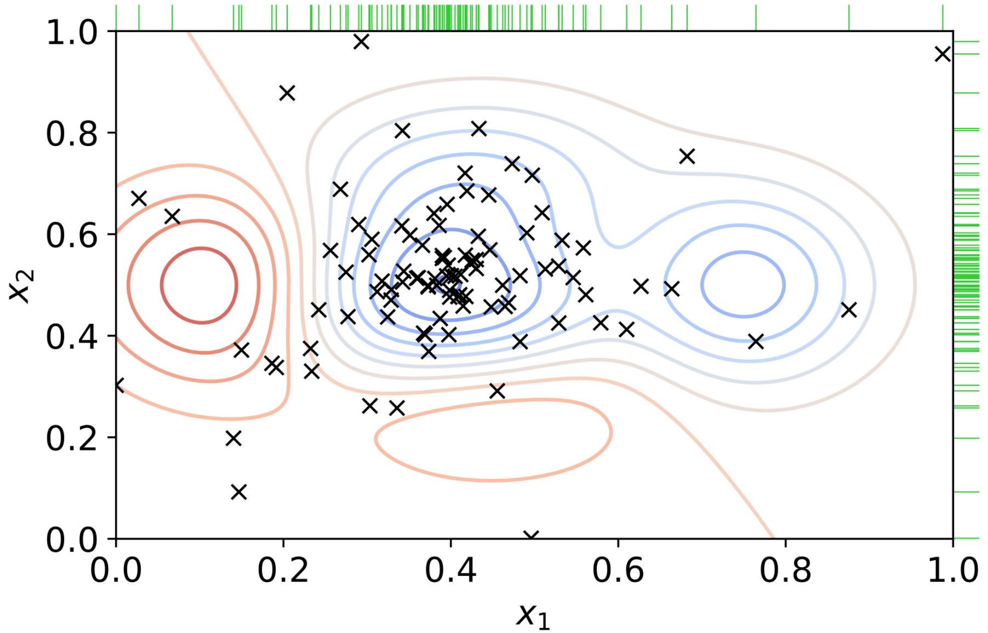


ML Process - Hyperparameters tuning

<u>Search approach</u>: **Bayesian optimization**

- Selects next set of hyperparameters to evaluate based on the performance of previous ones
  - Can be adjusted to favor exploring unknown regions or to focus on best regions found so far

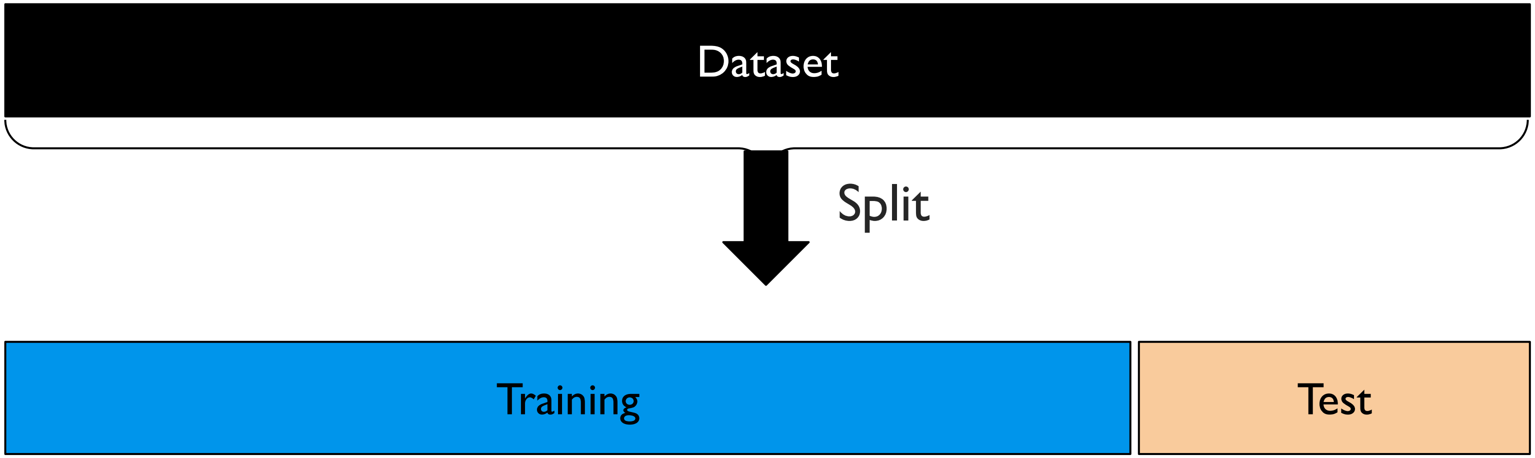
- Example:
  - $x_1 \in = [0.0, 1.0]$
  - $x_2 \in = [0.0, 1.0]$



Dataset splitting

ML Process - Dataset splitting

- On supervised learning tasks, the dataset is usually split into two subsets: training and test
    - Training set: used to train the model (i.e., adjust θ)
    - Test set: check the model generalization
        - Represents new/unseen data



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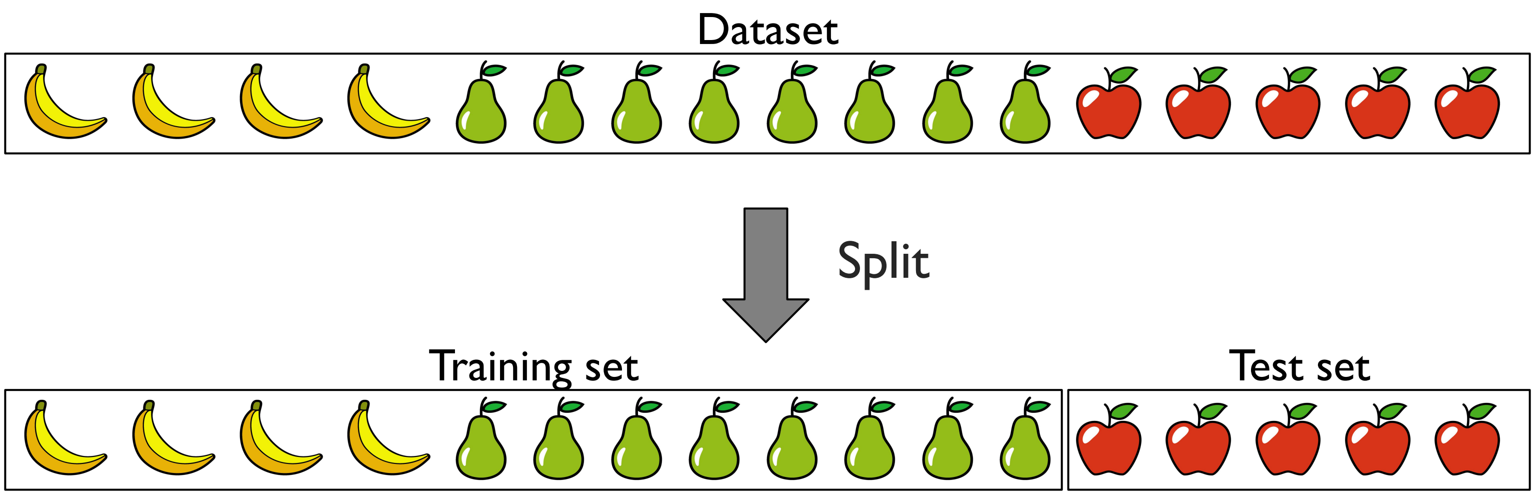

WARNING: Bad split!

ML Process - Dataset splitting

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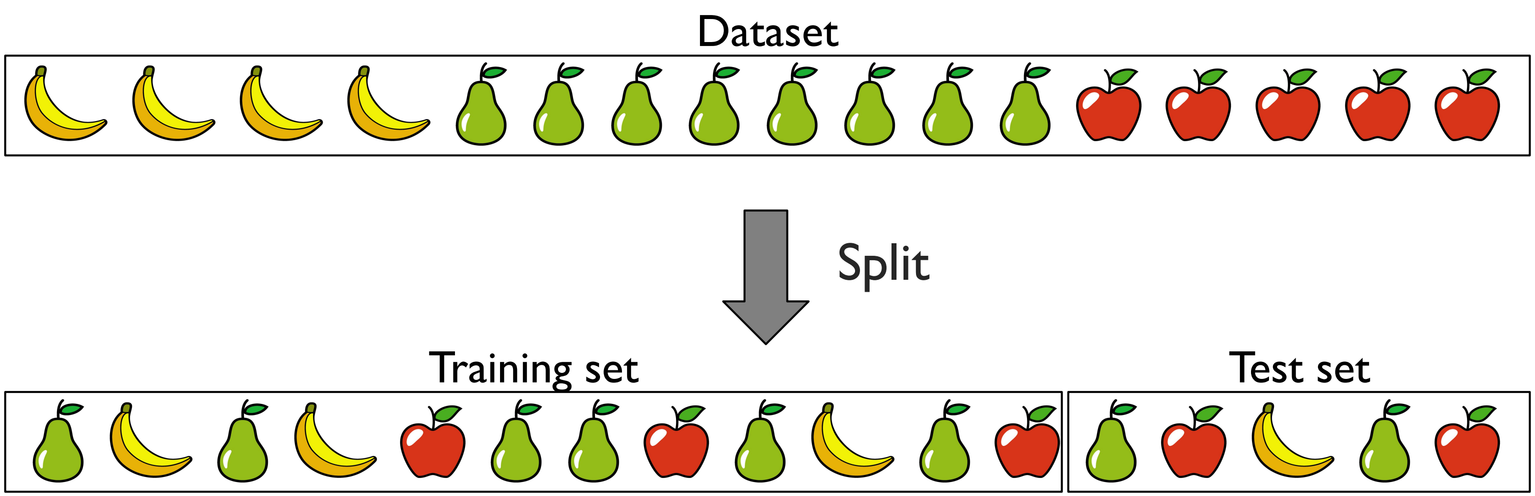

Random is better!

