Cross Validation

OLS Solution

- Ordinary Least Squares (OLS) Regression:

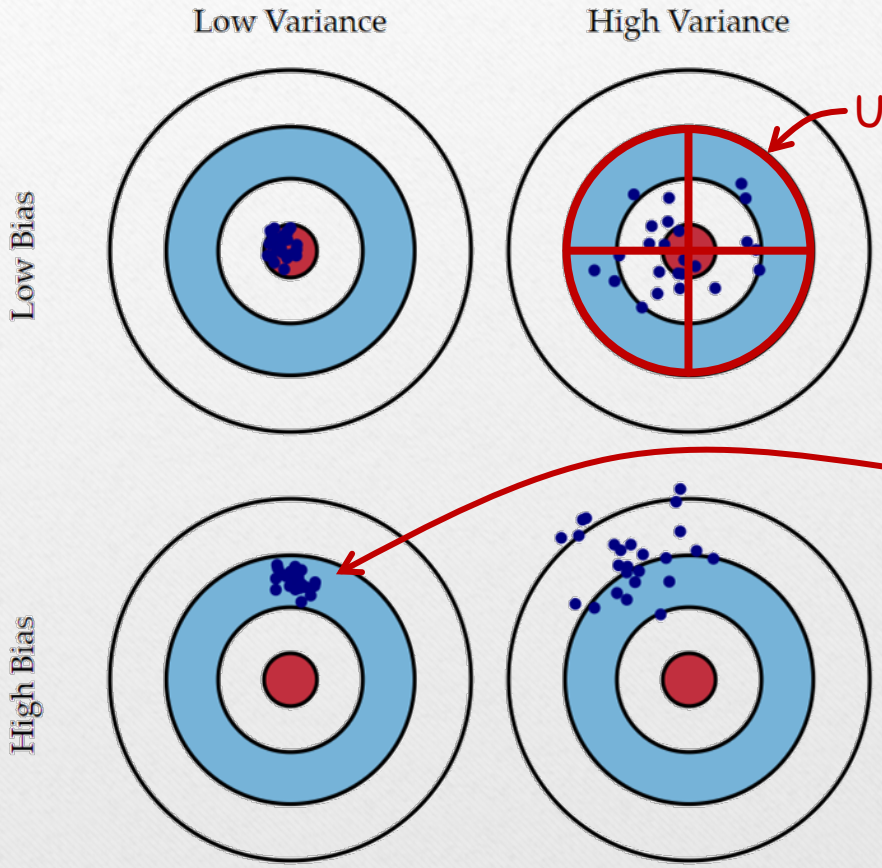
$$\min_{\beta_0 \dots \beta_k} \sum_i \left[y_i - \left(\beta_0 + \beta_1 x_{i,1} + \cdots + \beta_k x_{i,k} \right) \right]^2$$

where $x_{i,j}$ is the value in ith row and jth column of X. i.e. the ith value in the jth independent variable.

- Solution to this problem can be represented by the following matrix equation:

$$\vec{\beta} = (X^T X)^{-1} X^T \vec{y}$$

Variance vs Bias



Unbiased: $E[\hat{\beta}_j] = \beta_j$

OLS has the lowest variance among **unbiased estimators**.

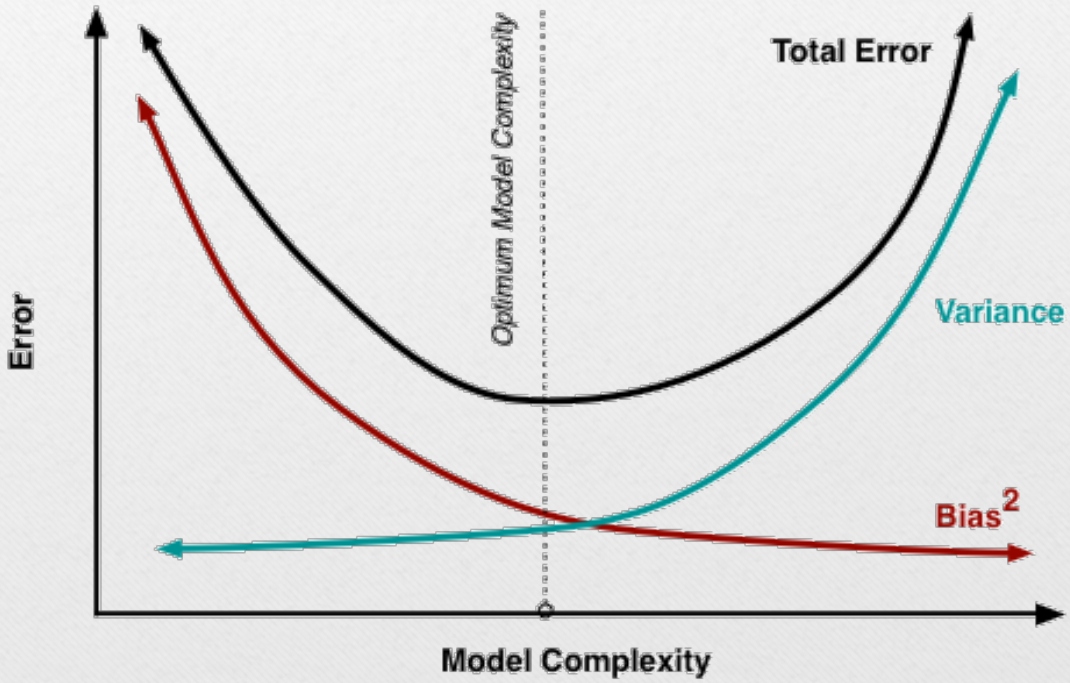
We can further lower variance if we are willing to consider **biased estimators**.

