

Linear regression

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YSDA, fall 2024

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

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



$$Y = X_1 + X_2 + X_3$$

The diagram illustrates the components of the linear model equation $Y = X_1 + X_2 + X_3$. A vertical arrow points from the variable Y down to the label 'Dependent Variable'. A horizontal bracket groups the variables X_1 , X_2 , and X_3 , with an arrow pointing from the center of the bracket down to the label 'Independent Variable'.

Dependent Variable

Independent Variable

Outcome Variable

Predictor Variable

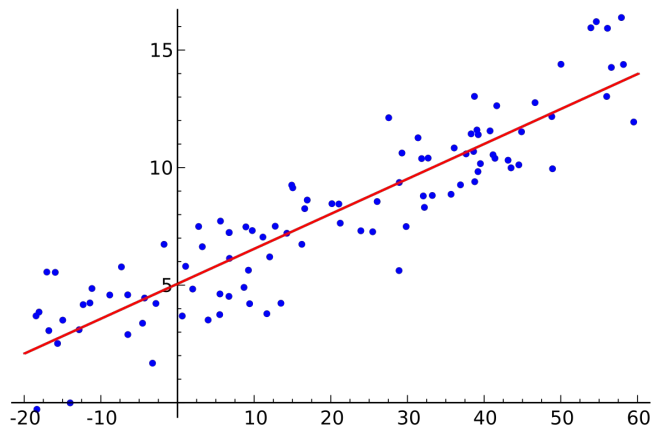
Response Variable

Explanatory Variable

Linear models



- Regression models



Estimated
(or predicted)
Y value for
observation i

Estimate of
the regression
intercept

Estimate of the
regression slope

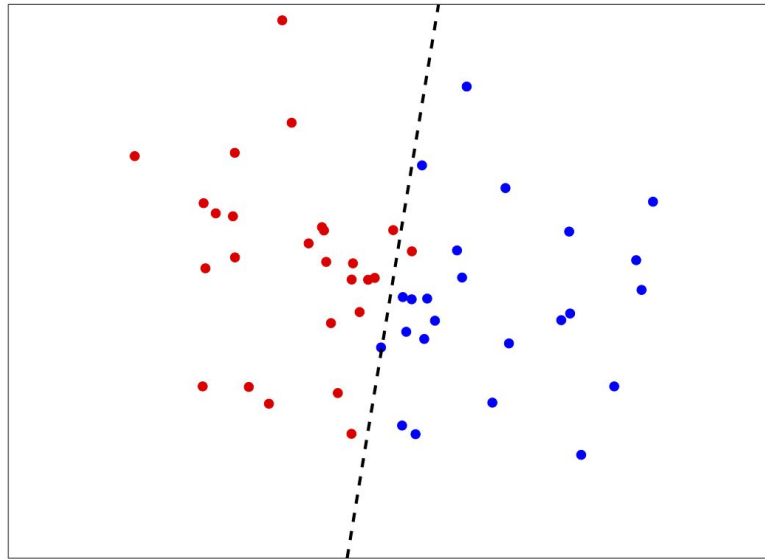
Value of X for
observation i

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

Linear models



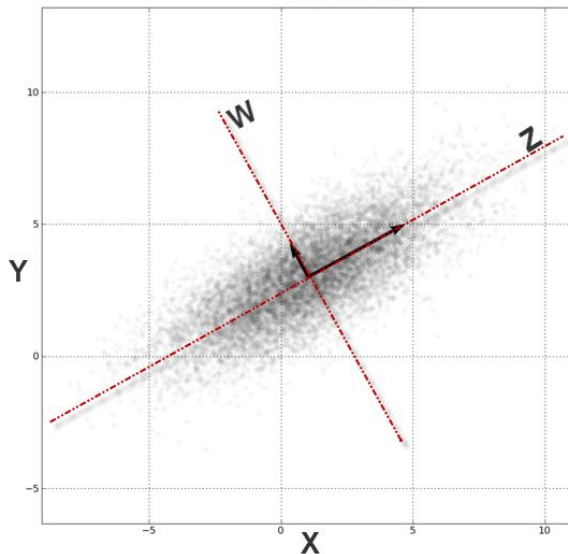
- Regression models
- Classification models



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 $\mathbf{x}_i \in \mathbb{R}^n$, $y_i \in \mathbb{R}$.



Linear regression

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- The model is linear:

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



Linear regression

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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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where $\mathbf{w} = (w_0, w_1, \dots, w_n)$, w_0 is bias term.

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

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

$$\begin{aligned}\nabla_{\mathbf{w}} Q(\mathbf{w}) &= \nabla_{\mathbf{w}} [Y^T Y - Y^T X \mathbf{w} - \mathbf{w}^T X^T Y + \mathbf{w}^T X^T X \mathbf{w}] = \\ &= 0 - X^T Y - X^T Y + (X^T X + X^T X) \mathbf{w} = 0\end{aligned}$$

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

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:

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

Gauss-Markov assumptions:

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



Gauss-Markov theorem

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

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
array([ 2.68027723, -186.0552577 , 184.41701118])
```

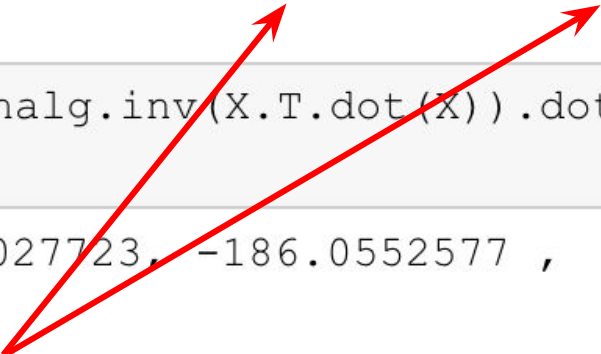


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```



corresponding features are almost collinear



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w_star  
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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:

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

Regularization



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Regularization

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

where $I = \text{diag}[1_1, \dots, 1_p]$.

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:

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

only works for Gauss-Markov theorem

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

Regularization terms:

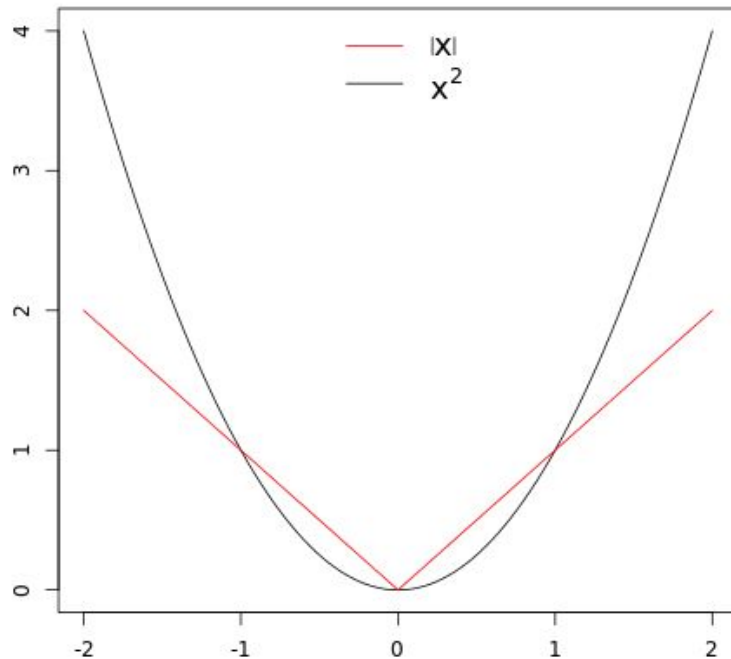
