Data Science 1

STAT/CS 287

Jim Bagrow, UVM Dept of Math and Statistics

LECTURE 18

Today

More on predictive models (*supervised learning*)

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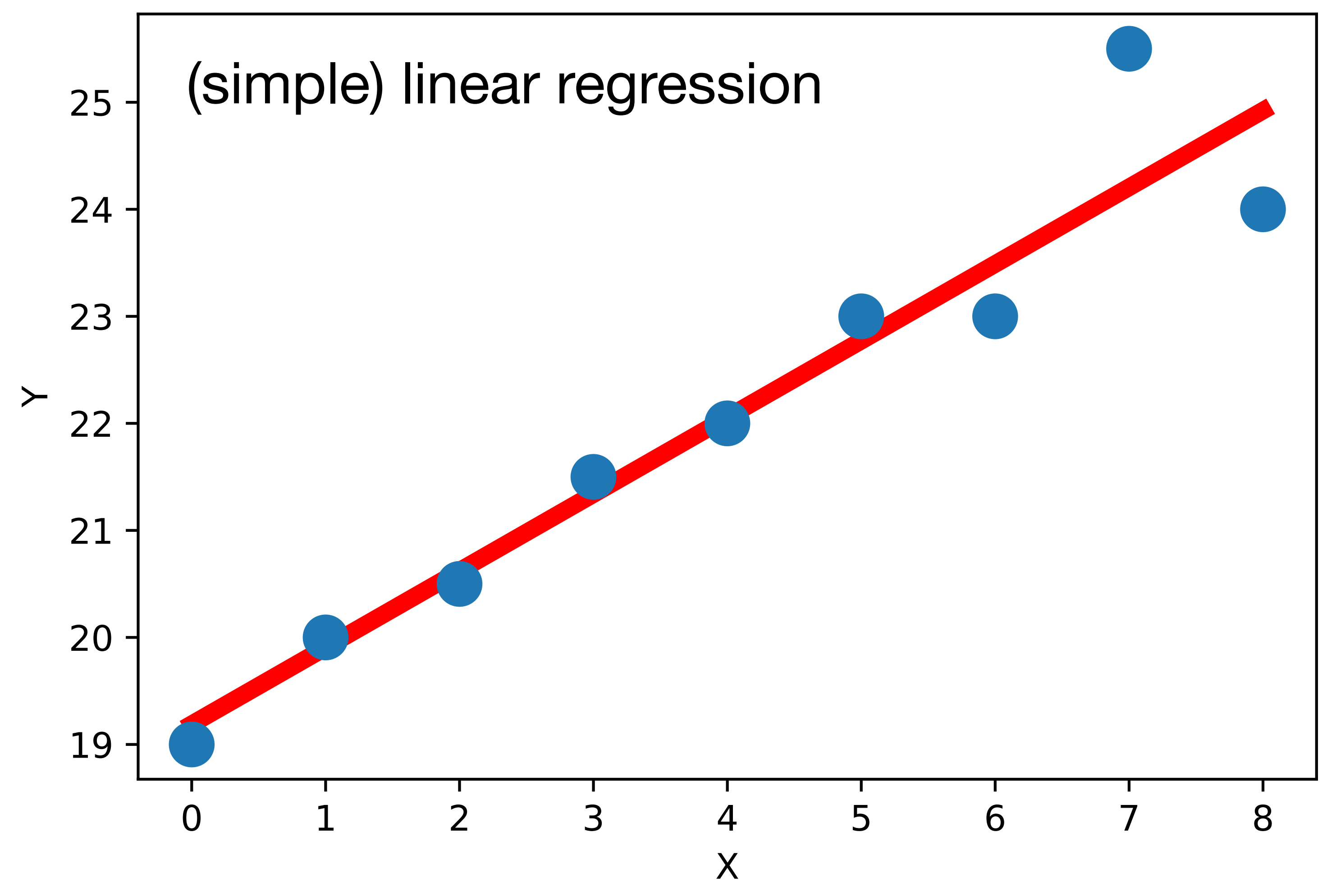
Prediction vs. Inference → Linear Regression

Prediction

new x comes in, predict y using $y = f(x) = \beta_0 + \beta_1 x$



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learn how changing x changes y by examining β's

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                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.999
Model:                            OLS   Adj. R-squared:                  0.999
Method:                 Least Squares   F-statistic:                 5.849e+04
Date:                Thu, 31 Oct 2019   Prob (F-statistic):          3.44e-150
Time:                        10:25:51   Log-Likelihood:                 153.19
No. Observations:                 100   AIC:                            -300.4
Df Residuals:                      97   BIC:                            -292.6
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          0.9926      0.016     60.925      0.000       0.960       1.025
x1             0.0562      2.517      0.022      0.982      -4.939       5.051
x2             0.5034      0.198      2.539      0.013       0.110       0.897
==============================================================================
Omnibus:                        4.957   Durbin-Watson:                   1.903
Prob(Omnibus):                  0.084   Jarque-Bera (JB):                2.704
Skew:                           0.153   Prob(JB):                        0.259
Kurtosis:                       2.255   Cond. No.                     3.53e+03
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```

Recall

Natural Language Processing Tasks & Semantic Similarity

Supervised Learning — Classifiers

Documents and labels:

$$\begin{array}{c c} & \text{— \# unique words (types) —} \\ \text{— \# documents —} & \underbrace{\begin{bmatrix} 0\ 0\ 0\ 7\ 3\ 0\ 0\ 1 \cdots 0\ 5\ 0\ 0\ 0 \\ \vdots \quad \ddots \qquad\qquad \vdots \\ \\ \\ \end{bmatrix}}_{X} \end{array} \qquad \underbrace{\begin{bmatrix} \text{spam} \\ \text{spam} \\ \vdots \\ \text{spam} \\ \text{ham} \\ \vdots \\ \text{ham} \end{bmatrix}}_{y}$$

— Labels vector

— Training data

$$y = f(X)$$

A new, unlabeled document comes in:

built a machine $\hat{f}$ to predict label given count vector —

$$\hat{f}([\,0\ 0\ 0\ 2\ 6\ 3\ 0\ 5 \cdots 0\ 0\ 11\ 0\ 0\,]) =$$

$$\arg\max\,[\Pr(\text{spam}), \Pr(\text{ham})] =$$

$$\arg\max\,[\,0.6, 0.4\,] =$$

spam

(for example)

$$y = \hat{f}(X)$$

Predictive Models

$$y \approx \hat{f}(X)$$

Use function $\hat{f}$ to predict an unknown y given a known X

Examples

	X	y
KIDS dataset:	features of hospitalizations	outcome of hospital stay
Image classification:	(raw) image features	label of subject of image
Finance:	values of stocks, bonds, foreign exchange	tomorrow's stock price of $IBM

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Why build a predictive model?

X **- readily available** y **- very hard to come by** **so approximate** y **with** $\hat{y} = \hat{f}(X)$

Predictive Models

$$y \approx \hat{f}(X)$$

Use function $\hat{f}$ to predict an unknown y given a known X

How to build a predictive model?

Invest in the effort to generate training data, many X, y pairs

Figure out a good $\hat{f}$ by comparing $\hat{f}(X)$ and y when both are known - training or learning

Predictive Models

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Never forget the **guiding principle** – **deployment**

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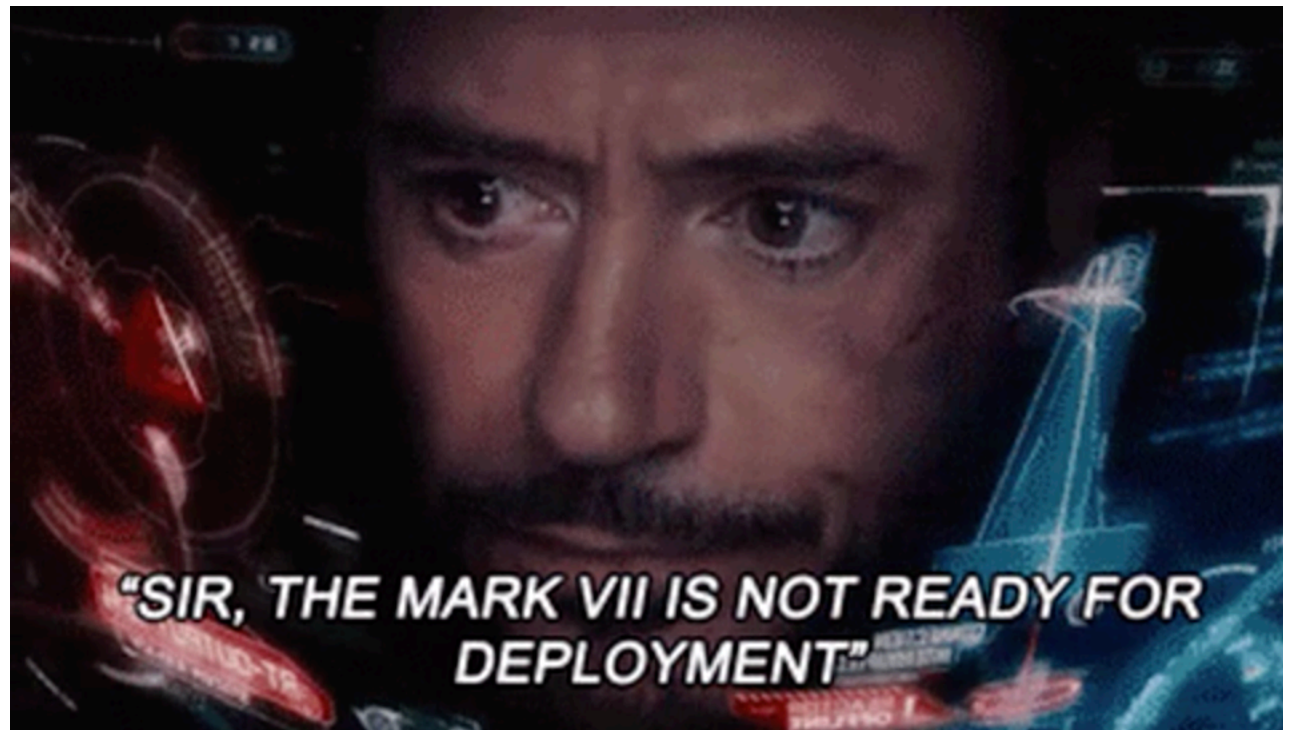

