# Machine Learning (in One Lecture) EC 607, Set 12

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# Prologue

## Schedule

### Last time

Resampling methods

### Today

A one-lecture introduction to machine-learning methods

### Upcoming

The end is near. As is the final.

# Prediction: What's the goal?

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### What's different?

Machine-learning methods focus on **prediction**. What's different?

Up to this point, we've focused on causal **identification/inference** of  $\beta$ , *i.e.*,

 $\mathbf{Y}_i = \mathbf{X}_i \boldsymbol{\beta} + u_i$ 

meaning we want an unbiased (consistent) and precise estimate  $\hat{\beta}$ .

With **prediction**, we shift our focus to accurately estimating outcomes.

In other words, how can we best construct  $\hat{\mathbf{Y}}_i$ ?

## Prediction: What's the goal?

#### ... so?

So we want "nice"-performing estimates  $\hat{y}$  instead of  $\hat{eta}$ .

**Q** Can't we just use the same methods (*i.e.*, OLS)?

**A** It depends. How well does your **linear**-regression model approximate the underlying data? (And how do you plan to select your model?)

*Recall* Least-squares regression is a great **linear** estimator.

Data data be tricky<sup>†</sup>—as can understanding many relationships.

**†** "Tricky" might mean nonlinear... or many other things...



#### Linear regression





#### Linear regression, linear regression $(x^4)$ , KNN (100)



#### Linear regression, linear regression $(x^4)$ , KNN (100), KNN (10)



#### Linear regression, linear regression $(x^4)$ , KNN (100), KNN (10), random forest



Note That example only had one predictor...

## What's the goal?

#### Tradeoffs

In prediction, we constantly face many tradeoffs, e.g.,

- **flexibility** and **parametric structure** (and interpretability)
- performance in **training** and **test** samples
- variance and bias

As your economic training should have predicted, in each setting, we need to **balance the additional benefits and costs** of adjusting these tradeoffs.

Many machine-learning (ML) techniques/algorithms are crafted to optimize with these tradeoffs, but the practitioner (you) still needs to be careful.

# What's the goal?

There are many reasons to step outside the world of linear regression...

Multi-class classification problems

- Rather than {0,1}, we need to classify  $y_i$  into 1 of K classes
- *E.g.*, ER patients: {heart attack, drug overdose, stroke, nothing}

#### Text analysis and image recognition

- Comb though sentences (pixels) to glean insights from relationships
- *E.g.*, detect sentiments in tweets or roof-top solar in satellite imagery

#### **Unsupervised learning**

- You don't know groupings, but you think there are relevant groups
- E.g., classify spatial data into groups



Stanford University (Stanford, CA) researchers have developed a deep-learning algorithm that can evaluate chest X-ray images for signs of disease at a level exceeding practicing radiologists.



Parking Lot Vehicle Detection Using Deep Learning



Gender Classifier	Darker Male	Darker Female	Lighter Male	Lighter Female	Largest Gap
Microsoft	94.0%	79.2%	100%	98.3%	20.8%
FACE**	99.3%	65.5%	99.2%	94.0%	33.8%
IBM	88.0%	65.3%	99.7%	92.9%	34.4%



Flexibility is huge, but we still want to avoid overfitting.

### What is it good for?

A lot of things. We tend to break statistical-learning into two(-ish) classes:

1. **Supervised learning** builds ("learns") a statistical model for predicting an **output** (y) given a set of **inputs**  $(x_1, \ldots, x_p)$ , *i.e.*, we want to build a model/function f

$$\mathbf{y} = \boldsymbol{f}(\mathbf{x}_1, \ldots, \mathbf{x}_p)$$

that accurately describes **y** given some values of  $\mathbf{x}_1, \ldots, \mathbf{x}_p$ .

2. **Unsupervised learning** learns relationships and structure using only **inputs**  $(x_1, \ldots, x_p)$  without any *supervising* output—letting the data "speak for itself."

