# Causality and supervised machine learning

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#### Introduction

What is the objective of empirical policy research?

- 1. causation: what is the effect of a particular variable on an outcome?
- 2. prediction: find some function that provides a good prediction of y as a function of

Χ

## Intution

$$y = \alpha + \beta x + \varepsilon$$

- causation: interested in  $\hat{\beta}$
- prediction: interested in  $\hat{y}$

## Preparation

```
In [1]: import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
import statsmodels.formula.api as smf # module for various regression models
sns.set()
%matplotlib inline
```

## **Causal Inference**

#### Introduction

Most statistical methods in social science theory is focused on estimating causal effects

Causal effect: how does the factor A affect B?

Examples of causal questions:

- what is the effect of being assigned to a shared group on communication?
- what is the effect of sterotypical names on job interview success?

#### Intuition

Variable of interest (often called treatment): Di

Outcome of interest: Yi

#### Potential outcome framework

$$Y_{i} = \begin{cases} Y_{1i} & \text{if } D_{i} = 1, \\ Y_{0i} & \text{if } D_{i} = 0 \end{cases}$$

The observed outcome Y<sub>i</sub> can be written in terms of potential outcomes as

$$Y_i = Y_{0i} + (Y_{1i} - Y_{0i})D_i$$

 $Y_{1i} - Y_{0i}$  is the *causal* effect of  $D_i$  on  $Y_i$ .

But we never observe the same individual i in both states. This is the **fundamental problem** of causal inference.

#### Selection Bias I

We need some way of estimating the state we do not observe (the *counterfactual*)

Usually, our sample contains individuals from both states

So why not do a naive comparison of averages by treatment status? i.e.

$$E[Y_i | D_i = 1] - E[Y_i | D_i = 0]$$

#### Selection Bias II

We can rewrite into:  $\left[Y_i|D_i=1\right] - E[Y_i|D_i=1] - E[Y_i|D_i=1] + \left[Y_i|D_i=1\right] - E[Y_i|D_i=1] + \left[Y_i|D_i=1\right] - E[Y_i|D_i=1] - E[Y_i|D_i=$ 

#### The decomposition:

- $E[Y_{1i}|D_i = 1] E[Y_{0i}|D_i = 1] = E[Y_{1i} Y_{0i}|D_i = 1]$ : the average causal effect of  $D_i$  on Y.
- $E[Y_{0i} | D_i = 1] E[Y_{0i} | D_i = 0]$ : difference in average  $Y_{0i}$  between the two groups. Likely to be different from 0 when individuals are allowed to self-select into treatment. Often referred to as **selection bias**.

## Random assignment solves the problem

Random assignment of  $D_i$  solves the problem because random assignment makes  $D_i$  independent of potential outcomes

That means that  $E[Y_{0i} | D_i = 1] = E[Y_{0i} | D_i = 0]$  and thus that the selection bias term is zero

Intuition: with random assignment, non-treated individuals can be used as counterfactuals for treated (what would have happened to individual i had he not received the treatment?)

This allows us to overcome the fundamental problem of causal inference

#### Randomization

Holland and Rubin (1986)

no causation without manipulation

As mentioned, we need to worry when individuals are allowed to self-select
This means that a lot of thought has to go into the *randomization phase*Randomization into treatment groups has to be manipulated by someone
But what about effect of *immutable characteristics* such as race, gender, etc.?

## **Quasi Experiments**

Quasi-experiments: randomization happens by "accident"

- Differences in Differences
- Regression Discontinuity Design
- Instrumental variables

#### **Randomized Controlled Trials**

Randomized controlled trials (RCT): randomization done by researcher

- Survey experiments
- Field experiments

Note: difficult to say one is strictly better than the other. Randomization can be impractical and/or unethical.

## **External & internal validity**

Internal validity: Refers to the validity of causal conclusions

External validity: Refers to the extent to which the conclusions of a particular study can be generalized beyond a particular setting

RCTs - external and internal validity

- Kosuke Imai (2016): There is tradeoff.
- Cyrus Samii (2016): No such tradeoff.