ML Process - Dataset splitting

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  - Training set: used to train the model (i.e., adjust θ)
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```
from sklearn.model_selection import train_test_split
X = ['y', 'y', 'y', 'r', 'r', 'r', 'r', 'g', 'g', 'g', 'g', 'g', 'g']
y = ['B', 'B', 'B', 'A', 'A', 'A', 'A', 'P', 'P', 'P', 'P', 'P', 'P']

# Split arrays or matrices into random train and test subsets.
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.2)

print(X_train, X_test)
print(y_train, y_test)
```

```
['r', 'y', 'g', 'r', 'g', 'g', 'y', 'r', 'g', 'g'] ['r', 'y', 'g']
['A', 'B', 'P', 'A', 'P', 'P', 'B', 'A', 'P', 'P'] ['A', 'B', 'P']
```

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print(X_train, X_test)
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```

```
['r', 'y', 'g', 'r', 'g', 'g', 'y', 'r', 'g', 'g
['A', 'B', 'P', 'A', 'P', 'P', 'B', 'A', 'P', 'P
```

Must be chosen carefully!

ML Process - Dataset splitting

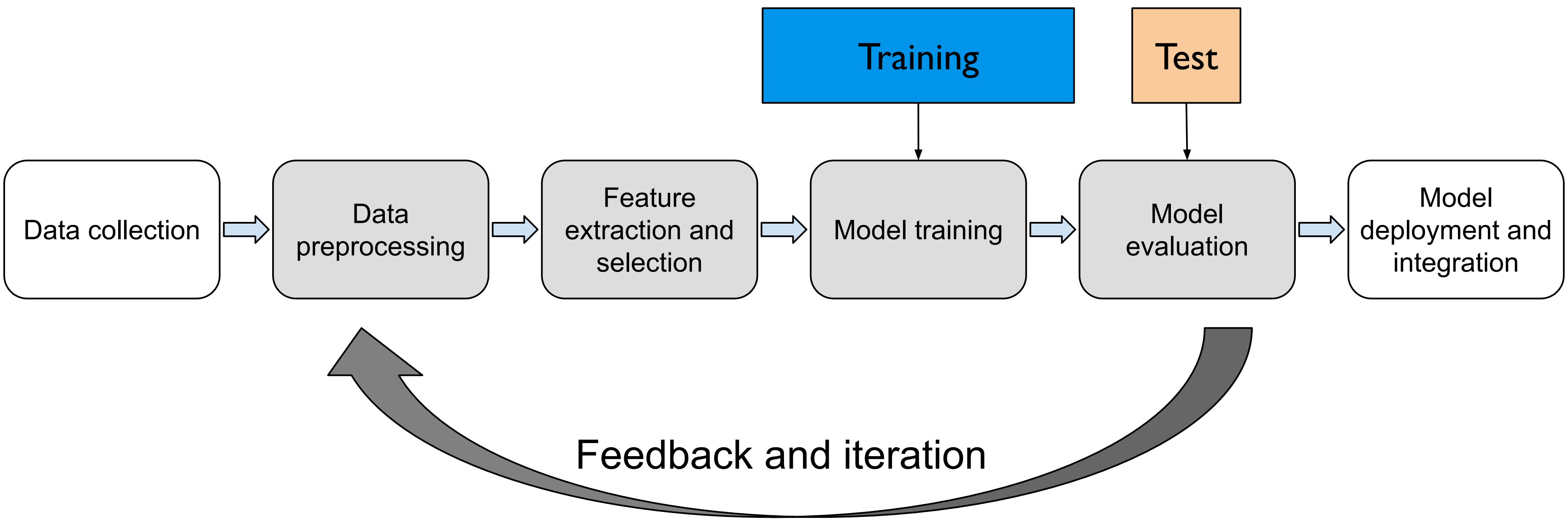
- On supervised learning tasks, the dataset is usually split into two subsets: training and test
  - Training set: used to train the model (i.e., adjust θ)
  - Test set: check the model generalization
    - Represents new/unseen data

Never train your model using the test data!

ML Process - Dataset splitting

<u>Test set and ML process iterations.</u>

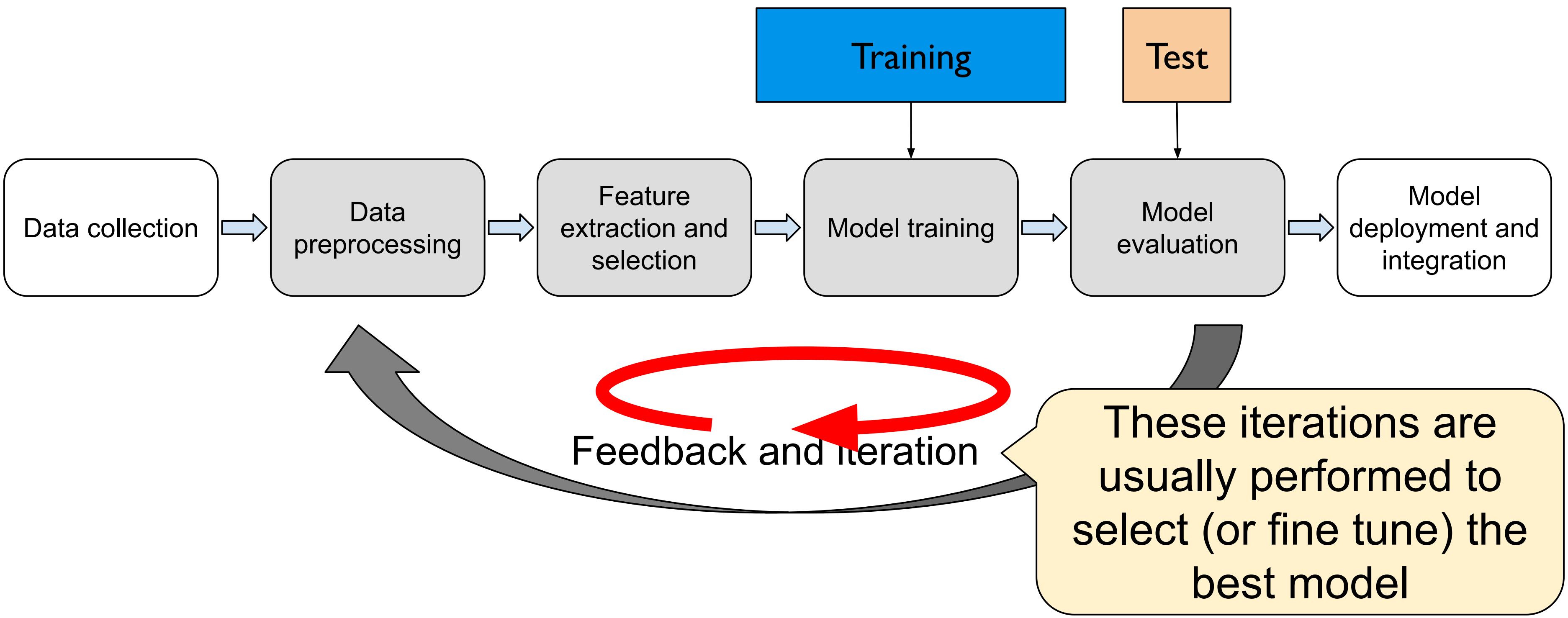
Previously…



ML Process - Dataset splitting

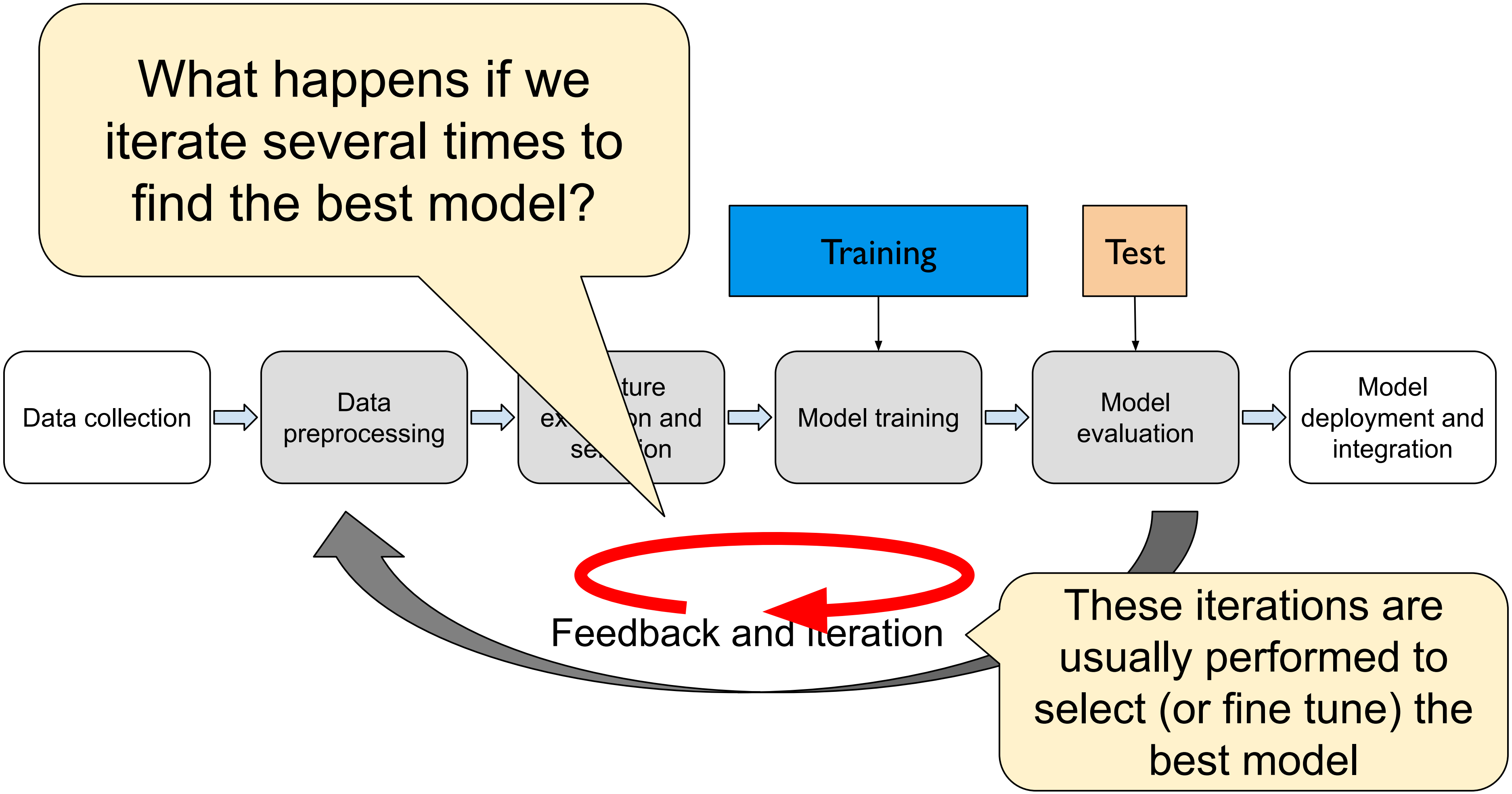
Test set and ML process iterations.

Previously…



ML Process - Dataset splitting

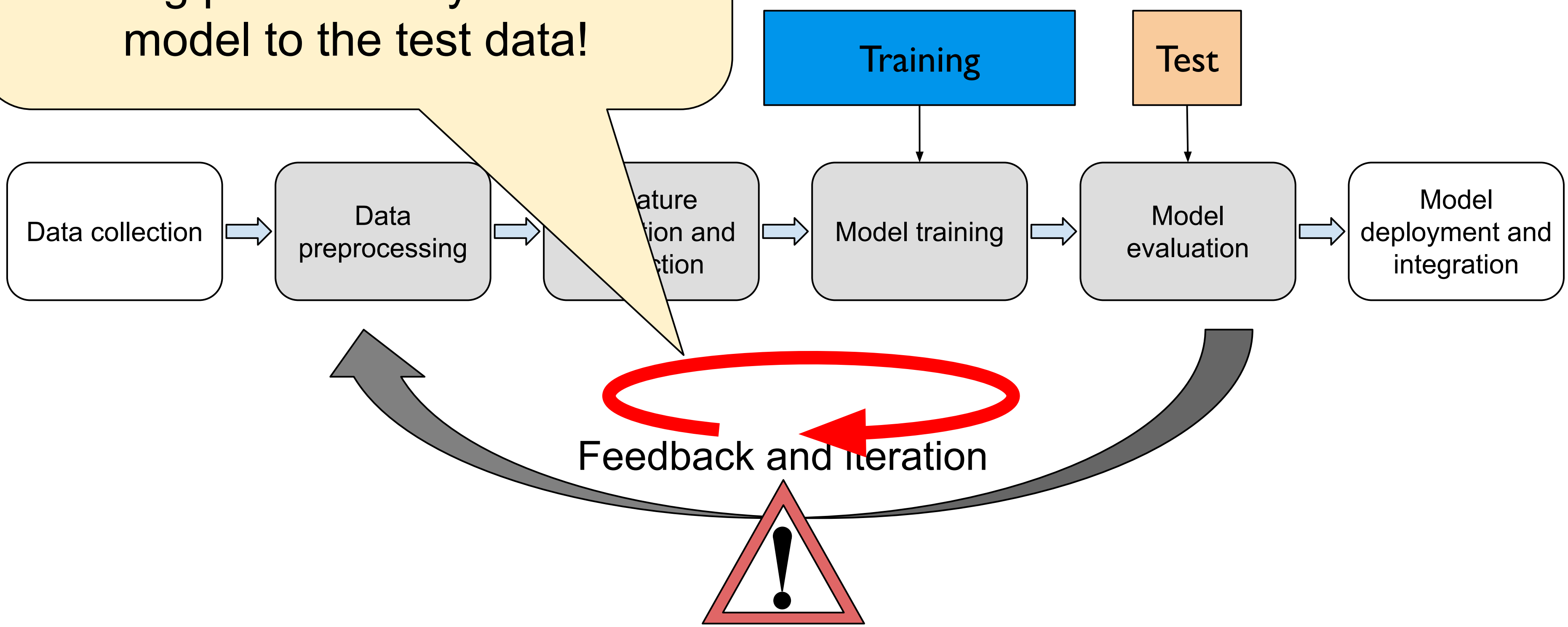
Test set and ML process iterations.



ML Process - Dataset splitting

Test set and ML process iterations.

Using the test results to repeatedly change/improve your learning process may overfit the model to the test data!

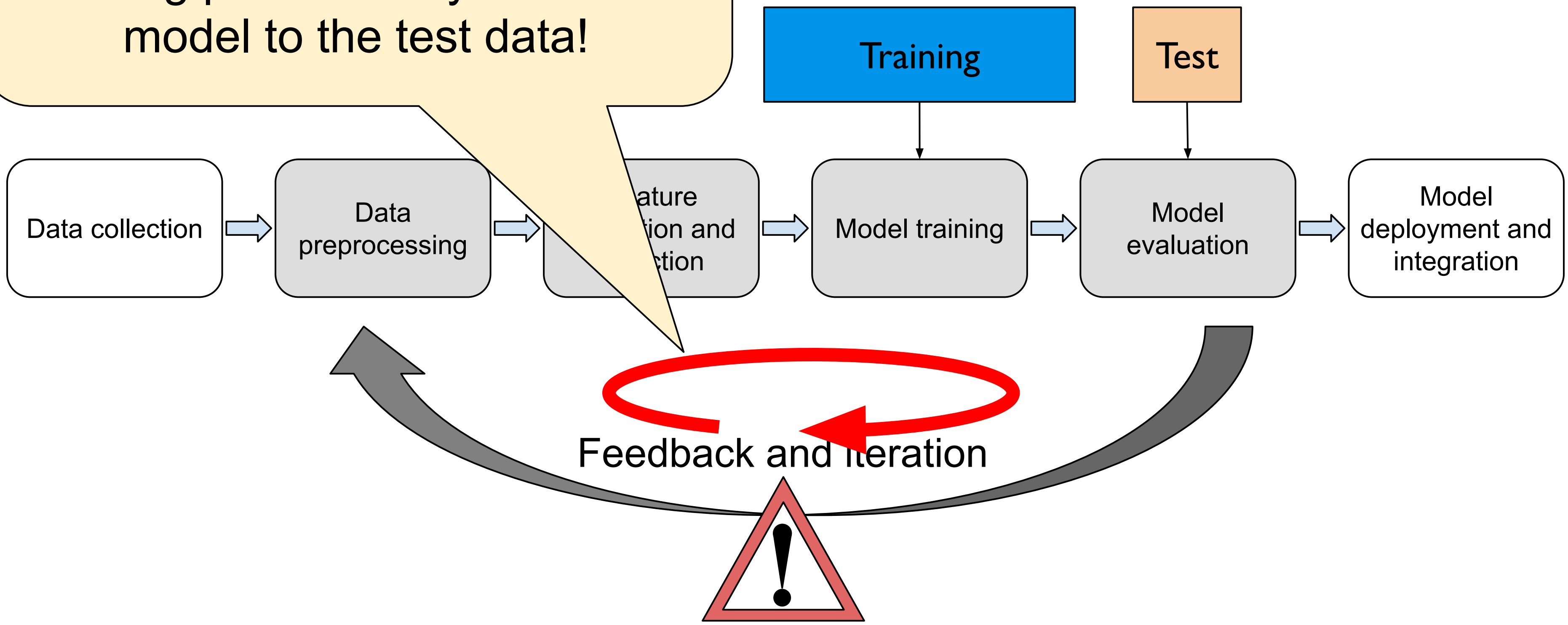


ML Process - Dataset splitting