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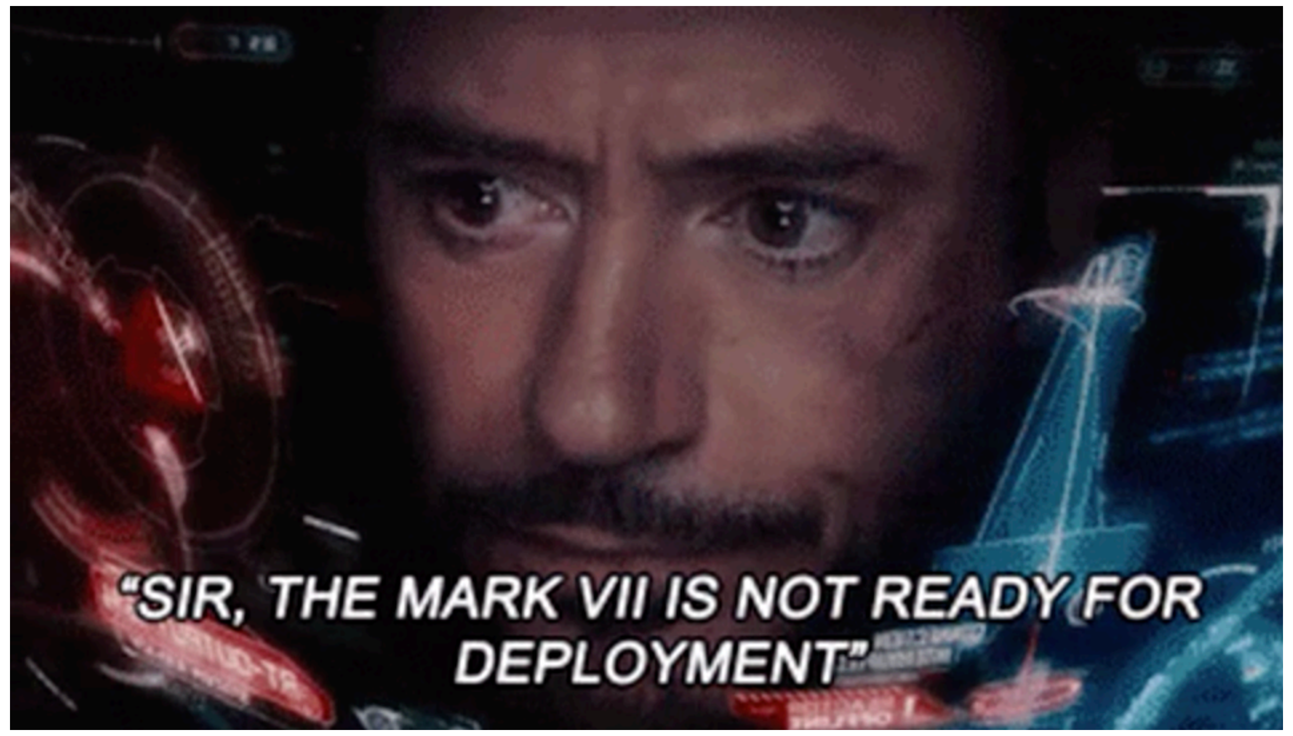

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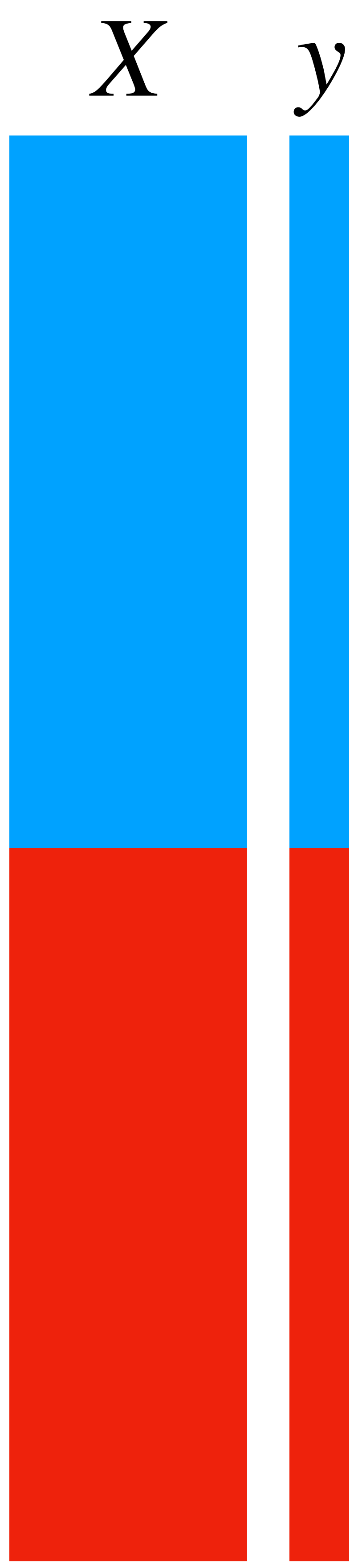
so approximate y with $\hat{y} = \hat{f}(X)$

Very easy, especially for beginners, to get lost fitting $\hat{f}$ to data (error metrics, cross-validation, hyperparameters) but remember: you are building a system that works without knowing y

Simulating Deployment: Training / Testing

50 / 50 split

(90/10 also common)



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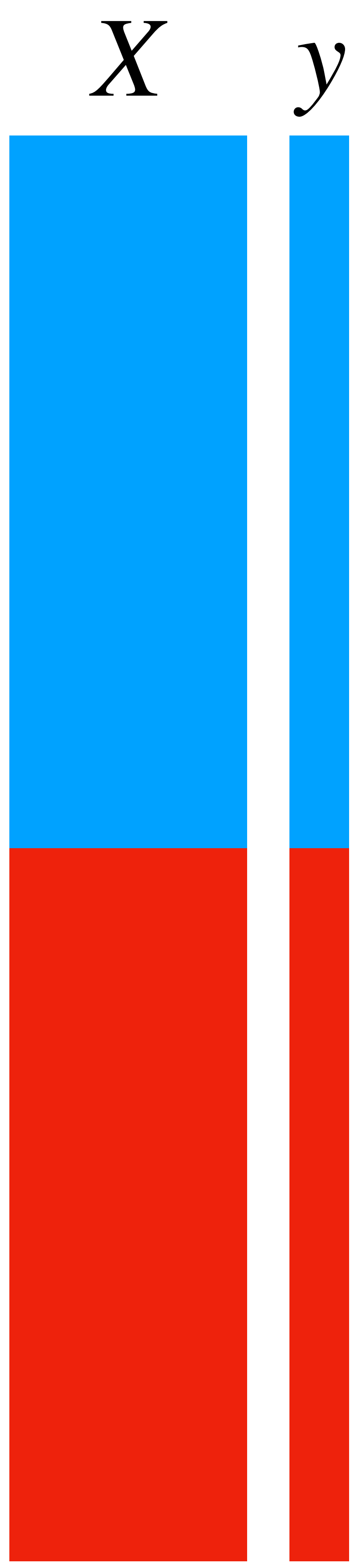

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Predictive model is given X_{tr} and y_{tr} to **learn**

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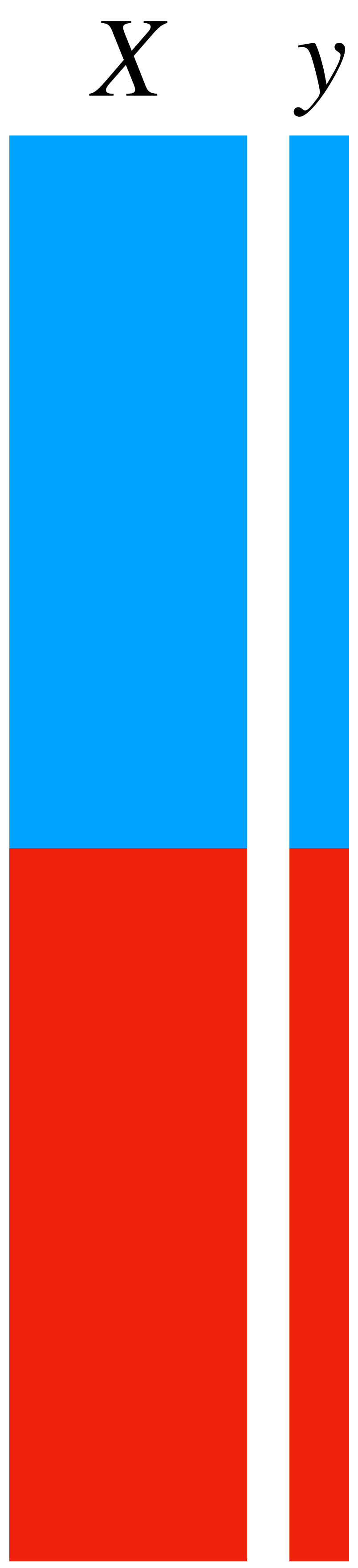


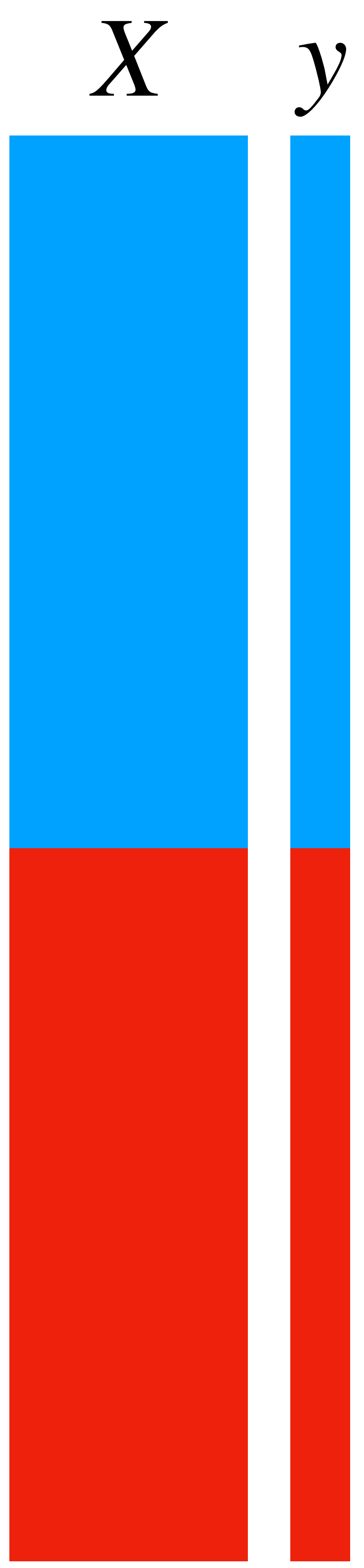
Predictive model is given X_{tr} and y_{tr} to **learn**

$$\hat{f}(X) \approx f(X)$$

Predictive model is **tested** with X_{te} and y_{te} by comparing $\hat{f}(X_{\text{te}})$ against y_{te}

- Example *error metric* (sum of squared errors): $\|\hat{f}(X) - y\|_2^2$

Simulating Deployment: Training / Testing



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maximize the information we have?