## Observational study

In many cases, social scientists are unable to randomize treatment assignment for ethical or logistic reasons

Observational study: No random manipulation of treatment

Strategy: Statistical control (control variables, fixed effects, matching, etc)

Risks: selection & confounding bias and endogeneity.

#### Case: Racial Discrimination in the Labor Market

Does racial discrimination exist in the labor market?

Experiment: In response to newspaper ads, researchers send out resumes of fictitious job candidates, varying only the names of the job applicants while leaving all other information in the resumes unchanges

Names were randomized between stereotypically black- and white-sounding names (Lakisha, Jamal, Emily, Greg, etc.)

### Case: Racial Discrimination in the Labor Market (2)

```
In [2]: gh_raw = "https://raw.githubusercontent.com/"
    user = "kosukeimai/"
    repo = 'qss/'
    branch = "master/"
    filepath = "CAUSALITY/resume.csv"
    url = gh_raw + user + repo + branch + filepath

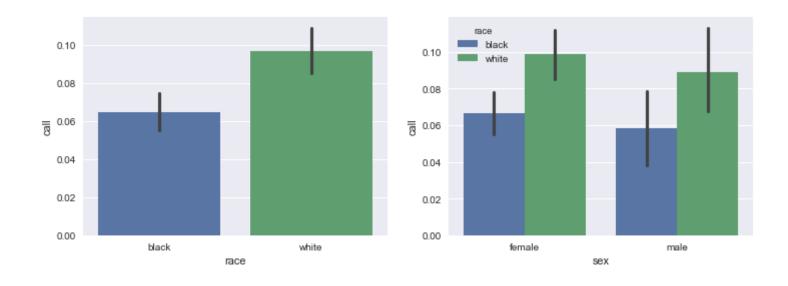
df = pd.read_csv(url,dtype={'race':'category','sex':'category'})
```

#### Case: Racial Discrimination in the Labor Market (3)

Can we use a boxplot?

```
In [3]: f, ax = plt.subplots(1,2,figsize=(12,4))
    sns.barplot(x='race', y='call', data=df, ax=ax[0])
    sns.barplot(x='sex', hue='race', y='call', data=df, ax=ax[1])
```

Out[3]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1d1e56a24e0>



Case: Racial Discrimination in the Labor Market (4)

```
In [4]: model = smf.ols(formula='call~race*sex', data=df)
    results = model.fit()
    results.summary()
```

#### Out[4]: OLS Regression Results

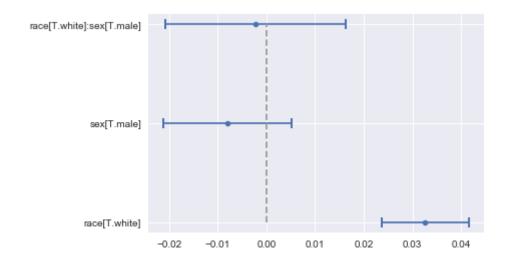
Dep. Variable:	call	R-squared:	0.004
Model:	OLS	Adj. R-squared:	0.003
Method:	Least Squares	F-statistic:	5.973
Date:	Sun, 13 Aug 2017	Prob (F-statistic):	0.000464
Time:	23:57:25	Log-Likelihood:	-561.75
No. Observations:	4870	AIC:	1131.
Df Residuals:	4866	BIC:	1157.
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P> t	[0.025	0.975]
Intercept	0.0663	0.006	10.595	0.000	0.054	0.079
race[T.white]	0.0326	0.009	3.677	0.000	0.015	0.050
sex[T.male]	-0.0080	0.013	-0.606	0.544	-0.034	0.018
race[T.white]:sex[T.male]	-0.0022	0.018	-0.121	0.904	-0.038	0.034

Omnibus:	2968.362	Durbin-Watson:	1.441
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#### Case: Racial Discrimination in the Labor Market (5)

Out[5]: [<matplotlib.lines.Line2D at 0x1d1e65c9c50>]



# Machine learning

## Topics in machine learning

Supervised Learning: Models designed to infer a relationship between input and labeled training data. These models are used for **prediction**.

