Linear regression

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Recap

1. ML and AI overview
2. Thesaurus and notation
   a. Dataset, observation, feature, target, design matrix
   b. i.i.d. property
   c. Model, prediction, loss/quality function
   d. Parameter, Hyperparameter
3. Maximum Likelihood Estimation
4. Some Machine Learning problems
   a. Classification
   b. Regression
   c. Dimensionality reduction
5. Naïve Bayes classifier
6. k Nearest Neighbours (kNN)

Outline

1. Linear models overview
2. Linear regression solution
3. Gauss-Markov theorem
4. Regularizations
5. Model validation and evaluation

Linear models overview

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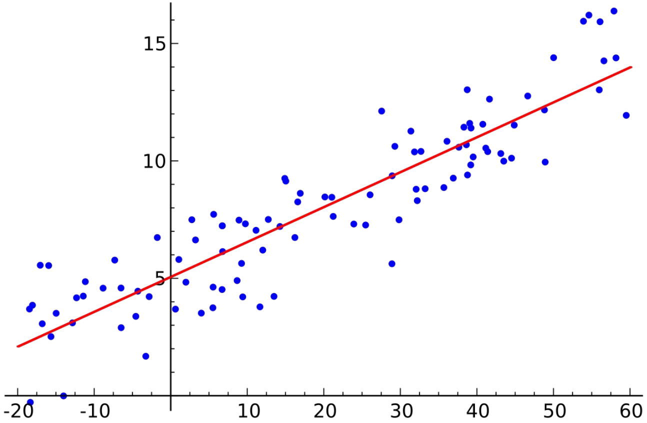
Linear models

$$Y = X_1 + X_2 + X_3$$

Dependent Variable	Independent Variable
Outcome Variable	Predictor Variable
Response Variable	Explanatory Variable

Linear models

- Regression models



Estimated (or predicted) Y value for observation i

Estimate of the regression intercept

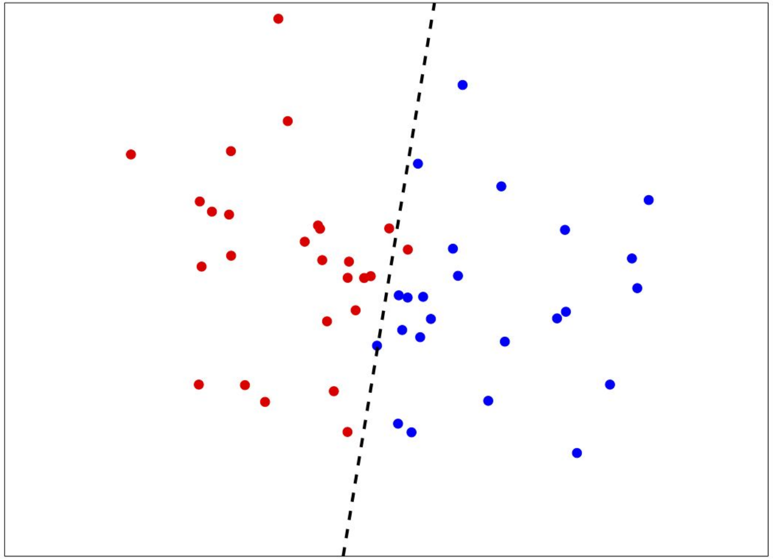
Estimate of the regression slope

Value of X for observation i

$$\hat{Y}_i = b_0 + b_1 X_i$$

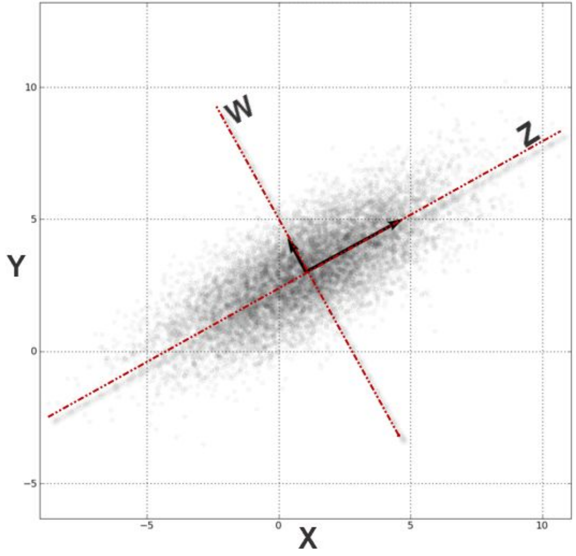
Linear models

- Regression models
- Classification models



Linear models

- Regression models
- Classification models
- Unsupervised models (e.g. PCA)



Linear models

- Regression models
- Classification models
- Unsupervised models (e.g. PCA)
- Building block of other models (ensembles, NNs, etc.)

Linear regression

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Linear regression

Linear regression problem statement:

- Dataset $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, where $\mathbf{x}_i \in \mathbb{R}^n, \quad y_i \in \mathbb{R}$.

Linear regression

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- The model is linear:

$$\hat{y} = w_0 + \sum_{k=1}^{p} x_k \cdot w_k = //\mathbf{x} = [1, x_1, x_2, \ldots, x_p]// = \mathbf{x}^T \mathbf{w}$$

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we added an additional column of 1's to the design matrix to simplify the formulas

Linear regression

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- Least squares method (MSE minimization) provides a solution:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|Y - \hat{Y}\|_2^2 = \arg\min_{\mathbf{w}} \|Y - X\mathbf{w}\|_2^2$$

Analytical solution

Denote quadratic loss function:

$$Q(\mathbf{w}) = (Y - X\mathbf{w})^T(Y - X\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2 \,,$$

where $X = [\mathbf{x}_1, \dots, \mathbf{x}_n], \quad \mathbf{x}_i \in \mathbb{R}^p \; Y = [y_1, \dots, y_n], \quad y_i \in \mathbb{R}$.

To find optimal solution let's equal to zero the derivative of the equation above:

$$\nabla_{\mathbf{w}} Q(\mathbf{w}) = \nabla_{\mathbf{w}}[Y^TY - Y^TX\mathbf{w} - \mathbf{w}^TX^TY + \mathbf{w}^TX^TX\mathbf{w}] =$$

$$= 0 - X^TY - X^TY + (X^TX + X^TX)\mathbf{w} = 0$$

$$\hat{\mathbf{w}} = \boxed{(X^TX)}^{-1}X^TY$$

what if this matrix is singular?