**Semi-supervised learning** falls somewhere between these supervised and unsupervised learning—generally applied to supervised tasks when labeled **outputs** are incomplete.



### **Supervised Learning**

### **Unsupervised Learning**

Source

#### Output

We tend to further break **supervised learning** into two groups, based upon the **output** (the outcome we want to predict):

- 1. **Classification tasks** for which the values of **y** are discrete categories *E.g.*, race, sex, loan default, hazard, disease, flight status
- Regression tasks in which y takes on continuous, numeric values.
   E.g., price, arrival time, number of emails, temperature

*Note*<sup>1</sup> The use of *regression* differs from our use of *linear* regression.

*Note*<sub>2</sub> Don't get tricked: Not all numbers represent continuous, numerical values—*e.g.*, zip codes, industry codes, social security numbers.<sup>†</sup>

† **Q** Where would you put responses to 5-item Likert scales?

### The goal

As defined before, we want to *learn* a model to understand our data.

- 1. Take our (numeric) output y.
- 2. Imagine there is a function f that takes inputs  $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_p$ and maps them, plus a random, mean-zero error term  $\varepsilon$ , to the output.

 $\mathbf{y} = f(\mathbf{X}) + \varepsilon$ 

## Learning from $\hat{f}$

There are two main reasons we want to learn about f

- Causal inference settings How do changes in X affect y?
   What we've done all quarter.
- 2. **Prediction problems** Predict **y** using our estimated *f*, *i.e.*,

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

our *black-box setting* where we care less about f than  $\hat{\mathbf{y}}$ .<sup>†</sup>

Similarly, in causal-inference settings, we don't particulary care about  $\hat{\mathbf{y}}$ .

<sup>+</sup> You shouldn't actually treat your prediction methods as total black boxes.

### Prediction errors

As tends to be the case in life, you will make errors in predicting y.

The accuracy of  $\hat{\mathbf{y}}$  depends upon **two errors**:

- 1. **Reducible error** The error due to  $\hat{f}$  imperfectly estimating f. *Reducible* in the sense that we could improve  $\hat{f}$ .
- 2. **Irreducible error** The error component that is outside of the model f. *Irreducible* because we defined an error term  $\varepsilon$  unexplained by f.

*Note* As its name implies, you can't get rid of *irreducible* error—but we can try to get rid of *reducible* errors.

### Prediction errors

Why we're stuck with *irreducible* error

$$egin{aligned} &Eigg[\{\mathbf{y}-\hat{\mathbf{y}}\}^2igg] = Eigg[igg\{f(\mathbf{X})+oldsymbol{arepsilon}+\hat{f}\left(\mathbf{X}
ight)igg\}^2igg] \ &= \underbrace{igg[f(\mathbf{X})-\hat{f}\left(\mathbf{X}
ight)igg]^2}_{ ext{Reducible}} + \underbrace{ ext{Var}(oldsymbol{arepsilon})}_{ ext{Irreducible}} \end{aligned}$$

In less math:

- If  $\varepsilon$  exists, then X cannot perfectly explain y.
- So even if  $\hat{f} = f$ , we still have irreducible error.

Thus, to form our **best predictors**, we will **minimize reducible error**.

## Model accuracy

#### MSE

**Mean squared error (MSE)** is the most common<sup>†</sup> way to measure model performance in a regression setting.

$$ext{MSE} = rac{1}{n}\sum_{i=1}^{n}\left[ oldsymbol{y}_{i} - \hat{f}\left( x_{i} 
ight) 
ight]^{2}$$

Recall:  $y_i - \hat{f}(x_i) = y_i - \hat{y}_i$  is our prediction error.

Two notes about MSE

MSE will be (relatively) very small when **prediction error** is nearly zero.
 MSE **penalizes** big errors more than little errors (the squared part).

*† Most common* does not mean best—it just means lots of people use it.