There is a tradeoff between bias and variance

Source: http://scott.fortmann-roe.com/docs/BiasVariance.html

Variance-Bias Tradeoff

- The tradeoff between a model's ability to minimize variance and to minimize bias



Source: http://scott.fortmann-roe.com/docs/BiasVariance.html

Regularization

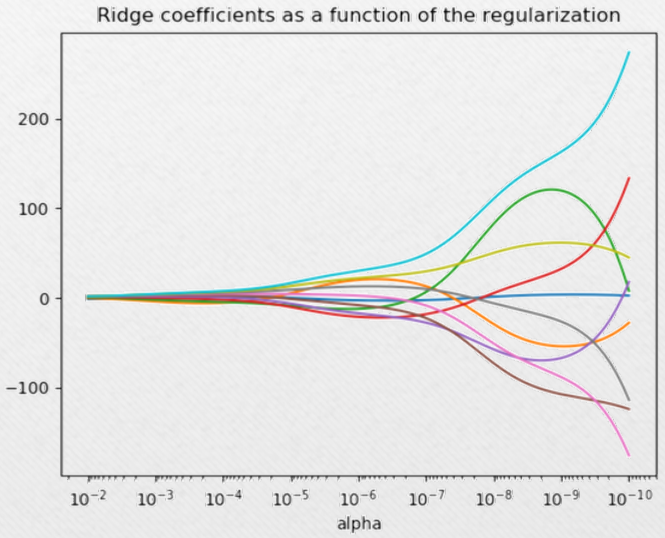
- **Regularization** penalizes large coefficients
- This reduce overfitting by making regression coefficients over different samples more similar to each other
  - In the most extreme case, all coefficients will be zero regardless of sample
- Regularized regression are biased, but they have smaller variance than OLS
- The two most regularized regressions are **ridge** and **lasso**

Regularization

- Ridge Regression, also called **Least Square with L2-regularization**, have the following objective:

$$\min_{\beta}\left\{\sum_{i}\left(y_i-\vec{\beta}\cdot\vec{x}_i\right)^2+\alpha\sum_{k}\beta_k^2\right\}$$

- Ridge regression pushes **all** coefficients **towards zero**
- Stronger regularization (higher α) leads to smaller coefficients



Regularization

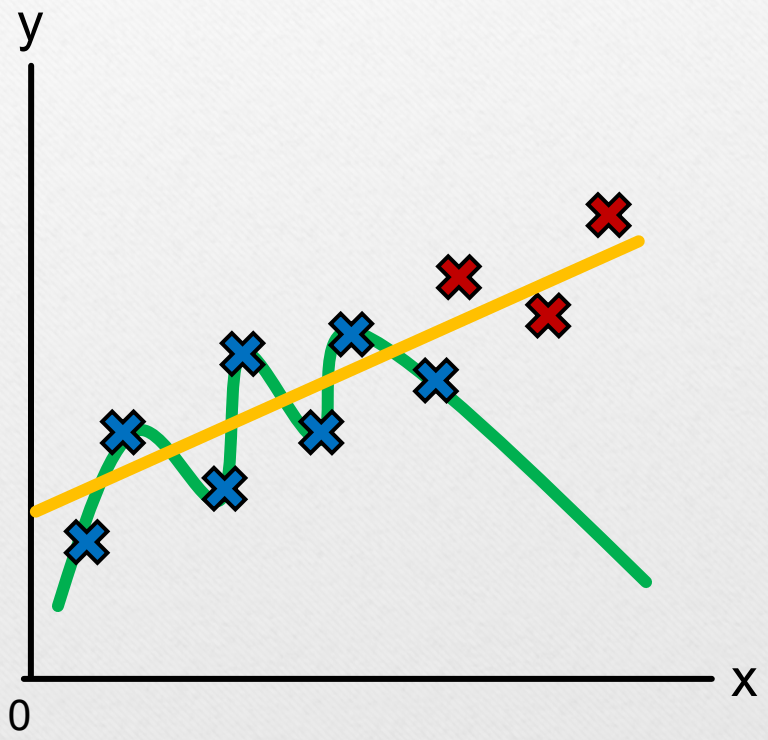
- Lasso Regression, also called **Least Square with L1-regularization**, have the following objective:

$$\min_{\beta} \left\{ \sum_{i} \left(y_i - \vec{\beta} \cdot \vec{x}_i \right)^2 + \alpha \sum_{k} |\beta_k| \right\}$$