Analytical solution

$$\hat{\mathbf{w}} = \boxed{(X^T X)}^{-1} X^T Y$$

what if this matrix is singular?

Gauss-Markov theorem

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Gauss-Markov theorem

Suppose target values are expressed in following form:

$Y = X\mathbf{w} + \boldsymbol{\varepsilon}$, where $\boldsymbol{\varepsilon} = [\varepsilon_1, \ldots, \varepsilon_N]$ are random variables

Gauss–Markov assumptions:

- $\mathbb{E}(\varepsilon_i) = 0 \quad \forall i$
- $\mathrm{Var}(\varepsilon_i) = \sigma^2 < \inf \quad \forall i$
- $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0 \quad \forall i \neq j$

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$$\boxed{\hat{\mathbf{w}} = (X^T X)^{-1} X^T Y}$$

delivers **B**est **L**inear **U**nbiased **E**stimator

Regularizations

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Unstable solution

In case of multicollinear features the matrix $X^T X$ is almost singular .

It leads to unstable solution:

```
w_true
```

```
array([ 2.68647887, -0.52184084, -1.12776533])
```

```
w_star = np.linalg.inv(X.T.dot(X)).dot(X.T).dot(Y)
w_star
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corresponding features are almost collinear

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```

the coefficients are huge and sum up to almost 0

Regularization

To make the matrix nonsingular, we can add a diagonal matrix:

$$\hat{\mathbf{w}} = (X^T X + \lambda I)^{-1} X^T Y,$$

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where $I = \mathrm{diag}[1_1, \ldots, 1_p]$.

Actually, it's a solution for the following loss function:

$$Q(\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2 + \lambda^2 \|\mathbf{w}\|_2^2$$

exercise: derive it by yourself

Loss functions in regression

$$MSE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N}\|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \frac{1}{N}\sum_i (y_i - \hat{y}_i)^2$$

$$MAE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N}\|\mathbf{y} - \hat{\mathbf{y}}\|_1 = \frac{1}{N}\sum_i |y_i - \hat{y}_i|$$

Different norms

Once more: loss functions:

$$\boxed{MSE = \frac{1}{n}\|\mathbf{x}^T\mathbf{w} - \mathbf{y}\|_2^2}$$

only works for Gauss-Markov theorem

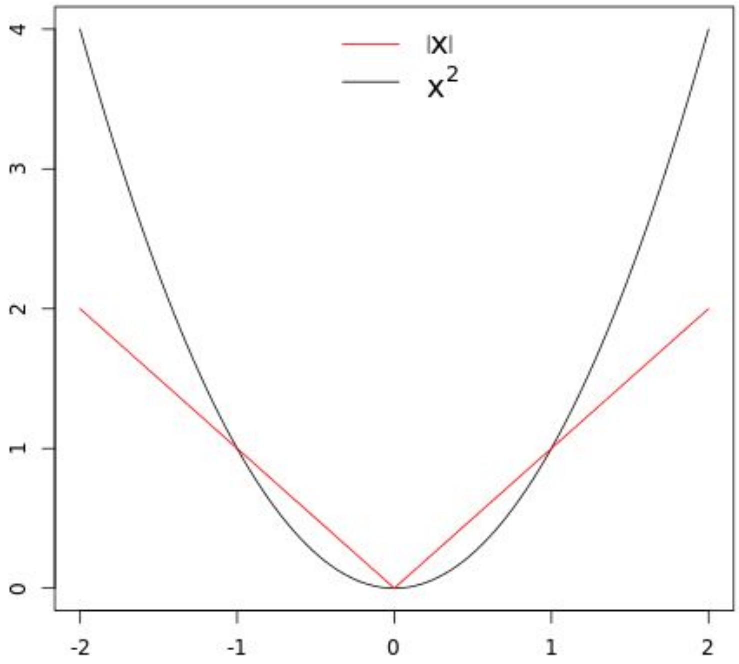
$$MAE = \frac{1}{n}\|\mathbf{x}^T\mathbf{w} - \mathbf{y}\|_1$$

Regularization terms:

- L2 $\|\mathbf{w}\|_2^2$
- L1 $\|\mathbf{w}\|_1$