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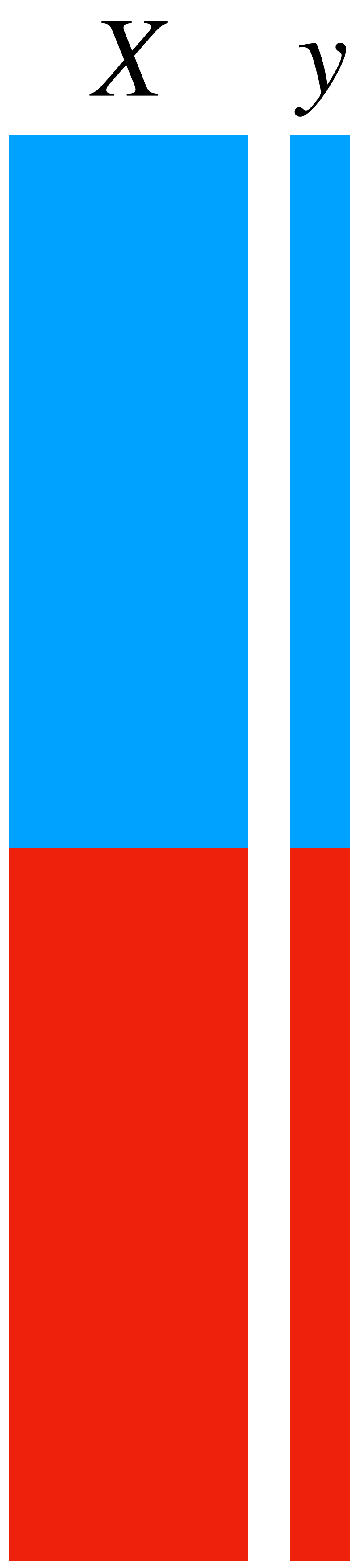
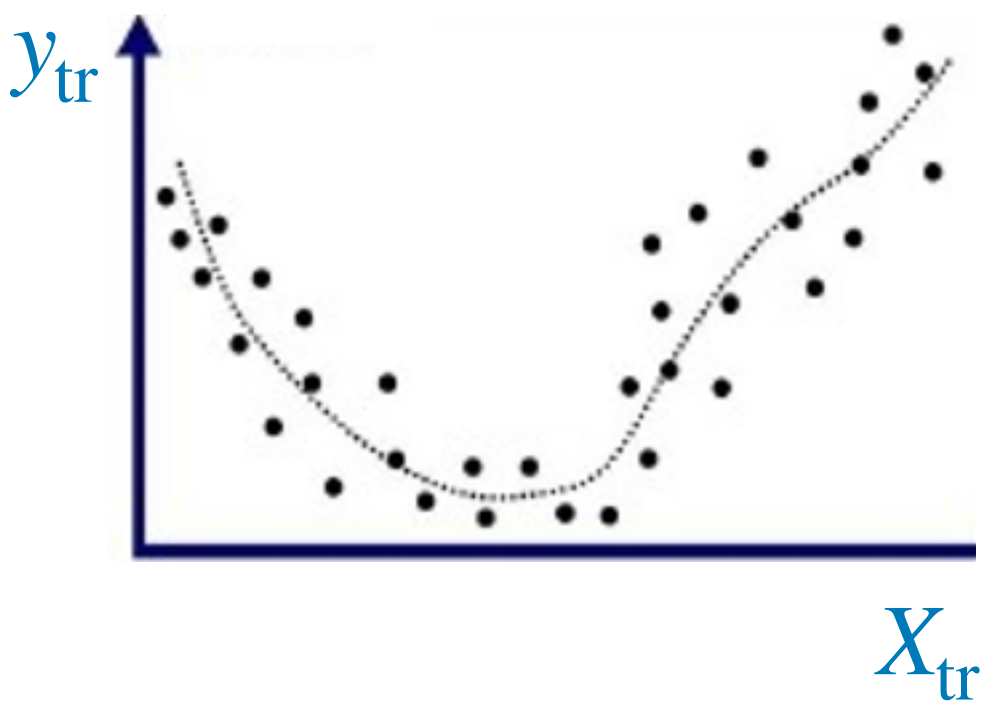


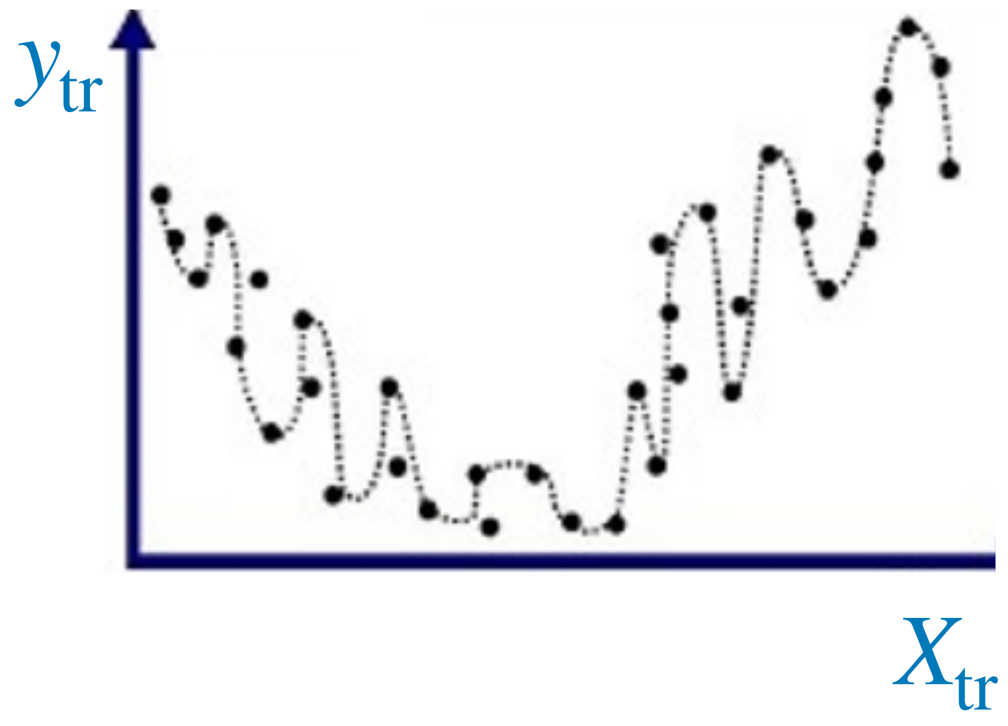
Why not use all the data to learn, maximize the information we have?

To prevent overfitting

Good fit (?)



Overfit!



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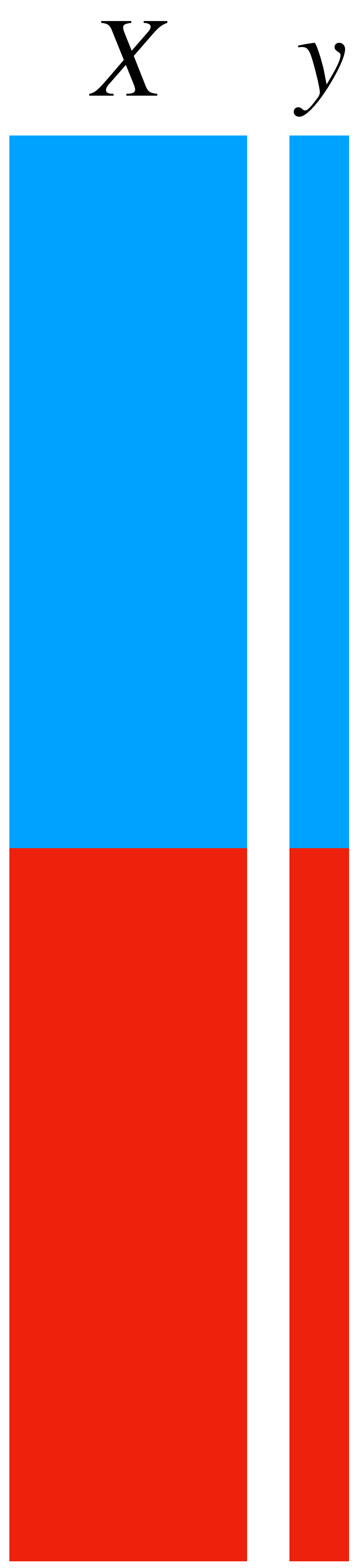

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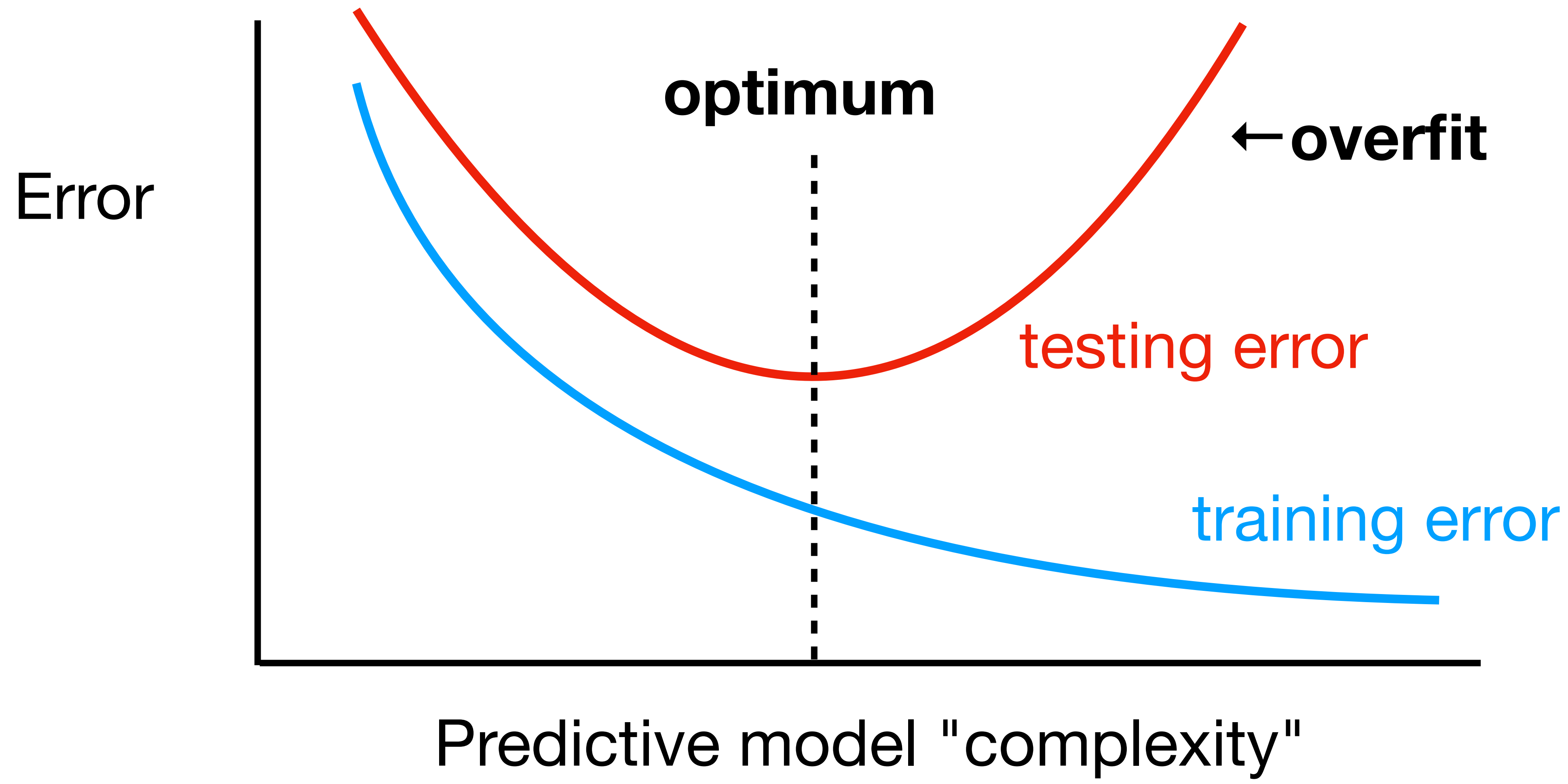