### Training or testing?

Low MSE (accurate performance) on the data that trained the model isn't actually impressive—maybe the model is just overfitting our data.<sup>†</sup>

What we want: How well does the model perform **on data it has never seen**?

This introduces an important distinction:

- 1. **Training data**: The observations  $(y_i, x_i)$  used to **train** our model  $\hat{f}$ .
- 2. **Testing data**: The observations  $(y_0, x_0)$  that our model has yet to see and which we can use to evaluate the performance of  $\hat{f}$ .

#### **Real goal: Low test-sample MSE** (not the training MSE from before).

<sup>+</sup> Recall the kNN performance for k=1.

#### Regression and loss

For **regression settings**, the loss is our prediction's distance from truth, *i.e.*,

$$ext{error}_i = y_i - \hat{y}_i \qquad ext{loss}_i = \left| y_i - \hat{y}_i \right| = \left| ext{error}_i \right|$$

Depending upon our ultimate goal, we choose **loss/objective functions**.

$$egin{aligned} ext{L1 loss} &= \sum_i ig| oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig| & ext{MAE} &= rac{1}{n} \sum_i ig| oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig| \ ext{L2 loss} &= \sum_i ig| oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig|^2 & ext{MSE} &= rac{1}{n} \sum_i ig| oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig| \ ext{MSE} &= rac{1}{n} \sum_i ig| oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig|^2 \end{aligned}$$

Whatever we're using, we care about **test performance** (*e.g.*, test MSE), rather than training performance.

## Model accuracy

#### Classification

For classification problems, we often use the test error rate.

$$rac{1}{n}\sum_{i=1}^n \mathbb{I}(y_i 
eq \hat{y}_i)$$

#### The Bayes classifier

- 1. predicts class j when  $\Pr(y_0 = j | \mathbf{X} = \mathbf{x}_0)$  exceeds all other classes.
- 2. produces the **Bayes decision boundary**—the decision boundary with the lowest test error rate.
- 3. is unknown: we must predict  $\Pr(y_0 = j | \mathbf{X} = \mathbf{x}_0)$ .

# Flexibility

### The bias-variance tradeoff

Finding the optimal level of flexibility highlights the **bias**-variance tradeoff.

**Bias** The error that comes from inaccurately estimating f.

- More flexible models are better equipped to recover complex relationships (*f*), reducing bias. (Real life is seldom linear.)
- Simpler (less flexible) models typically increase bias.

**Variance** The amount  $\hat{f}$  would change with a different **training sample** 

- If new **training sets** drastically change  $\hat{f}$ , then we have a lot of uncertainty about f (and, in general,  $\hat{f} \not\approx f$ ).
- More flexible models generally add variance to *f*.

# Flexibility

#### The bias-variance tradeoff

The expected value<sup>†</sup> of the **test MSE** can be written

$$E\left[\left(\mathbf{y_0} - \hat{f}\left(\mathbf{X}_0\right)\right)^2\right] = \underbrace{\operatorname{Var}\left(\hat{f}\left(\mathbf{X}_0\right)\right)}_{\operatorname{Variance}} + \underbrace{\left[\operatorname{Bias}\left(\hat{f}\left(\mathbf{X}_0\right)\right)\right]^2}_{\operatorname{Bias}} + \underbrace{\operatorname{Var}(\varepsilon)}_{\operatorname{Irr. \ error}}$$

The tradeoff in terms of model flexibility

- Increasing flexibility *from total inflexibility* generally **reduces bias more** than it increases variance (reducing test MSE).
- At some point, the marginal benefits of flexibility **equal** marginal costs.
- Past this point (optimal flexibility), we **increase variance more** than we reduce bias (increasing test MSE).

**U-shaped test MSE** with respect to model flexibility (KNN here). Increases in variance eventually overcome reductions in (squared) bias.