Unsupervised Learning: Models designed to infer a relationship from **unlabeled** training data. This may involve clustering, dimensionality reduction and more.

Supervised machine learning

#### **Prediction**

Many policy problems are not about causality but rather about prediction

Sometimes called *prediction policy problems* 

- How many people will sign up for Obamacare?
- Who will win the U.S general election in November?
- Who should the Department of Economics hire in the future?

#### Who predicts?

- Local governments -> crime, childcare usage, pension payments etc.
- FB/GOOG/AMZN/NTFL/etc. > estimating 'preferences' to improve customer experience / sales
  - ads, status updates, music, movies, news
- Insurance companies -> what your risk of death is
- Stock traders > to trade
- Robots -> understanding their environment (e.g. self-driving cars)
- You? -> will Social Data Science be a fun/rewarding/interesting course to follow?

# Why predict? Glory!



#### The Netflix Contest

Competition started in October 2006. Training data is ratings for 18K movies by 400K Netflix customers, each rating between 1 and 5

Training data is very sparse - about 98% missing

Objective is to predict the rating for a set of 1 million customer-movie pairs that are missing in the training data

Winner: Averaged 800 models

#### Why predict? Riches!



# Improve Healthcare, Win \$3,000,000.

http://www.heritagehealthprize.com/c/hhp (http://www.heritagehealthprize.com/c/hhp)

### **Prediction problem types**

Predicition problems are often described in terms of the data types they are predicting.

- The first is **regression** which uses numeric (continuous) variables.
- The second is **classification** which uses categorical (discrete) variables.

## Case: Predicting gender from body shape

```
In [6]: gh_raw = "https://raw.githubusercontent.com/"
    user = "johnmyleswhite/"
    repo = 'ML_for_Hackers/'
    branch = "master/"
    filepath = "02-Exploration/data/01_heights_weights_genders.csv"
    url = gh_raw + user + repo + branch + filepath

    body = pd.read_csv(url)
    body['Male'] = (body.Gender=='Male').astype(float)
    body.Height = body.Height*2.56
    body.Weight = body.Weight*0.454
```

## Case: Predicting gender from body shape (2)

Do we already know any machine learning models?

```
In [7]: from sklearn.linear_model import LogisticRegression

X = body[['Weight', 'Height']]
y = body.Male

clf = LogisticRegression().fit(X, y)

pd.Series(clf.coef_[0],index=['Weight', 'Height'])

Out[7]: Weight    0.433517
Height    -0.186886
dtype: float64
```

## Predicting gender from body shape (3)

Logit estimates

$$P(Y_i = 1 | X_i = x_i) = \frac{1}{1 + e^{-x_i \beta}}$$

This probability is .5 when  $x_i\beta = 0$ . Thus we can classify predicted gender based on height and weight with the following rule:

$$\hat{y} = \begin{cases} 1 & \text{if } x_i \beta \ge 0, \\ 0 & \text{otherwise} \end{cases}$$

Classifier threshold:

$$H = \frac{-\alpha - \beta_W W}{\beta_H}$$

Predicting gender from body shape (4)

```
In [8]: | xx, yy = np.mgrid[25:125:.1, 130:210:.08]
         grid = np.c [xx.ravel(), yy.ravel()]
         probs = clf.predict proba(grid)[:, 1].reshape(xx.shape)
        f, ax = plt.subplots(figsize=(13, 7))
         contour = ax.contourf(xx, yy, probs, 25, cmap="RdBu",
                               vmin=0, vmax=1)
         ax c = f.colorbar(contour)
         ax c.set label("P(y = 1)")
         ax c.set ticks([0, .25, .5, .75, 1])
         plt.scatter(X.iloc[:,0], X.iloc[:,1], c=y, s=10,
                     cmap="RdBu", vmin=-.2, vmax=1.2,
                     edgecolor="white", linewidth=.5, alpha=.3)
         ax.set(aspect="equal",
                xlim=(25, 125), ylim=(130, 210),
                xlabel="Weight", ylabel="Height")
```

