Day 2: Rethinking regression as a predictive tool

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Classification and prediction as goals

- Machine learning focuses on identifying classes (classification), while social science is typically interested"
 - estimating marginal effects
 - measuring things (latent trait scaling)
- Regression analysis is the workhorse of social science statistical analysis, but can also be used to predict out of sample
- "Statistical learning" view is that regression is a "supervised" machine learning method for continuously-valued outcomes

Supervised v. unsupervised methods compared

- Two different approaches:
 - Supervised methods require a training set that exmplify constrasting classes, identified by the researcher
 - Unsupervised methods scale differences and identify patterns, without requiring a training step
- Relative advantage of supervised methods: You set the input dimensions
- Relative disadvantage of supervised methods: You need to "know" in advance the dimensions being scaled, in order to train or fit the model

Supervised v. unsupervised methods: Examples

General examples:

- Supervised: Regression, logistic regression, Naive Bayes, k-Nearest Neighbor, Support Vector Machines (SVM)
- Unsupervised: correspondence analysis, IRT models, factor analytic approaches
- Lots of applications in text analysis
 - Supervised: Wordscores (LBG 2003); SVMs (Yu, Kaufman and Diermeier 2008); Naive Bayes (Evans et al 2007)
 - Unsupervised "Wordfish" (Slapin and Proksch 2008); Correspondence analysis (Schonhardt-Bailey 2008); two-dimensional IRT (Monroe and Maeda 2004)

How do we get "true" condition?

- For regression examples: We have a sample with a continuously-valued dependent variable
- In some domains: through more expensive or extensive tests
- May also be through expert annotation or coding
 - A scheme should be tested and reported for its reliability

Generalization and overfitting

- Generalization: A classifier or a regression algorithm learns to correctly predict output from given inputs not only in previously seen samples but also in previously unseen samples
- Overfitting: A classifier or a regression algorithm learns to correctly predict output from given inputs in previously seen samples but fails to do so in previously unseen samples. This causes poor prediction/generalization

How model fit is evaluated

- For discretely-valued outcomes (class prediction): Goal is to maximize the frontier of precise identification of true condition with accurate recall, defined in terms of false positives and false negatives
 - will define formally later
- For continuously-valued outcomes: minimize Root Mean Squared Error (RMSE)

Regression as a prediction method

- Training step: fitting a model to data for which the outcome variable Y_i is known
- Test step: predicting out of sample Y_i for a new configuration of data input values X_i
- Evaluation: based on RMSE, or average

$$\sqrt{\sum(Y_i - \hat{Y}_i)}$$

Example

par(mar=c(4,4,1,1))
x <- c(0,3,1,0,6,5,3,4,10,8)
y <- c(12,13,15,19,26,27,29,31,40,48)
plot(x, y, xlab="Number of prior convictions (X)",
 ylab="Sentence length (Y)", pch=19)
abline(l=c(10,20,30,40), col="grey70")</pre>



Number of prior convictions (X)

Least squares formulas

For the three parameters (simple regression):

the regression coefficient:

$$\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$$

the intercept:

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

• and the residual variance σ^2 :

$$\hat{\sigma}^2 = \frac{1}{n-2} \sum [y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)]^2$$

Least squares formulas continued

Things to note:

- the prediction line is $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$
- the value $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ is the predicted value for x_i
- the residual is $e_i = y_i \hat{y}_i$
- The residual sum of squares (RSS) = $\sum_i e_i^2$
- The estimate for σ^2 is the same as