Training / Validation / Testing

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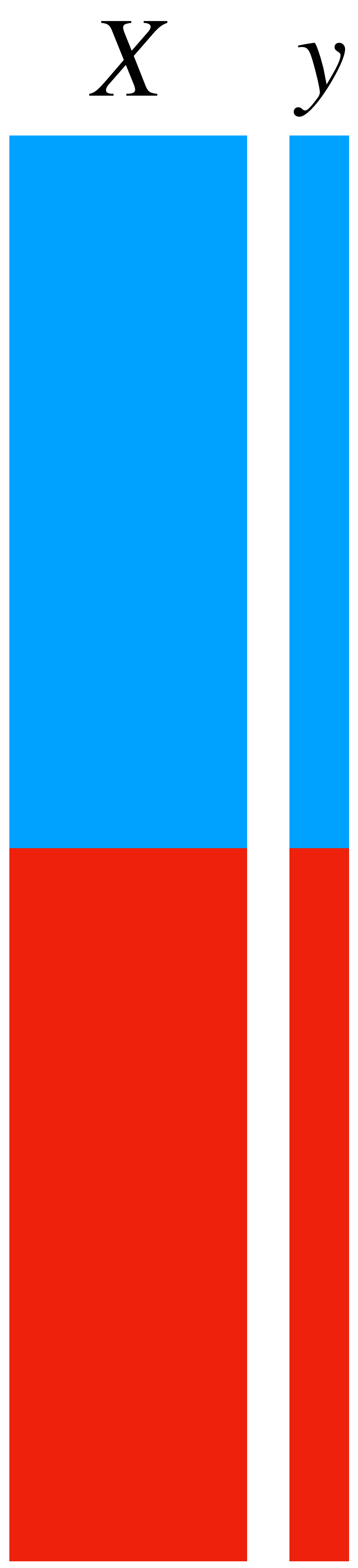

Many predictive models have both *parameters* and *hyperparameters*

Parameters: changed during/due to training

Hyperparameters: chosen <u>before</u> training

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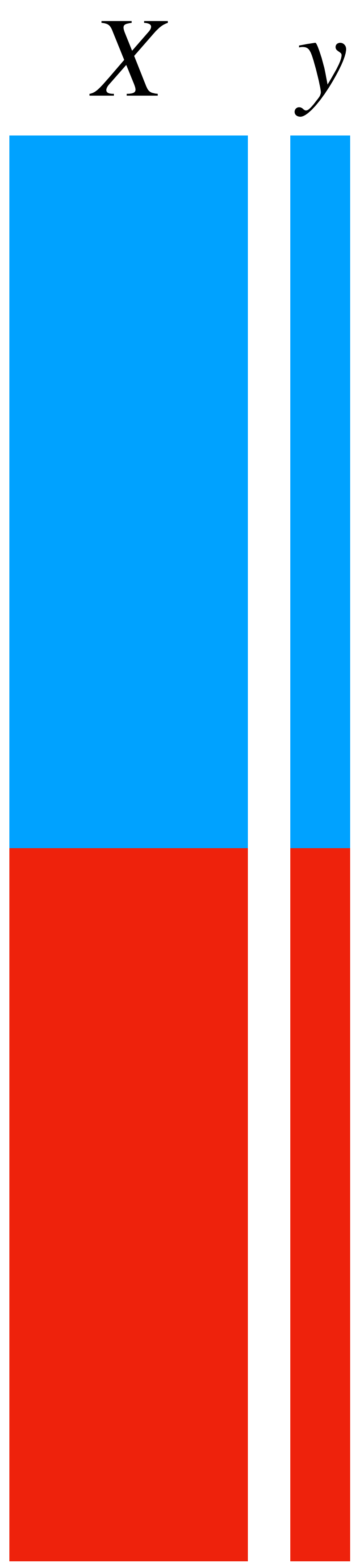

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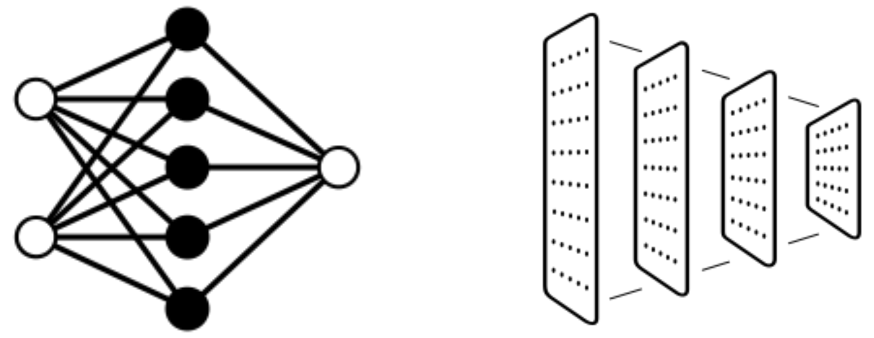
Polynomial regression

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_d x^d$$

Parameters: coefficients β_i

Hyperparameter: polynomial order d

Neural networks

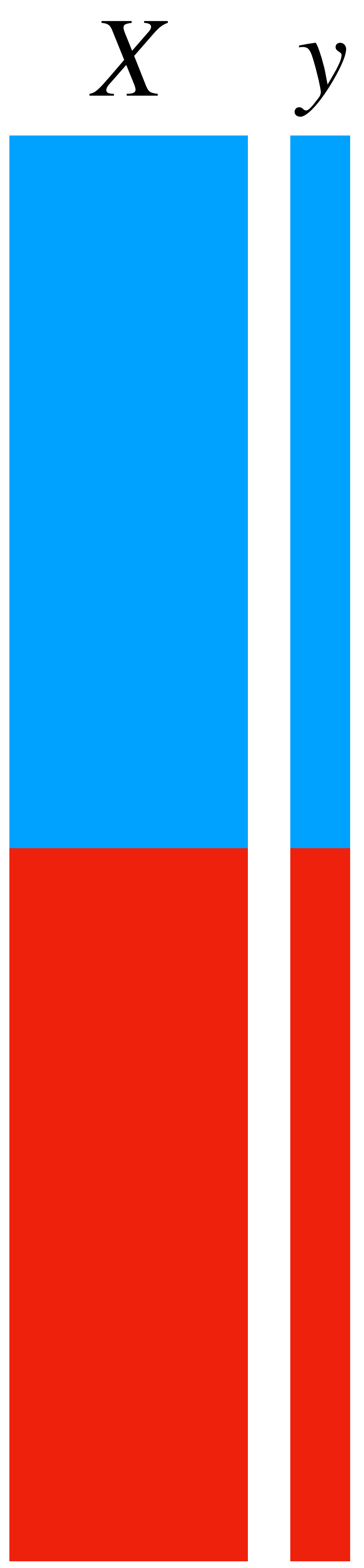


Parameters: weights on links

Hyperparameters:

Network architecture
Choice of activation function
…

Training / Validation / Testing



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Parameters: changed during/due to training

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You could:

1. Use training data to fit parameters
2. Use testing data to compare different hyperparameters

But:

- Risk overfitting again—all your data went into the model, nothing is left over for testing

Training / Validation / Testing

Many predictive models have both *parameters* and *hyperparameters*

Parameters: changed during/due to training
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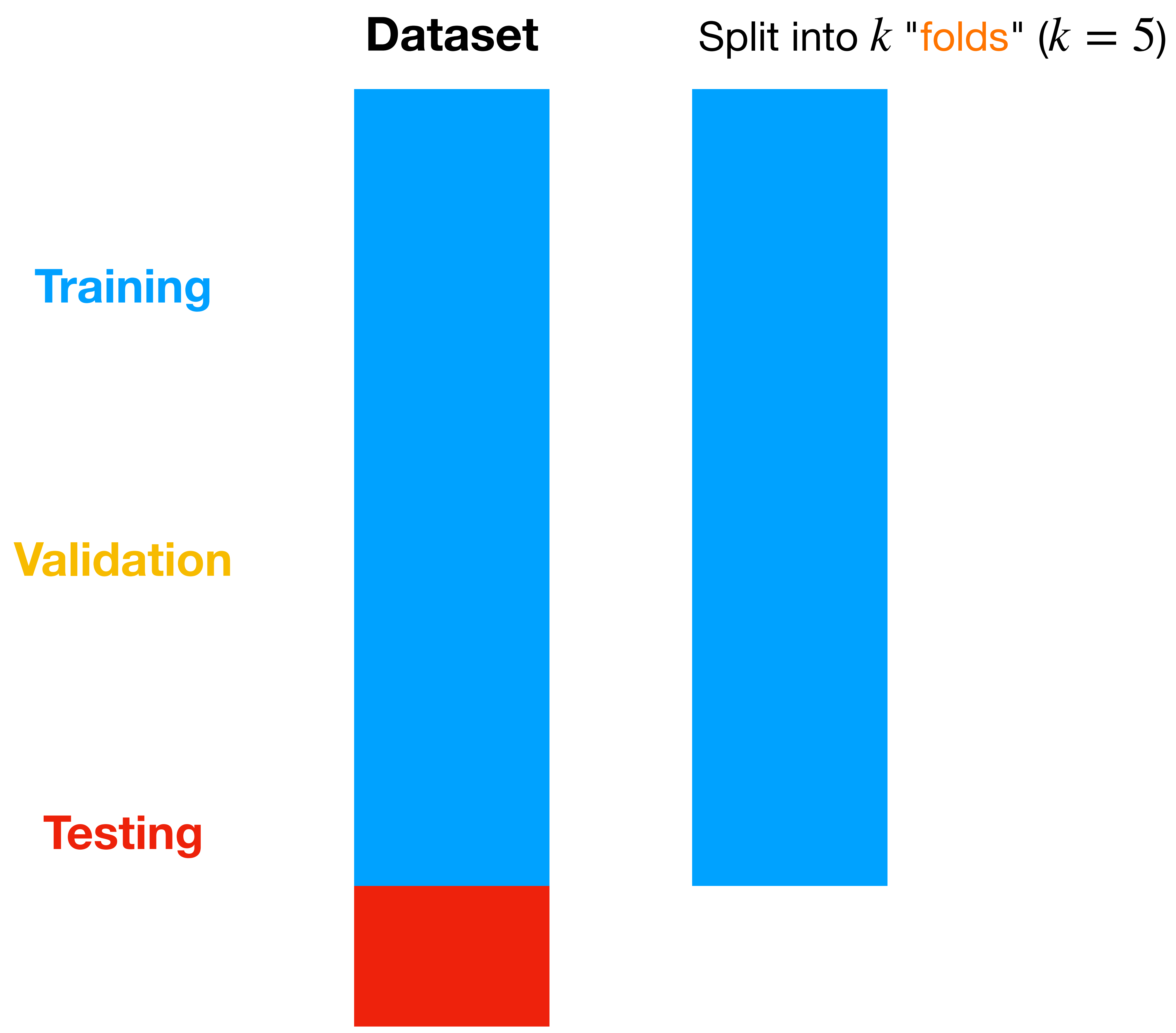
Instead:

1. Use **training data** to fit parameters
2. Use validation data to compare different hyperparameters
3. Use **testing data** to pick best model

One issue:

May need **multiple** training/validation splits, to get enough statistics (repetitions) to make good comparisons