[(130, 210),

(25, 125),

None]

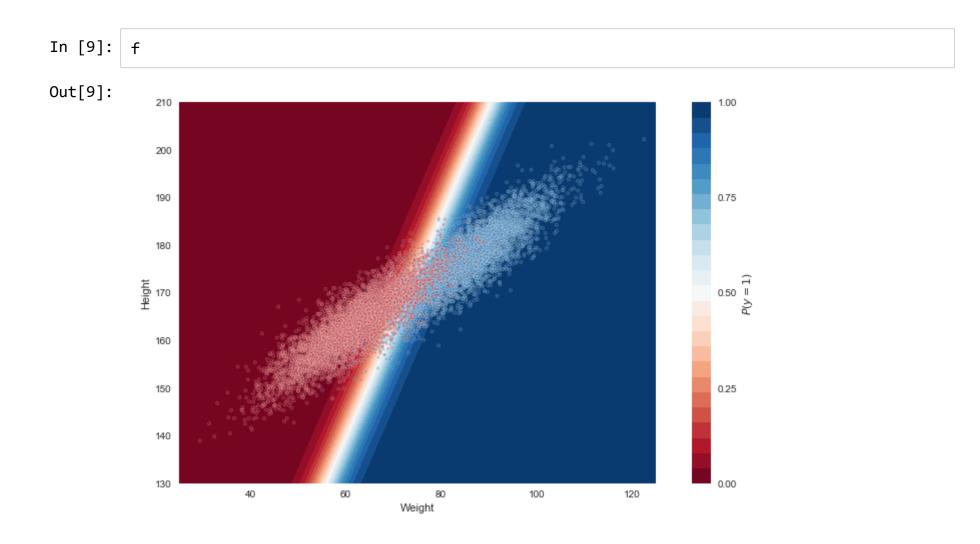
<matplotlib.text.Text at 0x1d1e88e6748>,

<matplotlib.text.Text at 0x1d1e88d1eb8>,

Out[8]:

## Predicting gender from body shape (5)

#### **Decision boundary**



### Predicting gender from body shape (6)

Another model: nearest neighbor

```
In [10]: from sklearn.ensemble import RandomForestClassifier
    from sklearn.neighbors import KNeighborsClassifier

X = body[['Weight', 'Height']]
y = body.Male

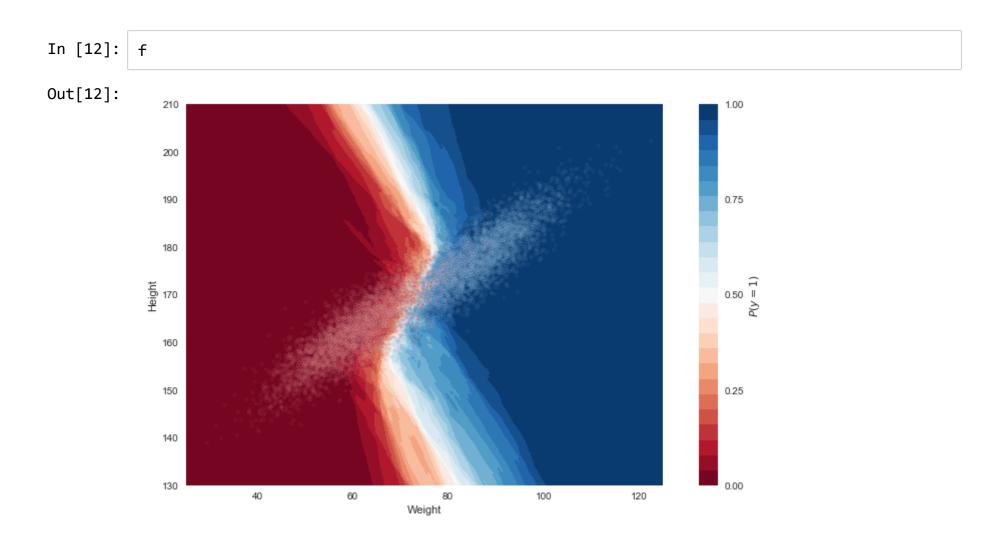
clf = KNeighborsClassifier(n_neighbors=50).fit(X, y)
```

# Predicting gender from body shape (7)

Computing nearest neighbor decision boundary

# Predicting gender from body shape (8)

#### **Decision boundary non-linear**



# Bias and variance

Are OLS and logistic regression good for prediction?