$$\hat{\sigma}^2 = \mathsf{RSS}/(n-2)$$

Example to show fomulas in R

```
> x <- c(0,3,1,0,6,5,3,4,10,8)
> y <- c(12,13,15,19,26,27,29,31,40,48)
> (data <- data.frame(x, y, xdev=(x-mean(x)), ydev=(y-mean(y)),</pre>
                     xdevydev=((x-mean(x))*(y-mean(y))),
+
                     xdev2=(x-mean(x))^2,
+
                     ydev2=(y-mean(y))^2)
+
      y xdev ydev xdevydev xdev2 ydev2
    х
   0 12
          -4 -14
                        56
                               16
1
                                   196
2
                        13
                                   169
   3 13 -1 -13
                               1
3
   1 15 -3 -11
                        33
                                   121
                               9
4
   0 19 -4 -7
                        28
                               16
                                   49
   6 26
        2 0
5
                         0
                               4
                                     0
6
   5 27
         1 1
                         1
                                1
                                     1
7
   3 29
         -1 3
                        -3
                                     9
                               1
8
   4 31
           0 5
                         0
                               0
                                     25
9
  10 40
         6
               14
                        84
                               36
                                   196
10 8 48
            4
               22
                        88
                                   484
                               16
> (SP <- sum(data$xdevydev))</pre>
[1] 300
> (SSx <- sum(data$xdev2))</pre>
[1] 100
> (SSy <- sum(data$ydev2))</pre>
[1] 1250
> (b1 <- SP / SSx)
[1] 3
```

```
(h0 \leq man(m) = h1 + man(m))
```

From observed to "predicted" relationship

- \blacktriangleright In the above example, $\hat{eta}_0=1$ 4, $\hat{eta}_1=3$
- This linear equation forms the regression line
- The regression line always passes through two points:

• the point
$$(x=0,y=\hat{eta}_0)$$

- the point (\bar{x}, \bar{y}) (the average X predicts the average Y)
- The residual sum of squares (RSS) = $\sum_i e_i^2$
- The regression line is that which minimizes the RSS

Ordinary Least Squares (OLS)

• Objective: minimize $\sum e_i^2 = \sum (Y_i - \hat{Y}_i)^2$, where

$$\hat{Y}_i = b_0 + b_1 X_i$$

$$\bullet \text{ error } e_i = (Y_i - \hat{Y}_i)$$

$$b = \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sum (X_i - \bar{X})}$$
$$= \frac{\sum X_i Y_i}{\sum X_i^2}$$

• The intercept is:
$$b_0 = ar{Y} - b_1 ar{X}$$

OLS rationale

- Formulas are very simple
- Closely related to ANOVA (sums of squares decomposition)
- Predicted Y is sample mean when Pr(Y|X) = Pr(Y)
 - In the special case where Y has no relation to X, b₁ = 0, then OLS fit is simply Ŷ = b₀
 - Why? Because $b_0 = \bar{Y} b_1 \bar{X}$, so $\hat{Y} = \bar{Y}$
 - Prediction is then sample mean when X is unrelated to Y
- Since OLS is then an extension of the sample mean, it has the same attractice properties (efficiency and lack of bias)
- Alternatives exist but OLS has generally the best properties when assumptions are met

OLS in matrix notation

• Formula for coefficient β :

$$Y = X\beta + \epsilon$$

$$X'Y = X'X\beta + X'\epsilon$$

$$X'Y = X'X\beta + 0$$

$$(X'X)^{-1}X'Y = \beta + 0$$

$$\beta = (X'X)^{-1}X'Y$$

- ▶ Formula for variance-covariance matrix: $\sigma^2(X'X)^{-1}$
 - In simple case where $y = \beta_0 + \beta_1 * x$, this gives $\sigma^2 / \sum (x_i \bar{x})^2$ for the variance of β_1
 - Note how increasing the variation in X will reduce the variance of β₁

The "hat" matrix

The hat matrix H is defined as:

$$\hat{\beta} = (X'X)^{-1}X'y$$

$$X\hat{\beta} = X(X'X)^{-1}X'y$$

$$\hat{y} = Hy$$

• $H = X(X'X)^{-1}X'$ is called the *hat-matrix*

- ► Other important quantities, such as ŷ, ∑ e_i² (RSS) can be expressed as functions of H
- Corrections for heteroskedastic errors ("robust" standard errors) involve manipulating H

Some important OLS properties to understand

Applies to $y = \alpha + \beta x + \epsilon$

- If β = 0 and the only regressor is the intercept, then this is the same as regressing y on a column of ones, and hence α = ȳ −− the mean of the observations
- ▶ If $\alpha = 0$ so that there is no intercept and one explanatory variable x, then $\beta = \frac{\sum xy}{\sum x^2}$
- If there is an intercept and one explanatory variable, then

$$\beta = \frac{\sum_{i} (x_{i} - \bar{x})(y_{i} - \bar{y})}{\sum (x_{i} - \bar{x})^{2}}$$
$$= \frac{\sum_{i} (x_{i} - \bar{x})y_{i}}{\sum (x_{i} - \bar{x})^{2}}$$

Some important OLS properties (cont.)

