# CS 171: Intro to ML and DM

Christian Shelton

**UC** Riverside

Slide Set 5: Cross Validation



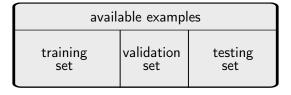
### Slides from CS 171

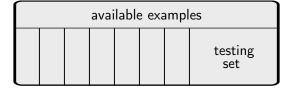
- From UC Riverside
  - CS 171: Introduction to Machine Learning and Data Mining
  - Professor Christian Shelton
- DO NOT REDISTRIBUTE
  - ► These slides contain copyrighted material (used with permission) from
    - ► Elements of Statistical Learning (Hastie, et al.)
    - Pattern Recognition and Machine Learning (Bishop)
    - An Introduction to Machine Learning (Kubat)
    - Machine Learning: A Probabilistic Perspective (Murphy)
  - ► For use only by enrolled students in the course

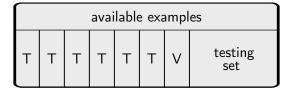
So, how to pick  $\lambda$ ?

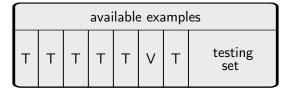
So, how to pick  $\lambda$ ? Cross validation! (or n-fold cross validation)

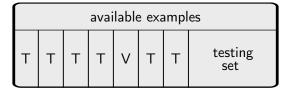
available examples	
training	testing
set	set

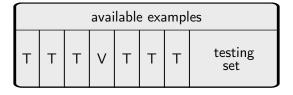


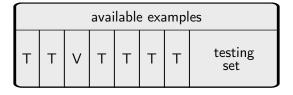


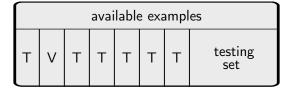


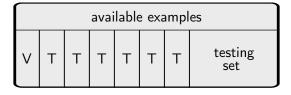












#### Cross Validation:

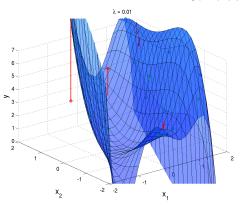
- Split Training data into two parts: Train and Validation
- $\bullet$  For each version (different k), train on train and check performance on validate
- Pick the version that does best on validation set

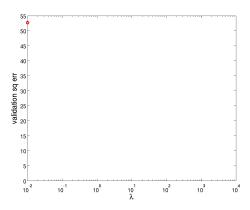
#### *n*-fold Cross Validation:

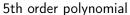
- ullet Do cross validation n times (n different train/validation splits)
- ullet Pick version (value of k) that does best on average across these n different trails
- ullet Most common: partition data into n equal-sized sets and use each one as validation once (and other n-1 sets as train)

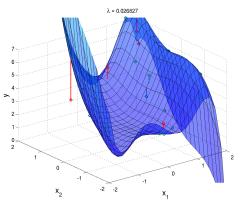
### Leave-one-out Cross Validation (LOO CV):