#### The bias-variance tradeoff

OLS is designed to minimize *in sample error*: the error rate you get on the same data set you used to build your predictor.

$$\underset{i=1}{\text{arg min}} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2 = \underset{\beta}{\text{arg min}} (V(\hat{f}(x_0)) + \sigma^2)$$

But for prediction we are interested in minimizing *out of sample error*: the error rate you get on a new data set

#### **Prediction**

Too see this, consider a prediction at a new point (out-of-sample),  $x_0$ . Our prediction for  $y_0$  is then  $\hat{f}(x_0)$  and the mean squared error (MSE) can be decomposed as

$$E[(y_0 - \hat{f}(x_0))^2] = E[\hat{f}(x_0) - f(x_0)]Bias(\hat{f}(x))^2 + E[\hat{f}(x_0)^2] - E[\hat{f}(x_0)]^2 Var(\hat{f}(x)) + \sigma^2$$

By ensuring zero bias within sample, OLS picks a solution which not be optimal for prediction

• in many cases we can lower variance while increasing bias a little.

#### Bias and variance

What do we mean by the *variance* and *bias* of an estimator?

- *Bias*: Comes from using erroneous model assumptions, e.g. fitting non-linear fct. f with linear fct. f.
  - Can lead to missing relevant patterns in data, i.e. underfitting.
- Variance: Refers to model complexity. If the model is too complex then small changes to the data will cause the solution to change a lot.
  - Can lead to finding spurious patterns in data, i.e. overfitting.

Machine learning techniques were developed specifically to maximize prediction performance by providing an empirical way to make this bias-variance trade off

#### Bias and variance (2)

So why do we care about bias?

- By not modelling bias: allows *inference*, i.e. testing hypotheses! (model parameters converge to true parameters)
- By modelling bias: allows better predictive models as they trade off bias and variance.

**Out-of-sample measures** 

### **Key concepts**

- Training data: where we estimate our model
- Test data: where we evaluate the model's accuracy

#### **Error**

Statistical learning models are designed to minimize *out of sample error*: the error rate you get on a new data set

Key ideas

- Out of sample error is what you care about
- In sample error < out of sample error
- The reason is overfitting (matching your algorithm to the data you have)

#### Error measures (continuous variables)

Mean absolute error (MAE):

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |\hat{y}_i - y_i|$$

Mean squared error (MSE):

MSE = 
$$\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$$

Root mean squared error (RMSE):

$$\sqrt{\text{MSE}}$$

**Question:** what is the difference?

#### Case: Longevity

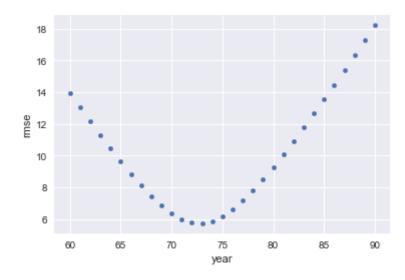
```
In [14]: gh_raw = "https://raw.githubusercontent.com/"
    user = "johnmyleswhite/"
    repo = "ML_for_Hackers/"
    branch = "master/"
    filepath = "05-Regression/data/longevity.csv"
    url = gh_raw + user + repo + branch + filepath
    longevity = pd.read_csv(url)
    print(longevity.head())
```

	Smokes	AgeAtDeath
0	1	75
1	1	72
2	1	66
3	1	74
4	1	69

#### Case: Longevity (2)

Best guess: 73

Out[15]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1d18289b0b8>



# **Cross validation (CV)**

#### Test and training data

Accuracy on the training set (resubstitution accuracy) does not capture bias and therefore is optimistic. A better estimate comes from an independent set (test set accuracy). Strategy:

- Use share of observations for training
- Use other of observations for testing model (out-of-sample)

So we estimate the test data accuracy with the model calibrated on training data.