- ▶ If the observations are expressed as deviations from their means, $y* = y \bar{y}$ and $x^* = x \bar{x}$, then $\beta = \sum x^* y^* / \sum x^{*2}$
- ► The intercept can be estimated as ȳ βx̄. This implies that the intercept is estimated by the value that causes the sum of the OLS residuals to equal zero.
- The mean of the ŷ values equals the mean y values together with previous properties, implies that the OLS regression line passes through the overall mean of the data points

Normally distributed errors



OLS in R

```
> dail <- read.dta("dail2002.dta")</pre>
> mdl <- lm(votes1st ~ spend_total*incumb + minister, data=dail)</pre>
> summary(mdl)
Call:
lm(formula = votes1st ~ spend_total * incumb + minister, data = dail)
Residuals
   Min
           1Q Median 3Q Max
-5555.8 -979.2 -262.4 877.2 6816.5
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)
                 469.37438 161.54635 2.906 0.00384 **
spend_total
                     0.20336 0.01148 17.713 < 2e-16 ***
incumb
                  5150.75818 536.36856 9.603 < 2e-16 ***
minister
                  1260 00137 474 96610 2 653 0 00826 **
spend total:incumb -0.14904 0.02746 -5.428 9.28e-08 ***
---
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 ` ' 1
Residual standard error: 1796 on 457 degrees of freedom
  (2 observations deleted due to missingness)
Multiple R-squared: 0.6672, Adjusted R-squared: 0.6643
F-statistic: 229 on 4 and 457 DF, p-value: < 2.2e-16
```

OLS in Stata

. use dail2002 (Ireland 2002 Dail Election - Candidate Spending Data)

```
. gen spendXinc = spend_total * incumb
(2 missing values generated)
```

. reg votes1st spend_total incumb minister spendXinc

Source	1	SS	df		MS		Number of obs	=	462
	+-						F(4, 457)	=	229.05
Model	1	2.9549e+09	4	738	8728297		Prob > F	=	0.0000
Residual	1	1.4739e+09	457	3225	5201.58		R-squared	=	0.6672
	+-						Adj R-squared	=	0.6643
Total	1	4.4288e+09	461	960	7007.17		Root MSE	=	1795.9
votes1st	1	Coef.	Std.	Err.	t	P> t	[95% Conf.	In	terval]
	+-				47.74		4000004		
spena_totai		.2033637	.0114	807	1/./1	0.000	.1808021	•	2259252
incumb		5150.758	536.3	686	9.60	0.000	4096.704	6	204.813
minister	1	1260.001	474.9	661	2.65	0.008	326.613		2193.39
spendXinc	1	1490399	.0274	584	-5.43	0.000	2030003		0950794
_cons	L	469.3744	161.5	6464	2.91	0.004	151.9086	7	86.8402

Sums of squares (ANOVA)

TSS Total sum of squares $\sum (y_i - \bar{y})^2$

ESS Estimation or Regression sum of squares $\sum (\hat{y}_i - \bar{y})^2$ RSS Residual sum of squares $\sum e_i^2 = \sum (\hat{y}_i - y_i)^2$ The key to remember is that TSS = ESS + RSS

Examining the sums of squares

```
> yhat <- mdl$fitted.values
                               # uses the lm object mdl from previous
> ybar <- mean(mdl$model[,1])</pre>
> y <- mdl$model[,1]</pre>
                               # can't use dail$votes1st since diff N
> TSS <- sum((y-ybar)^2)
> ESS <- sum((yhat-ybar)^2)</pre>
> RSS <- sum((yhat-y)^2)</pre>
> RSS
[1] 1473917120
> sum(mdl$residuals^2)
[1] 1473917120
> (r2 <- ESS/TSS)
[1] 0.6671995
> (adjr2 <- (1 - (1-r2)*(462-1)/(462-4-1)))
[1] 0.6642865
> summary(mdl)$r.squared  # note the call to summary()
[1] 0.6671995
> RSS/457
[1] 3225202
> sqrt(RSS/457)
[1] 1795.885
> summary(mdl)$sigma
[1] 1795.885
```

Regression model return values

Here we will talk about the quantities returned with the lm() command and lm class objects.