Test set and ML process itera

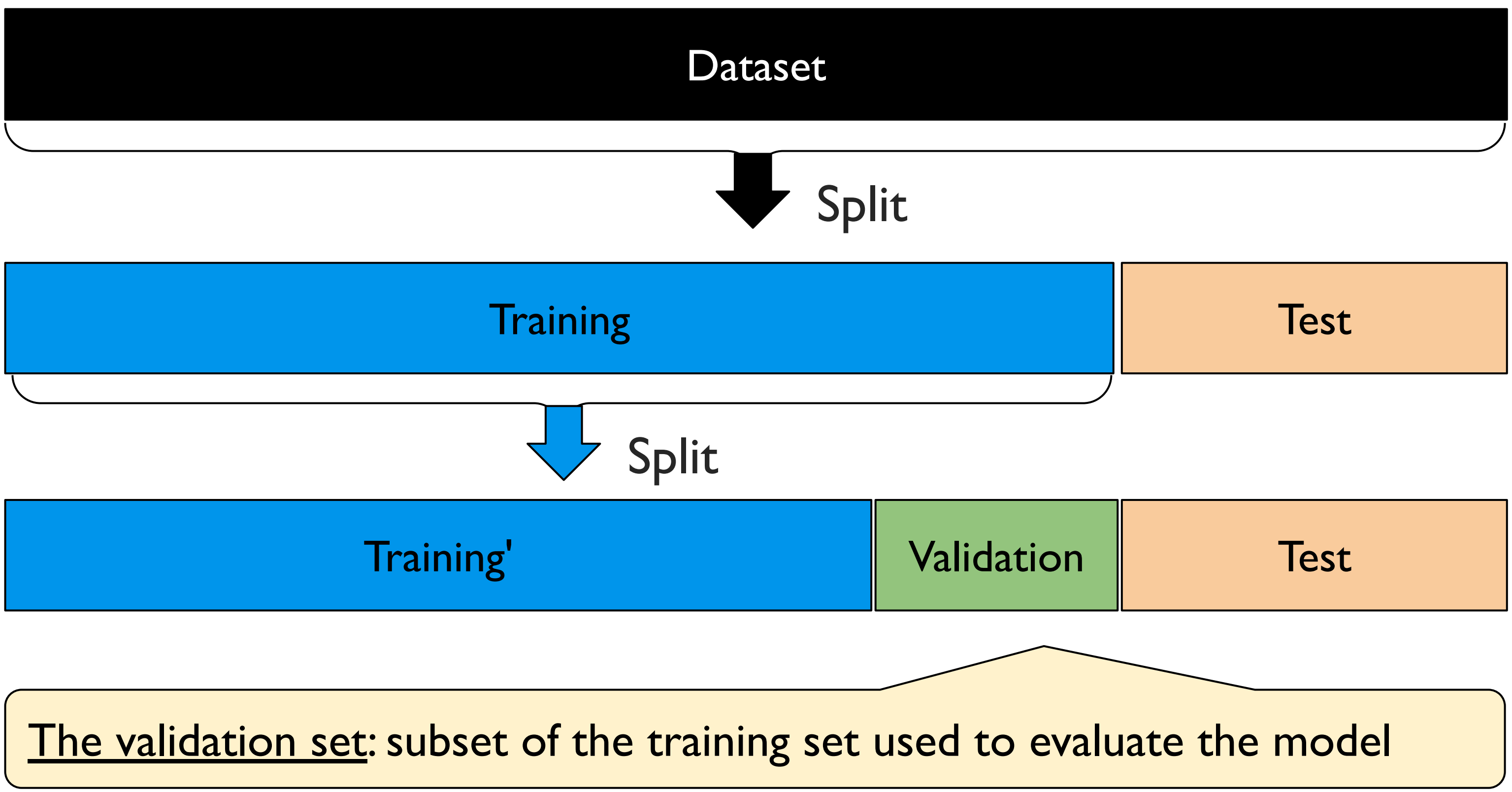
Using the test results to repeatedly change/improve your learning process may overfit the model to the test data!

Test set wears out and cannot be used to evaluate generalization anymore



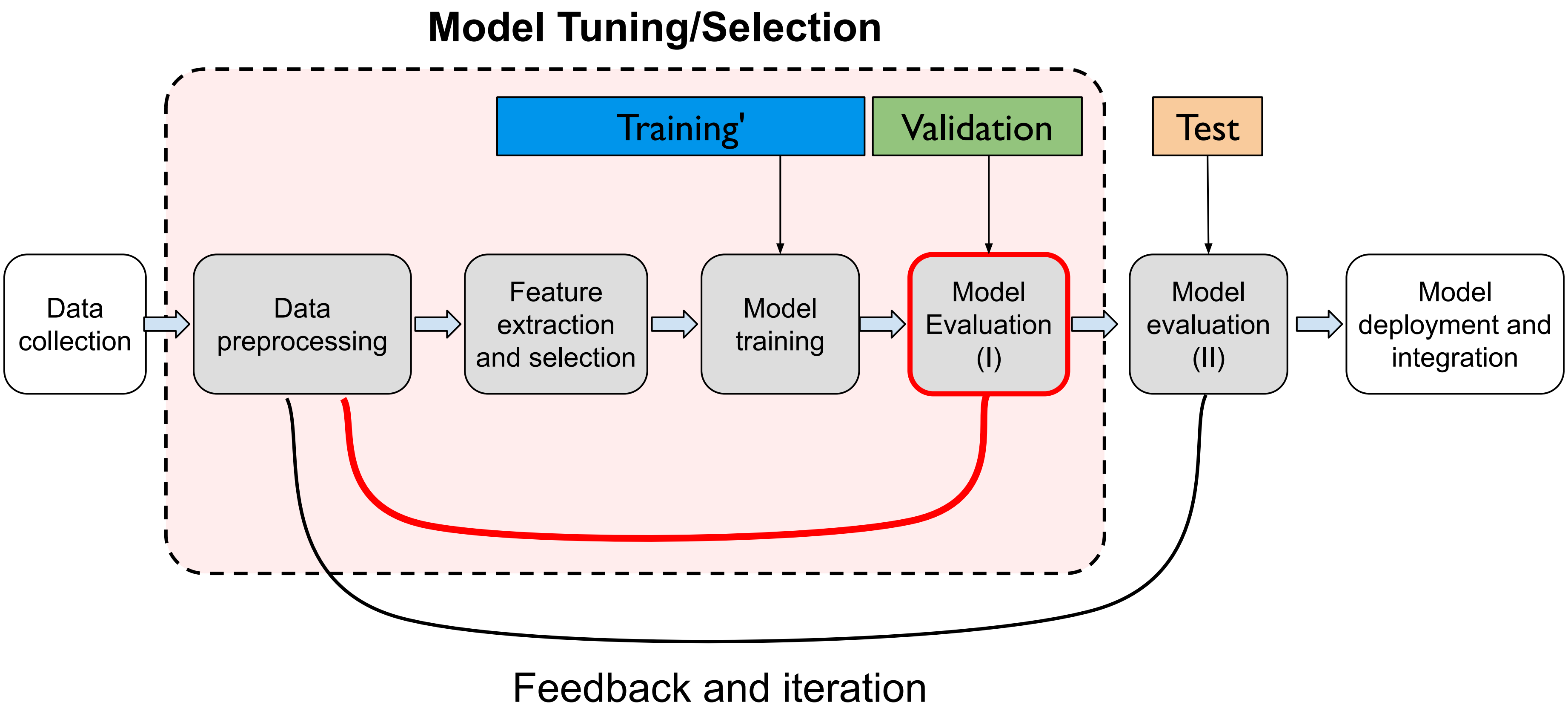
ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model



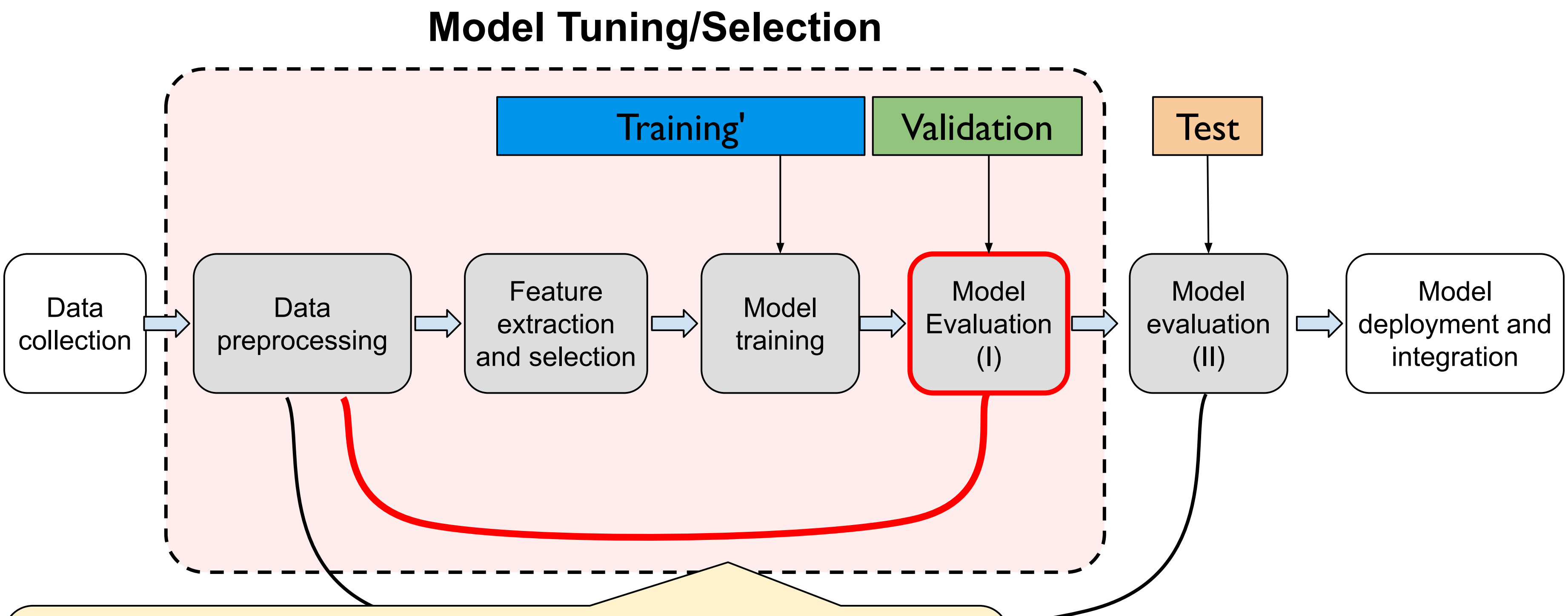
ML Process - Dataset splitting

<u>Cross-validation</u>: use different portions of the training set to train and to evaluate the model



ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

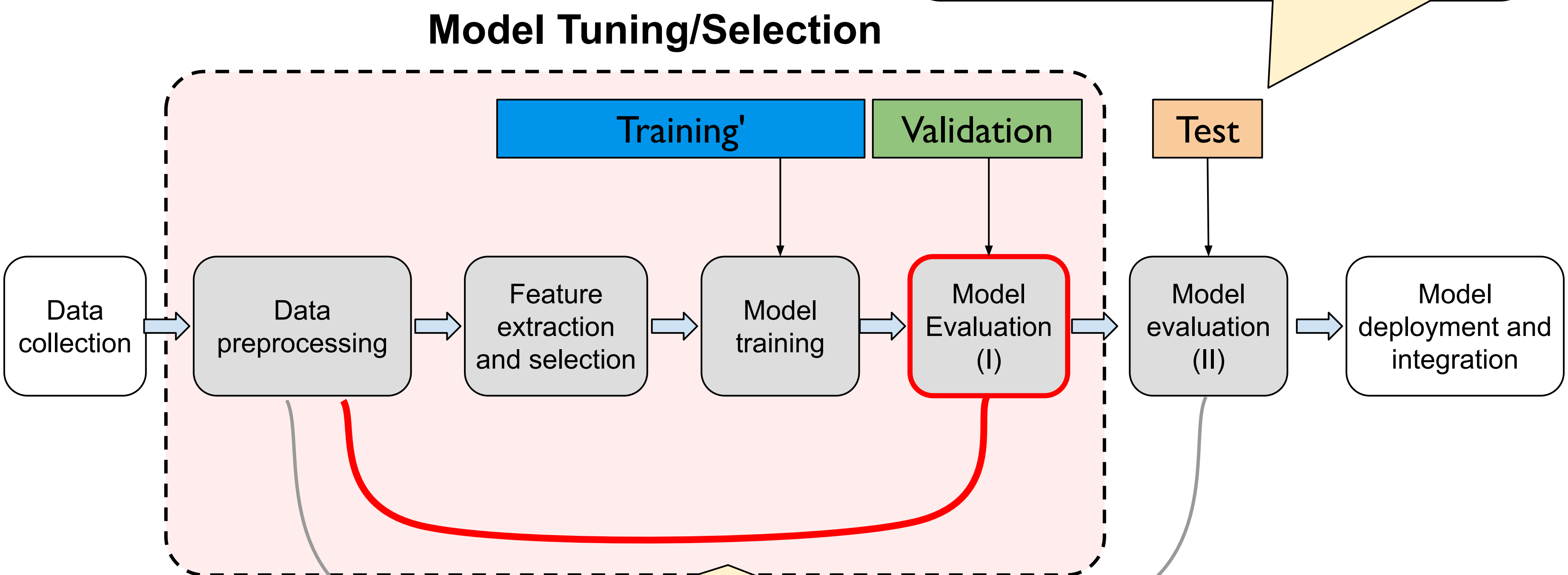


Pick model using validation set results and "double-check" it using the test set.

ML Process - Dataset splitting

Cross-validation: use different p... set to train and to evaluate the...

Unfrequently used!
Ideally, only once!



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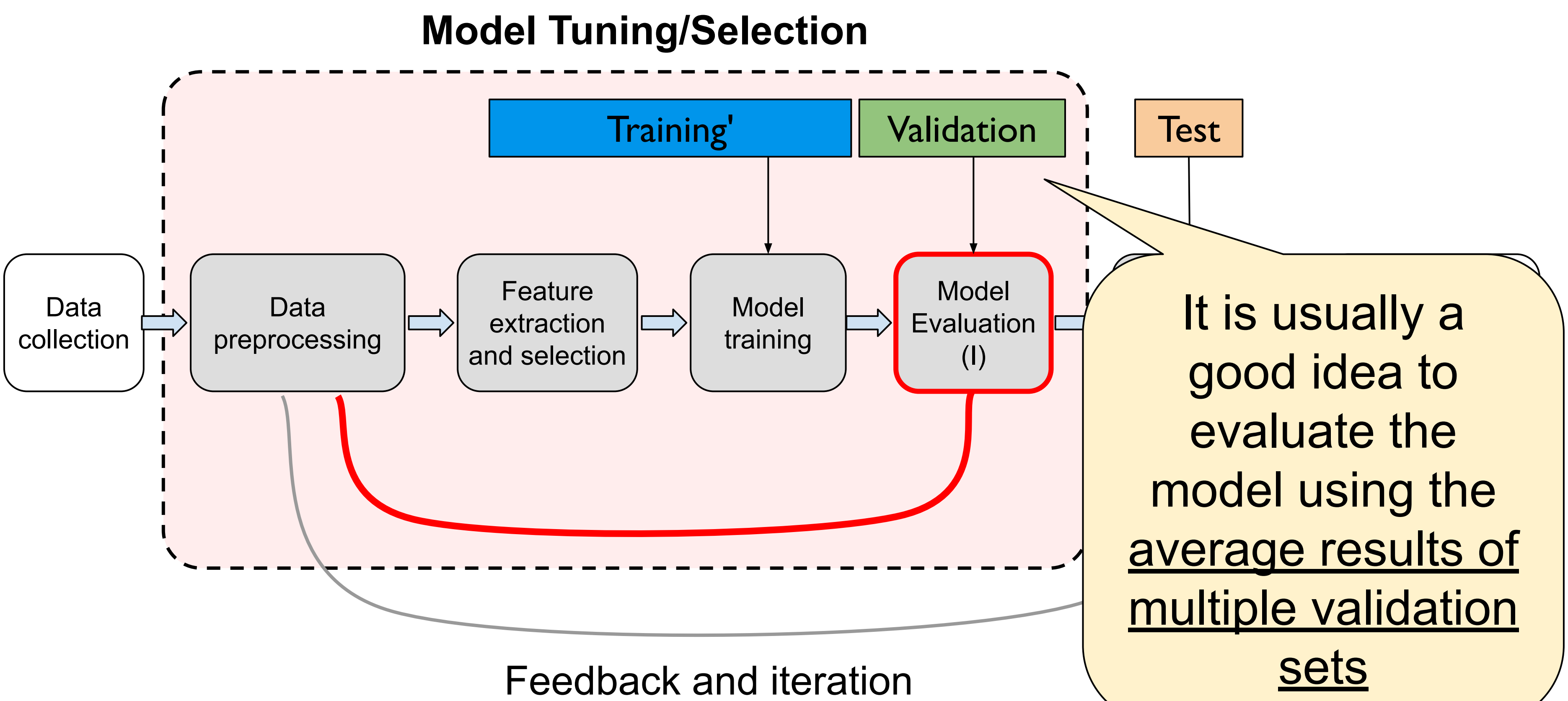
ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model



ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

Several approaches:

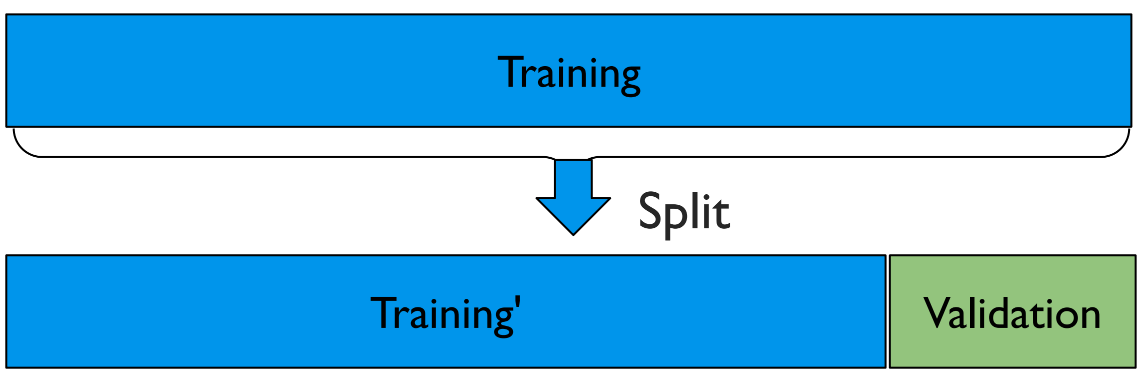
- **Holdout method**
- **Leave-one-out cross-validation**
- **k-fold cross-validation**
- Leave-p-out cross-validation
- repeated random sub-sampling validation
- k*l-fold cross validation
- …

ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

Several approaches:

- **Holdout method**: single train/validation partition randomly selected



ML Process - Dataset splitting

<u>Cross-validation</u>: use different p g
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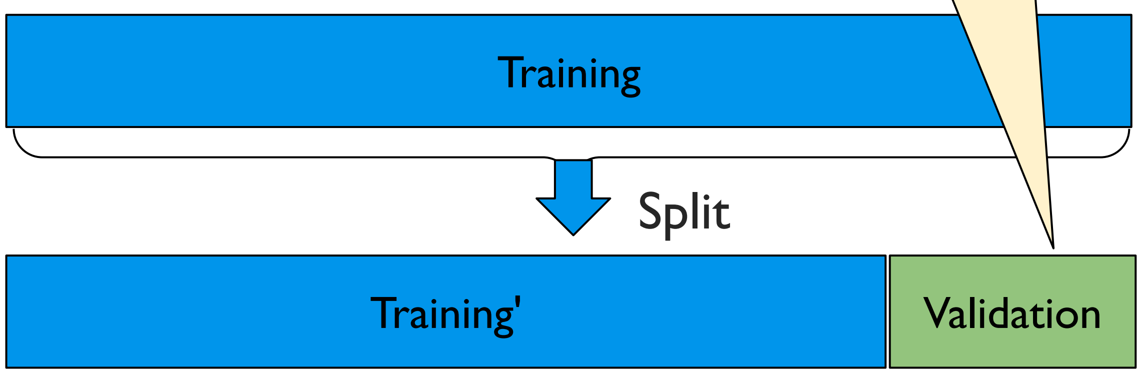
Several approaches:

- **Holdout method**: single train/validatio tion randomly selected

Single partition may cause evaluation bias.

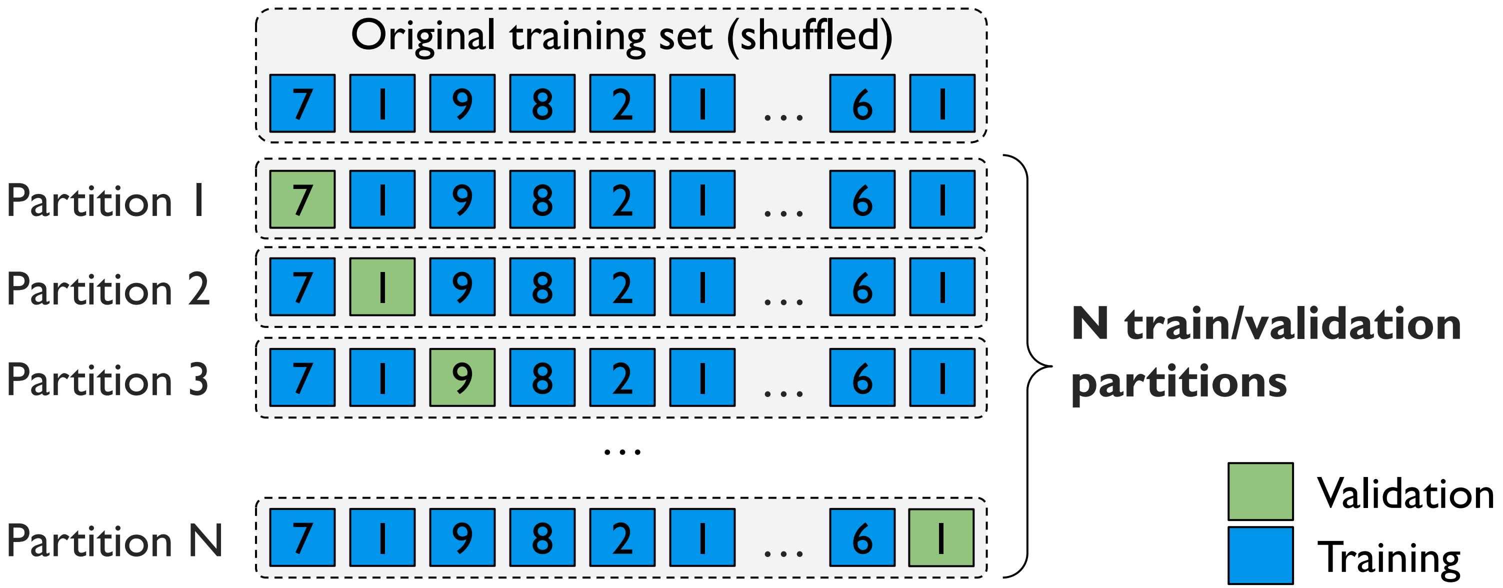


ML Process - Dataset splitting

<u>Cross-validation</u>: use different portions of the training set to train and to evaluate the model