(k-Fold) Cross-validation



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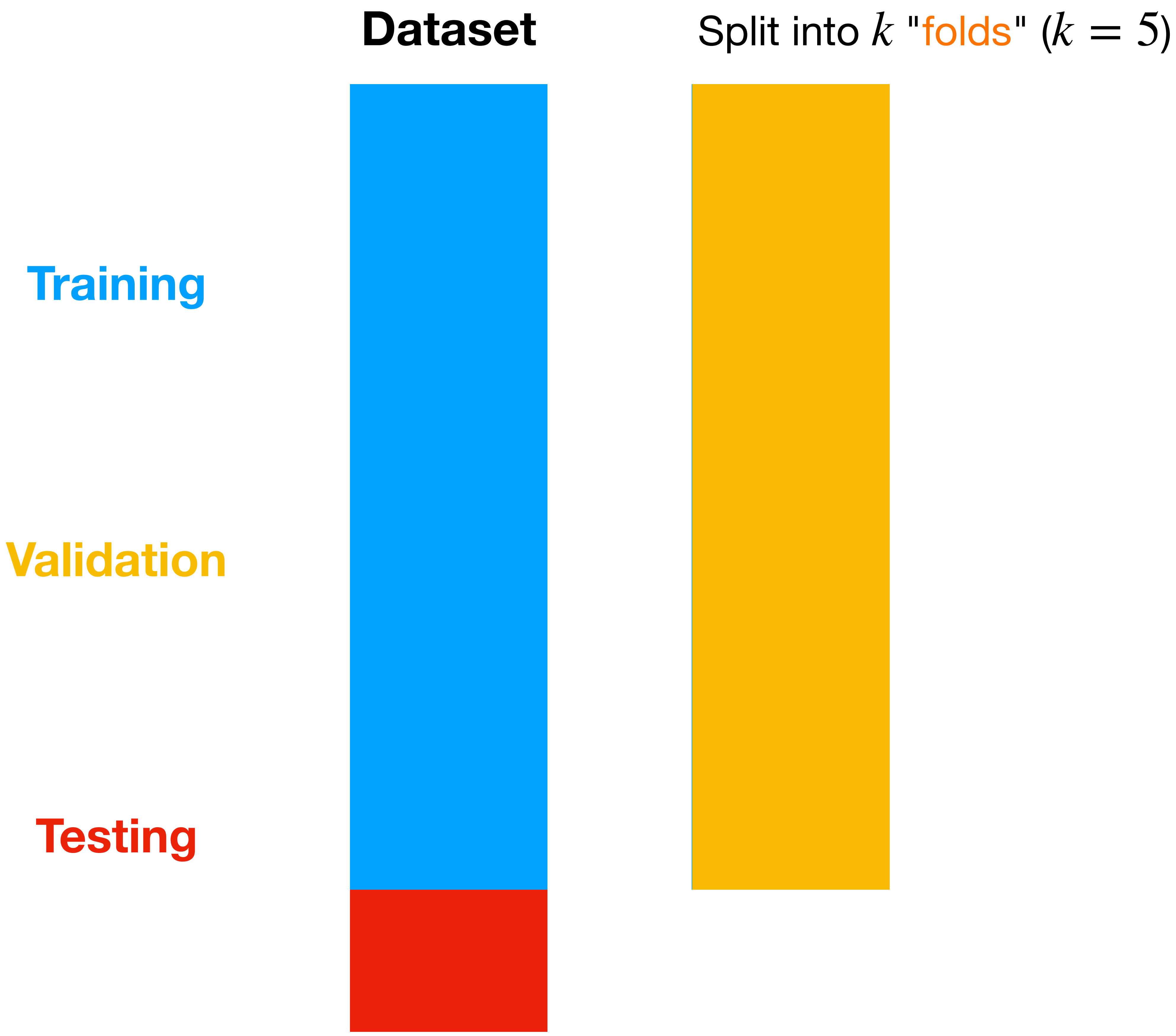

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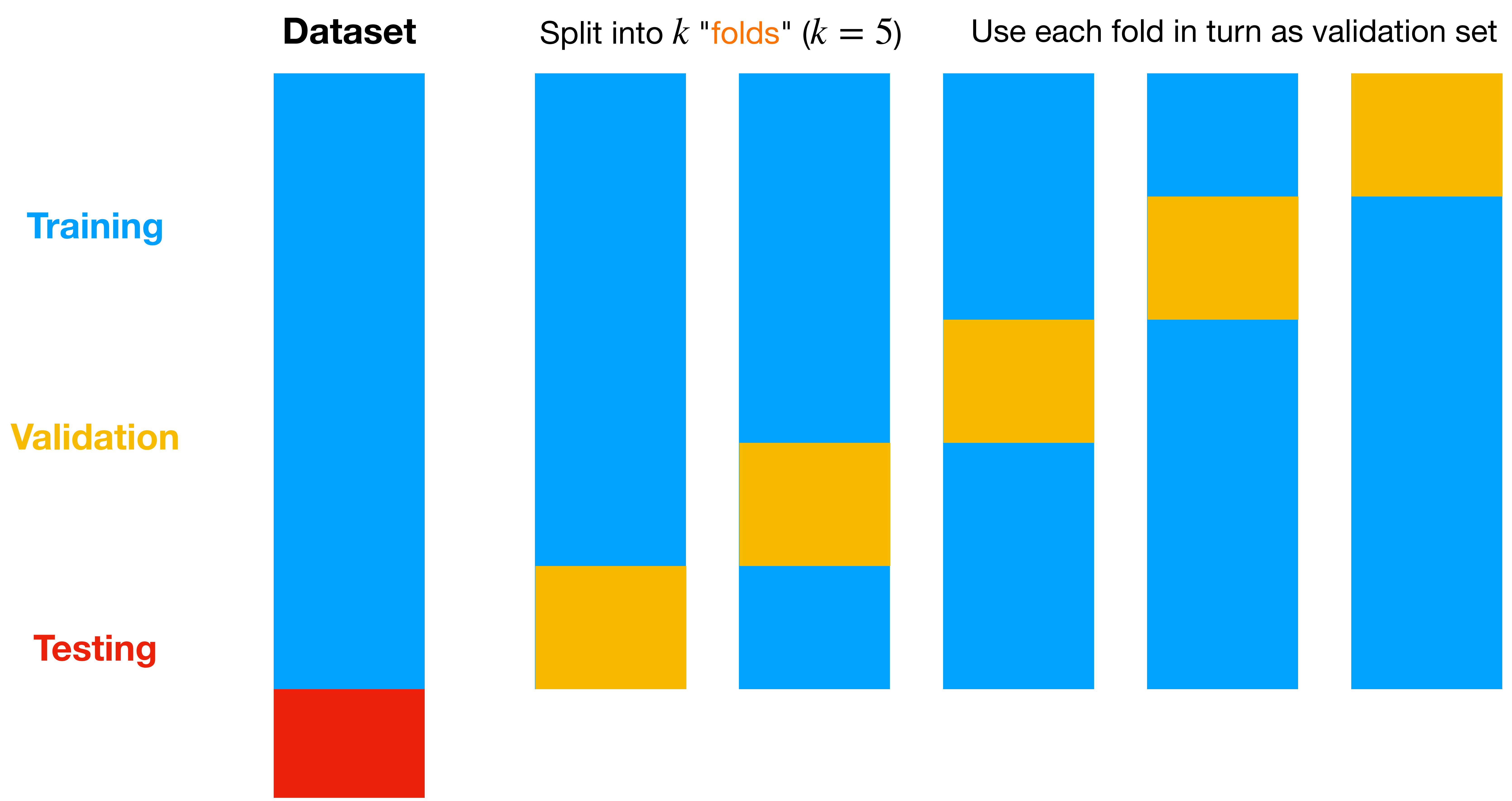

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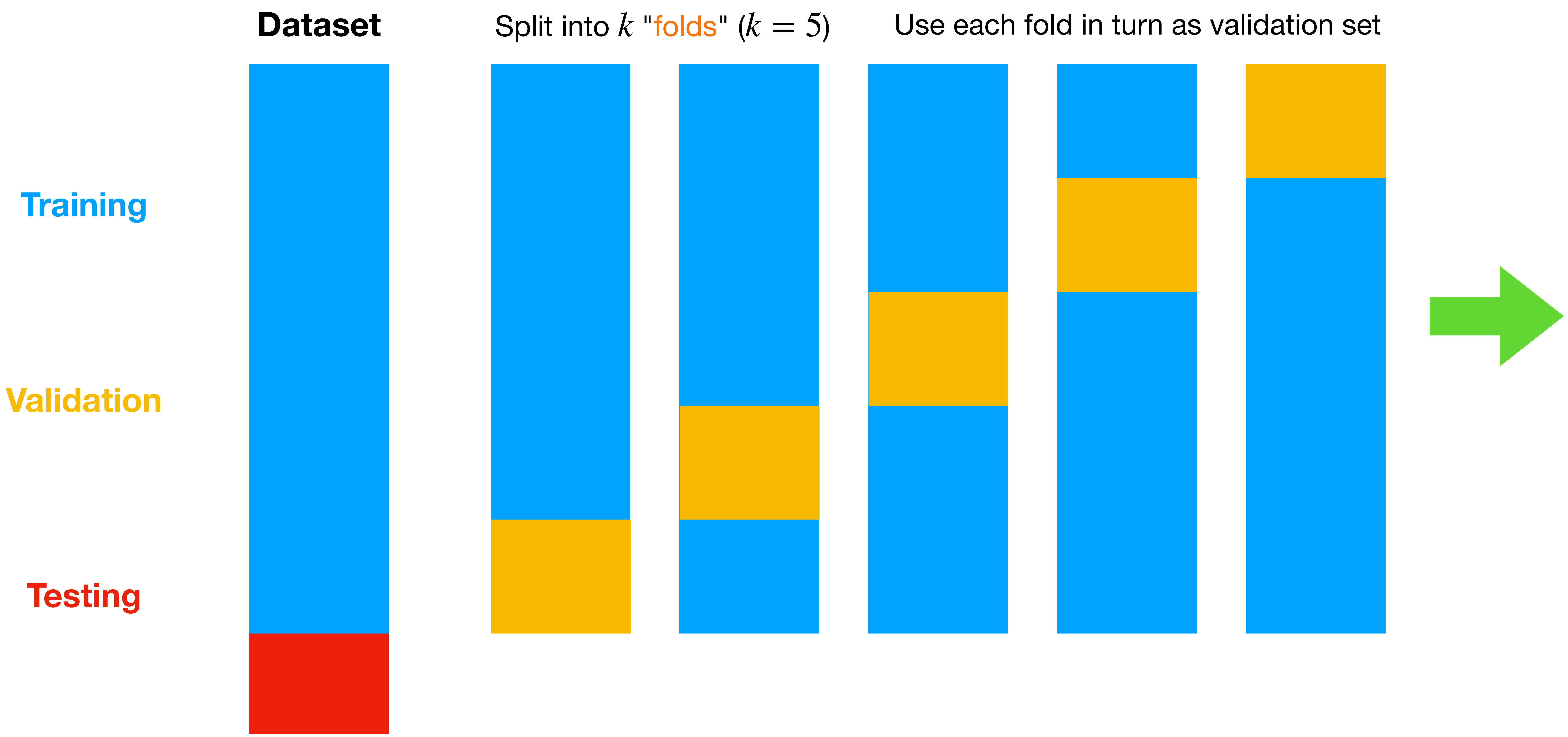