- $L_2 \quad \|\mathbf{w}\|_2^2$

- $L_1 \quad \|\mathbf{w}\|_1$

Loss function properties



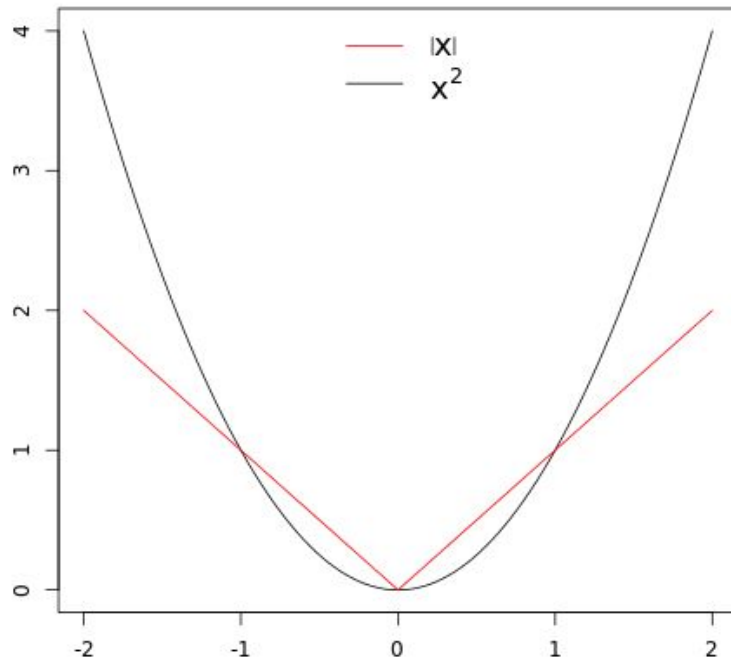
- MSE (L_2)
 - delivers BLUE according to Gauss-Markov theorem
 - differentiable
 - sensitive to noise
- MAE (L_1)
 - non-differentiable
 - not a problem
 - much more prone to noise



Regularization properties



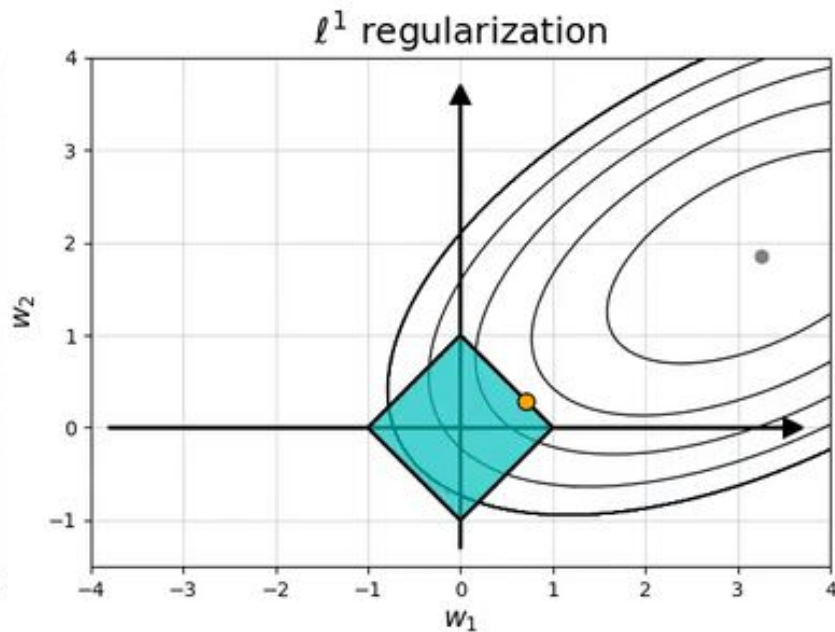
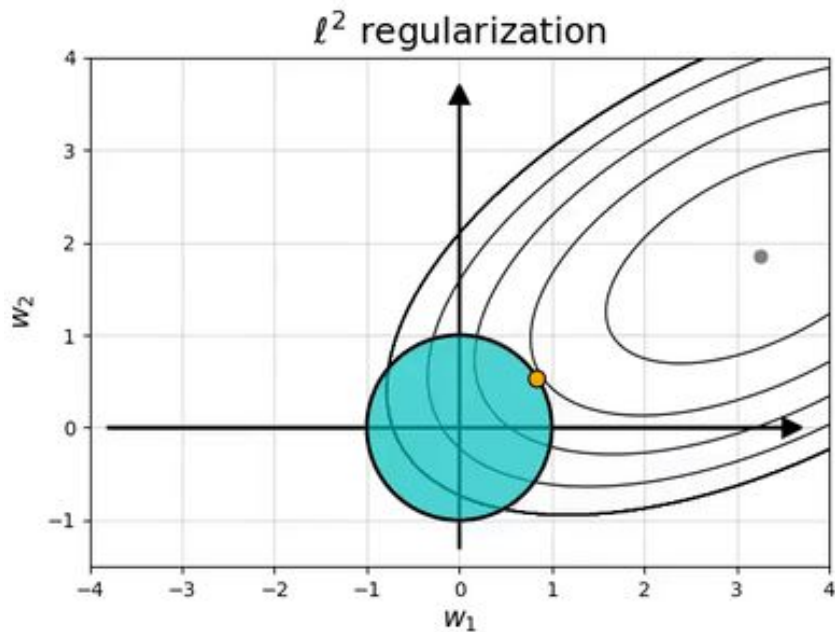
- L2 regularization
 - constraints weights
 - delivers more stable solution
 - differentiable
- L1 regularization