Table 10.1 Extractor functions for the result of lm()

<pre>summary()</pre>	returns summary information about the regression
plot()	makes diagnostic plots
coef()	returns the coefficients
residuals()	returns the residuals (can be abbreviated resid())
fitted()	returns fitted values, \hat{y}_i
deviance()	returns RSS
<pre>predict()</pre>	performs predictions
anova()	finds various sums of squares
AIC()	is used for model selection

Uncertainty in regression models: the linear case revisited

- Suppose we regress y on X to produce $b = (X'X)^{-1}X'y$
- Then we set explanatory variables to new values X^p to predict Y^p
- The prediction Y^p will have two forms of uncertainty:
 - 1. estimation uncertainty that can be reduced by increasing the sample size. Estimated a $\hat{y}^p = X^p b$ and depends on sample size through b
 - 2. fundamental variability comes from variability in the dependent variable around the expected value $E(Y^p) = \mu = X^p\beta$ even if we knew the true β

Estimation uncertainty and fundamental variability

We can decompose this as follows:

$$Y^{p} = X^{p}b + \epsilon^{p}$$

Var(Y^p) = Var(X^pb) + Var(\epsilon^{p})
= X^{p}Var(b)(X^{p})' + \sigma^{2}I
= \sigma^{2}X^{p}((X^{p})'X^{p})^{-1} + \sigma^{2}I

= estimation uncertainty + fundamental variability

• It can be shown that the distribution of \hat{Y}^p is:

$$\hat{Y}^{p} \sim \mathcal{N}(X^{p}eta, X^{p}\mathsf{Var}(b)(X^{p})')$$

▶ and that the unconditional distribution of Y^p is:

$$Y^p \sim N(X^p \beta, X^p \operatorname{Var}(b)(X^p)' + \sigma^2 I)$$

Confidence intervals for predictions

- ► For any set of explanatory variables x_0 , the predicted response is $\hat{y_0} = x'_0 \hat{\beta}$
- But this prediction also comes with uncertainty, and by extension, with a confidence interval
- Two types:
 - ▶ predictions of future observations: based on the prediction plus the variance of \epsilon (Note: this is what we usually want)

$$\hat{y}_0 \pm t_{n-k-1}^{\alpha/2} \hat{\sigma} \sqrt{1 + x_o'(X'X)^{-1} x_0}$$

prediction of mean response: the average value of a y₀ with the characteristics x₀ - only takes into account the variance of β

$$\hat{y_0} \pm t_{n-k-1}^{\alpha/2} \hat{\sigma} \sqrt{x_0'(X'X)^{-1} x_0}$$

Confidence intervals for predictions in R

```
> summarv(m1)$coeff
                                 Std. Error t value
                      Estimate
                                                          Pr(>|t|)
(Intercept)
                  464.5955332 162.59752848 2.857335 4.466694e-03
spend total
                     0.2041449
                                 0.01155236 17.671273 1.154515e-53
incumb
                  4493.3251289 478.80828470 9.384393 2.962201e-19
spend_total:incumb -0.1068943 0.02254283 -4.741832 2.832798e-06
> fivenum(dail$spend_total)  # what is typical spending profile
[1]
       0.00 5927.32 14699.12 20812.66 51971.28
> x0 <- c(1, 75000, 1, 75000) # set some predictor values
> (y0 <- sum(x0*coef(m1)))
                              # compute predicted response
[1] 12251.71
> fivenum(dail$votes1st)
                              # how typical is this response?
[1]
       19.0 1151.5 3732.0 6432.0 14742.0
> guantile(dail$votes1st, .99, na.rm=T) # versus 99th percentile
    99%
11138.44
> x0.df <- data.frame(incumb=1. spend total=75000)</pre>
> predict(m1, x0.df)
       1
12251.71
> predict(m1, x0.df, interval="confidence")
      fit
               lwr
                         upr
1 12251.71 10207.33 14296.09
> predict(m1, x0.df, interval="prediction")
       fit
               lwr
                         upr
1 12251.71 8153.068 16350.36
```