- Lasso regression makes **some** coefficients **exactly zero**
- Stronger regularization (higher α) leads to more coefficients becoming zero
- **Lasso can help you select variables**

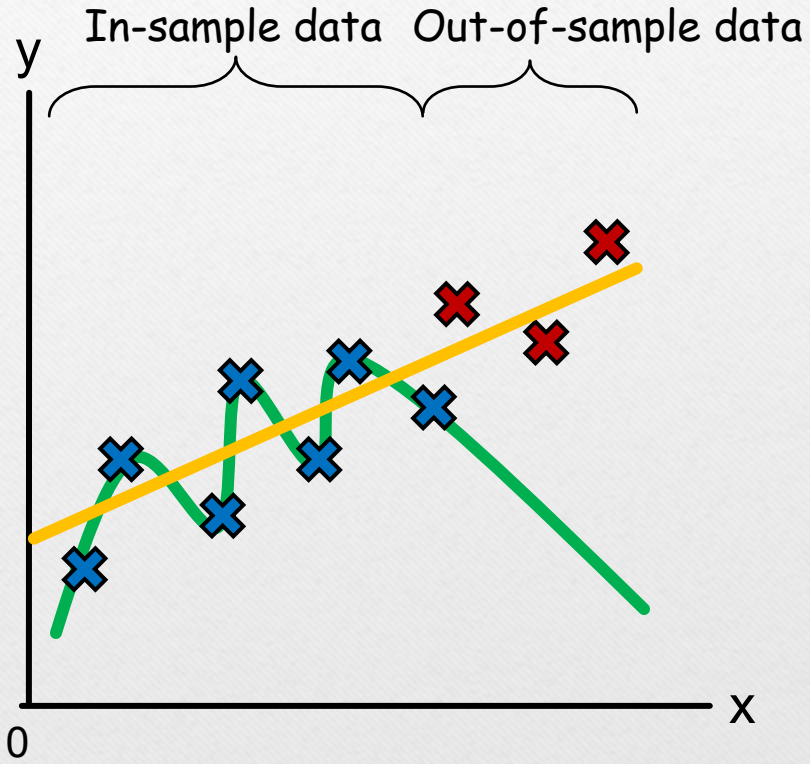
Out-of-Sample Test

- We want accurate prediction
- Given enough complexity, a model will always do well with data it has seen
- We want to know if the model does well with data it has **not yet seen**



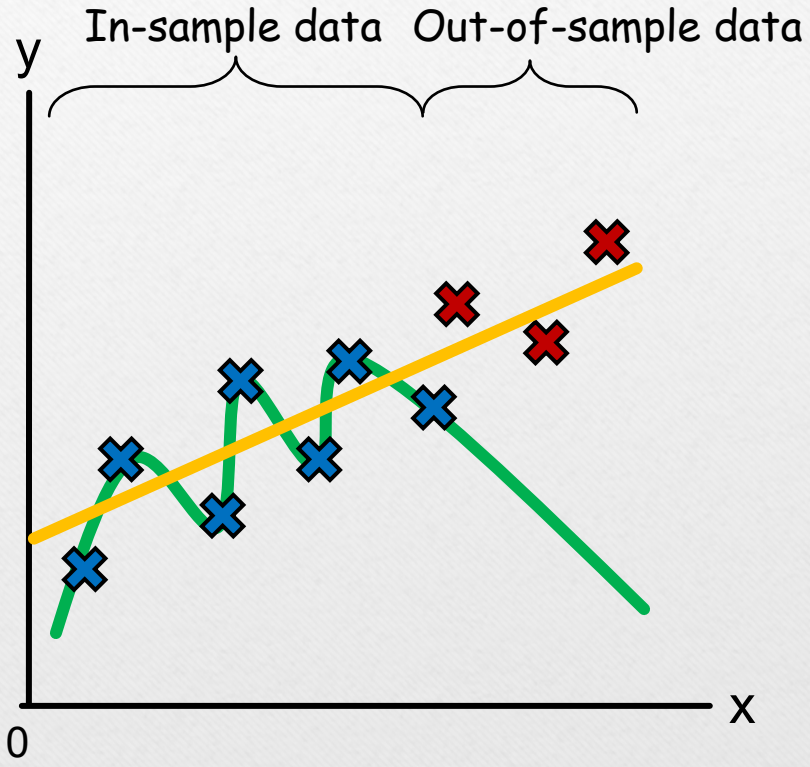
Out-of-Sample Test

- We will intentionally keep part of the data from the model training process
- This reserved data is not seen by the model during training, allowing us to conduct an **out-of-sample test**
- We pick the model (or model parameters) that has the highest out-of-sample prediction accuracy