Several approaches:

- **Leave-one-out cross-validation**: 1 partition per item

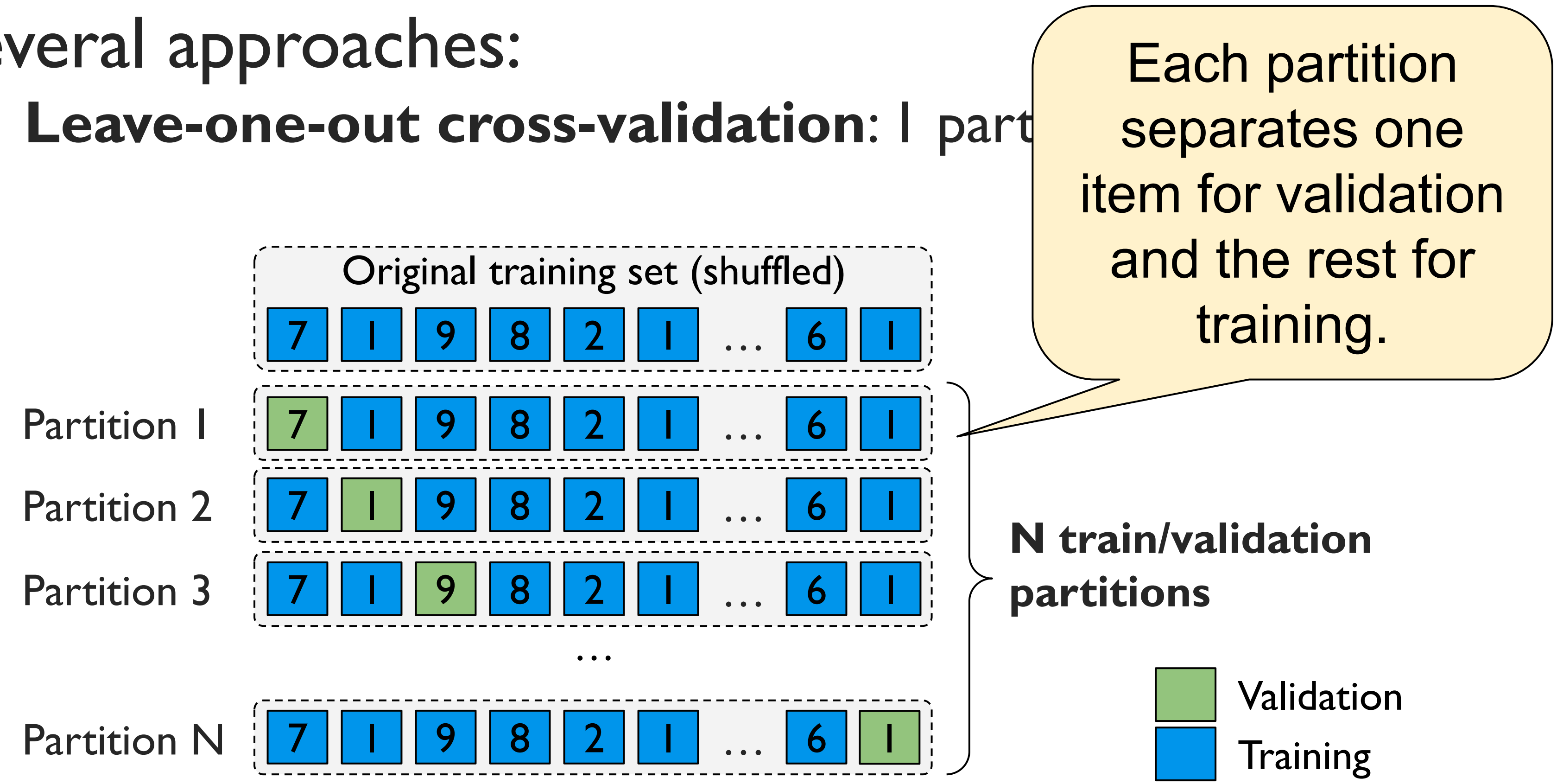


ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

Several approaches:

- **Leave-one-out cross-validation**: 1 part



ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

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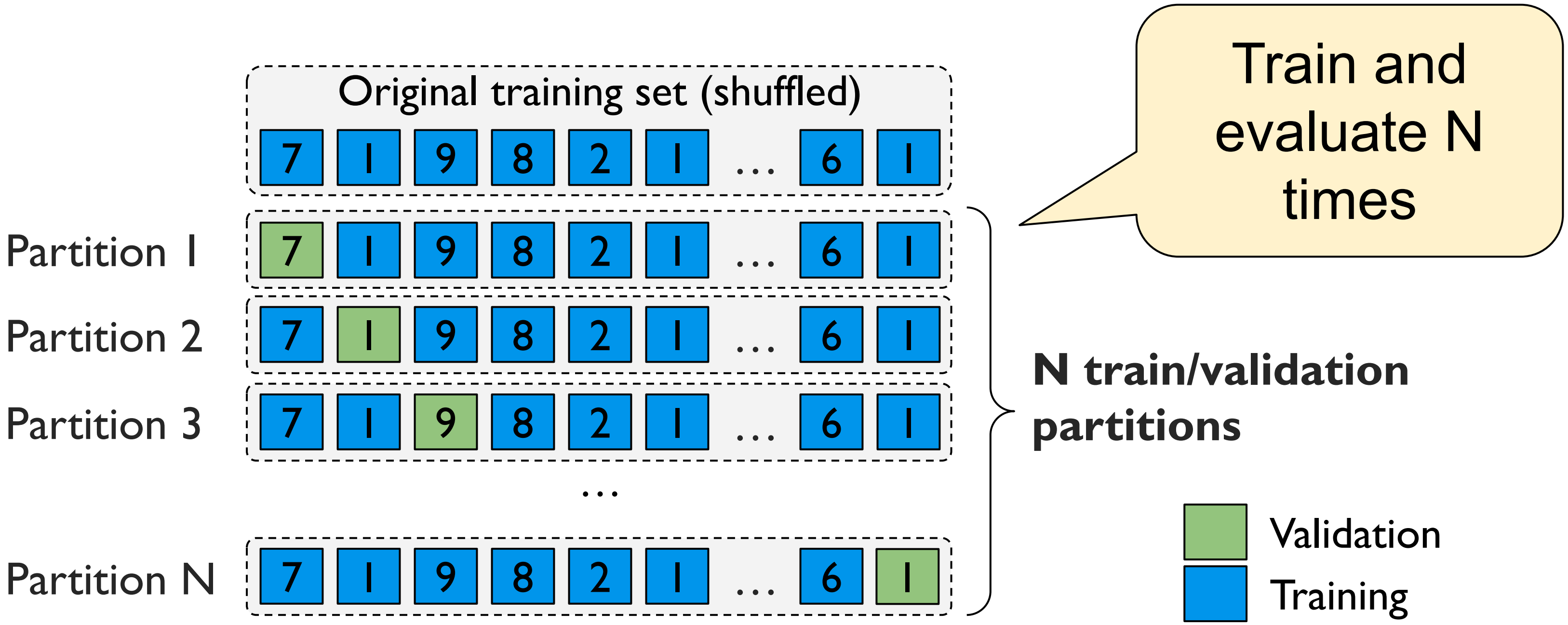


ML Process - Dataset splitting

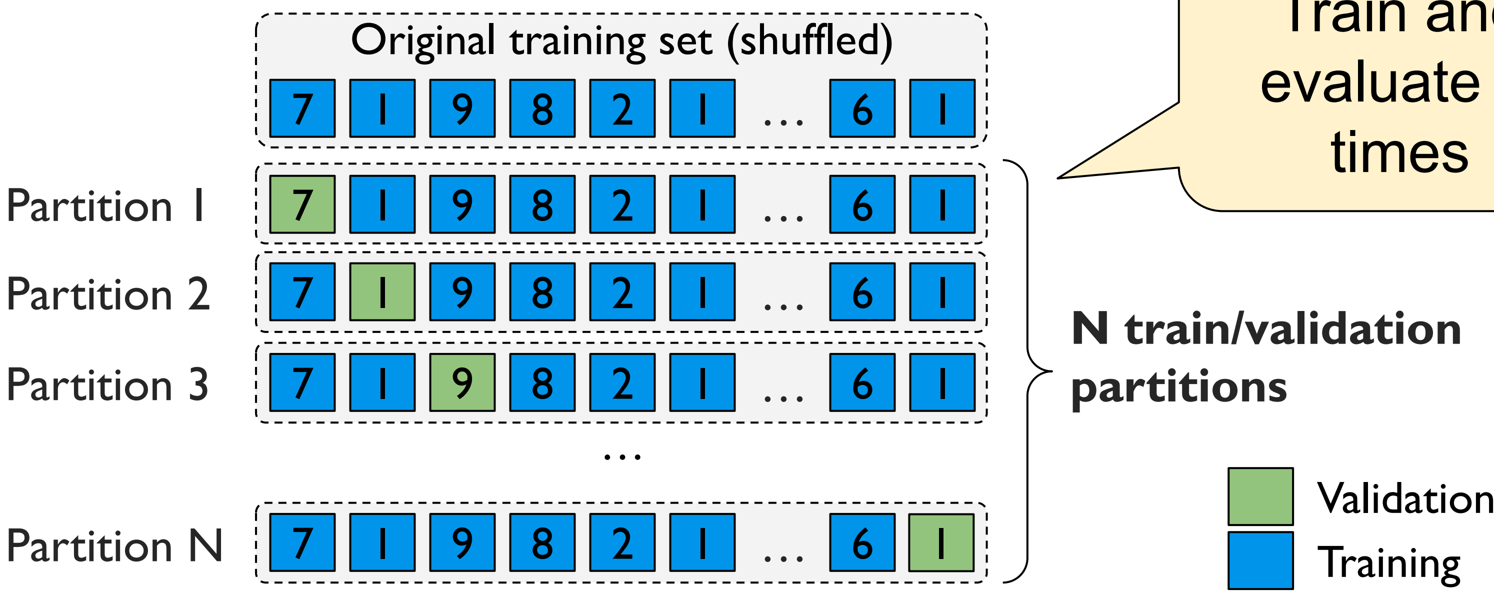
<u>Cross-validation</u>: use different portions g set to train and to evaluate the model

Several approaches:

- **Leave-one-out cross-validation**: 1 partition per item

Report average and stdev

Train and evaluate N times



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Cross-validation: use different portions g set to train and to evaluate the model

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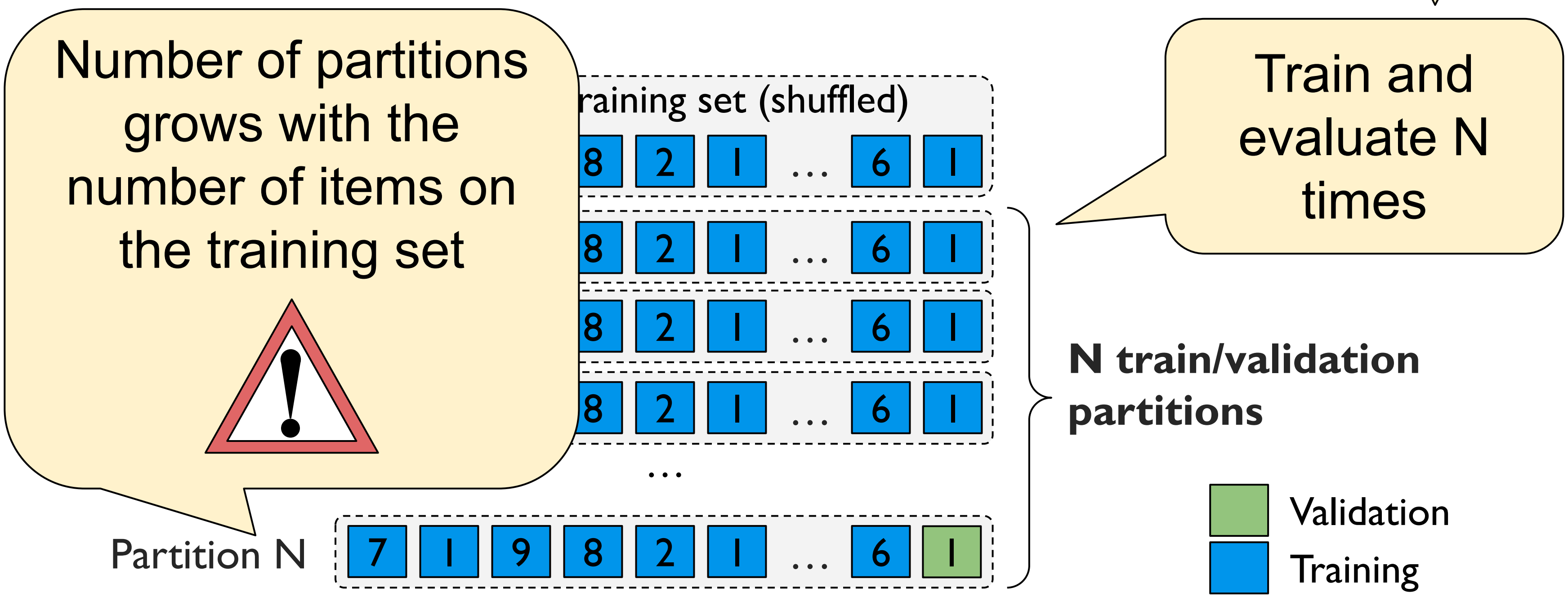
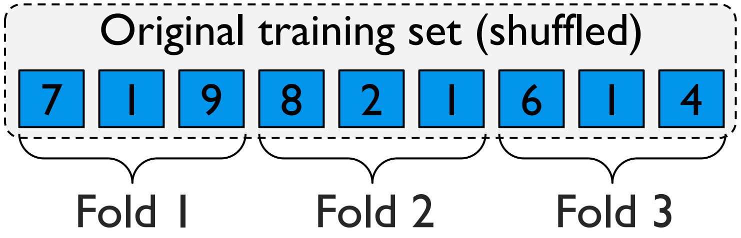


ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

Several approaches:

- **k-fold cross-validation**: split the data in K folds and generate 1 partition per fold
- Example: 3-fold cross-validation



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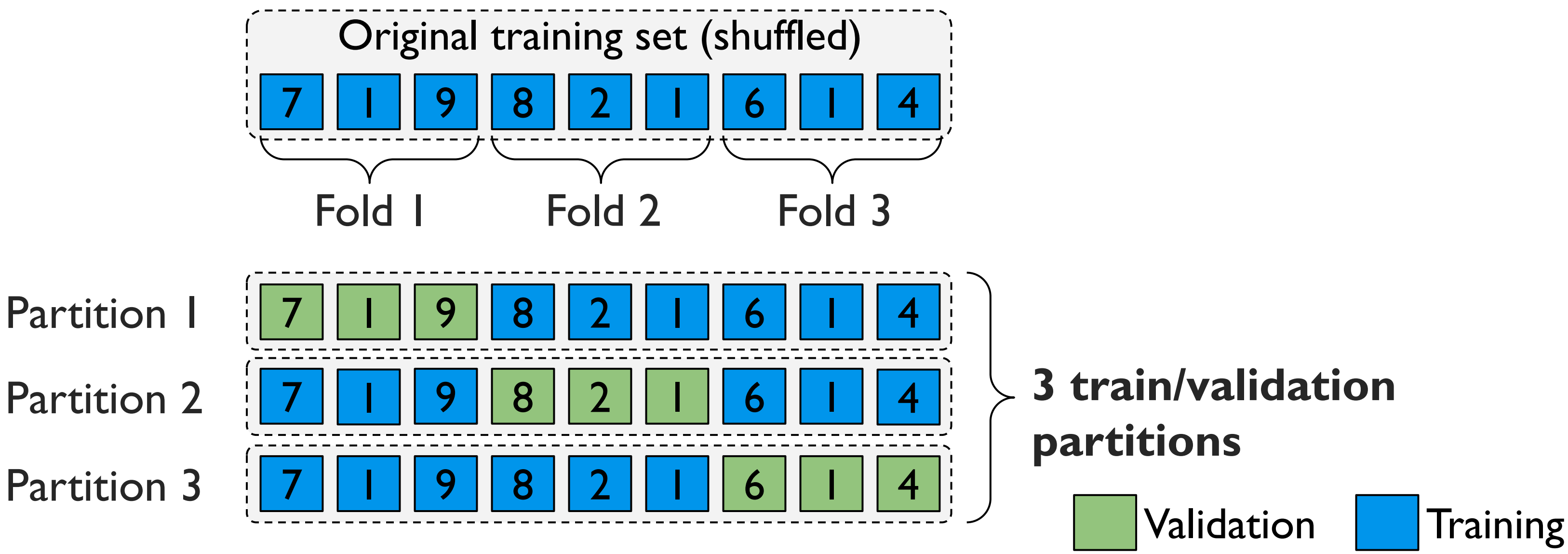


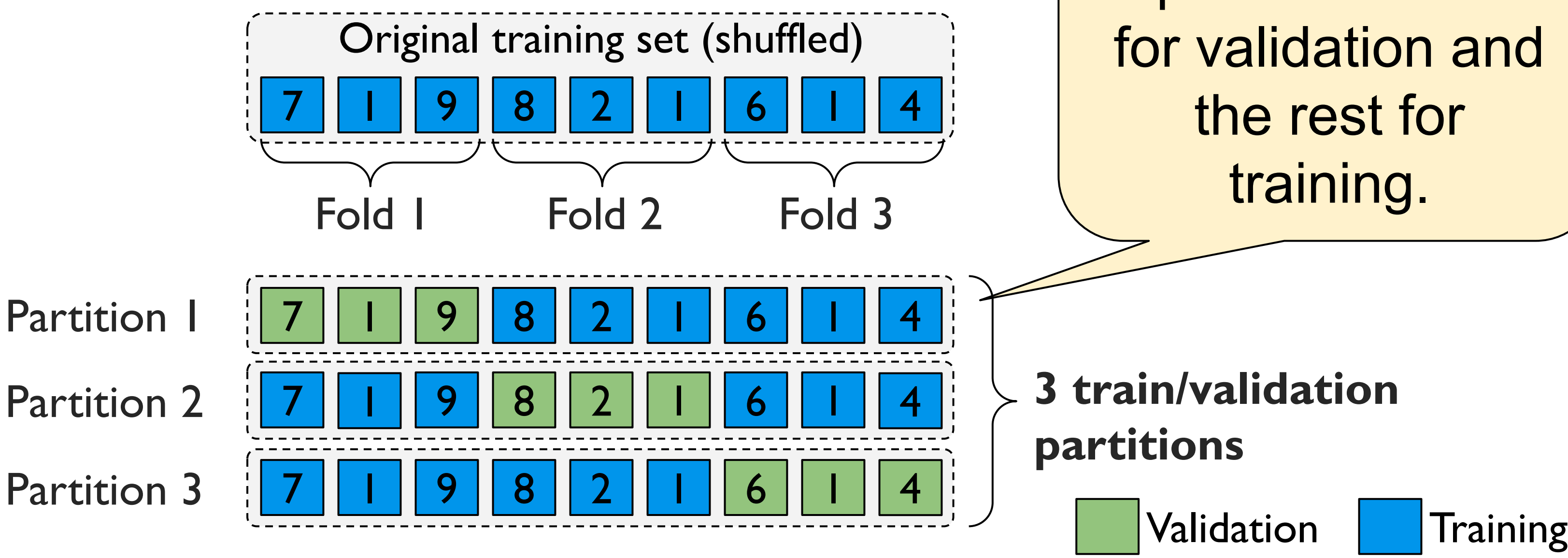
ML Process - Dataset splitting

Cross-validation: use different portions of the training set to train and to evaluate the model

Several approaches:

- **k-fold cross-validation**: split the data in K folds and generate 1 partition per fold
- Example: 3-fold cross-validation

Each partition separates one fold for validation and the rest for training.



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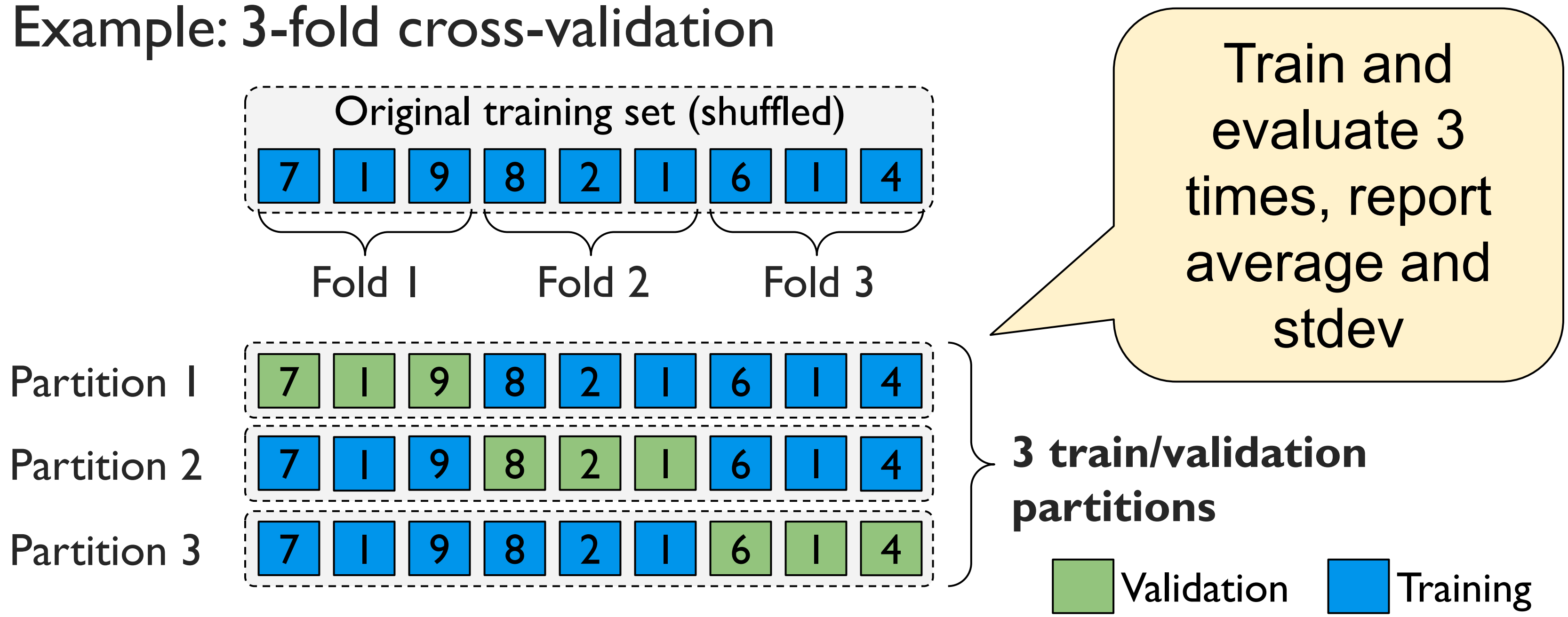


ML Process - Dataset splitting

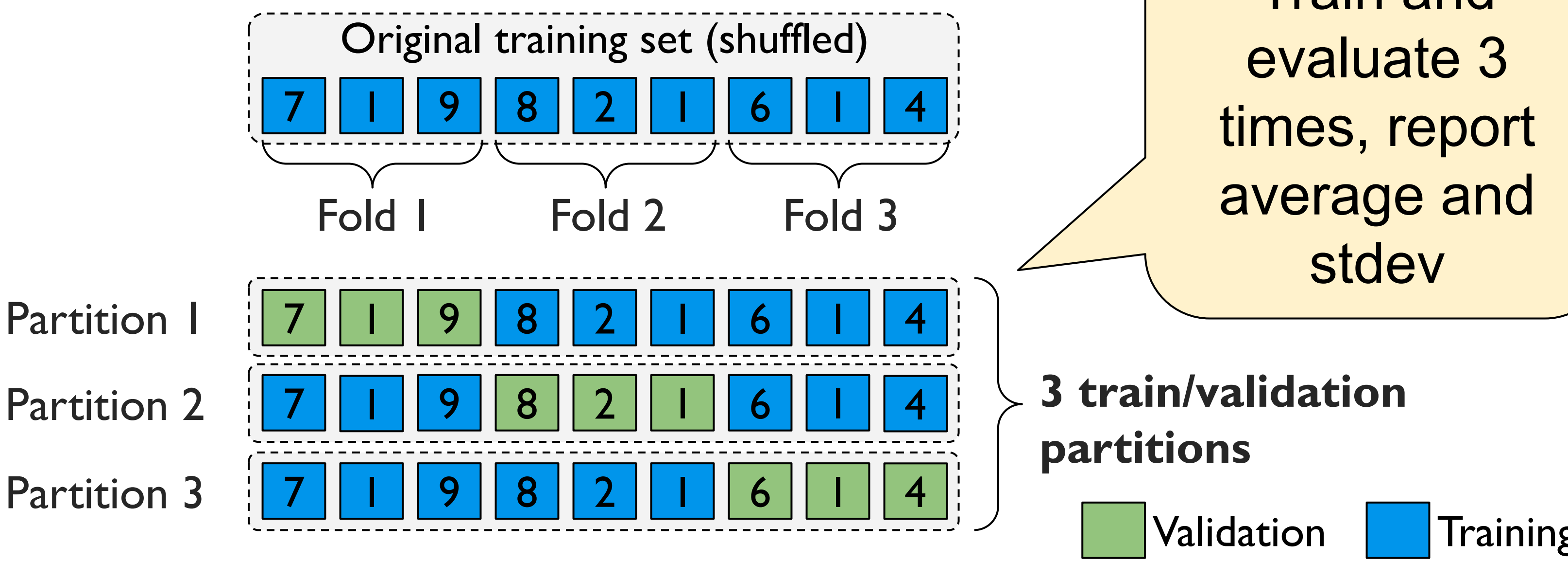
Cross-validation: use different portions of the training set to train and to evaluate the

Several approaches:

- **k-fold cross-validation**: split the ... nerate 1 partition per fold
- Example: 3-fold cross-validation

Number of partitions and training/validation operations = K

Train and evaluate 3 times, report average and stdev



ML Process - Dataset splitting

Key takeaways

- Training Set: part of the dataset used to train the model
- Validation Set: part of the dataset used to evaluate the model when searching for the best model or best set of hyperparameters
- Test set: part of the dataset set aside for final model evaluation. Ideally, should be used only once!
- Cross-validation: resampling method that uses different portions of the training set to train and evaluate models on different iterations
  - k-fold cross-validation: split the data in K folds and generate k partitions - each one using a different fold for validation and the remaining ones for training

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Machine Learning Overview

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