Fundamental and estimation variability for non-linear forms

- For well-known cases, we known both the expectation and the fundamental variability, e.g.
 - Poisson $E(Y) = e^{\chi_{\beta}}$, $Var(Y) = \lambda$
 - logistic $E(Y) = \frac{1}{1+e^{-X\beta}}$, $Var(Y) = \pi(1-\pi)$
- Calculating the estimation variability is harder, but can be done using a linear approximation from the Taylor series. The Taylor series approximation of ŷ^p = g(b) is:

$$\hat{y}^{p} = g(b) = g(\beta) + g'(\beta)(b - \beta) + \cdots$$

where $g'(\beta)$ is the first derivative of the functional form $g(\beta)$ with respect to β

If we drop all but the first two terms, then

$$egin{array}{rcl} {\sf Var}(\hat{Y}^p) &pprox & {\sf Var}[g(eta)] + {\sf Var}[g'(eta)(b-eta)] \ &= & g'(eta){\sf Var}(b)g'(eta)' \end{array}$$

This is known as the Delta method for calculating standard errors of predictions

Precision and recall

Illustration framework

		True condition		
		Positive	Negative	
	Positive	True Positive	False Positive (Type I error)	
Prediction	Negative	False Negative (Type II error)	True Negative	

Precision and recall and related statistics

Precision: true positives true positives + false positives

Recall: true positives true positives + false negatives

Accuracy: Correctly classified Total number of cases

Example: Computing precision/recall

Assume:

- We have a sample in which 80 outcomes are really positive (as opposed to negative, as in sentiment)
- Our method declares that 60 are positive
- ▶ Of the 60 declared positive, 45 are actually positive

Solution:

$$\begin{aligned} \text{Precision} &= (45/(45+15)) = 45/60 = 0.75\\ \text{Recall} &= (45/(45+35)) = 45/80 = 0.56 \end{aligned}$$

Accuracy?



add in the cells we can compute

		True condition		
		Positive	Negative	
	Positive	45	15	60
Freulction	Negative	35		

80

but need True Negatives and N to compute accuracy

		True condition		
		Positive	Negative	
	Positive	45	15	60
Freuction	Negative	35	???	

80

assume 10 True Negatives:



now assume 100 True Negatives:



Receiver Operating Characteristic (ROC) plot



Estimating uncertainty through simulation

- King, Timz, and Wittenberg (2000) propose using statistical simulation to estimate uncertainty
- Notation:

stochastic component $Y_i \sim f(\theta_i, \alpha)$ systmatic component $\theta_i = g(X_i, \beta)$ For example in a linear-normal model, $Y_i = N(\mu_i, \sigma^2)$ and $\mu_i = X_i\beta$ simulated parameter vector $\hat{\gamma} = \text{vec}(\hat{\beta}, \hat{\alpha})$

The central limit theorem tells us we can simulate $\boldsymbol{\gamma}$ as

 $\tilde{\gamma} \sim \mathsf{N}(\hat{\gamma}, \hat{V}(\hat{\gamma}))$

Simulating predicted values

- 1. Using the algorithm in the previous subsection, draw one value of the vector $\tilde{\gamma} = \text{vec}(\tilde{\beta}, \tilde{\alpha})$.
- 2. Decide which kind of predicted value you wish to compute, and on that basis choose one value for each explanatory variable. Denote the vector of such values X_c .
- 3. Taking the simulated effect coefficients from the top portion of $\tilde{\gamma}$, compute $\tilde{\theta}_c = g(X_c, \tilde{\beta})$, where $g(\cdot, \cdot)$ is the systematic component of the statistical model.
- 4. Simulate the outcome variable \tilde{Y}_c by taking a random draw from $f(\tilde{\theta}_c, \tilde{\alpha})$, the stochastic component of the statistical model.

