Prediction and Crossvalidation

Mark M. Fredrickson (mfredric@umich.edu)

Computational Methods in Statistics and Data Science (Stats 406)

Cross Validation

Prediction

Suppose we have a sample of the form

$$(Y_i, \mathbf{X}_i) \overset{\text{iid}}{\sim} F$$

where $\mathbf{X}$ is a vector of **predictors** or **features**. We may or may not assume F

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Goal: **predict $\hat{Y}$ at certain $\mathbf{X}$**

- $\mathbf{X}$ may be cheap/easy to sample, but Y is expensive/difficult
- Wish to get understanding of Y where we have not observed $\mathbf{X}$

In many cases we will **condition on $\mathbf{X} = \mathbf{x}$** and **model $Y \mid \mathbf{X} = \mathbf{x}$** using some function $f(\mathbf{x})$.

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- Linear regression: $f(x_1, x_2, \ldots) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \ldots$
- Machine learning technique (support vector machines, deep learners, random forests)

Predictions and Loss Functions

A **loss function** scores how close a prediction and the true value are:

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The goal of the loss function is to capture **how expensive is an error**?

We'll come back to loss functions, but for now a concrete example is **squared error loss**:

$$l(f(\mathbf{x}^*), y \mid \mathbf{x}^*) = (y - f(\mathbf{x}^*))^2$$

Notice, f implicitly **depends on the original sample**:

$$f(\mathbf{x}^*) = f(\mathbf{x}^*, Y_1, \mathbf{X}_1, \ldots, Y_n, \mathbf{X}_n)$$

so I^* is a random quantity.

Sources of Randomness

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so I^* is a random quantity.

Additionally, if we are thinking about a new observation $Y^* = Y \mid \mathbf{x}^*$, then

$$I(f(\mathbf{x}^*), Y^*)$$

has **two sources of randomness** (the original sample and Y^*).

Operating Characteristics

As you might expect, we want to understand **operating characteristics** of loss functions. We could look at many things, but we'll focus on **expected loss**:

$$E\left(l(f(\mathbf{x}^*), Y^*)\right)$$

where the expectation is taken over the joint distribution of the original sample and a new observation (equiv.: by IID assumption, a sample of size $n+1$).

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Notice: when using **squared error loss** this is **similar but different than MSE**:

$$\mathrm{E}\left((\hat{\theta} - \theta)^2\right)$$

because θ is **fixed**.

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Want to note one way **not to compute**: use the sample:

$$\frac{1}{n}\sum_{i=1}^{n} l(f(\mathbf{x}_i), Y_i)$$

Since f and Y are **not independent** we risk **under estimating prediction error (overfitting)**.

Overfitting Example

Suppose we are predicting $Y \mid \mathbf{X} = \mathbf{x}$ using **an estimator of the conditional mean**: $\mu(\mathbf{x}) = \mathrm{E}\left(Y \mid \mathbf{x}\right)$.

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We'll see some examples later in the semester of **smoothing estimators** $\hat{\mu}(\mathbf{x})$ that are **unbiased for the conditional mean**:

$$\mathrm{E}\left(\hat{\mu}(\mathbf{x})\right) = \mu(\mathbf{x})$$

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Consider the case of using **squared error loss** and a new observation Y^*. What is our (true) expected loss?

True Expected Loss

$$\mathrm{E}\left((Y^* - \hat{\mu}(\mathbf{x}^*))^2\right) = \mathrm{E}\left({Y^*}^2\right) - 2\mathrm{E}\left(Y^*\hat{\mu}(\mathbf{x}^*)\right) + \mathrm{E}\left(\hat{\mu}(\mathbf{x}^*)^2\right)$$