MSE

Model flexibility
# Resampling refresher

**Resampling methods** help understand uncertainty in statistical modeling.

The process behind the magic of resampling methods:

- 1. Repeatedly draw samples from the training data.
- 2. **Fit your model**(s) on each random sample.
- 3. Compare model performance (or estimates) across samples.
- 4. Infer the **variability/uncertainty in your model** from (3).

# Resampling

### Hold out

*Recall:* We want to find the model that **minimizes out-of-sample test error**.

If we have a large test dataset, we can use it (once).

Q<sub>1</sub> What if we don't have a test set?

Q<sub>2</sub> What if we need to select and train a model?

 $Q_3$  How can we avoid overfitting our training<sup>†</sup> data during model selection?

A<sub>1,2,3</sub> Hold-out methods (*e.g.*, cross validation) use training data to estimate test performance—holding out a mini "test" sample of the training data that we use to estimate the test error.

### Option 1: The validation set approach

To estimate the **test error**, we can *hold out* a subset of our **training data** and then **validate** (evaluate) our model on this held out **validation set**.

- The validation error rate estimates the test error rate
- The model only "sees" the non-validation subset of the **training data**.

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#### Initial training set

### Option 1: The validation set approach

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### Option 1: The validation set approach

*Example* We could use the validation-set approach to help select the degree of a polynomial for a linear-regression model.

The goal of the validation set is to **estimate out-of-sample (test) error**.

**Q** So what?

- Estimates come with **uncertainty**—varying from sample to sample.
- Variability (standard errors) is larger with **smaller samples**.

**Problem** This estimated error is often based upon a fairly small sample (<30% of our training data). So its variance can be large.

#### Validation MSE for 10 different validation samples



#### **True test MSE** compared to validation-set estimates



### Option 1: The validation set approach

Put differently: The validation-set approach has  $(\geq)$  two major drawbacks:

- 1. **High variability** Which observations are included in the validation set can greatly affect the validation MSE.
- 2. **Inefficiency in training our model** We're essentially throwing away the validation data when training the model—"wasting" observations.

(2)  $\implies$  validation MSE may overestimate test MSE.

Even if the validation-set approach provides an unbiased estimator for test error, it is likely a pretty noisy estimator.

#### Option 2: Leave-one-out cross validation

**Cross validation** solves the validation-set method's main problems.

- Use more (= all) of the data for training (lower variability; less bias).
- Still maintains separation between training and validation subsets.

**Leave-one-out cross validation** (LOOCV) is perhaps the cross-validation method most similar to the validation-set approach.

- Your validation set is exactly one observation.
- New You repeat the validation exercise for every observation.
- *New* Estimate MSE as the mean across all observations.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation 1's turn for validation produces MSE<sub>1</sub>.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation 2's turn for validation produces MSE<sub>2</sub>.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation 3's turn for validation produces MSE<sub>3</sub>.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation 4's turn for validation produces MSE<sub>4</sub>.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation 5's turn for validation produces MSE<sub>5</sub>.

Each observation takes a turn as the **validation set**, while the other n-1 observations get to **train the model**.

Observation n's turn for validation produces MSE<sub>n</sub>.

Because **LOOCV uses n-1 observations** to train the model,<sup>†</sup> MSE<sub>i</sub> (validation MSE from observation i) is approximately unbiased for test MSE.

Problem MSE<sub>i</sub> is a terribly noisy estimator for test MSE (albeit ≈unbiased).
Solution Take the mean!

$$\mathrm{CV}_{(n)} = rac{1}{n}\sum_{i=1}^n \mathrm{MSE}_i$$

 LOOCV reduces bias by using n-1 (almost all) observations for training.
 LOOCV resolves variance: it makes all possible comparison (no dependence upon which validation-test split you make).

† And because often n-1 ≈ n.

#### True test MSE and LOOCV MSE compared to validation-set estimates



Leave-one-out cross validation is a special case of a broader strategy: **k-fold cross validation**.

- 1. **Divide** the training data into *k* equally sized groups (folds).
- 2. **Iterate** over the k folds, treating each as a validation set once (training the model on the other k 1 folds).
- 3. **Average** the folds' MSEs to estimate test MSE.