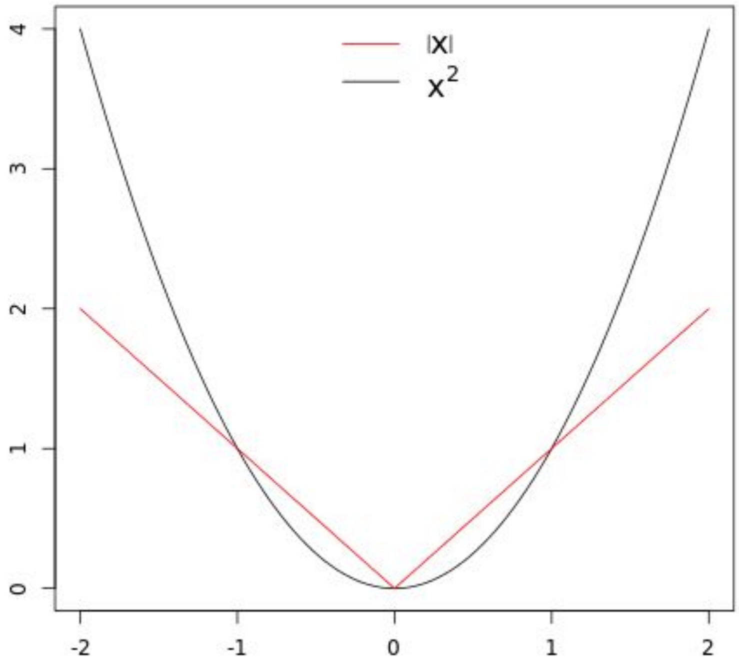
Loss function properties

- MSE (L_2)
  - delivers BLUE according to Gauss-Markov theorem
  - differentiable
  - sensitive to noise
- MAE (L_1)
  - non-differentiable
    - not a problem
  - much more prone to noise

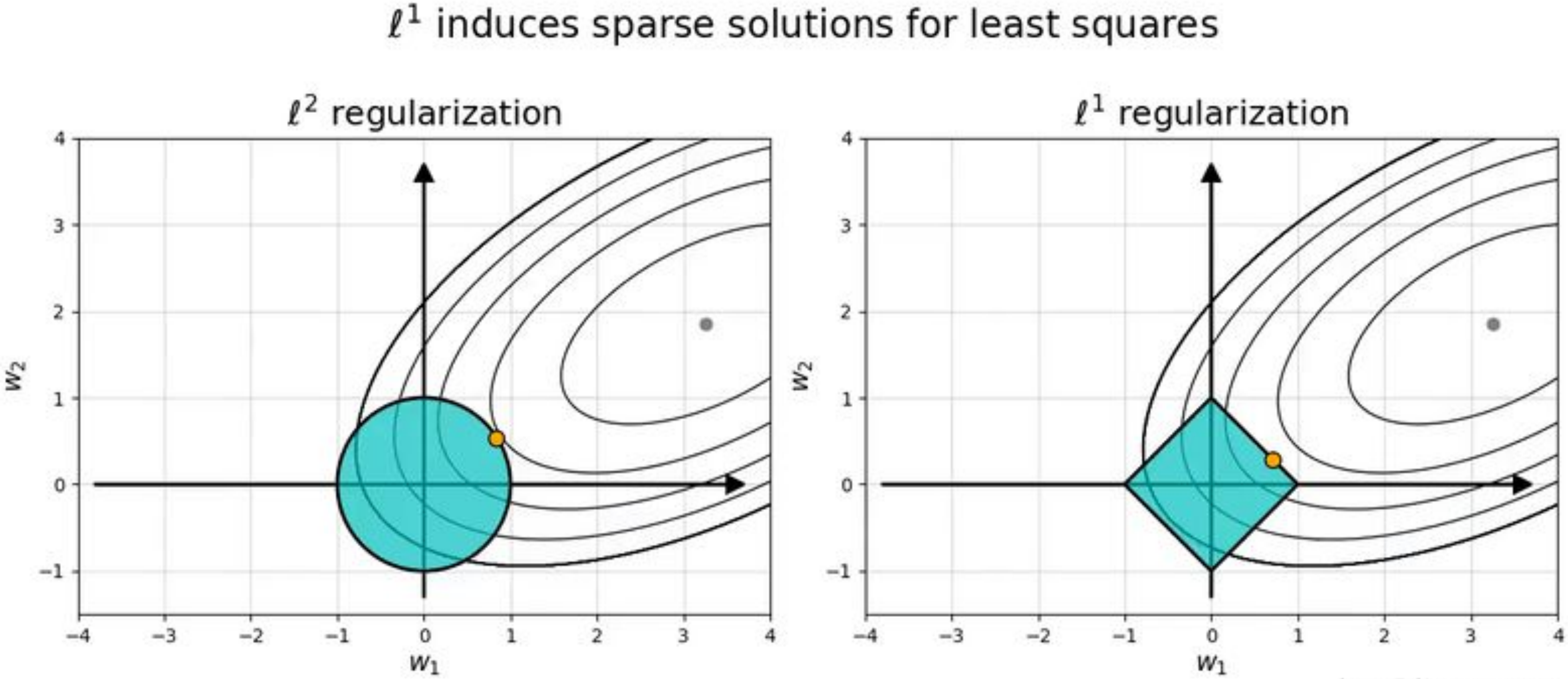


Regularization properties

- L_2 regularization
  - constraints weights
  - delivers more stable solution
  - differentiable
- L_1 regularization
  - non-differentiable
  - not a problem
  - selects features



L1 vs L2 regularization



Loss functions in regression

Other functions to measure the quality in regression:

- R2 score
- MAPE
- SMAPE
- …

Conclusion

- Linear models are simple yet quite effective models
- Regularization incorporates some prior assumptions/additional constraints

Model validation and evaluation