 - non-differentiable
 - not a problem
 - selects features



L1 vs L2 regularization



ℓ^1 induces sparse solutions for least squares



Loss functions in regression



Other functions to measure the quality in regression:

- R^2 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

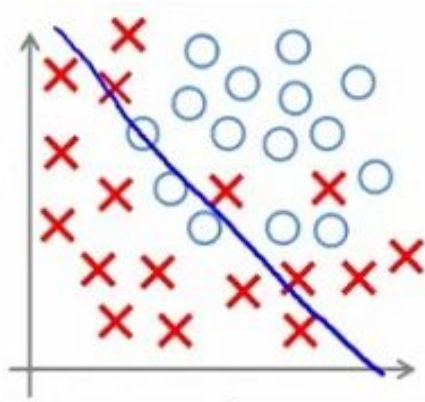
Let's denote:

- 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

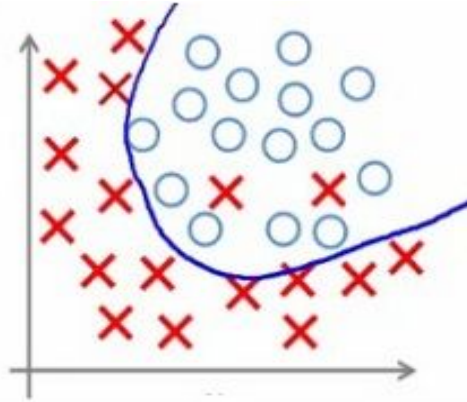
Loss function $Q(\mathbf{x}, y, f)$ that should be minimized

Overfitting vs. underfitting