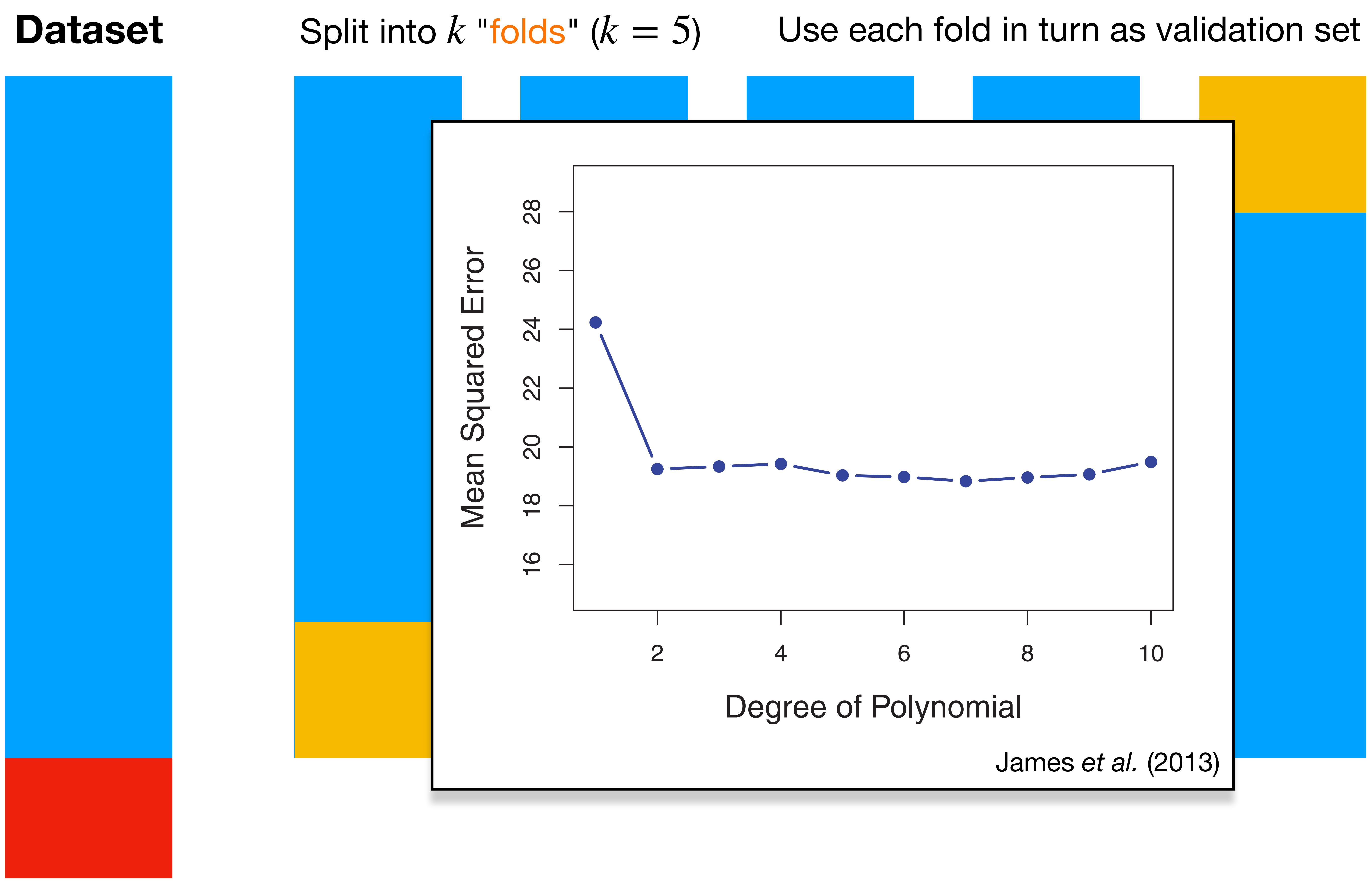
Use measure of performance (error metric?) **averaged over folds** to select best model

(k-Fold) Cross-validation

Training

Validation

Testing



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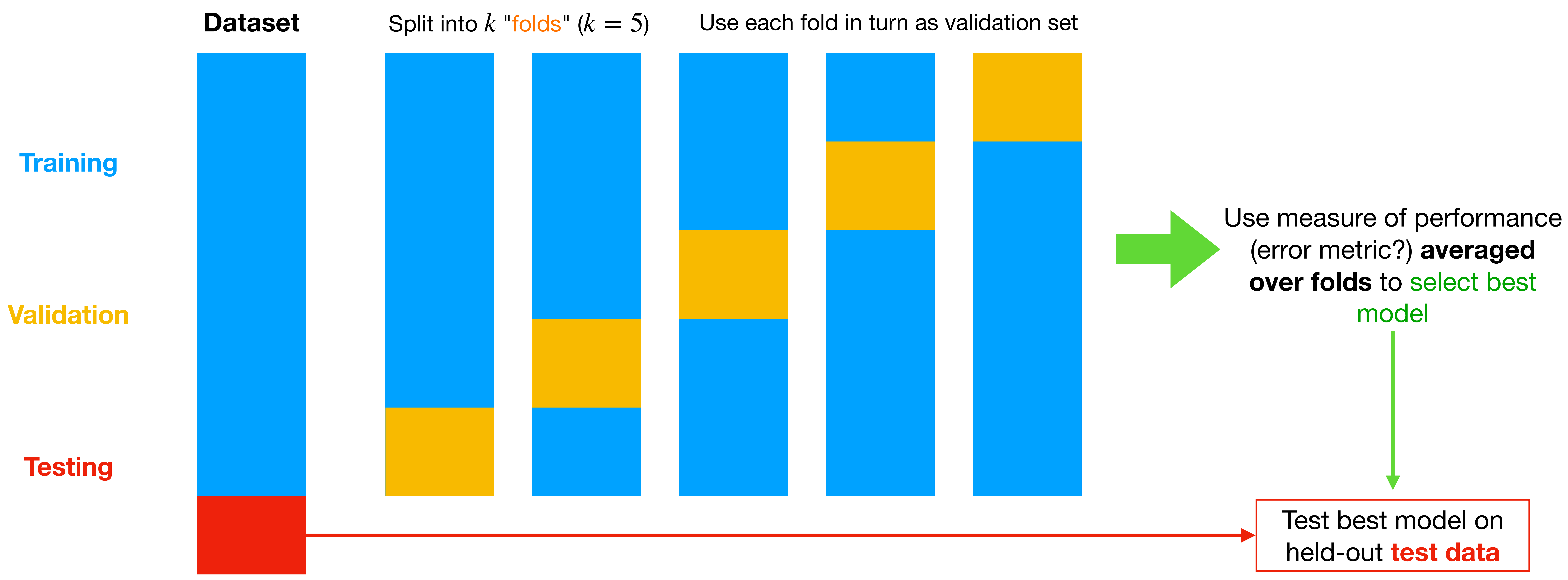

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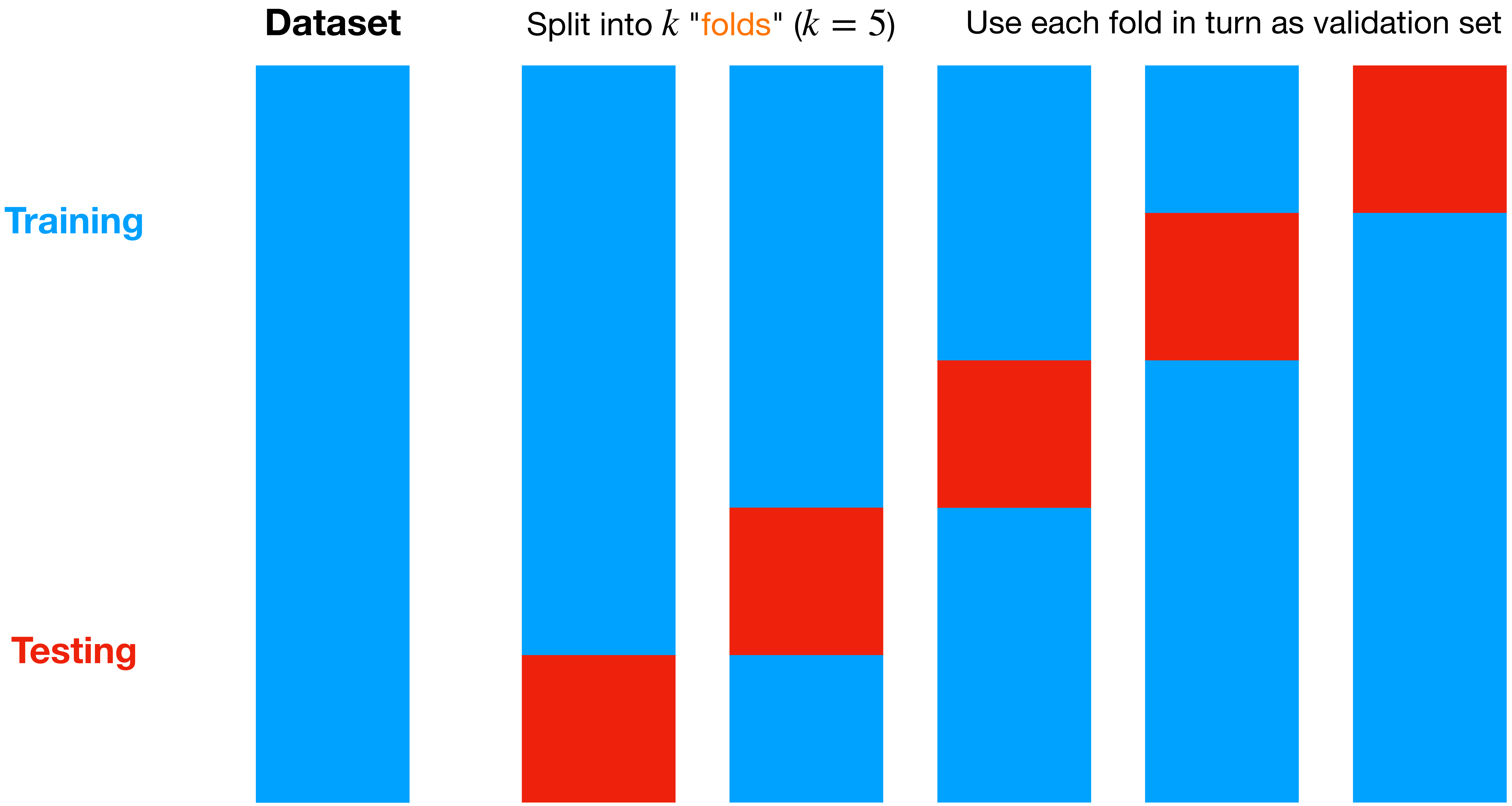

Often common to dispense with the validation split altogether!

