S&DS 355 / 365 / 565

Data Mining and Machine Learning

Bias, Variance and Cross Validation

Tuesday, September 17th

Yale

Outline

- Finish off SGD
- Bias/variance redux
- Cross validation

SGD for general loss

SGD update:

$$\boldsymbol{\beta} \longleftarrow \boldsymbol{\beta} - \eta \nabla L(y, \boldsymbol{\beta}^T x)$$

$$\beta_j \longleftarrow \beta_j - \eta \frac{\partial L(y, \boldsymbol{\beta}^T x)}{\partial \beta_j}$$

- η is the *learning rate* or "step size"
- Needs to be chosen carefully, getting smaller over time

SGD: choice of learning rate

A conservative choice of learning rate is

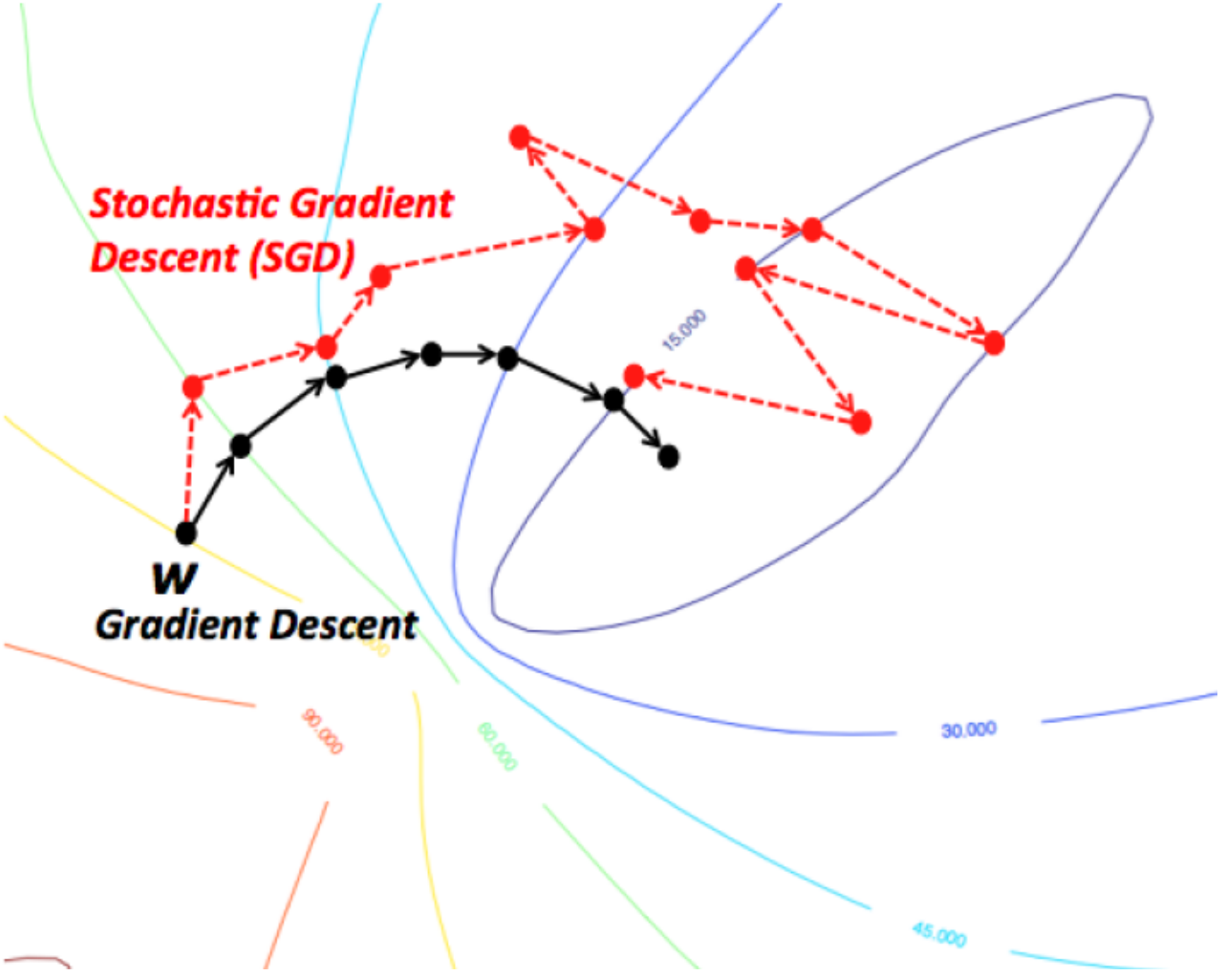
$$\eta_t = \frac{1}{t}$$

A more agressive choice is

$$\eta_t = \frac{1}{\sqrt{t}}$$

Which is more appropriate for GD?
Which is more appropriate for SGD?