#### Data split

Why not just divide data randomly the data into a test and training set?

Two drawbacks

- 1. RMSE is very sensitive to which observations are used for test and training.
- 2. RMSE is artificially large as not all observations are used for training model (model becomes more accurate for more observations)

One very useful refinement of the test-training data approach is *cross-validation* use multiple splits.

#### K-fold Cross Validation

- 1. Divide the data into k roughly equal subsets and label them s = 1, ..., k.
- 2. Fit your model using the k 1 subsets other than subset s
- 3. Predict for subset s and calculate RMSE
- 4. Stop if s = k, otherwise increment s by 1 and continue

The k fold CV estimate is computed by averaging the mean squared errors (  $MSE_1, ..., MSE_k$ )

$$CV_k = \frac{1}{k} \sum_{i=1}^{k} MSE_i$$

Common choices for k are 3, 5 and 10.

CV can (and should) be used both to decide hyperparameters and to report goodness-of-fit measures.

#### K-fold Cross Validation (2)

<img src="http://sebastianraschka.com/images/faq/evaluate-a-model/k-fold.png
(http://sebastianraschka.com/images/faq/evaluate-a-model/k-fold.png)", width="1000" >

#### Fitting polynomial

### Fitting polynomial (2)

```
In [27]: from sklearn.linear_model import LinearRegression

X_s = []
    rmse_in_sample = []

for i in range(1,10):
        X_s.append(x_range**i)
        X = np.vstack(X_s).T

    model = LinearRegression().fit(X,y)
    y_pred = model.predict(X)

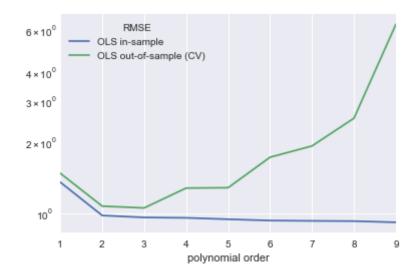
    rmse_in_sample.append(np.sqrt(mse(y, y_pred)))
```

#### Fitting polynomial (3)

```
In [28]:
         from sklearn.model_selection import KFold
         kf = KFold(n splits=10, random state=123)
         X s = []
         rmse CV = []
         for i in range(1,10):
             X s.append(x_range**i)
             X = np.vstack(X s).T
              rmse fold = []
              # cross validation loop
              for train_index, test_index in kf.split(X):
                 X train, X test = X[train index], X[test index]
                 y train, y test = y[train index], y[test index]
                  model = LinearRegression().fit(X_train,y_train)
                 y pred = model.predict(X test)
                  rmse = np.sqrt(mse(y_test, y_pred))
                  rmse fold.append(rmse)
              rmse CV.append(np.mean(rmse fold))
```

#### Fitting polynomial (4)

Why does in-sample and out-of-sample estimates of RMSE diverse?



#### Regularization

Why do we regularize?

• To avoid overfitting and thus have better predictions

How do we regularize?

We make models which are less complex by reducing the number and/or size of the coefficients.

### Regularization (2)

What does regularization look like?

We add a penalty term our optimization procedure:

$$\arg \min_{\beta} E[(y_0 - \hat{f}(x_0))^2]MSE + \lambda \cdot R(\beta)$$
 penalty

Introduction of penalties implies that increased model complexity has to be met with high increases precision of estimates.

# Regularization (3)

What are some used penalty functions?