True Expected Loss

$$
\begin{aligned}
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&= \mathrm{E}\left(Y^{*2}\right) - \mathrm{E}\left(Y^*\right)^2 + \mathrm{E}\left(Y^*\right)^2 + \\
&\quad \mathrm{E}\left(\hat{\mu}(\mathbf{x}^*)^2\right) - \mathrm{E}\left(\hat{\mu}(\mathbf{x}^*)\right)^2 + \mathrm{E}\left(\hat{\mu}(\mathbf{x}^*)\right)^2 - 2\mathrm{E}\left(Y^*\hat{\mu}(\mathbf{x}^*)\right)
\end{aligned}
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&= \mathrm{Var}\left(Y^*\right) + \mathrm{Var}\left(\hat{\mu}(\mathbf{x}^*)\right)
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Using the same sample to estimate prediction error

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$$\frac{1}{n}\sum_{i=1}^{n}\left[\hat{\mu}(\mathbf{x}_i) - Y_i\right]^2$$

This is generally **not unbiased** for the true prediction error because the $\hat{\mu}$ and Y_i are not independent and

$$\mathrm{E}\left(\hat{\mu}(\mathbf{x}_i) Y_i\right) \neq \mathrm{E}\left(\hat{\mu}(\mathbf{x}_i)\right) \mathrm{E}\left(Y_i\right)$$

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Solution: find another sample that is independent of the original to make our prediction error estimate.

Leave-one-out prediction

Recall, the **jackknife** estimates bias by **repeatedly dropping one observation**.

$$T_j = T(X_1, \ldots, X_{j-1}, X_{j+1}, \ldots, X_n)$$

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Since we assumed the observations were **independent**:

$$X_j \perp X_1, \ldots, X_{j-1}, X_{j+1}, \ldots X_n$$

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Idea: we could **predict** each X_j with T_j and **average over all** n. We call this "leave-one-out" (LOO) prediction.

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Differences between Hispanic and non-Hispanic families in social capital and child development: First-year findings from an experimental study

Adam Gamoran[a,*], Ruth N. López Turley[b], Alyn Turner[a], Rachel Fish[a]

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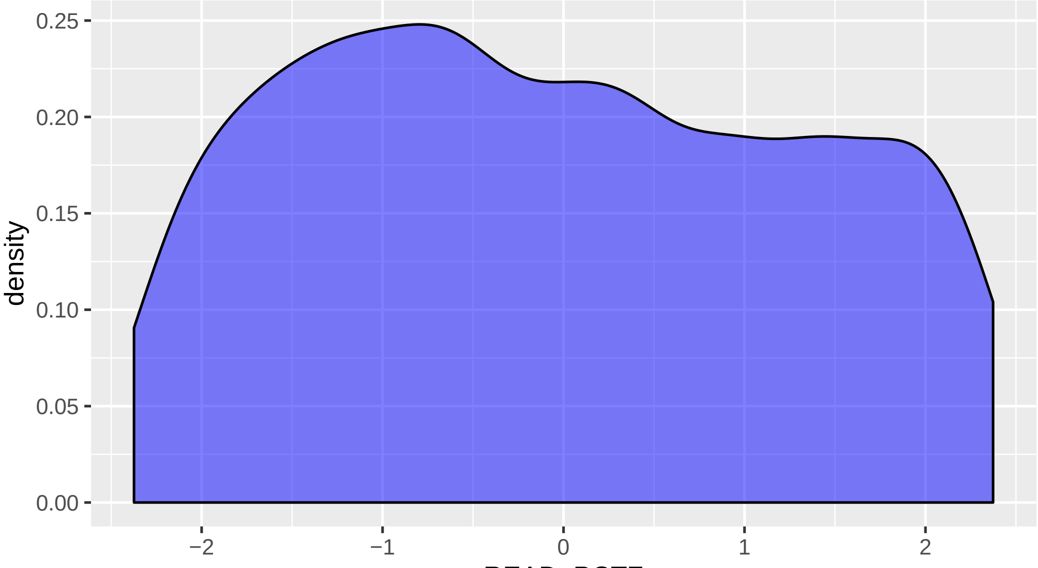
Reading test scores



Question: what would have less prediction error, the mean or mode?