Benefits?

- 1. Less computationally demanding (fit model k = 5 or 10 times; not n).
- 2. **Greater accuracy** (in general) due to bias-variance tradeoff!
  - $\circ$  Somewhat higher bias, relative to LOOCV: n-1 vs. (k-1)/k.
  - Lower variance due to high-degree of correlation in LOOCV MSE<sub>i</sub>. ☜

With k-fold cross validation, we estimate test MSE as

$$\mathrm{CV}_{(k)} = rac{1}{k}\sum_{i=1}^k \mathrm{MSE}_i$$



Our k = 5 folds.

With k-fold cross validation, we estimate test MSE as

$$\mathrm{CV}_{(k)} = rac{1}{k}\sum_{i=1}^k \mathrm{MSE}_i$$

Each fold takes a turn at **validation**. The other k-1 folds **train**.

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$



For k = 5, fold number 1 as the **validation set** produces MSE<sub>k=1</sub>.

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$



For k = 5, fold number 2 as the **validation set** produces  $MSE_{k=2}$ .

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$

 $\bullet$ 

For k = 5, fold number 3 as the **validation set** produces MSE<sub>k=3</sub>.

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$



For k = 5, fold number 4 as the **validation set** produces MSE<sub>k=4</sub>.

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$



For k = 5, fold number 5 as the **validation set** produces MSE<sub>k=5</sub>.

## Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$ext{CV}_{(k)} = rac{1}{k} \sum_{i=1}^k ext{MSE}_i$$

**Test MSE** *vs.* estimates: LOOCV, 5-fold CV (20x), and validation set (10x)



Note: Each of these methods extends to classification settings, e.g., LOOCV

$$\mathrm{CV}_{(n)} = rac{1}{n}\sum_{i=1}^n \mathbb{I}(y_i 
eq \hat{y}_i)$$

#### Caveat

So far, we've treated each observation as separate/independent from each other observation.

The methods that we've defined so far actually need this independence.

#### Goals and alternatives

You can use CV for either of two important **modeling tasks:** 

- Model selection Choosing and tuning a model
- Model assessment Evaluating a model's accuracy

Alternative approach: Shrinkage methods

- fit a model that contains all *p* predictors
- simultaneously: shrink<sup>†</sup> coefficients toward zero

*Idea*: Penalize the model for coefficients as they move away from zero.

# Shrinkage

## Why?

Q How could shrinking coefficients twoard zero help or predictions?

A Remember we're generally facing a tradeoff between bias and variance.

- Shrinking our coefficients toward zero **reduces the model's variance**.<sup>+</sup>
- **Penalizing** our model for **larger coefficients** shrinks them toward zero.
- The **optimal penalty** will balance reduced variance with increased bias.

Now you understand shrinkage methods.

- Ridge regression
- Lasso
- Elasticnet

† Imagine the extreme case: a model whose coefficients are all zeros has no variance.

# Ridge regression

# Ridge regression

### Back to least squares (again)

Recall Least-squares regression gets  $\hat{\beta}_j$ 's by minimizing RSS, *i.e.*,

$$\min_{\hat{eta}} \mathrm{RSS} = \min_{\hat{eta}} \sum_{i=1}^{n} e_i^2 = \min_{\hat{eta}} \sum_{i=1}^{n} \left( y_i - \underbrace{\left[ \hat{eta}_0 + \hat{eta}_1 x_{i,1} + \dots + \hat{eta}_p x_{i,p} 
ight]}_{= \hat{y}_i} 
ight)^2$$

Ridge regression makes a small change

- adds a shrinkage penalty = the sum of squared coefficients  $\left(\lambda \sum_{j} \beta_{j}^{2}\right)$
- minimizes the (weighted) sum of RSS and the shrinkage penalty

$$\min_{\hat{eta}^R} \sum_{i=1}^n \left( {y_i - \hat{y}_i } 
ight)^2 + \lambda \sum_{j=1}^p eta_j^2$$