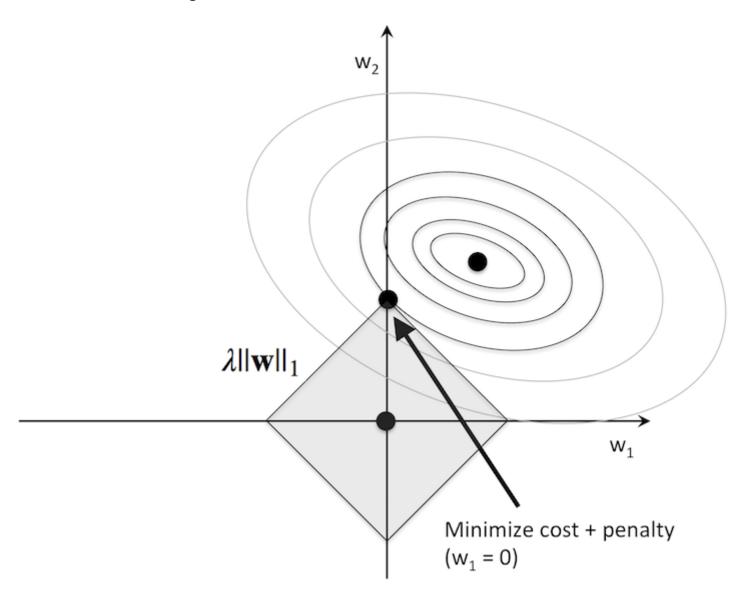
The two most common penalty functions are L1 and L2 regularization.

- L1 regularization (*Lasso*):  $R(\beta) = \sum_{j=1}^{p} |\beta_j|$ 
  - Makes coefficients sparse, i.e. selects variables by removing some (if  $\lambda$  is high)
- L2 regularization (*Ridge*):  $R(\beta) = \sum_{j=1}^{p} \beta_j^2$ 
  - Reduce coefficient size
  - Fast due to analytical solution

To note: The Elastic Net uses a combination of L1 and L2 regularization.

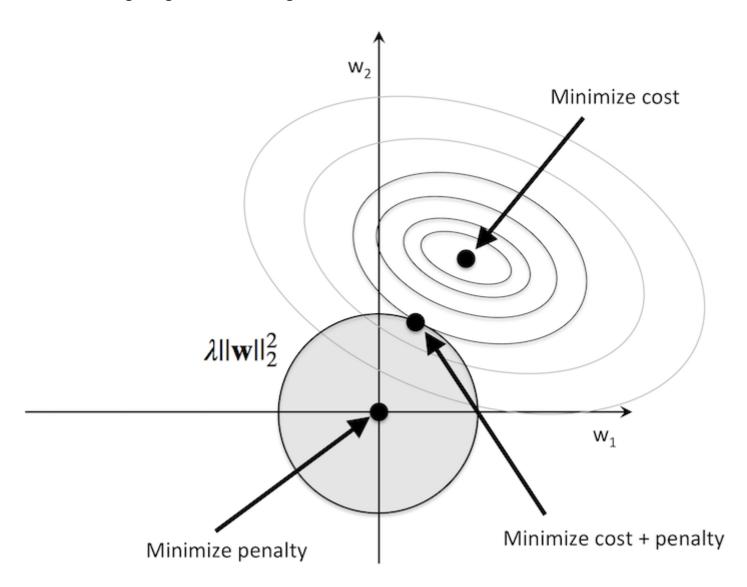
# Regularization (4)

How the Lasso (L1 reg.) deviates from OLS



# Regularization (5)

How the Ridge regression (L2 reg.) deviates from OLS



Models for supervised machine learning

#### Model overview

#### Parametric models

- linear models
  - unbiased: OLS
  - biased: *Lasso* (L1), *Ridge* (L2) (regulariation)
- classifier
  - unbiased: logistic

#### Other models

- random forest
- nearest neighbor
- neural networks

#### Fitting polynomial (5)

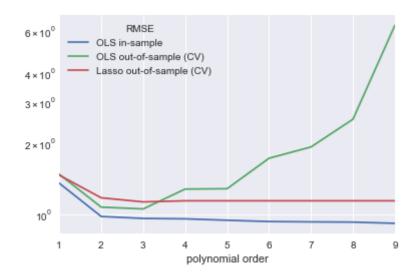
Training the model with Lasso

```
In [30]:
         from sklearn.model_selection import KFold
         from sklearn.linear_model import Lasso
         kf = KFold(n splits=10, random state=123)
         X s = []
         rmse CV L = []
         for i in range(1,10):
             X s.append(x range**i)
             X = np.vstack(X s).T
             rmse fold = []
             # cross validation loop
             for train index, test index in kf.split(X):
                 X train, X test = X[train index], X[test index]
                 y train, y test = y[train index], y[test index]
                 y pred = Lasso(alpha=0.05).fit(X train,y train).predict(X test)
                  rmse = np.sqrt(mse(y_test, y_pred))
                  rmse fold.append(rmse)
              rmse CV L.append(np.mean(rmse fold))
```