Diagramatic Differences



SGD: choice of learning rate

Learning rate should scale as

$$\eta_t = \frac{1}{\sqrt{t}}$$

Problem: Some of the updates may be on different scales.

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Problem: Some of the updates may be on different scales.

Solution: Let $g_{tj} = \frac{\partial L(y_t, \beta^T x_t)}{\partial \beta_j}$

Scale gradients to get update rule

$$\beta_j \longleftarrow \beta_j - \eta \frac{g_{tj}}{\sqrt{\sum_{s=1}^{t} g_{sj}^2}}$$

SGD: scaling issues

For a linear model, the SGD update is

$$\beta_j \longleftarrow \beta_j - c_t x_j$$

If x_j increases by a factor of two, the weight β_j should decrease by a factor of two.

This update doesn't respect that scaling

SGD: scaling issues

Usual solution is to "standardize" each variable — subtract out the mean and divide by the standard deviation

$$x_j \leftarrow \frac{x_j - \text{mean}(x_j)}{\sqrt{\text{var}(x_j)}}$$

But this involves "looking ahead" to compute the mean and variance, and destroys the online property of the algorithm

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Solution: The mean and variance can be updated in an online manner, in constant time, by storing auxiliary variables for each component j.

SGD: Regularization

A "ridge" penalty $\lambda \sum_{j=1}^{d} \beta_j^2$ is easily handled.

Gradient changes by an additive term $2\lambda\beta_j$. Update becomes

$$\begin{aligned} \beta_j &\longleftarrow \beta_j + \eta\{(y-\pi)x_j - \lambda\beta_j\} \\ &= (1-\eta\lambda)\beta_j + \eta(y-\pi)x_j \end{aligned}$$

$$\beta_j x_j \longleftarrow (1-\eta\lambda)\beta_j x_j + \eta(y-\pi)x_j^2$$

Observe that this "does the right thing" whether β_j wants to be large positive or negative.

- *The penalty shrinks β_j toward zero*

Batch GD vs. SGD

- In a “batch” algorithm, we compute the exact gradient by summing over the entire training set
- In a “stochastic” algorithm, we tolerate noise in the estimate of the gradient, in exchange for speed
- Could also compute the gradient over “mini batches”
- Note: SGD is (apparently) difficult to parallelize

SGD: Linear regression

Batch gradient descent update step (using all $\{(x_i, y_i)\}_{i=1}^n$ observations):

$$\beta_j \leftarrow \beta_j + \rho \sum_{i=1}^{n} (y_i - x_i^t \beta) x_{ij}.$$

Stochastic gradient descent update (using a single observation (x, y)):

$$\beta_j \leftarrow \beta_j + \rho (y - x^t \beta) x_j.$$

SGD: Linear regression

Batch gradient descent update step (using all $\{(x_i, y_i)\}_{i=1}^n$ observations):

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Stochastic gradient descent update (using a single observation (x, y)):

$$\beta_j \leftarrow \beta_j + \rho (y - x^t \beta) x_j.$$

Equivalently,

$$\beta_j \leftarrow \beta_j + \rho (y - \widehat{y}) x_j.$$

SGD: Linear regression

$$\beta_j \leftarrow \beta_j + \rho(y - \widehat{y})x_j.$$

In words:

- Initialize all coefficients β_j to 0.
- For observation x:
  - Predict $\widehat{y} = x^t\beta$.
  - Observe true response y.
  - Update β so that $\widehat{y}$ is closer to y.

Stochastic Gradient Descent

Key points:

- Randomize data beforehand
- ρ (the learning rate) needs to be selected in a way that decreases with time
  - e.g. $\rho_t = \frac{1}{t}$, $\rho_t = \frac{1}{\sqrt{t}}$
- Scaling data can ensure that variance of variables don't interfere

$$x_j \leftarrow \frac{x_j - \text{mean}(x_j)}{\sqrt{\text{var}(x_j)}}$$

- Takes a windier path, and may not actually converge to the global minimum.

Model Selection

For purposes of prediction, **minimizing test error** is priority.