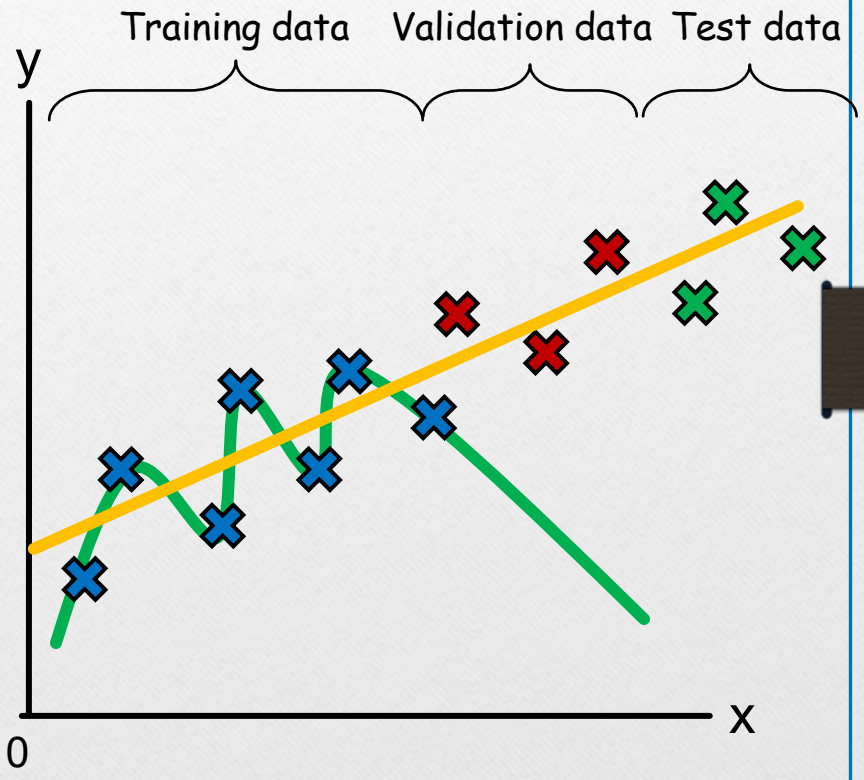
How to Find the Best α?

- Idea: we pick the model (or model **hyperparameters** such as α) that has the highest out-of-sample prediction accuracy
- Problem: If we pick α this way, the model has seen the reserved data, so it is no longer out of sample



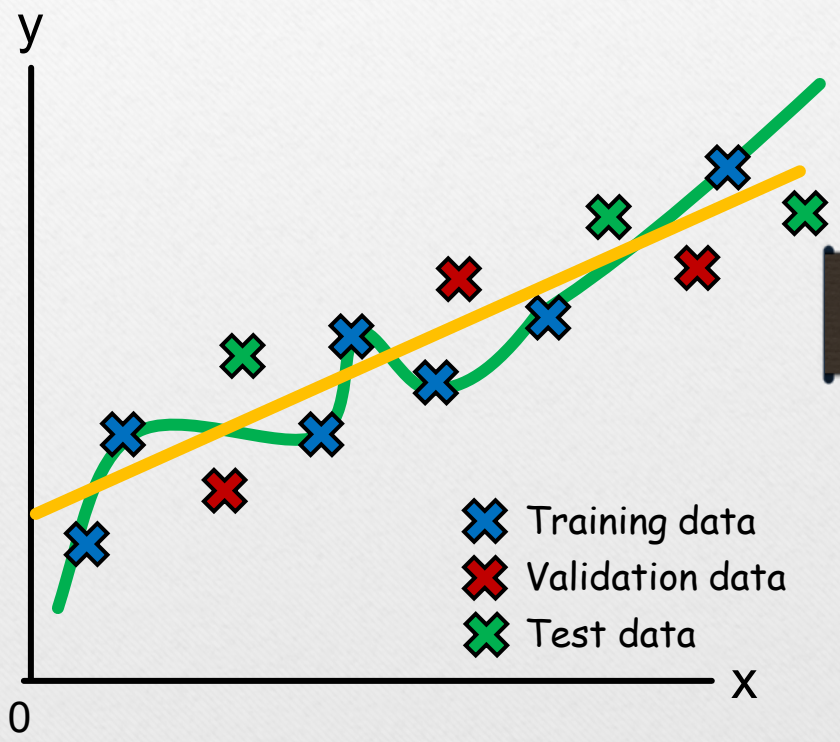
How to Find the Best Model

- Solution: split the data into three parts:
  1. **Training set** for training the model
  2. **Validation set** for choosing models and hyperparameters
  3. **Test set** for reporting out-of-sample performance