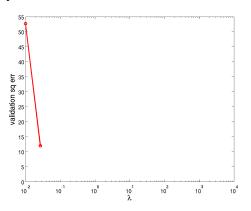
• n-fold Cross Validation where n=m

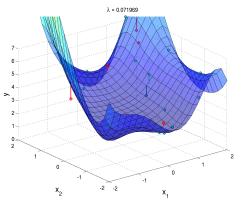


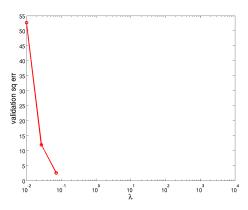


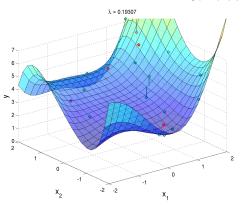


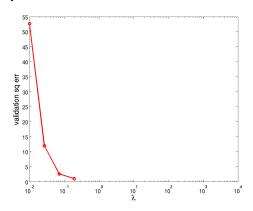


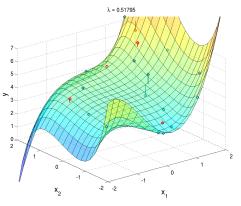


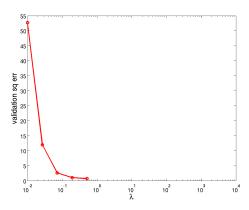


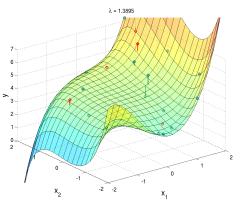


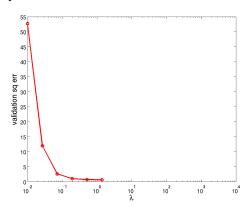


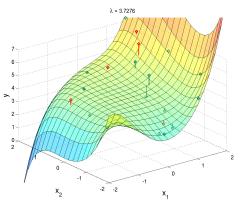


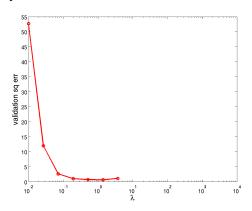


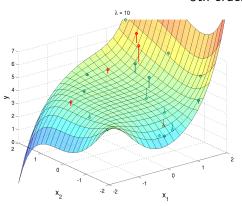


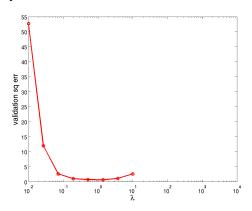


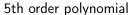


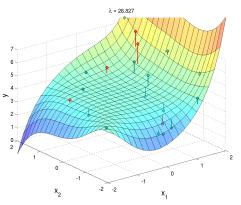


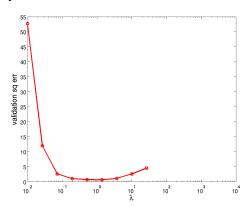


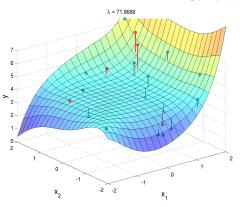


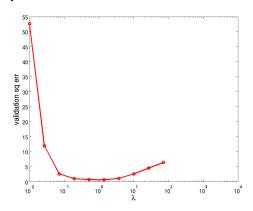


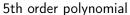


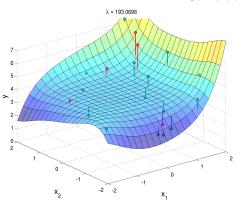


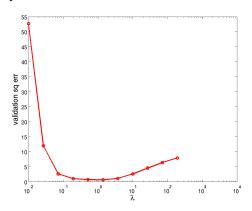


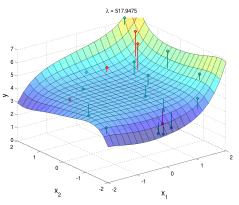


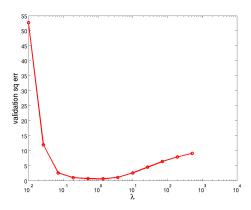


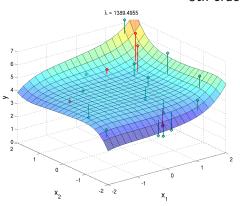


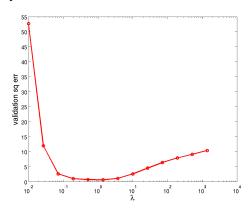


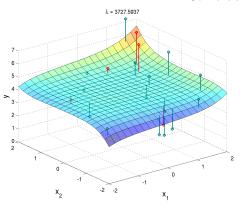


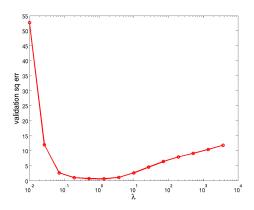


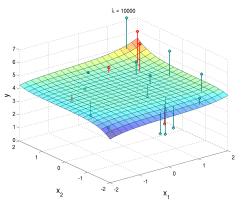


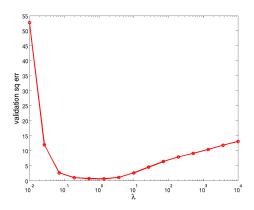












#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y, f) = (y - f)^2$$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

• Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

• Write down total loss/cost:

$$L = \sum_{i} l(y_i, f(x_i)) + R(w)$$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

• Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

• Write down total loss/cost:

$$L = \sum_{i} l(y_i, f(x_i)) + R(w)$$

ullet Figure out how to minimize L:

$$w = (X^{\top}X + \lambda I)^{-1}X^{\top}Y$$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

• Write down total loss/cost:

$$L = \sum_{i} l(y_i, f(x_i)) + R(w)$$

ullet Figure out how to minimize L:

$$w = (X^\top X + \lambda I)^{-1} X^\top Y$$

#### Algorithm Use:

- Pick a set of  $\lambda$ s,  $\Lambda$
- Divide Data into Training and Testing
- Divide Training into Training and Validation

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

• Write down total loss/cost:

$$L = \sum_{i} l(y_i, f(x_i)) + R(w)$$

ullet Figure out how to minimize L:

$$w = (X^\top X + \lambda I)^{-1} X^\top Y$$

#### Algorithm Use:

- Pick a set of  $\lambda$ s,  $\Lambda$
- Divide Data into Training and Testing
- Divide Training into Training and Validation
- For each  $\lambda \in \Lambda$ :
  - ▶ Train on Training set using  $\lambda$
  - Check average per-item loss on Validation set
  - If best loss so far, remember w and  $\lambda$

#### Algorithm Development:

• Pick form of function to be estimated:

$$f(x) = w^{\top} x$$

• Pick per-item loss/cost function:

$$l(y,f) = (y-f)^2$$

Pick regularizer:

$$R(w) = \lambda w^{\top} w$$

• Write down total loss/cost:

$$L = \sum_{i} l(y_i, f(x_i)) + R(w)$$

ullet Figure out how to minimize L:

$$w = (X^\top X + \lambda I)^{-1} X^\top Y$$

#### Algorithm Use:

- Pick a set of  $\lambda$ s,  $\Lambda$
- Divide Data into Training and Testing
- Divide Training into Training and Validation
- For each  $\lambda \in \Lambda$ :
  - ▶ Train on Training set using  $\lambda$
  - Check average per-item loss on Validation set
  - If best loss so far, remember w and  $\lambda$
- (Optional) Retrain on Training+Validation with best  $\lambda$
- ullet Report best w
- (If testing) Check average per-item loss on Testing set