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Supervised learning problem statement

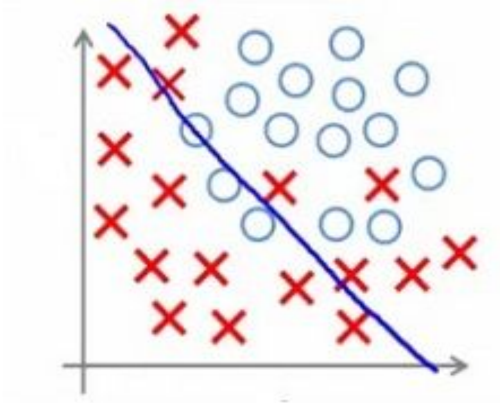
Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^n$, where
  - $(\mathbf{x} \in \mathbb{R}^p,\ y \in \mathbb{R}\ )$ for regression
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{+1, -1\}$ for binary classification

Model $f(\mathbf{x})$ predicts some value for every object

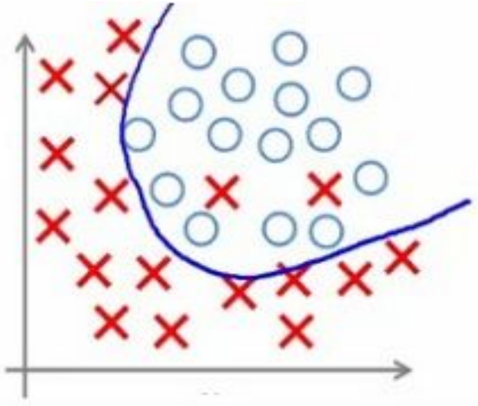
Loss function $Q(\mathbf{x}, y, f)$ that should be minimized

Overfitting vs. underfitting

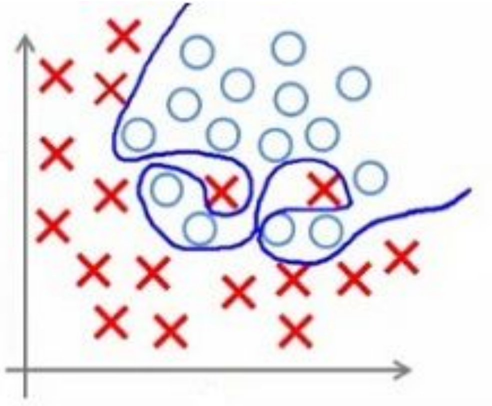


Under-fitting

(too simple to explain the variance)



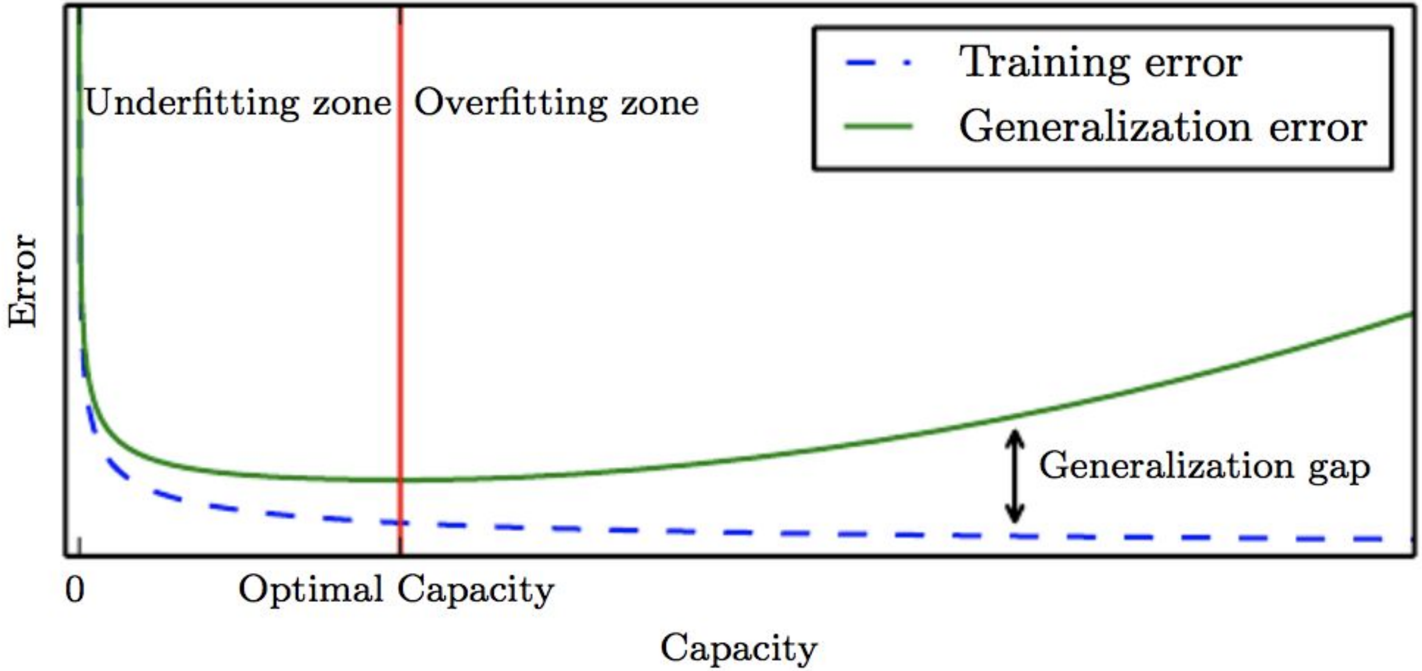
Appropriate-fitting



Over-fitting

(forcefitting -- too good to be true)

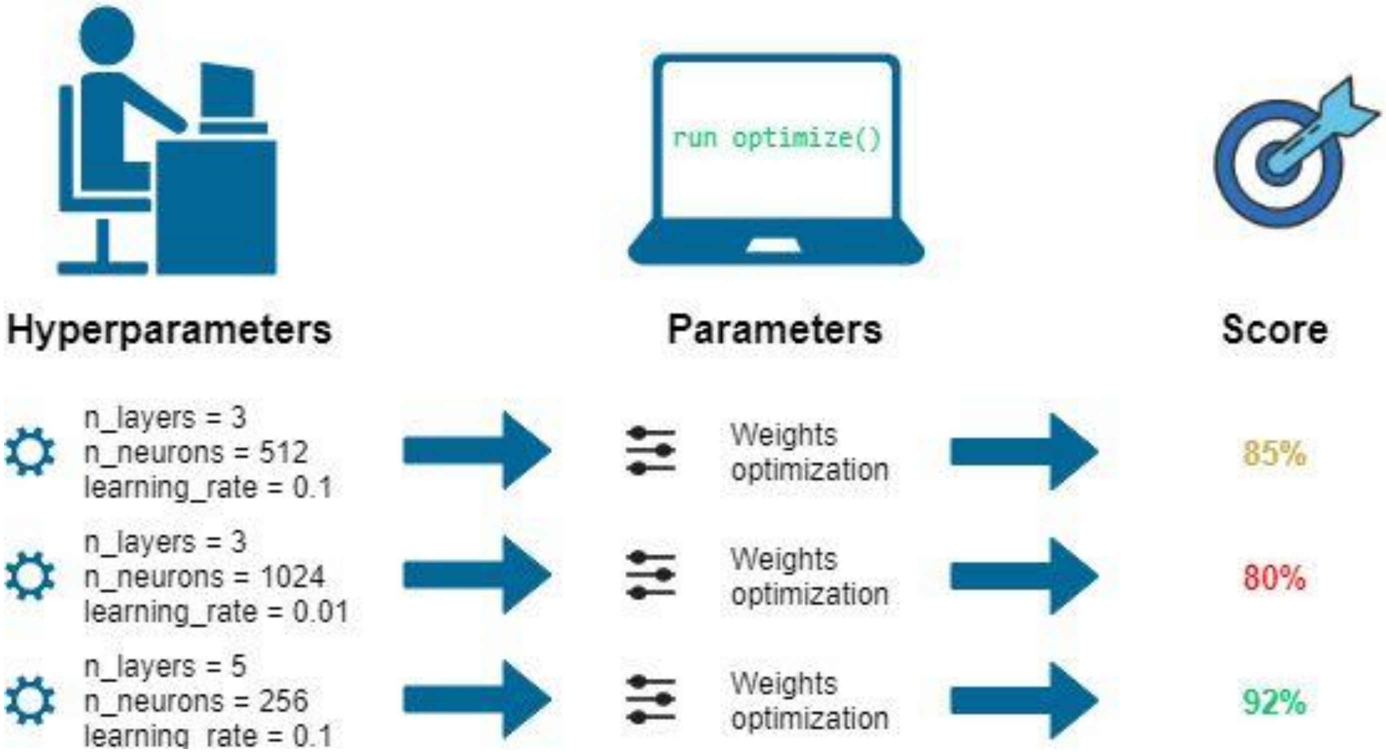