# Fitting polynomial (6)

Lasso vs OLS performance

```
In [31]: f,ax = plt.subplots()
    rmse_df['Lasso out-of-sample (CV)'] = rmse_CV_L
    rmse_df.plot(ax=ax)
    ax.set_yscale('log')
```



# Fitting polynomial (7)

Tuning The Lasso

```
In [32]:
        X = np.vstack(X s).T
         rmse CV lambda = []
         coef CV lambda = []
         for 1 in np.arange(.0001,.01,.0001):
             # cross validation loop
             rmse fold = []
             for train index, test index in kf.split(X):
                 X train, X test = X[train_index], X[test_index]
                 y train, y test = y[train index], y[test index]
                 model = Lasso(alpha=1).fit(X train,y train)
                 y pred = model.predict(X test)
                  rmse = np.sqrt(mse(y_test, y_pred))
                  rmse fold.append(rmse)
              coef CV lambda.append(model.coef )
              rmse CV lambda.append([1, np.mean(rmse fold)])
```

C:\Users\bvq720\AppData\Local\Continuum\Miniconda3\lib\site-packages\sklearn\linear\_m odel\coordinate\_descent.py:484: ConvergenceWarning: Objective did not converge. You m ight want to increase the number of iterations. Fitting data with very small alpha may cause precision problems.

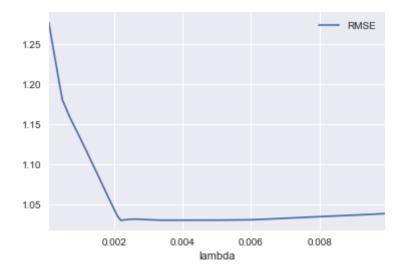
ConvergenceWarning)

## Fitting polynomial (8)

We search the  $\lambda$  grid : 0.0001-0.01 to find the optimal  $\lambda$  parameter

```
In [33]: rmse_lambda_df = pd.DataFrame(rmse_CV_lambda,columns=['lambda', 'RMSE']).set_index('lambda')
    rmse_lambda_df.plot()
```

Out[33]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1d18295ccc0>



# Fitting polynomial (9)

#### Model for optimal lambda

```
In [34]: lambda_opt = rmse_lambda_df.idxmin()
lambda_opt
```

Out[34]: RMSE 0.0022 dtype: float64

#### Parameters for optimal lambda

```
In [35]: coefs =
    pd.DataFrame(coef_CV_lambda,columns=range(1,10),index=np.arange(.0001,.01,.0001))
    coefs.loc[lambda_opt]
```

#### Out[35]:

	1	2	3	4	5	6	7	8	9
0.0022	-0.077694	0.0	6.793418	0.0	0.0	-0.0	-0.0	-0.0	-0.0

#### **Summary causality**

Selection bias: Issue for observational studies where treatment is correlated with baseline outcome.

Randomization: Enactment of treatments that are assigned randomly and thus do not suff selection biases.

#### Summary supervised learning

Prediction/postdiction: Application of model to estimate response/output associated with input.

Bias-variance tradeoff: There exist models beside OLS which can improve better at out-of-sample predictions, however, they have biased parameter estimates.

**Prediction types:** 

- when the response is numeric (continuous) the problem is called *regression*
- when response is categorical (discrete) the problem is called classification

MAE/RMSE: measures of prediction accuracy for regression problems

Cross validation: Split data in test and training data. Train model on training data, test it on test data.

Regularization: A technique used to model bias in an attempt to solve overfitting problems