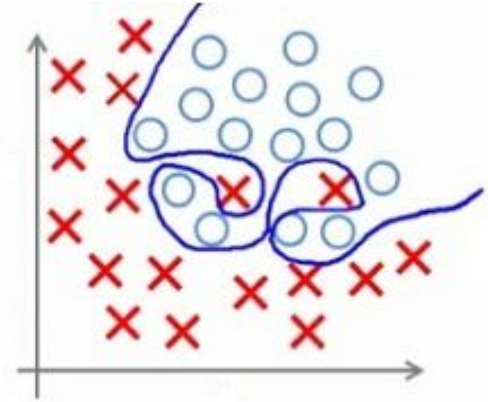


Under-fitting

(too simple to
explain the
variance)



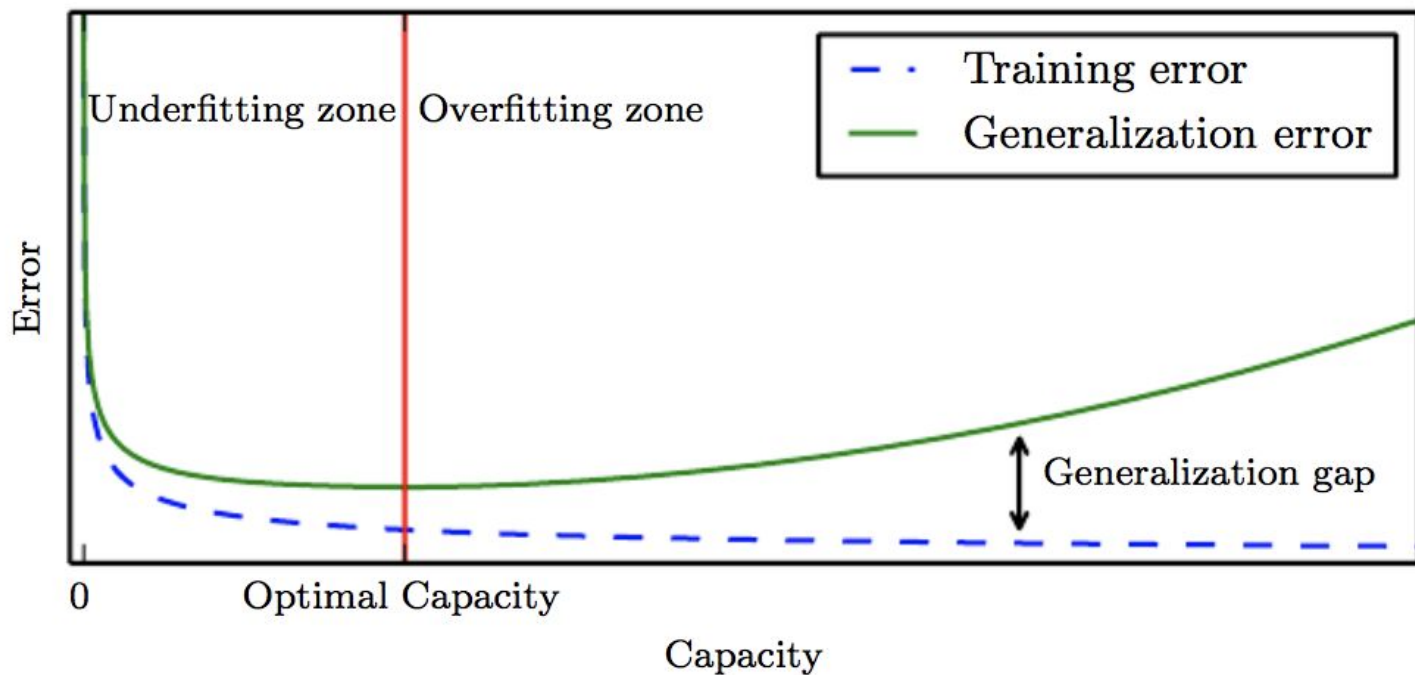
Appropriate-fitting



Over-fitting

(forcefitting -- too
good to be true)

Overfitting vs. underfitting



Evaluating the quality



Dataset

Training

Testing

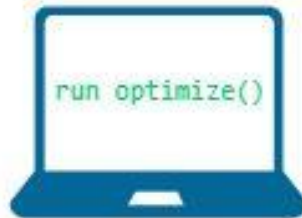
Holdout Method

Is it good enough?

Parameters and hyperparameters



Hyperparameters



Parameters



Score



Comparison

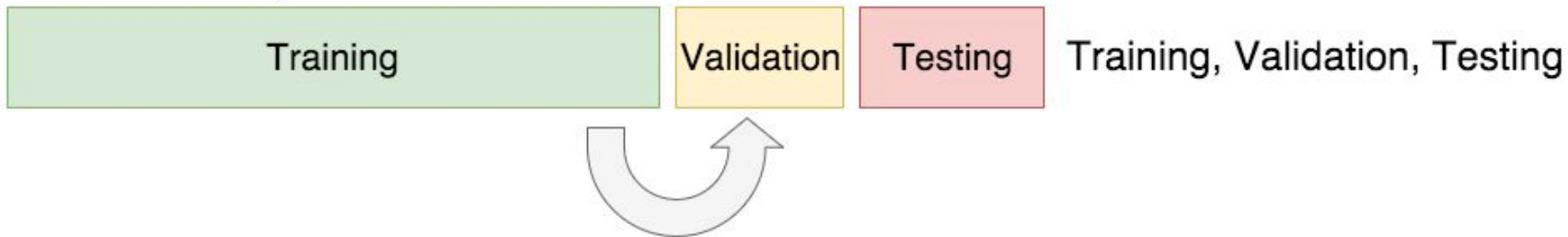