Overfitting vs. underfitting



Evaluating the quality

Is it good enough?

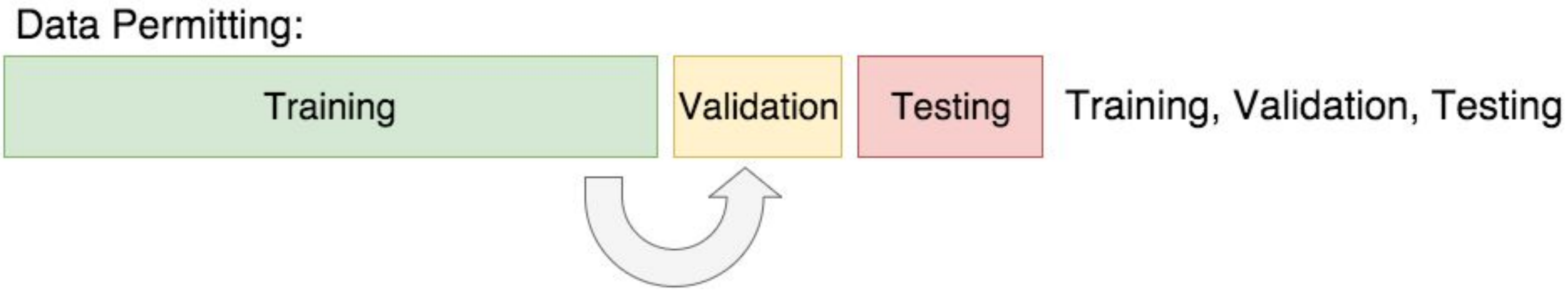
Parameters and hyperparameters



Comparison

	Defined by	Depend on the training data	Order of optimization methods	Required for	Affect the complexity of the model
Parameters	during the training	yes	first (gradient)	predictions	no
Hyperparameters	before the start of training	no	zero (manual, Bayesian)	training	yes

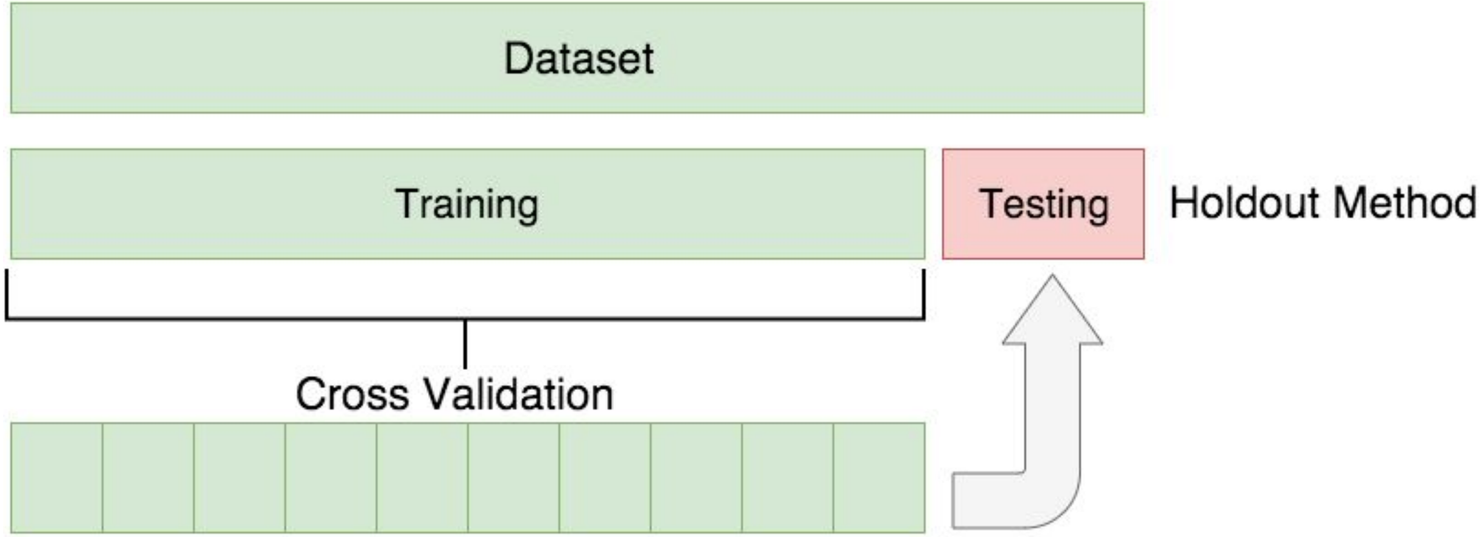
Dataset splits



Stages of model training

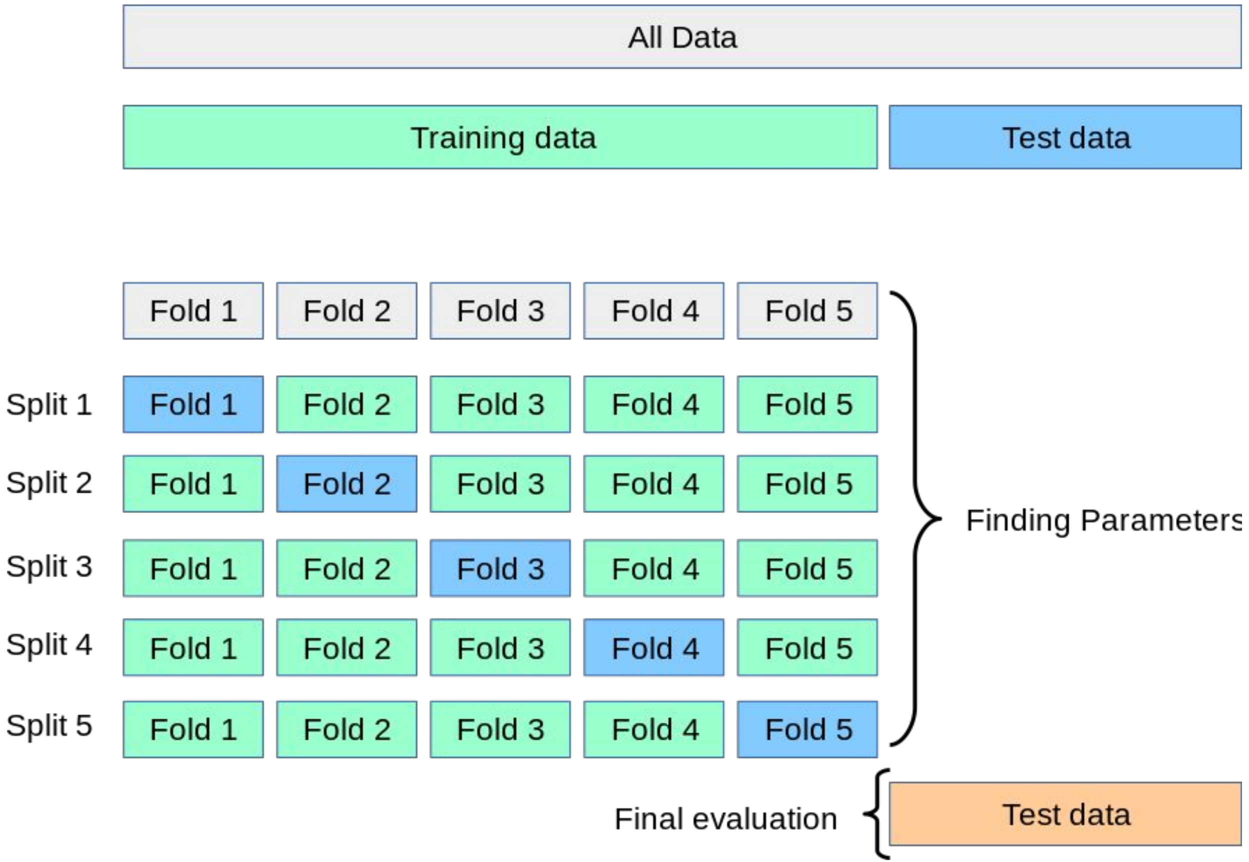
Split	training	validation	test
Used for	parameters optimization	hyperparameters selection	quality measurement
Overfitting level	high	average	low

Cross-validation

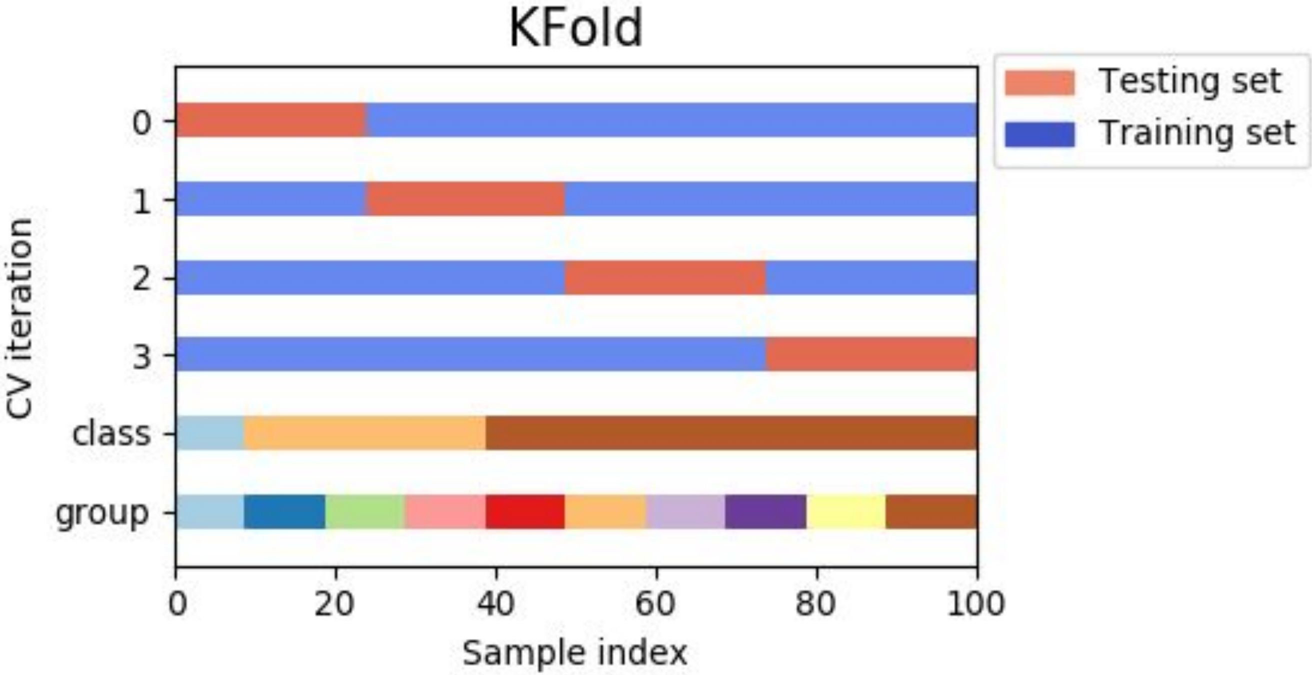