# **Ridge regression**

**Ridge regression** 

Least squares

$$\min_{\hat{eta}^R} \sum_{i=1}^n \left( {y_i - \hat{y}_i } 
ight)^2 + \lambda \sum_{j=1}^p eta_j^2$$

$$\min_{\hat{eta}} \sum_{i=1}^n \left( y_i - \hat{y}_i 
ight)^2$$

 $\lambda \ (\geq 0)$  is a tuning parameter for the harshness of the penalty.  $\lambda = 0$  implies no penalty: we are back to least squares. Each value of  $\lambda$  produces a new set of coefficients.

Ridge's approach to the bias-variance tradeoff: Balance

- reducing **RSS**, *i.e.*,  $\sum_{i} (y_i \hat{y}_i)^2$
- reducing **coefficients** (ignoring the intercept)

 $\lambda$  determines how much ridge "cares about" these two quantities.<sup>†</sup>

† With  $\lambda=0$ , least-squares regression only "cares about" RSS.
# **Ridge regression**

### $\lambda$ and penalization

Choosing a *good* value for  $\lambda$  is key.

- If  $\lambda$  is too small, then our model is essentially back to OLS.
- If  $\lambda$  is too large, then we shrink all of our coefficients too close to zero.

**Q** So what do we do?

A Cross validate!

(You saw that coming, right?)

## Penalization and standardization

Important Predictors' units can drastically affect ridge regression results.

**Why?** Because  $\mathbf{x}_j$ 's units affect  $\beta_j$ , and ridge is very sensitive to  $\beta_j$ .

Example Let  $x_1$  denote distance.

#### Least-squares regression

If  $x_1$  is *meters* and  $\beta_1 = 3$ , then when  $x_1$  is km,  $\beta_1 = 3,000$ . The scale/units of predictors do not affect least squares' estimates.

**Ridge regression** pays a much larger penalty for  $\beta_1 = 3,000$  than  $\beta_1 = 3$ . You will not get the same (scaled) estimates when you change units.

Solution Standardize your variables, *i.e.*, x\_stnd = (x - mean(x))/sd(x).

### Lasso

### Lasso

#### Intro

**Lasso** simply replaces ridge's *squared* coefficients with absolute values.

**Ridge regression** 

$$\min_{\hat{eta}^R} \sum_{i=1}^n ig( oldsymbol{y}_i - \hat{oldsymbol{y}}_i ig)^2 + \lambda \sum_{j=1}^p eta_j^2$$

Lasso

$$\min_{\hat{eta}^{L}}\sum_{i=1}^{n}\left(y_{i}-\hat{y}_{i}
ight)^{2}+\lambda\sum_{j=1}^{p}\left|eta_{j}
ight|$$

Everything else will be the same—except one aspect...

## Shrinkage

Unlike ridge, lasso's penalty does not increase with the size of  $\beta_j$ .

You always pay  $\lambda$  to increase  $|\beta_j|$  by one unit.

The only way to avoid lasso's penalty is to **set coefficents to zero**.

This feature has two **benefits** 

1. Some coefficients will be **set to zero**—we get "sparse" models.

2. Lasso can be used for subset/feature **selection**.

We will still need to carefully select  $\lambda$ .

#### **Ridge regression coefficents** for $\lambda$ between 0.01 and 100,000



#### **Lasso coefficents** for $\lambda$ between 0.01 and 100,000



# Machine learning

#### Wrap up

Now you understand the basic tenants of machine learning:

- How **prediction** differs from causal inference
- Bias-variance tradeoff (the benefits and costs of flexibility)
- Cross validation: Performance and tuning
- In- vs. out-of-sample **performance**

# Sources

Sources (articles) of images

- Deep learning and radiology
- Parking lot detection
- New Yorker writing
- Gender Shades

I pulled the comic from Twitter.