	Defined by	Depend on the training data	Order of optimization methods	Required for	Affect the complexity of the model
Parameters	during the training	yes	first (gradient)	predictions	no
Hyperparameters	before the start of training	no	zero (manual, Bayesian)	training	yes

Dataset splits



Data Permitting:



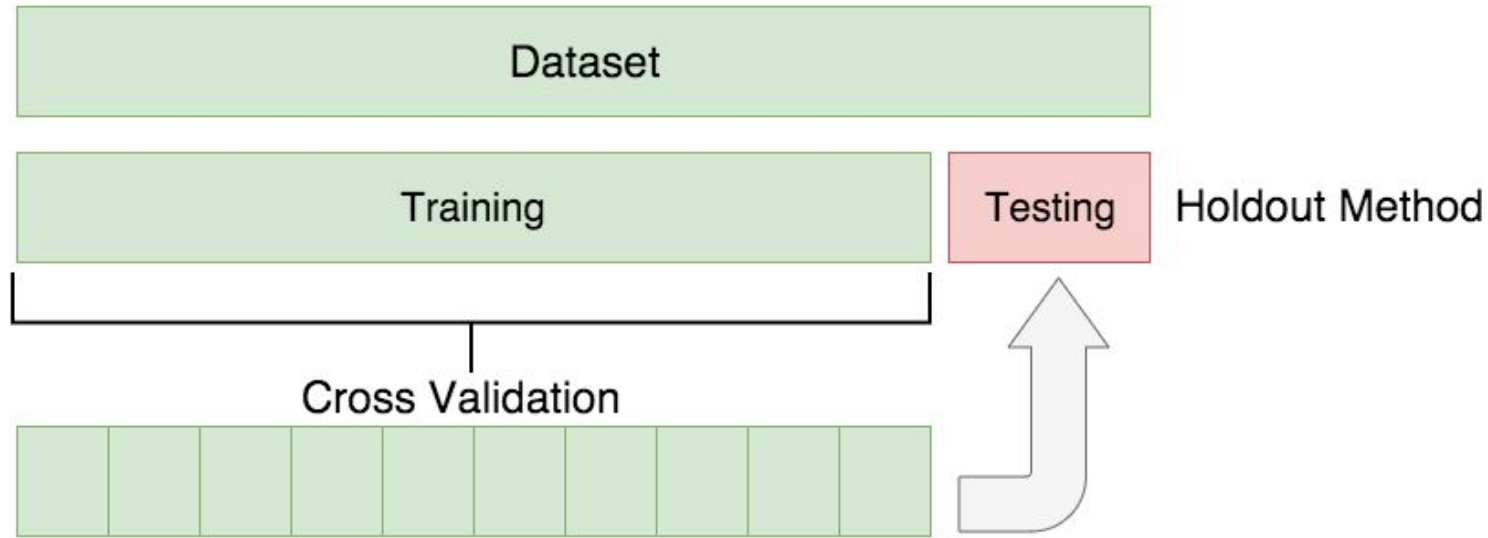
Stages of model training



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

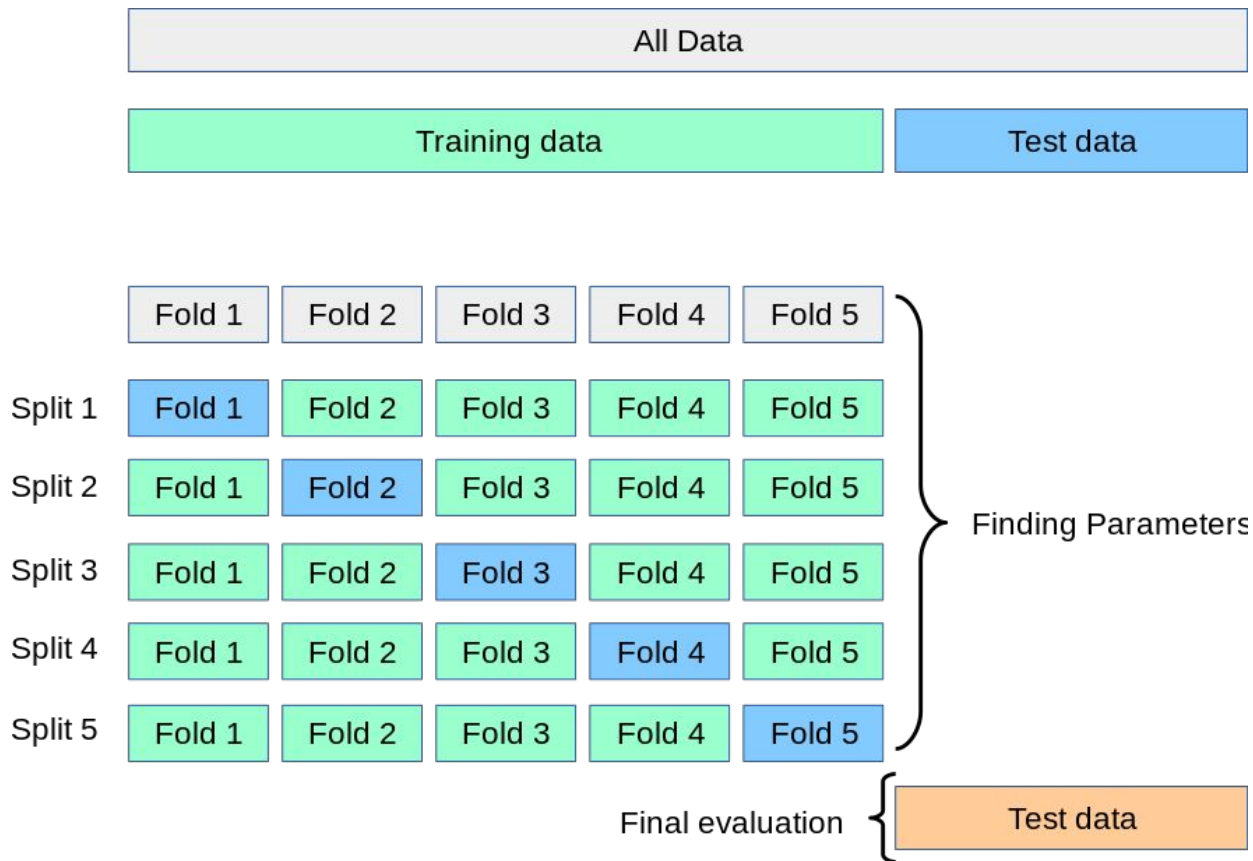


Cross-validation

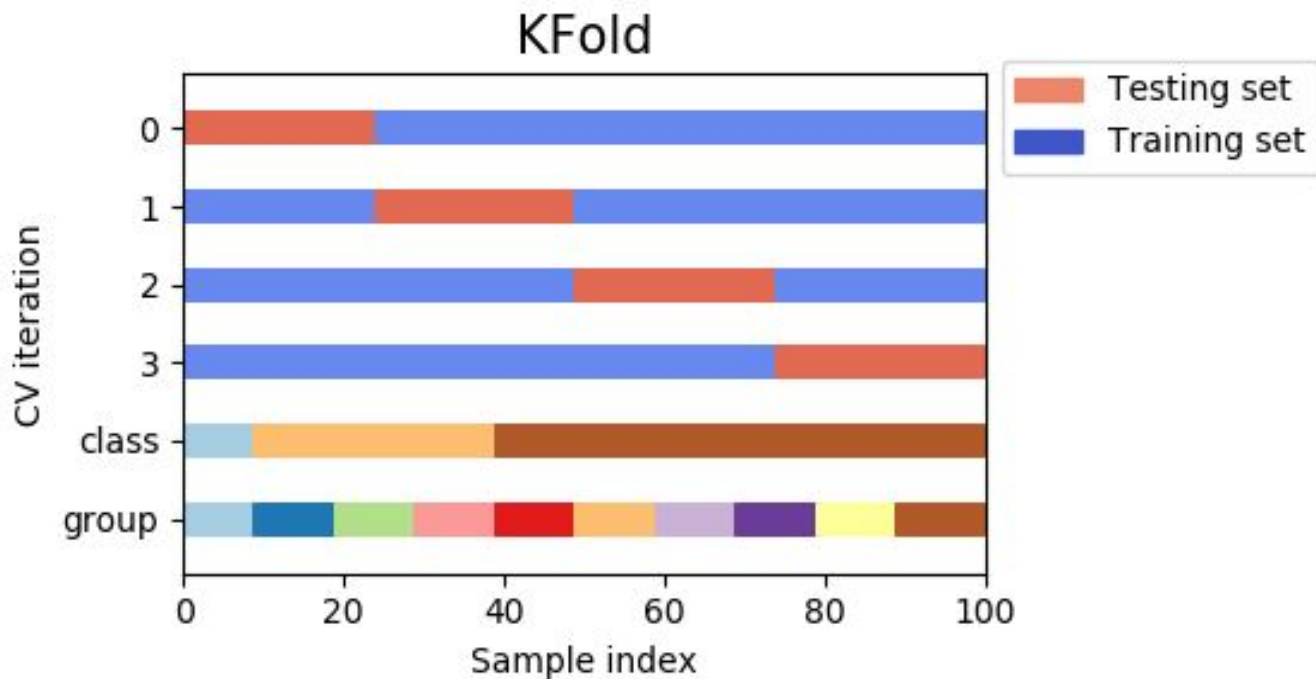


In real life is used only on **small datasets** ($<10^4$ samples)