In real life is used only on **small datasets** (<10^4 samples)

Cross-validation

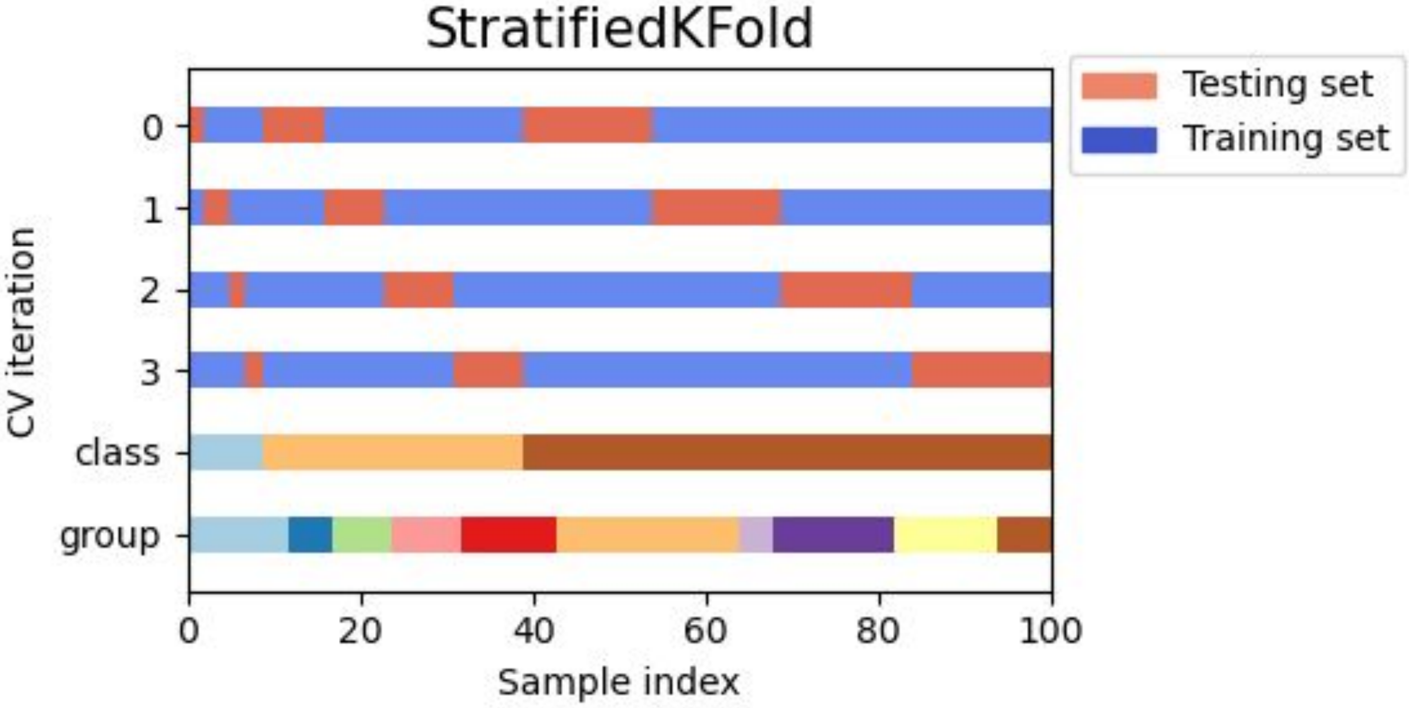


More validations



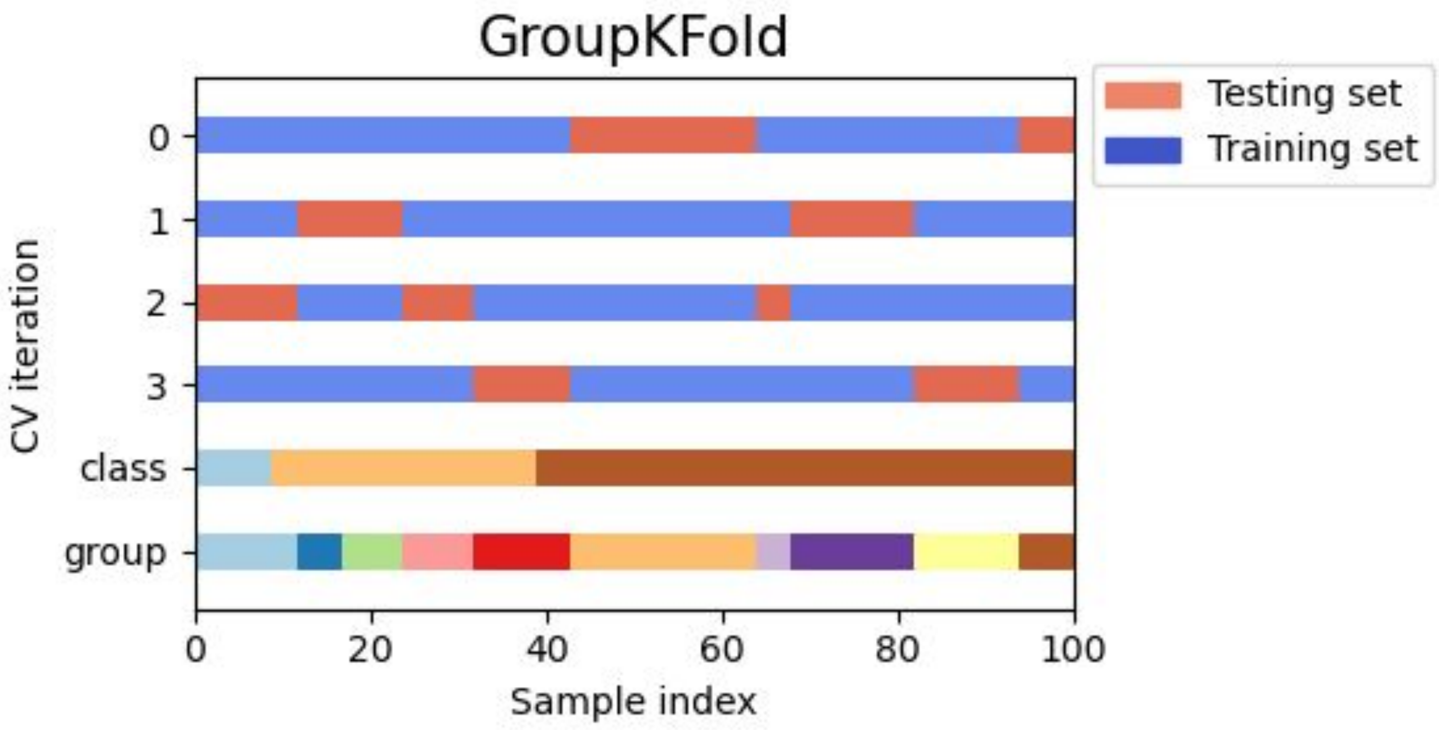
Special case: Leave One Out (LOO) - good for tiny datasets

More validations



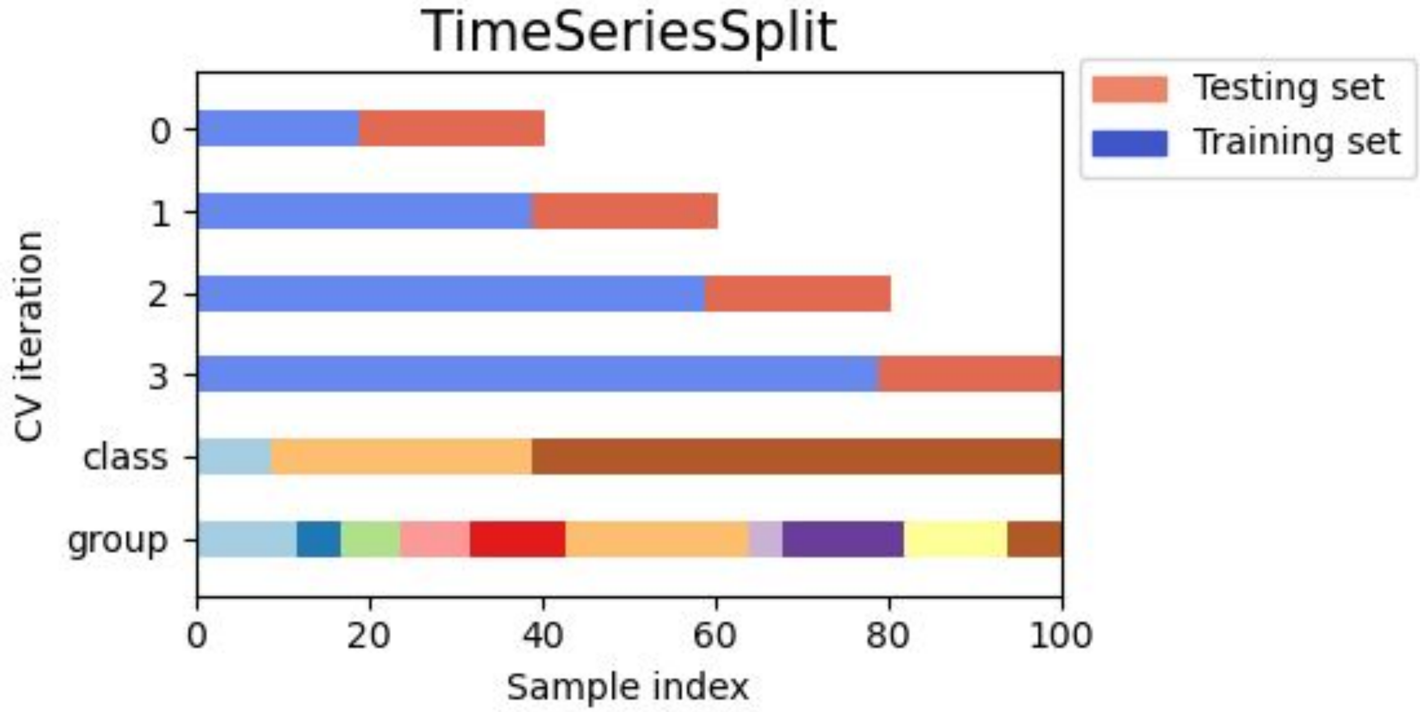
Preserve class ratio for each split. Default for sklearn methods

More validations



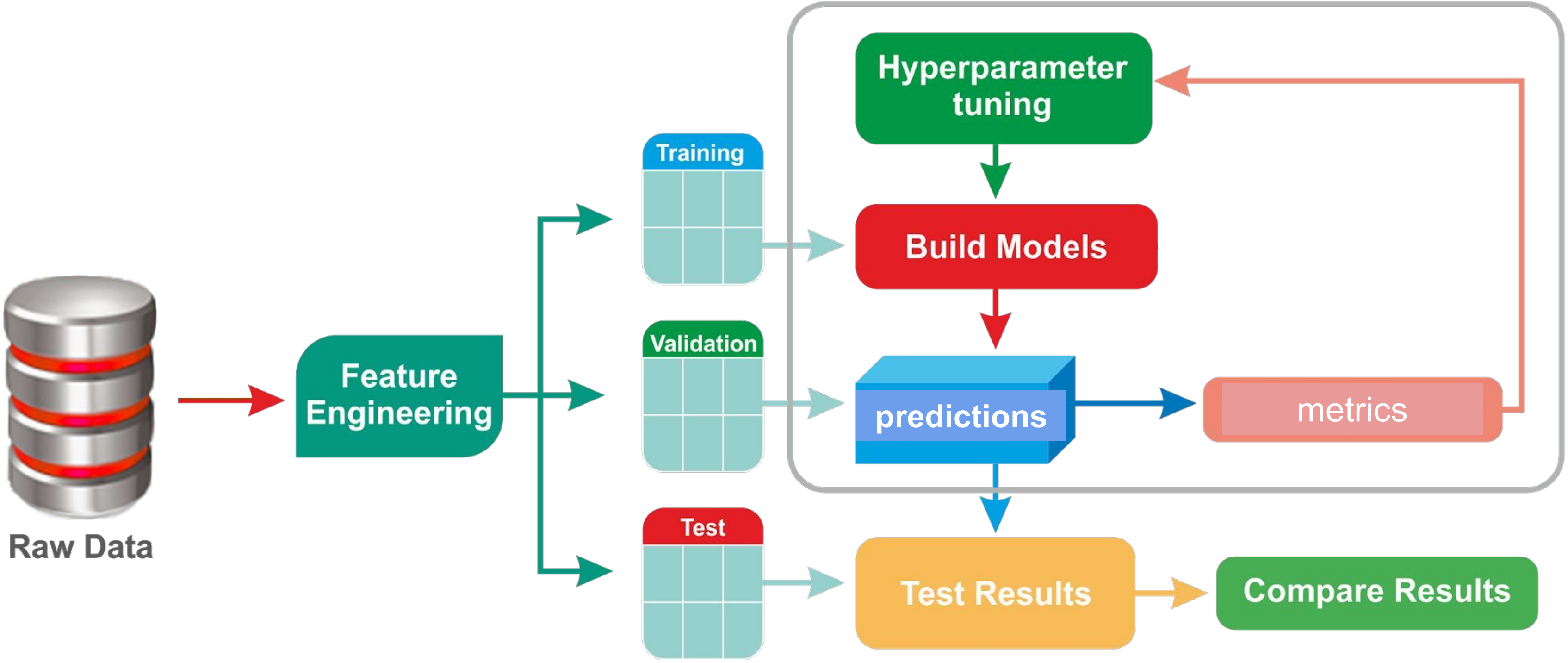
Set whole group either to train or validation

More validations



Never use train_test_split in this case!!!

Stages of model training



Revise

1. Linear models overview
2. Linear Regression under the hood
3. Gauss-Markov theorem
4. Regularization in Linear regression
5. Model validation and evaluation

Thanks for attention!

Questions?

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