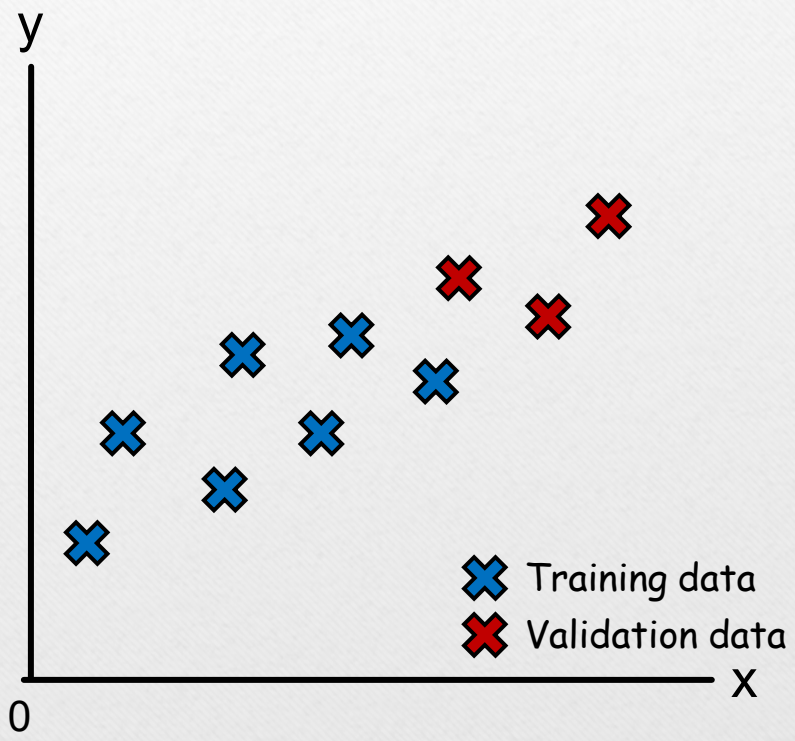
How to Find the Best Model

- To ensure that each set of data is representative, we generally want to split the data randomly rather than sequentially
- The exception is time series data. We must split such data sequentially to avoid hindsight bias



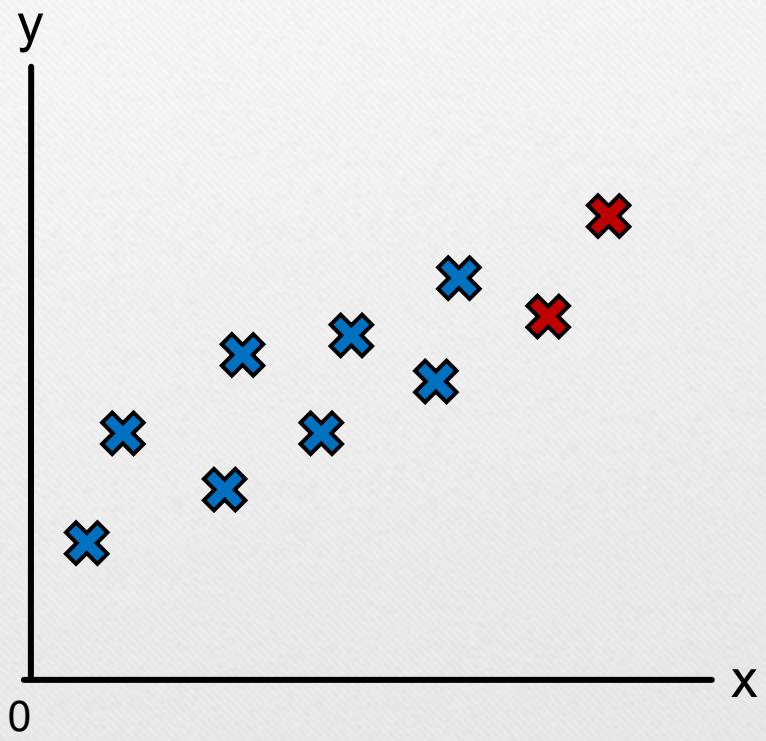
K-Fold Cross Validation

- We might question the representativeness of the validation set, particularly when the sample size is small
- At the same time, we might be unwilling to increase its size since that makes the training set smaller
- What to do in this case?