Cross-validation

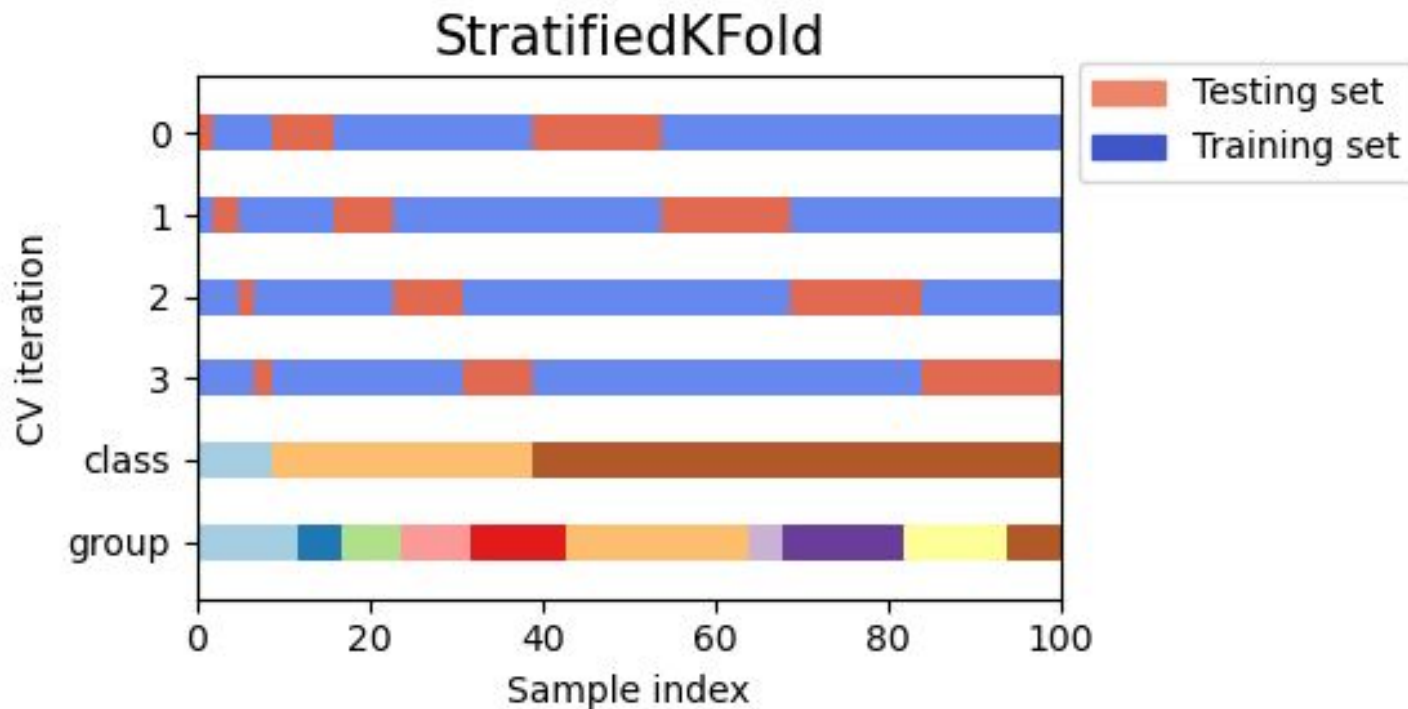


More validations



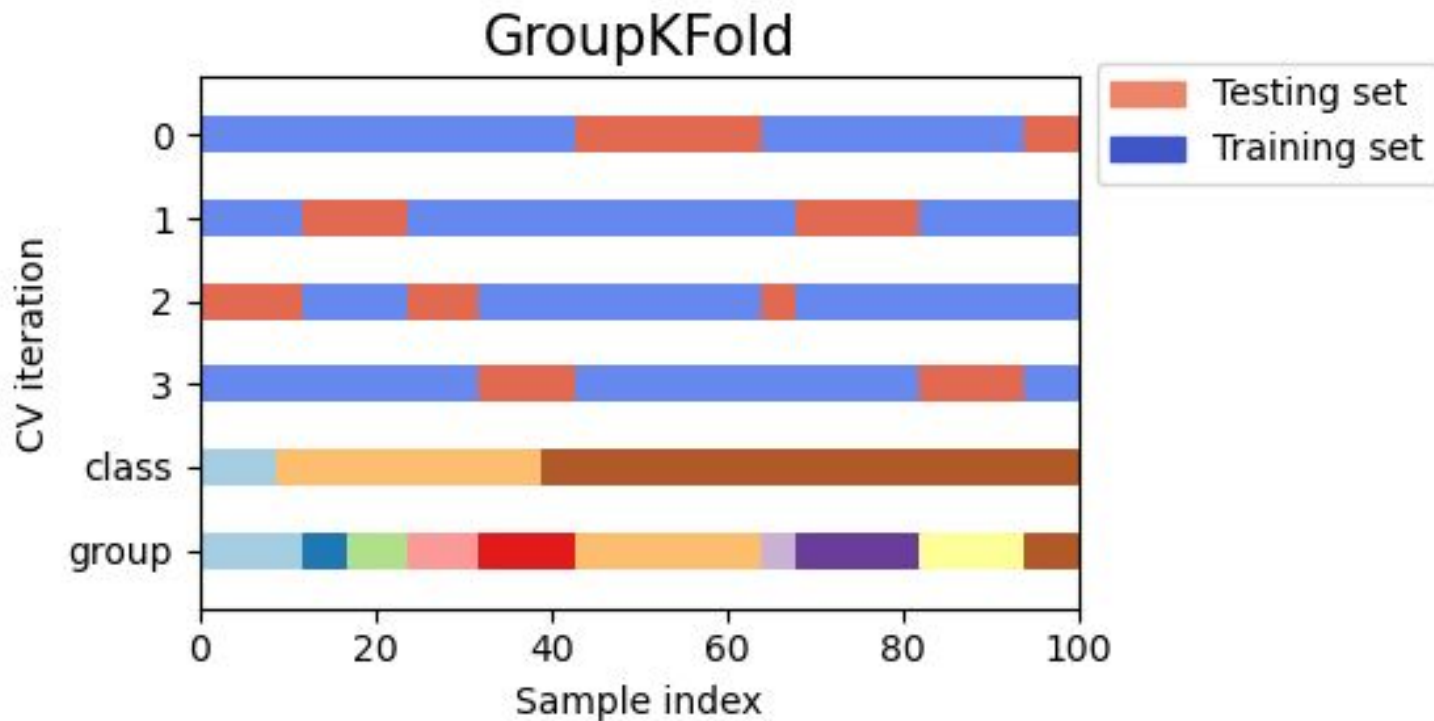
Special case: Leave One Out (LOO) - good for tiny datasets

More validations



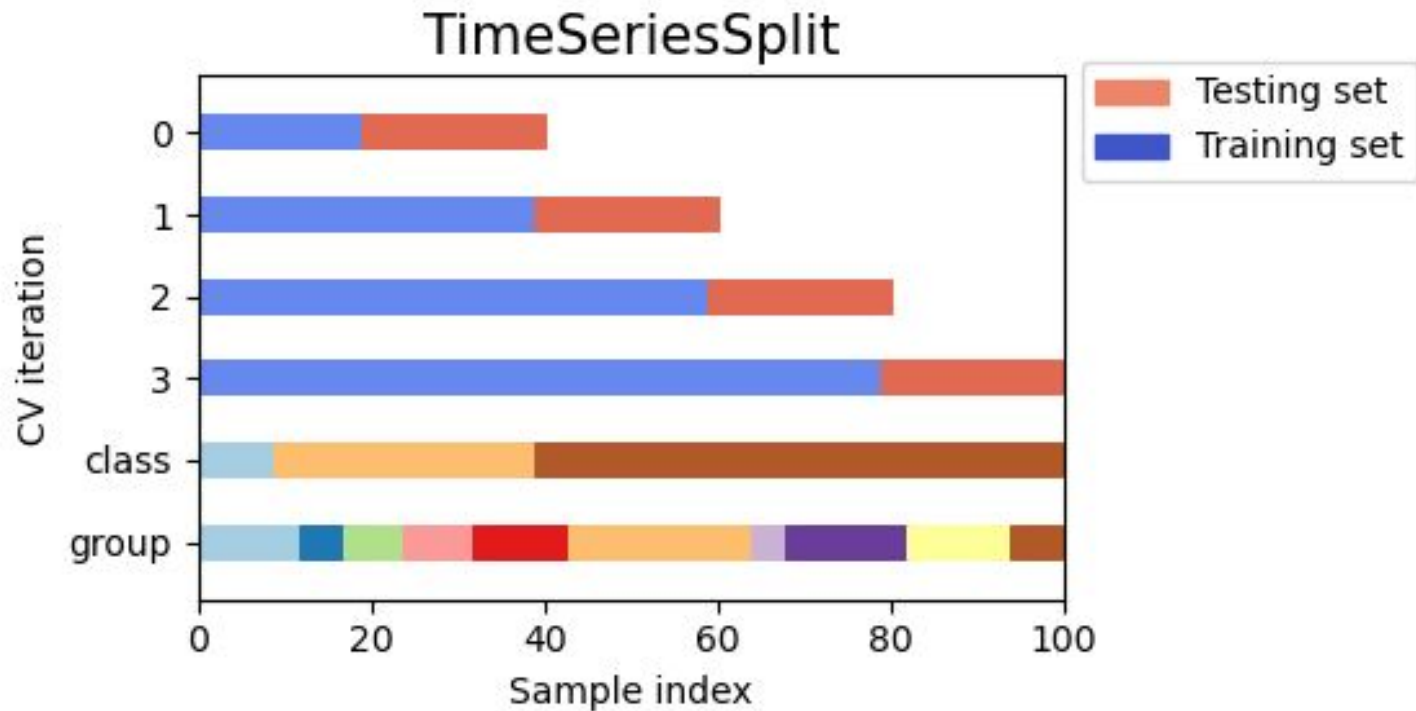
Preserve class ratio for each split. Default for sklearn methods

More validations



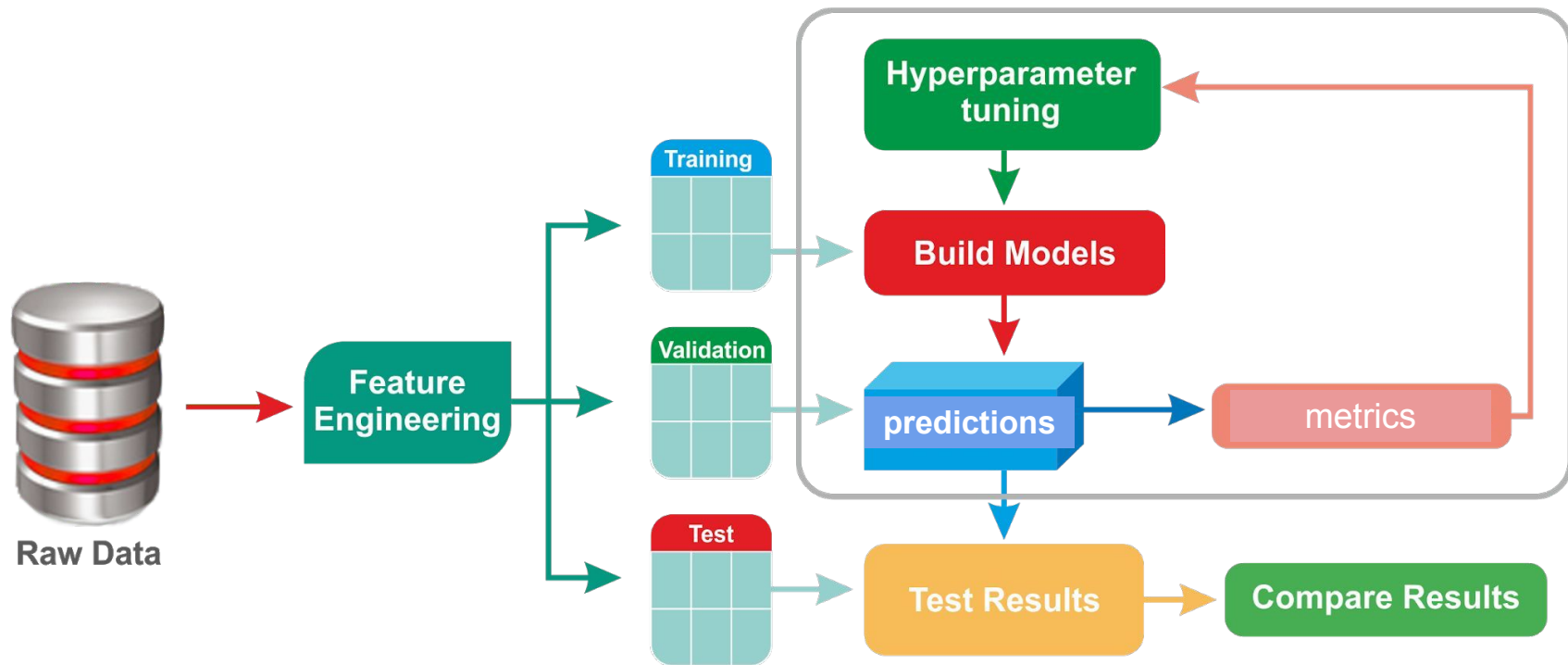
Set whole group either to train or validation

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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