Suppose we want to predict the reading score of a student not in the original study. What would have smaller error:

- The sample mean of the students in the study?

```
> mean(reading, na.rm = TRUE)
[1] -0.04814175
```

- The sample mode of a smoothed density?

```
> d <- density(reading)
> d$x[which.max(d$y)]
[1] -0.790038
```

Using the mean

Observe that if we drop X_j from the mean, we get:

$$\bar{X}_j = \frac{1}{n-1} \sum_{i \neq j} X_i = \frac{1}{n-1} \left(\left[\sum_{i=1}^{n} X_i \right] - X_j \right)$$

```
> n <- length(reading)
> barxj <- 1 / (n - 1) * (sum(reading) - reading)
```

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```
> n <- length(reading)
> barxj <- 1 / (n - 1) * (sum(reading) - reading)
```

We will estimate our squared error with the average of $(\bar{X}_j - X_j)^2$.

```
> err_mean <- barxj - reading
> (err2_mean <- mean(err_mean^2))
[1] 1.800303
```

Using the mode

```
> modej <- sapply(1:n, function(i) {
+     d <- density(reading[-i])
+     d$x[which.max(d$y)]
+ })
> err_mode <- modej - reading
> (err2_mode <- mean(err_mode^2))
```

```
[1] 2.349879
```

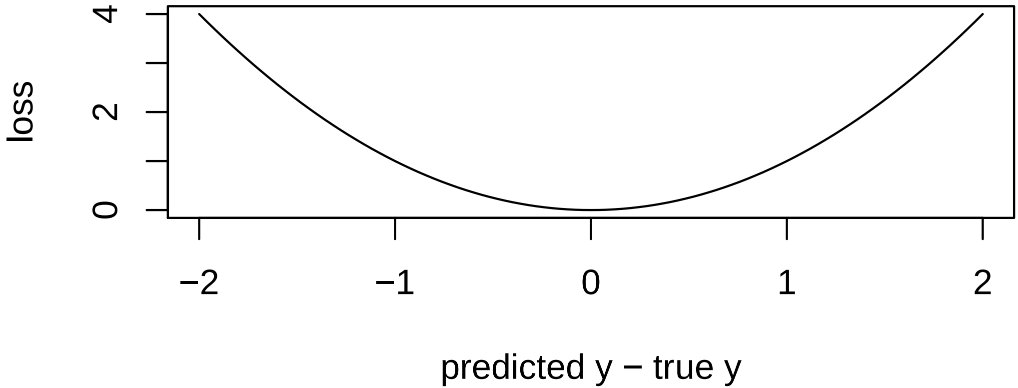
Which is larger than the predicted error using the mean:

```
> err2_mean / err2_mode
```

```
[1] 0.7661257
```

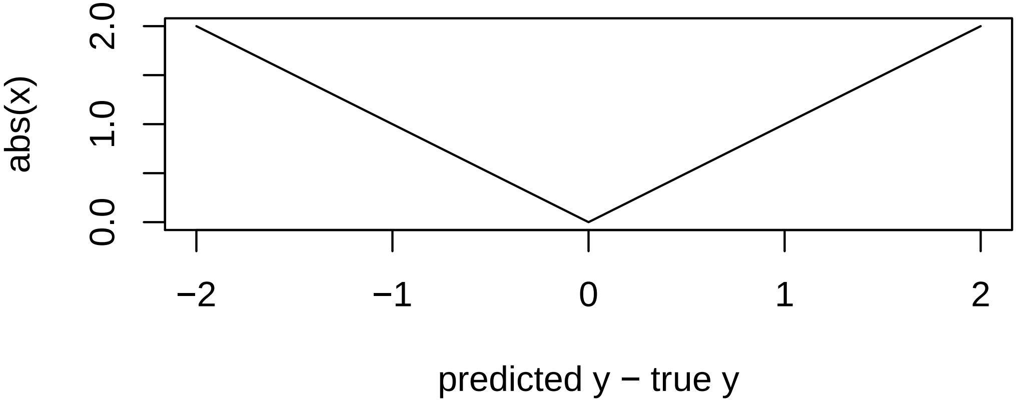
More on loss functions

We have been using **squared loss**

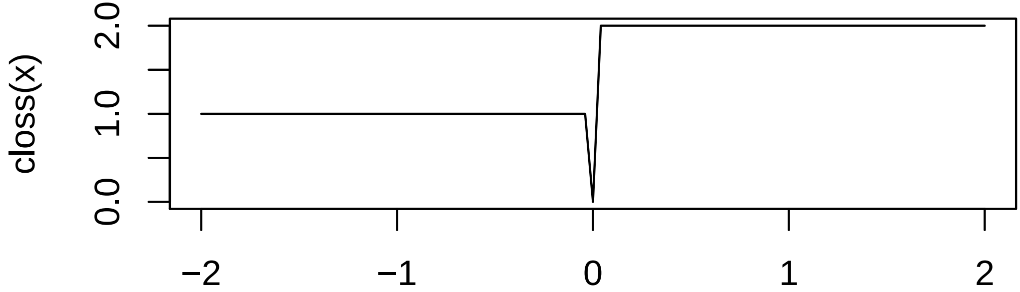


but we could consider other loss functions.

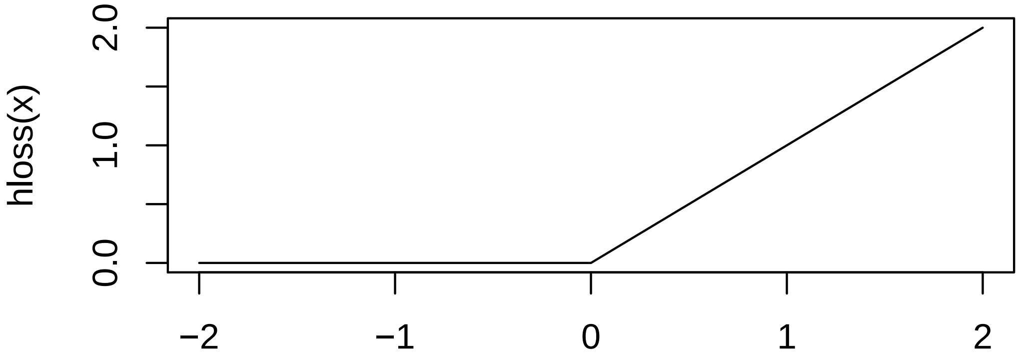
Absolute loss: $|Y^* - f(\mathbf{x}^*)|$



Constant loss: $a \times I(\hat{Y} > Y^*) + b \times I(\hat{Y} < Y^*)$



Hinge loss: $\max(0, \hat{Y} - Y^*)$



Different Loss, Different Conclusion