Recall our two error metrics for evaluating predictions $\widehat{f}(x_i)$:

- Regression:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{f}(x_i))^2$$

- Classification:

$$Err = \frac{1}{n}\sum_{i=1}^{n}\mathbb{1}\left\{\widehat{f}(x_i) \neq y_i\right\}$$

Bias-Variance Tradeoff

(Regression case)

Given $Y = f(X) + \epsilon$, where $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$, consider a predictor $\widehat{f}$.

Expected MSE for predicting a new Y at $X = x$ can be decomposed into:

$$E[(Y - \widehat{f}(x))^2] = Var(\widehat{f}(x)) + [Bias(\widehat{f}(x))]^2 + \sigma^2$$

Bias-Variance Tradeoff

$$E[(Y - \widehat{f}(x))^2] = Var(\widehat{f}(x)) + [Bias(\widehat{f}(x))]^2 + \sigma^2$$

- $Var(\widehat{f})$ is the amount of variability in our predictor with different training set.
- $Bias(\widehat{f})$ is the systematic error introduced by model approximation.
- σ^2 is *irreducible error*, inherent in the error term ϵ.

Bias-Variance Tradeoff

$$E[(Y - \widehat{f}(x))^2] = Var(\widehat{f}(x)) + [Bias(\widehat{f}(x))]^2 + \sigma^2$$

- $Var(\widehat{f})$ is the amount of variability in our predictor with different training set. Increases with increasing model flexibility.
- $Bias(\widehat{f})$ is the systematic error introduced by model approximation. Decreases with increasing model flexibility.
- σ^2 is *irreducible error*, inherent in the error term ϵ. Cannot get rid of this!

Need to balance bias and variance.

Bias-Variance

How does this apply to the k-NN algorithm?