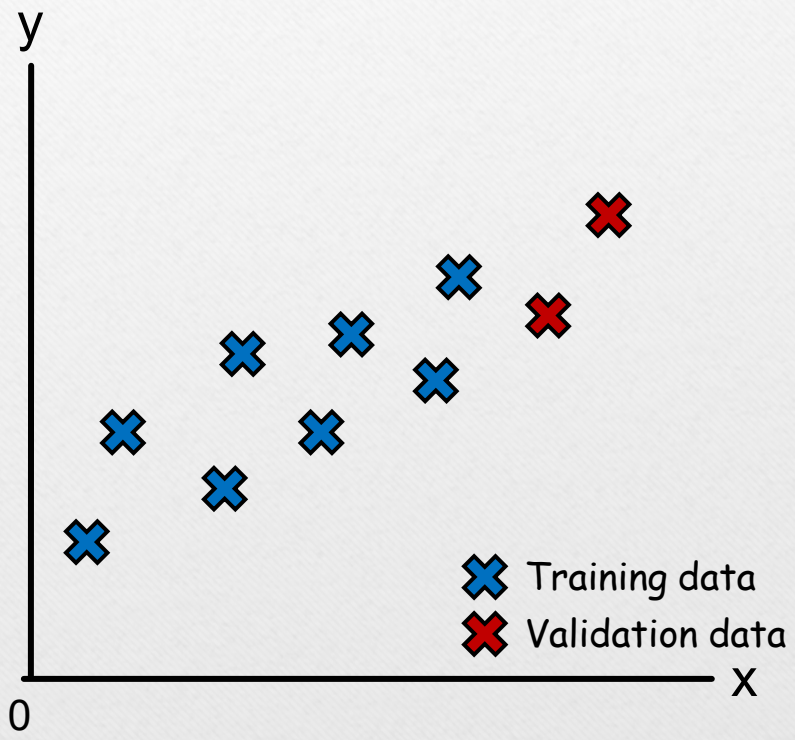
K-Fold Cross Validation

- We can handle this problem by using ***k*-fold cross validation**
- We first divide the data we intend to use for training and validation into *k* equal-sized folds. Five is a common choice
- We repeat the training process for *k* times. Each time we use one fold for validation and the rest for training