```
> mean(err_mean^2) / mean(err_mode^2) # squared error
[1] 0.7661257
> mean(abs(err_mean)) / mean(abs(err_mode)) # absolute error
[1] 0.9217158
> mean(closs(err_mean)) / mean(closs(err_mode)) # constant loss
[1] 1.121518
> mean(hloss(err_mean)) / mean(hloss(err_mode)) # hinge loss
[1] 2.268704
```

Picking a loss function

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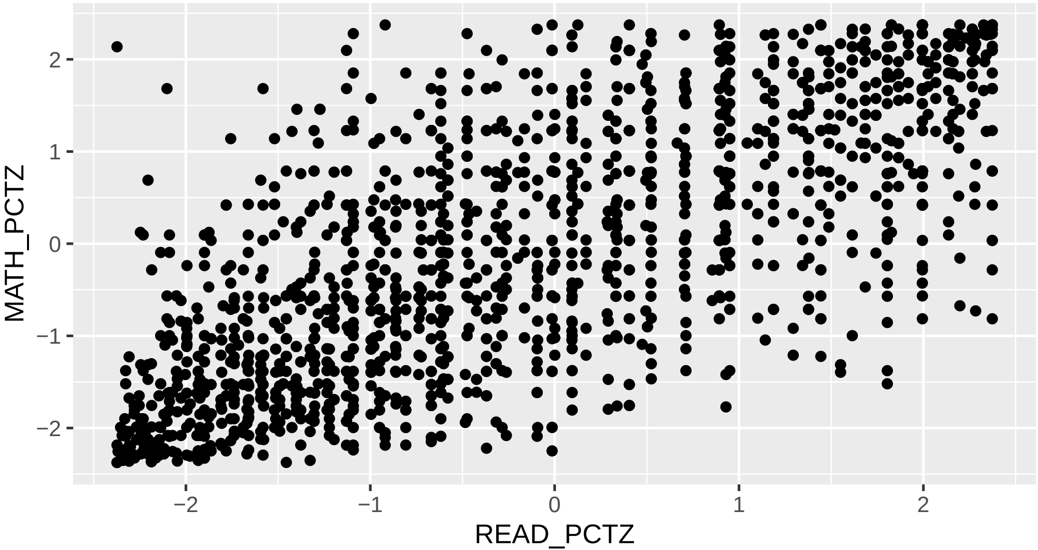
Best way: write down how costly mistakes are and deduce proper loss function.

More commonly, we use loss functions that are common to a discipline or industry.
(Similar to picking $\alpha = 0.05$ or $\alpha = 0.001$)

Predicting Math from Reading Scores



Using a linear model

We recently spent time working with a **linear model**:

$$Y = \beta_0 + \beta_1 X + R$$

where Y is an **outcome**, X is a **predictor**, and R is a **residual term**.

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If the **residual terms are Normal**, then OLS minimizes prediction error, but what if errors aren't Normal?

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For this example, we’ll generalize this idea by **leaving out half of the sample** and **predicting on the other half**.

We could just use a single split into a **training set** and a **testing set**.

We will repeat this process many times, **cross validation**.

Basic model fitting

```
> mod_lm <- lm(math ~ read, data = read_math)
> coef(mod_lm)