(If you don't need to find hyperparameters)

More **robust estimate** of model performance by averaging over **multiple** training/testing splits

Splits/Cross-Validation are biased

Compare

A) Take a single dataset and split it into two datasets

B) Generate a dataset and, later, generate a second dataset

Splits/Cross-Validation are biased

Compare

A) Take a single dataset and split it into two datasets

B) Generate a dataset and, later, generate a second dataset

It's likely there is **unaccounted variation(s)** that is changing the two datasets in option B that is not present in option A

→ Larger difference between the two B datasets than the two A datasets

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It's likely there is **unaccounted variation(s)** that is changing the two datasets in option B that is not present in option A

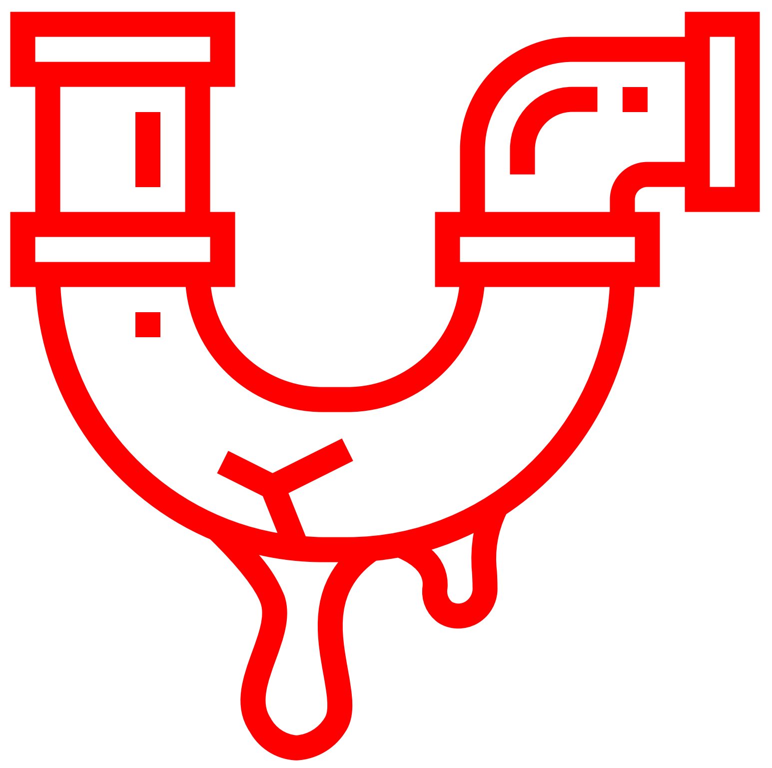
→ Larger difference between the two B datasets than the two A datasets

Therefore, training/testing or cross-validation will likely overestimate the true performance of a predictive model

Underestimates the error of the model

Data Leakage

Failure to simulate deployment



Information from the held out test set was used during training

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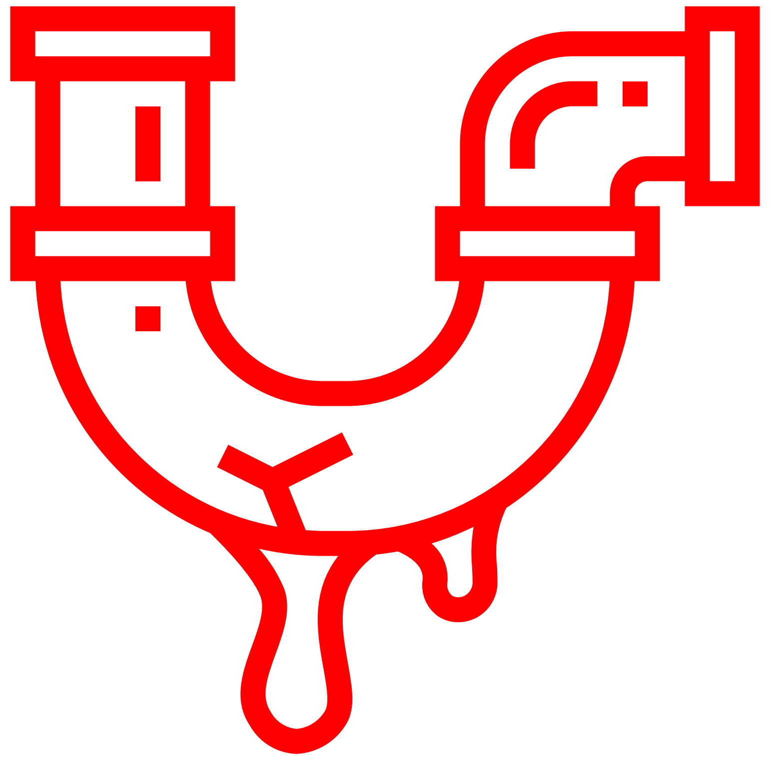

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Example

Suppose I want to rescale (one of) my predictive features:

$$X_i \text{ becomes } \frac{X_i - \bar{X}_i}{\sigma_{X_i}}$$

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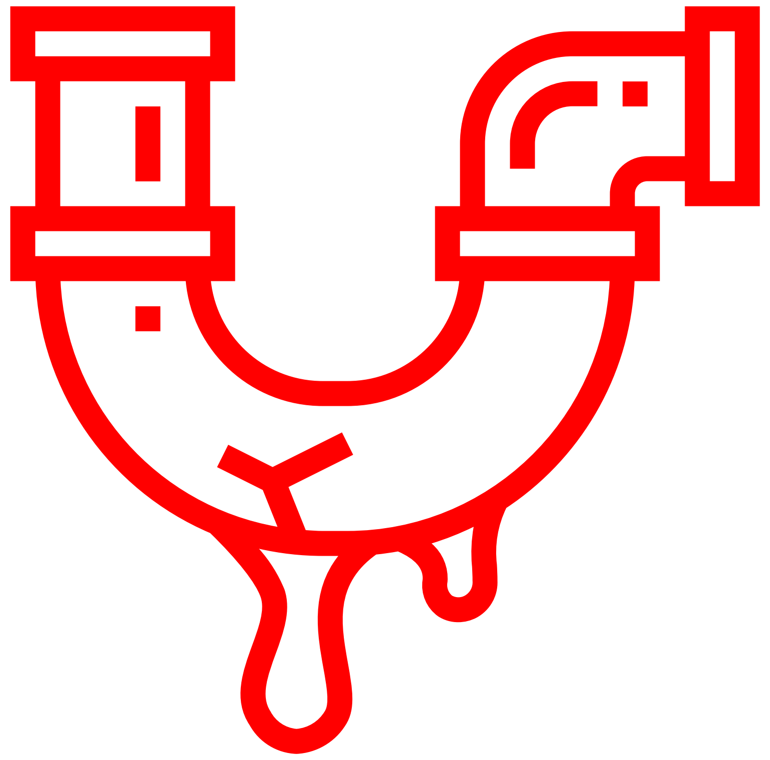

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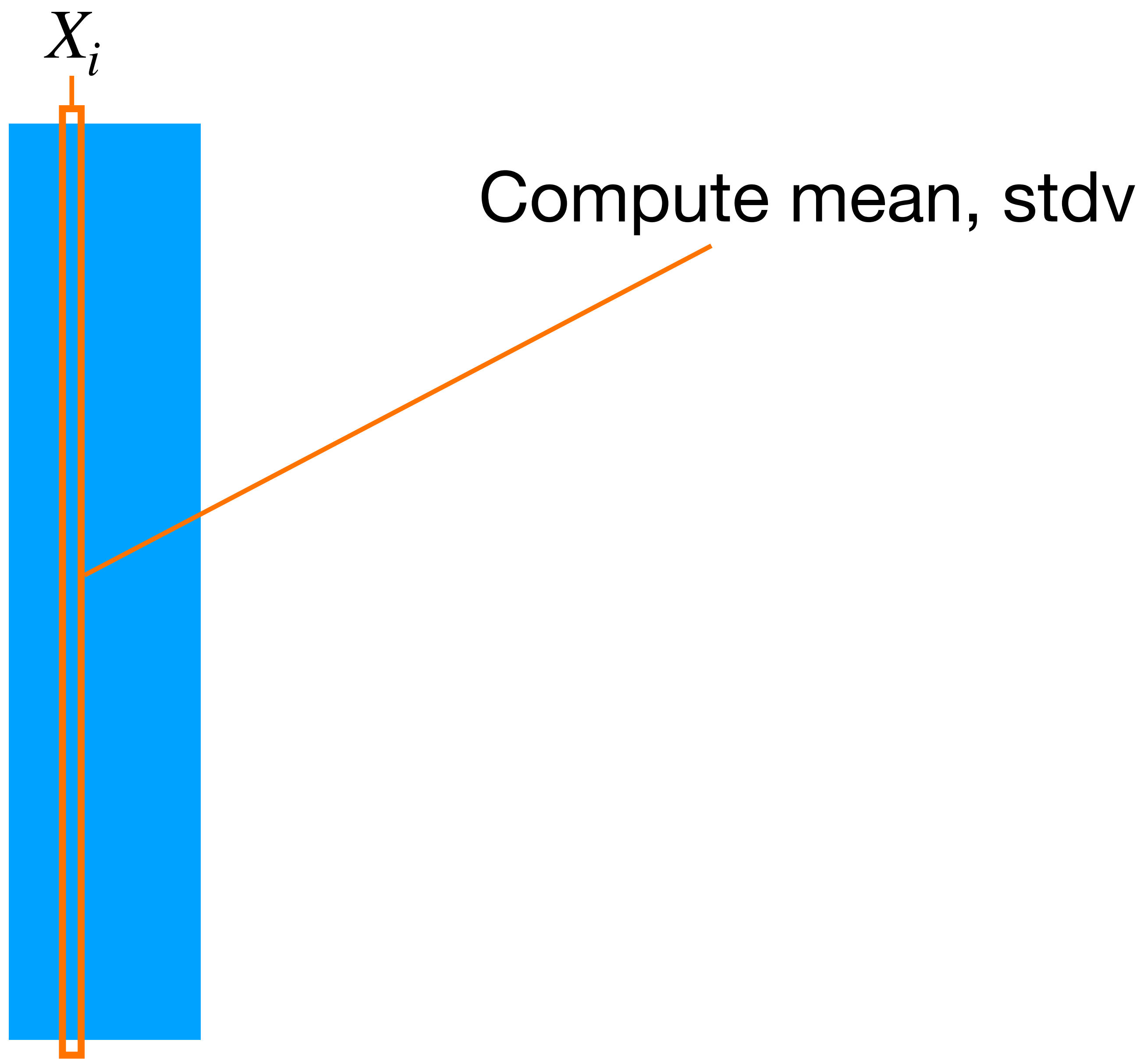

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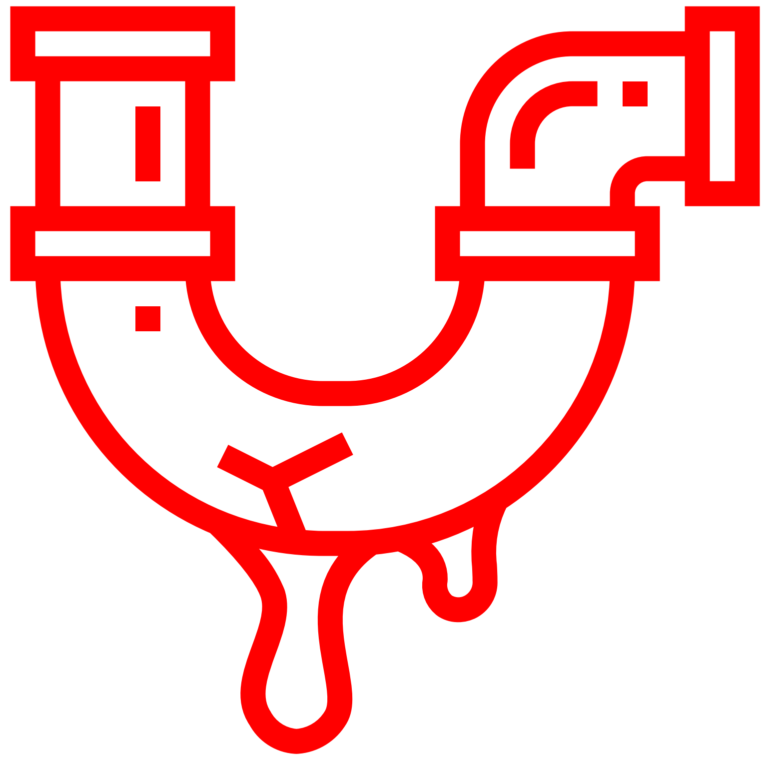