Repeat this M = 1000 times to approximate the entire probability distribution of Y_c . Using this estimated distribution we can compute mean and SDs which will approximate the predicted values and their error.

Simulating expected values

- Following the procedure for simulating the parameters, draw one value of the vector γ = vec(β, α).
- 2. Choose one value for each explanatory variable and denote the vector of values as *X_c*.
- 3. Taking the simulated effect coefficients from the top portion of $\tilde{\gamma}$, compute $\tilde{\theta}_c = g(X_c, \tilde{\beta})$, where $g(\cdot, \cdot)$ is the systematic component of the statistical model.
- 4. Draw *m* values of the outcome variable $\tilde{Y}_{c}^{(k)}$ (*k* = 1,..., *m*) from the stochastic component $f(\tilde{\Theta}_{c}, \tilde{\alpha})$. This step simulates fundamental uncertainty.
- 5. Average over the fundamental uncertainty by calculating the the mean of the *m* simulations to yield one simulated expected value $\tilde{E}(Y_c) = \sum_{k=1}^{m} \tilde{Y}_c^{(k)} / m$.

Note: It is m that approximates the fundamental variability but Step 5 averages it away. A large enough m will purge the simulated result of any fundamental uncertainty.

Repeat the entire process M = 1000 times to estimate the full probability distribution of $E(Y_c)$.

Calculating standard errors in Zelig

Calculating standard errors in Zelig

```
> summary(s.out <- sim(z.out, x=x.leo, x1=x.kate))</pre>
Values of X
  (Intercept) ageadults sexman classsecond classthird classcrew
1
            1
                      1
                             1
                                          0
                                                     1
                                                               0
Values of X1
  (Intercept) ageadults sexman classsecond classthird classcrew
1
            1
                      1
                             0
                                          0
                                                               0
                                                     Ω
Expected Values: E(Y|X)
                   2.5% 97.5%
   mean
             sd
1 0.105 0.01205 0.08251 0.1290
Predicted Values: Y|X
     0
        1
1 0.888 0.112
First Differences in Expected Values: E(Y|X1)-E(Y|X)
              sd 2.5% 97.5%
    mean
1 0.7791 0.02423 0.7291 0.8227
Risk Ratios: P(Y=1|X1)/P(Y=1|X)
           sd 2.5% 97.5%
  mean
1 8.538 1.062 6.723 10.89
```

More standard errors in Zelig

```
## economic bills data
ecbills <- read.dta("economic_bills.dta")</pre>
z.out <- zelig(status ~ cabinet + vpdi_LH92economic + xland,</pre>
               model="logit", data=ecbills)
x.out <- setx(z.out)</pre>
x.out[1,] <- c(1,0,0,0,0,1)
summary(sim(z.out, x.out))
# for comparison:
predict(log2,new=data.frame(cabinet=0,vpdi_LH92economic=0,xland="UK"),
        type="response", se=T)
## economic_bills data qn4c
x.out[1,] <- c(1,1,5,1,0,0)
summary(sim(z.out, x.out))
# for comparison:
predict(log2,new=data.frame(cabinet=1,vpdi_LH92economic=5,xland="FRA"),
        type="response",se=T)
## economic_bills data qn4d
(x.out <- setx(z.out, vpdi_LH92economic=seq(0,10.4,.1)))</pre>
x.out[,2] <- 0
x.out[,5] <- 1
s.out <- sim(z.out, x.out)</pre>
plot.ci(s.out)
lines(seq(0,10.4,.1), apply(s.out$qi$ev,2,mean))
```

Plot from Economic bills data



Replicate Benoit and Marsh (PRQ, 2009) Figure 2

```
## replicate Figure 2 Benoit and Marsh (2009) PRQ
require(foreign)
```

```
## Loading required package: foreign
```



Replicate Benoit and Marsh (PRQ, 2009) Figure 2



% Candidate Spending in Constituency

Compare models fits using a Receiver Operating Characteristic (ROC) plot



Replicate Benoit and Marsh (PRQ, 2009) Figure 2