(Intercept)        read
 0.08581827  0.72495925
```

Cross validating

```
> k <- 1000
> n <- dim(read_math)[1]
> half <- round(n/2)
> err_lm <- replicate(k, {
+     rand.order <- sample.int(n)
+     train.idx <- rand.order[1:half]
+     test.idx <- rand.order[(half + 1):n]
+
+     mod <- lm(math ~ read, read_math[train.idx, ])
+     preds <- predict(mod, newdata = read_math[test.idx, ])
+     read_math$math[test.idx] - preds
+ })
```

Alternative to OLS

Let's compare the error we get from prediction using OLS to that we would get if pick β_0 and β_1 to minimize **absolute error** (**median regression**):

$$\min_{\beta} \sum_{i=1}^{n} |y_i - (\beta_0 + \beta_1 x_i)|$$

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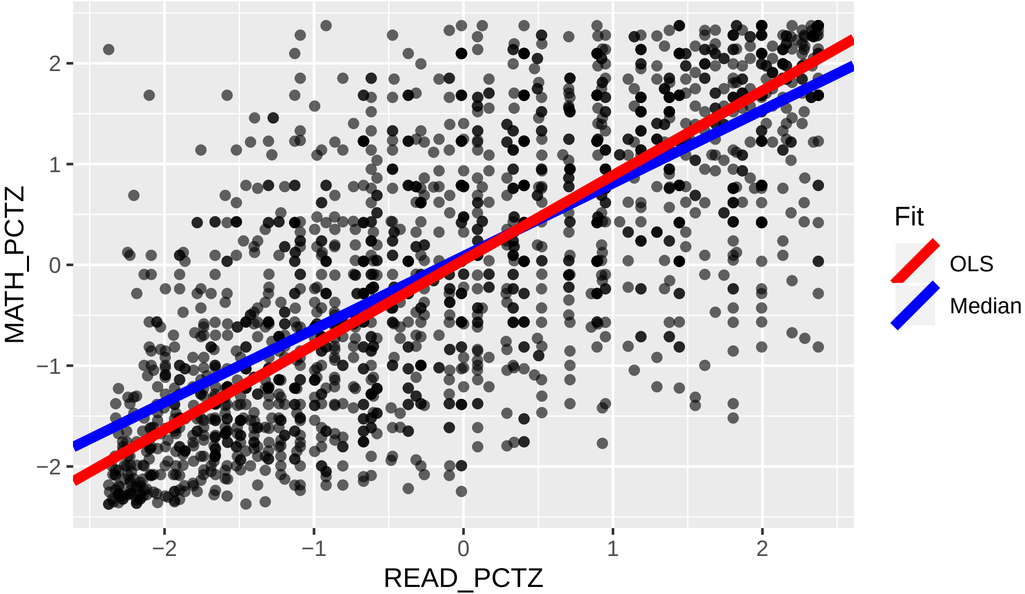
The `quantreg` package provides a routine to find β_0 and β_1:

```
> library(quantreg)
> mod_rq <- rq(math ~ read, data = read_math)
> coef(mod_rq)
```

```
(Intercept)        read
 0.04719007  0.84076874
```


MATH_PCTZ
2
1
0
−1
−2
−2
−1
0
1
2
READ_PCTZ
Fit
OLS
Median

```
> err_abs <- replicate(k, {
+     rand.order <- sample.int(n)
+     train.idx <- rand.order[1:half]
+     test.idx <- rand.order[(half + 1):n]
+
+     mod <- rq(math ~ read, data = read_math[train.idx, ]) # only differen
+     preds <- predict(mod, newdata = read_math[test.idx, ])
+     read_math$math[test.idx] - preds
+ })
```

Comparing OLS and median regression

```
> mean(err_lm^2) / mean(err_abs^2)
[1] 0.9712884
```

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```
> mean(err_lm^2) / mean(err_abs^2)
[1] 0.9712884
> mean(abs(err_lm)) / mean(abs(err_abs))
[1] 1.019969
```

Other Cross Validation Uses: Picking a model

We've used cross validation for **estimating prediction error**. Other uses include selecting a model to fit:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \quad \text{vs.} \quad Y = \beta_3 + \beta_4 x_1$$

The first model will always have smaller **in-sample prediction error**, but can **overfit** if x_2 actually is not important.

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The first model will always have smaller **in-sample prediction error**, but can **overfit** if x_2 actually is not important.

Also, using the same data set to pick a model as **perform inference** can lead to biased estimates, improper coverage rates, etc. **Post-selection inference** is a hot topic today, and many techniques boil down to cross-validation.

Tuning parameters

Many statistical methods have **tuning parameters**. For example the **LASSO shrinkage estimator**:

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We'll see examples later, for example picking a **"bandwidth" for density estimation.**

Summary

- **Prediction** guesses an unobserved Y^* based on observed $\mathbf{x}^*$ based on a prediction function $f(\mathbf{x}^*)$ which is created using a sample $(Y_i, \mathbf{X}_i)$.
- The quality of the prediction is given by **loss function** $l(Y^*, f(x^*))$
- There are **two sources of randomness**, the original sample and the Y^*.
- Key operating characteristic: **expected loss**
- Loss functions encode **costs of making mistakes** in predictions.
- Estimating expected loss can be achieved using **independent training and test sets**
- Many training/test splits are called **crossvalidation**.