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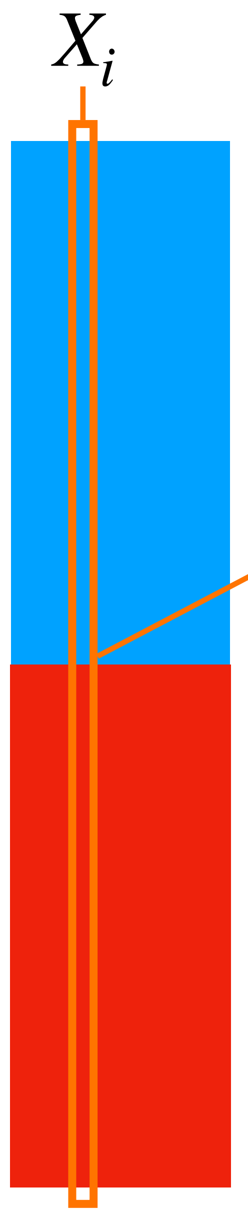

Compute mean, stdv

I haven't split training and testing yet

→ $\bar{X}_i, \sigma_{X_i}$ **used test points**. ***Leakage!***

Data Leakage

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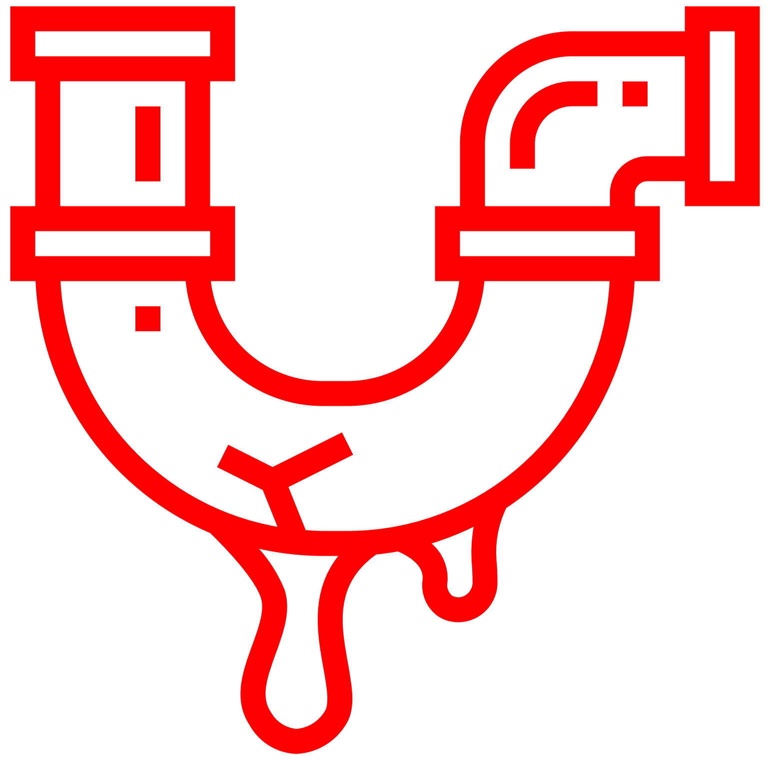

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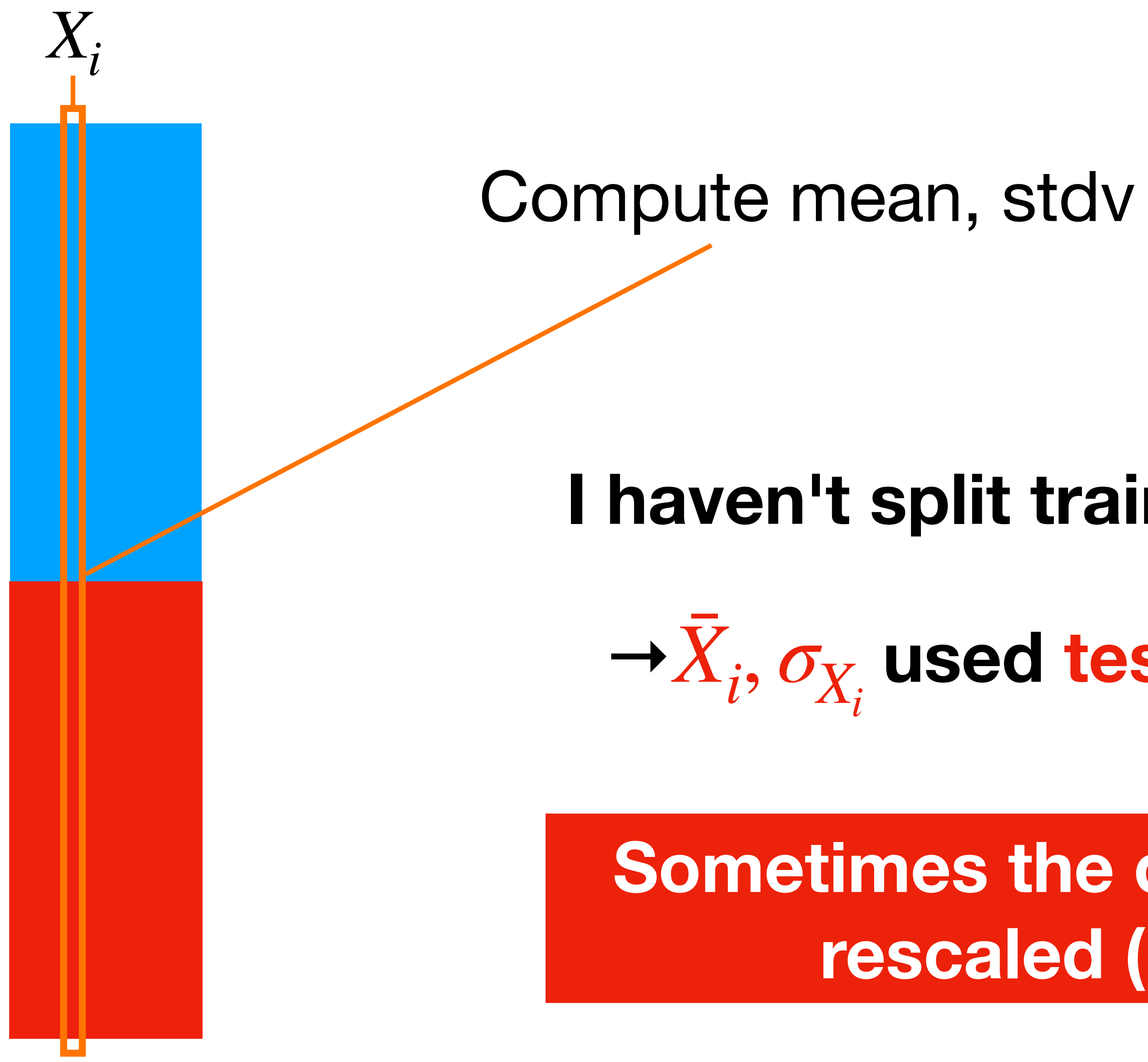

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Sometimes the data already come rescaled (pre-leaked!)

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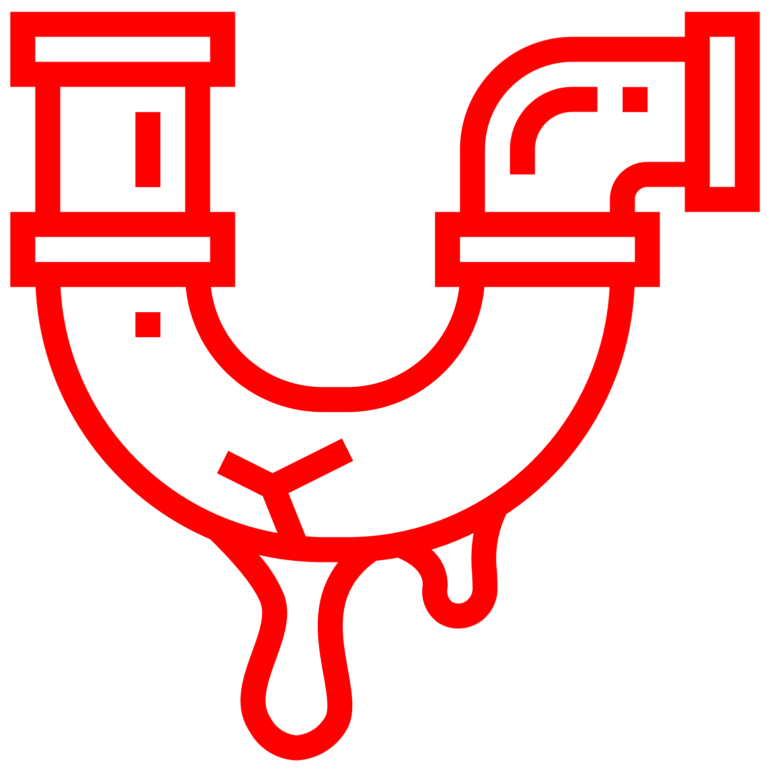

Amazing model performance?
Too-good-to-be-true performance?
Might be leakage!

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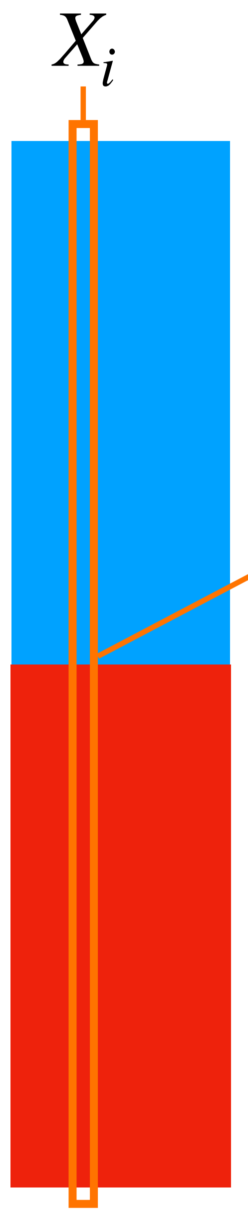

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→$\bar{X}_i, \sigma_{X_i}$ used test points. *Leakage!*

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Summary — Predictive Models

- Prediction vs inference
- Prediction with supervised learning $y = \hat{f}(X)$
  - dominant form of machine learning
  - use pre-existing X, y (*training data*) to figure out $\hat{f}$
- Why build predictive models?
  - X is cheap, y expensive, so use $\hat{f}(X)$ instead of y
- Deployment - how will model work when there is no y?
  - Simulate deployment with cross-validation
  - Take care—data leakage!