Cross-Validation

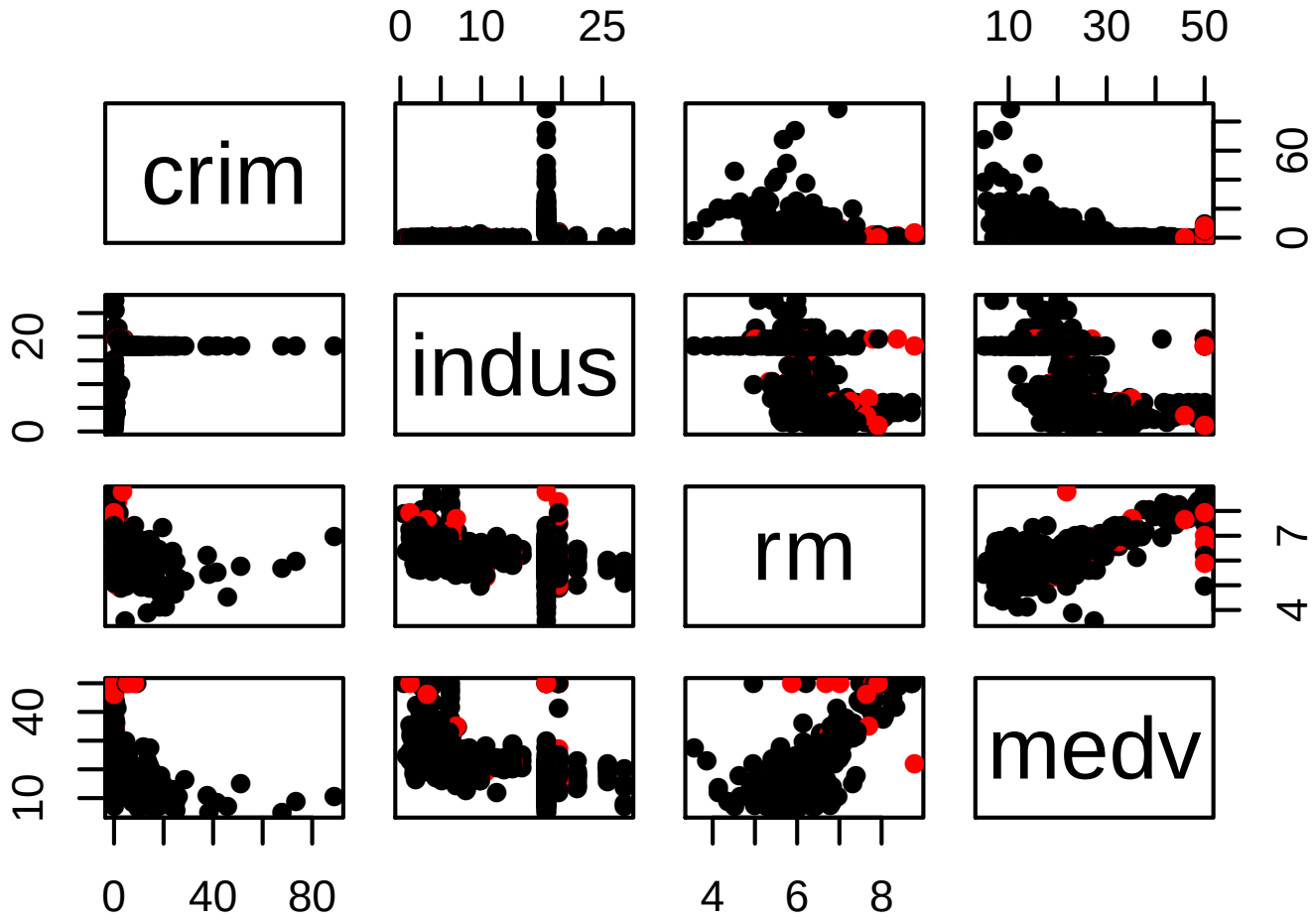
Data Bytes Podcast
Susan Wang

Cross-validation is an intuitive, widely-applicable approach for:

- model assessment
- model selection

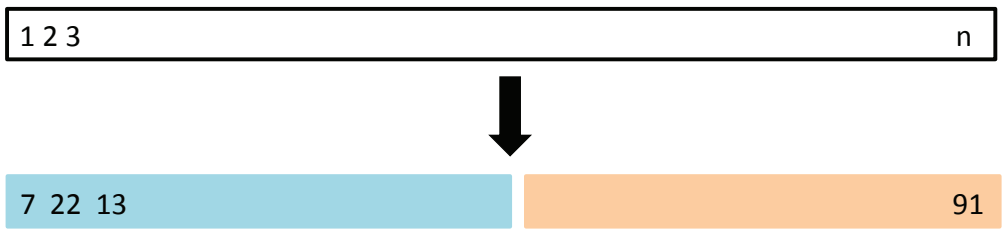
cross-validation is an extension of train-test split

Example: Boston Housing



Validation Sets

We've been doing this:



test/

1. Divide dataset randomly into a training set and a validation set.
2. Fit the model on the training set.
3. Use the validation set to obtain estimated test error.
4. Repeat!

Validation Sets

```
set.seed(365)
train <- sample(1:nrow(Boston), nrow(Boston)/2, replace=FALSE)
test <- Boston[-train,]
train <- Boston[train,]
m1 <- lm(medv ~ lstat, data=train)
p1 <- predict(m1, test)
```

Validation Sets

Example:

$$\widehat{medv} = \widehat{\beta}_0 + \widehat{\beta}_1 lstat$$

Estimated test error:

MSE ?

```
mean((p1 - test$medv)^2)
```

```
## [1] 43.57431
```

Validation Sets

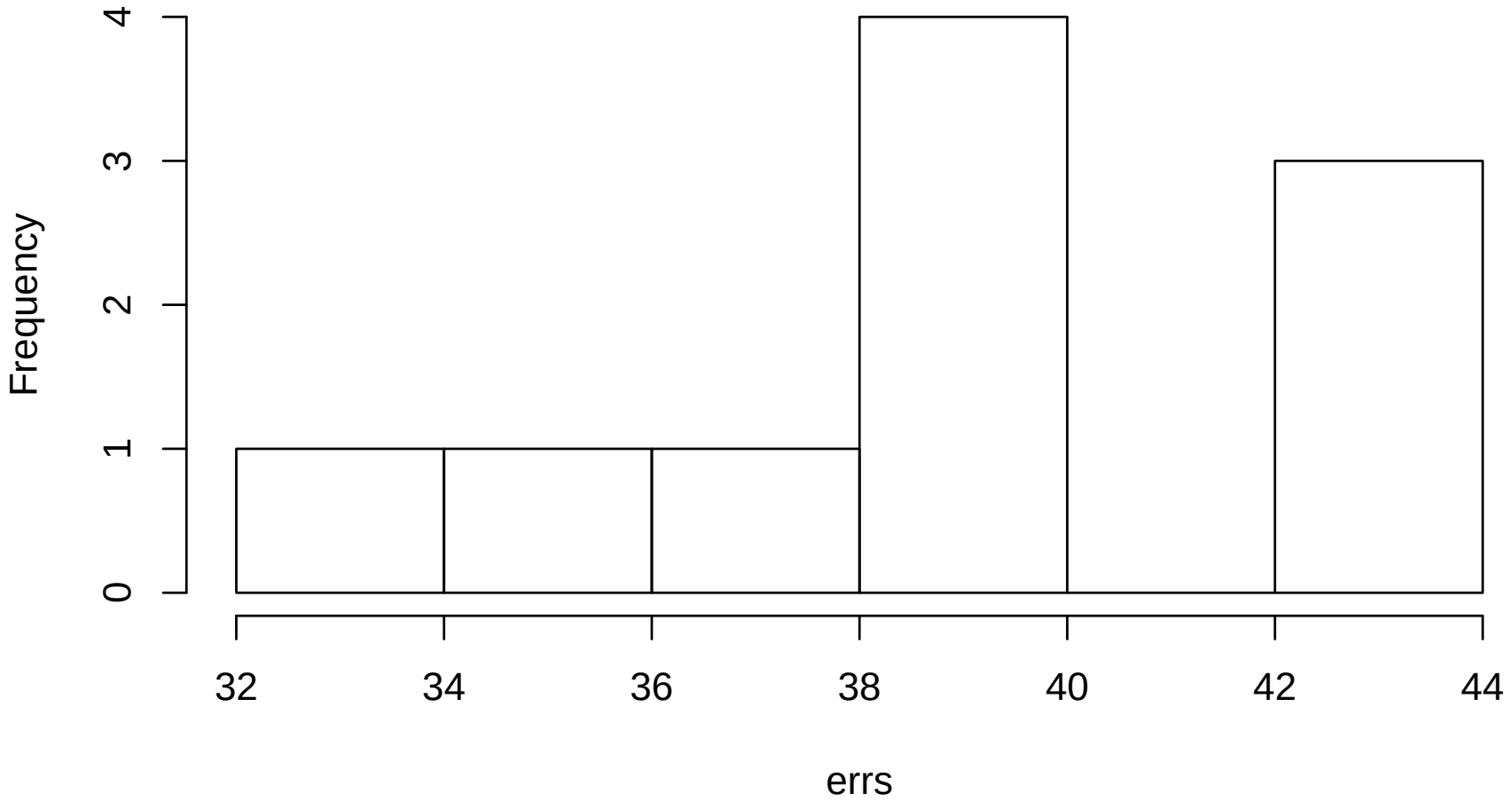
Repeat x 10:

```
set.seed(665)
errs <- rep(NA, 10)
for (i in 1:10) {
  train <- sample(1:nrow(Boston), nrow(Boston)/2, replace=FALSE)
  test <- Boston[-train,]
  train <- Boston[train,]
  m1 <- lm(medv ~ lstat, data=train)
  summary(m1)
  p1 <- predict(m1, test)
  errs[i] <- mean((p1 - test$medv)^2)
}
```

Histogram of errors

```
hist(errs, main="")
```

strange test errors



Validation Sets

- highly variable validation error
- only uses a fraction of the training set

Leave-One-Out Cross-Validation

How do we use more data to train with?

- Use a tiny validation set (e.g. (x_1, y_1))
- Train with the rest (e.g. $\{(x_2, y_2), \ldots, (x_n, y_n)\}$)

How do we feel about error rate evaluated on a single observation?

Leave-One-Out Cross-Validation

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How do we feel about error rate evaluated on a single observation?

Not good, but we can iterate through the dataset, each time using a different (x_i, y_i) as the validation set and obtaining an error MSE_i.

train using all data except 1 point (test) } do this for all n points

Leave-One-Out Cross-Validation

	Iteration					
Obs	1	2	3	4	...	n
1	valid	train	train	train	...	train
2	train	valid	train	train	...	train
3	train	train	valid	train	...	train
4	train	train	train	valid	...	train
...	...	...	...	...	...	...
n	train	train	...	...	...	valid
MSE	MSE_1	MSE_2	MSE_3	MSE_4	...	MSE_n

} take an average of all the MSE at the end

Leave-One-Out Cross-Validation

LOOCV estimate of test error is given by:

$$CV_{(n)} = \frac{1}{n} \sum_i MSE_i$$

MSE average

Leave-One-Out Cross-Validation

LOOCV estimate of test error is given by:

$$CV_{(n)} = \frac{1}{n} \sum_i MSE_i$$

For our example, a single number:

```
##        1
## 38.8901
```

Leave one out is computationally expensive → n times

k-fold Cross-Validation

Split data into k bins e.g k = 10 : 10 bins

A potentially faster approach:

- Randomly divide the dataset into k *folds*.
- For $b = 1, \ldots, k$:
  - Use b-th fold ("batch") as validation set.
  - Use everything else as training set.
  - Compute validation error on b-th fold.
- Estimate test error using:

(Leave one out is a special k-fold where k == n)

$$CV_{(k)} = \sum_b \frac{n_b}{n} MSE_b,$$

where n_b is the total # observations in the b-th fold, and n is the total # observations in the entire dataset.

k-fold Cross-Validation

	Iteration						
Obs	1	2	3	4	...	k	
1	valid	train	train	train	...	train	fold 1
2	valid	train	train	train	...	train	
3	valid	train	train	train	...	train	
4	train	valid	train	train	...	train	
...	...	...	...	...	...	...	
$n-2$	train	train	...	...	...	valid	fold v
$n-1$	train	train	...	...	...	valid	
n	train	train	...	...	...	valid	
MSE	MSE_1	MSE_2	MSE_3	MSE_4	...	MSE_k	

k-fold Cross-Validation

in iteration 1, the first fold is validation set

second fold is validation etc.

	Iteration						
Obs	1	2	3	4	...	k	
1	valid	train	train	train	...	train	fold 1
2	valid	train	train	train	...	train	
3	valid	train	train	train	...	train	
4	train	valid	train	train	...	train	
...	...	...	...	...	...	...	
$n-2$	train	train	...	...	...	valid	fold v
$n-1$	train	train	...	...	...	valid	
n	train	train	...	...	...	valid	
MSE	MSE_1	MSE_2	MSE_3	MSE_4	...	MSE_k	

n-fold CV is just LOOCV.

k-fold Cross-Validation

Running $k = 5$ and $k = 10$:

10 fold is usually the standard → computationally cheaper

```
set.seed(665)
kvals <- c(5, 10)
errs <- rep(0, length(kvals))
z <- Boston[sample(1:nrow(Boston)),]
for (j in 1:length(kvals)) {
  k <- kvals[j]
  folds <- as.numeric(cut(1:nrow(z), k))
  for (i in 1:k) {
    train <- z[folds != i,]
    valid <- z[folds == i,]
    m1 <- lm(medv ~ lstat, data=train)
    p1 <- predict(m1, test)
    errs[j] <- errs[j] +
         sum(folds==i)/nrow(z)*mean((p1-test$medv)^2)
  }
}
errs[1]/nrow(z)
```

```
## [1] 0.4546264
```

k-fold Cross-Validation

Estimated error for $k = 5$ and $k = 10$:

```
errs[1]/nrow(z)
```

```
## [1] 0.4546264
```

```
errs[2]/nrow(z)
```

```
## [1] 0.4546724
```

A slick shortcut

Suppose that the fitted values can be written $\widehat{Y} = LY$ where L is an $n \times n$ matrix.

This is the case for least squares regression

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This is the case for least squares regression

Then the leave-one-out-cross-validation error is

In the homework

$$R_{LOO} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{Y}_{(-i)})^2$$

$$\frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i - \widehat{Y}_i}{1 - L_{ii}}\right)^2$$

where L_{ii} is the ith diagonal entry.

In linear regression, you can do LOOCV without iterating through the entire dataset

A slick shortcut

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$$\frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i - \widehat{Y}_i}{1 - L_{ii}}\right)^2$$

where L_{ii} is the ith diagonal entry.

So, no need to fit n regressions!

Model Selection

So far, we've used it to estimate the test error. It's also useful for model selection.

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Suppose we are interested in comparing the following 3 models:

Model 1:

$$\widehat{medv} = \widehat{\beta}_0 + \widehat{\beta}_1 lstat$$

Model 2:

$$\widehat{log(medv)} = \widehat{\beta}_0 + \widehat{\beta}_1 lstat$$

Model 3:

$$\widehat{medv} = \widehat{\beta}_0 + \widehat{\beta}_1 lstat + \widehat{\beta}_2 lstat^2$$

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Model 3:

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We can use cross-validation to estimate the test error for each of these models, and select the model with the lowest test error.

What did we learn today?

- Cross validation is a practical way of estimating the variability of test error. Used for model selection.
- Leave-one-out CV is the most important version of CV. Has a shortcut formula.