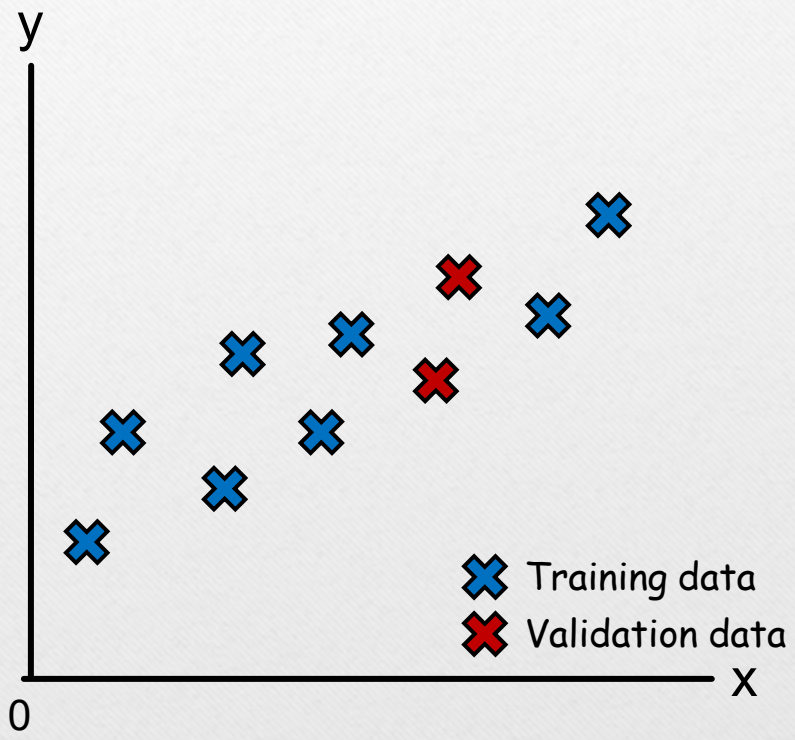
K-Fold Cross Validation

- Iteration 1



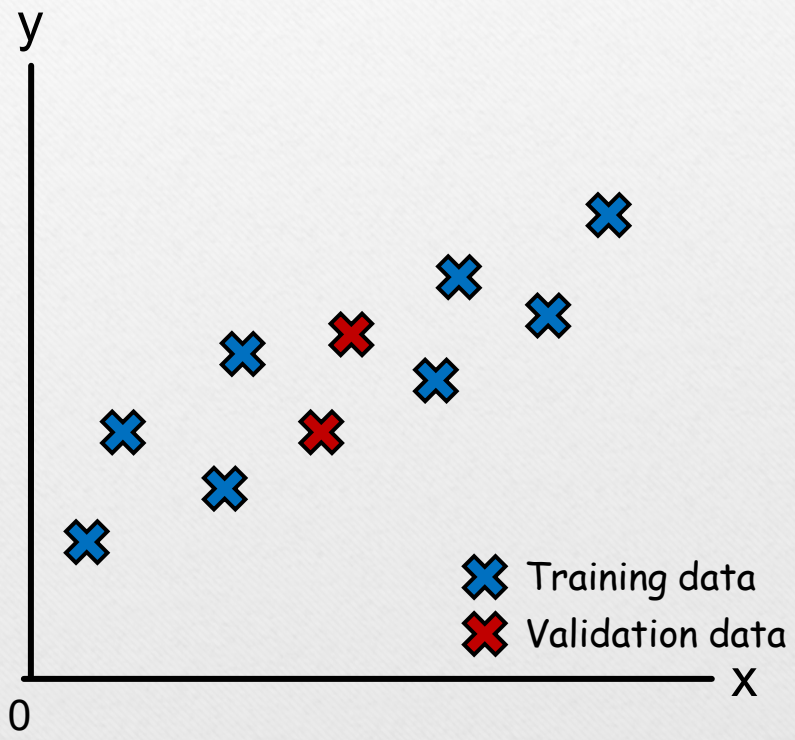
K-Fold Cross Validation

- Iteration 2



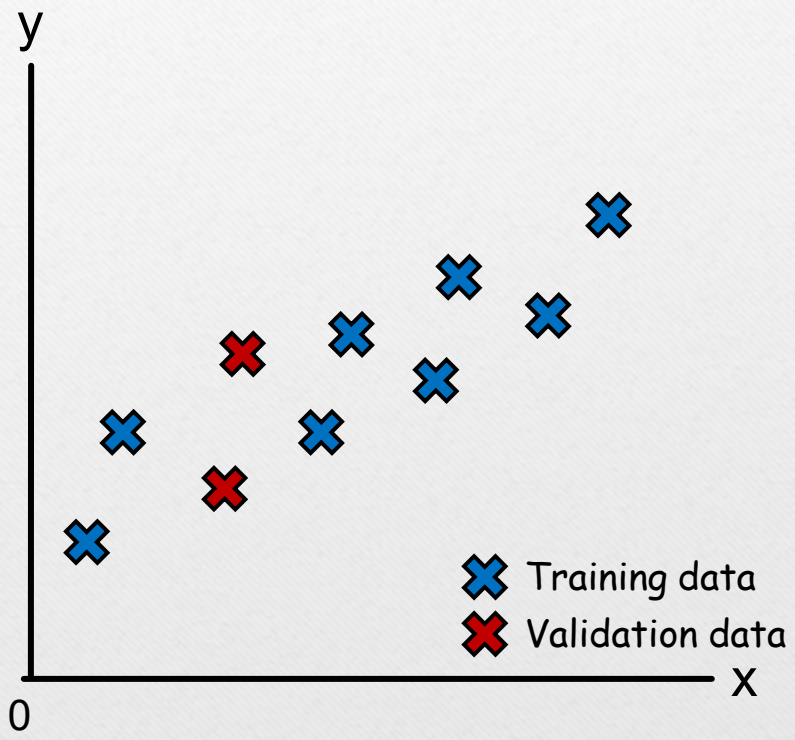
K-Fold Cross Validation

- Iteration 3



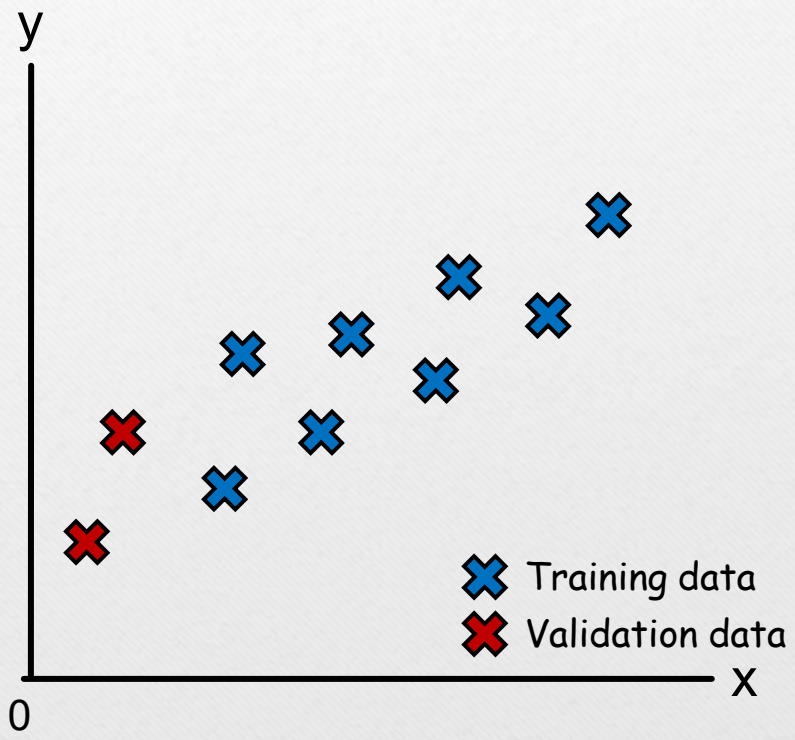
K-Fold Cross Validation

- Iteration 4



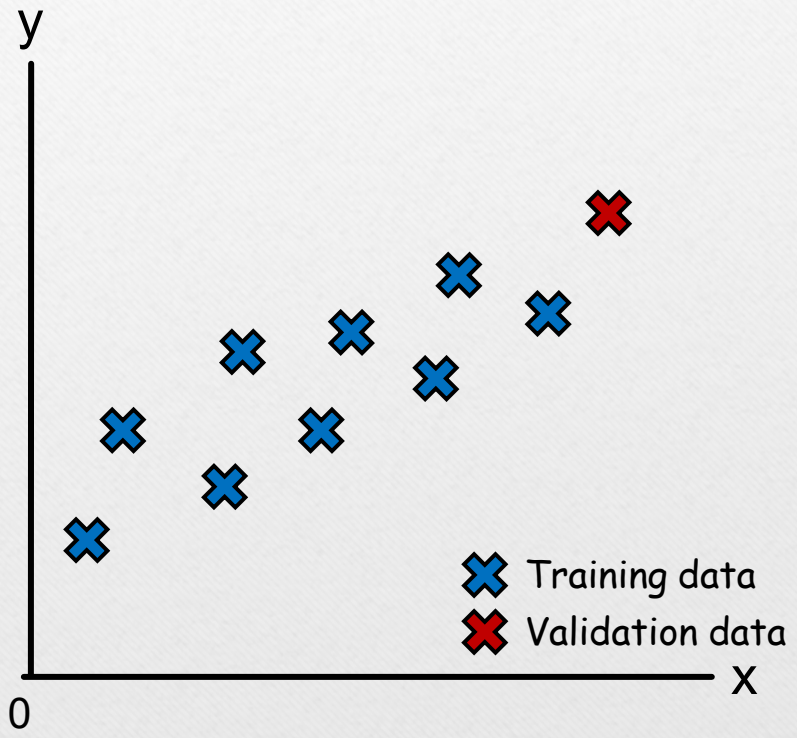
K-Fold Cross Validation

- Iteration 5



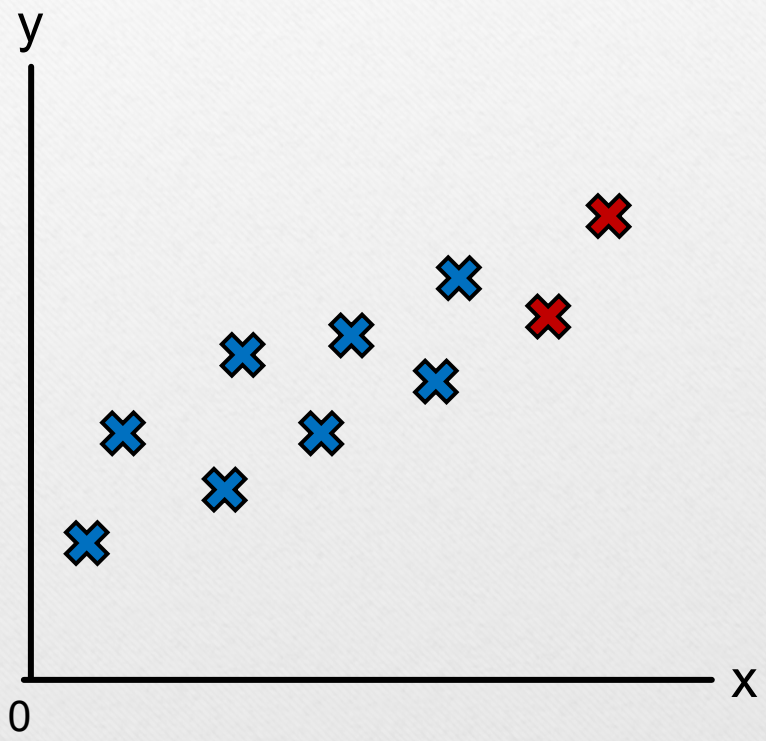
Leave-One-Out Validation

- If each fold only has one sample, the process is called leave-one-out validation (LOOV)



K-Fold Cross Validation

- Performance measures are averaged across folds
- K-fold cross validation trades training time for representativeness of validation data
- Might not be feasible when model is time consuming to train



Lasso Inference Models

- Have you ever had trouble figuring what control variables to add?
- Regression with automated control variable selection.
- Utilizes Lasso to select control variables. Strength of regularization can be selected through cross validation.
- Works even if the set of potential control variables is larger than the number of observations.

Lasso Inference Models

- Model $y = \mathbf{d}\alpha + \mathbf{x}\beta + \epsilon$
  - **d** is independent variables of interest
  - **x** is potential control variables
- **Double Selection Lasso Linear Regression**
  1. Run a Lasso for each d in **d** on **x**.
  2. Run a Lasso of y on **x**.
  3. Run OLS of y on **d** and **x** selected in step 1 and 2.