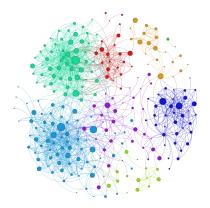
Classification

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Classification

Classification is a predictive task in which the response variable y is discrete or categorical 1 .

Examples:

- Is a credit card user going to default?
- Is a project going to be successful?
- Which product will a consumer buy?
- Which market will a firm enter?
- Which political candidate will an individual vote for?

 $^{^{1}}y$ is **discrete** if it takes on a set of discrete numerical values. y is **categorical** if it belongs to a set of **categories** (also called **classes**).

Binary Classification

For binary classification problems, let $y \in \{0,1\}$. One approach to predict y is to first estimate p(y|x) and then let

$$\widehat{y}(x) = \underset{c \in \{0,1\}}{\arg \max} \left\{ \widehat{p}(y = c|x) \right\}$$

$$= \begin{cases} 1 & \text{if } \widehat{p}(y = 1|x) > 0.5 \\ 0 & \text{o.w.} \end{cases}$$

$$(1)$$

(1) is the Bayes classifier.

Linear Regression

Notice that when $y \in \{0, 1\}$,

$$E(y|x) = 1 \cdot \Pr(y = 1|x) + 0 \cdot \Pr(y = 0|x) = \Pr(y = 1|x)$$

Hence if we assume

$$\Pr\left(y=1|x\right) = x'\beta\tag{2}$$

, then we obtain the linear regression model:

$$y = x'\beta + e \tag{3}$$

Is the model reasonable? p(y=1|x) is bounded by [0,1], but $x'\beta$ is not. So (2) may not be a good assumption. But let's see how well the model performs...

Linear Regression

Given data $\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\}$, we have:

$$y_i = x_i'\beta + e_i \tag{4}$$

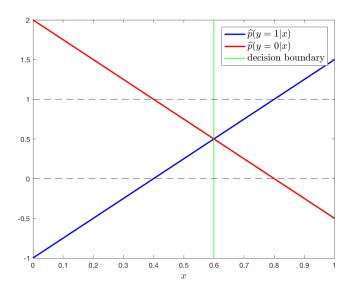
Fitting (4) $\Rightarrow \hat{\beta}$. $x_i'\hat{\beta}$ gives us an estimate of $\hat{E}(y_i|x_i) = \hat{p}(y_i = 1|x_i)$.

Therefore, given a new data point x_0 , we predict y_0 to be

$$\widehat{y}_0 = \begin{cases} 1 & \text{if } x_0' \widehat{\beta} > 0.5 \\ 0 & \text{o.w.} \end{cases}$$

, which yields the decision boundary: $x'\hat{\beta} - 0.5 = 0$.

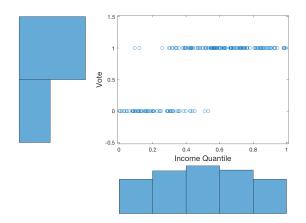
Linear Regression

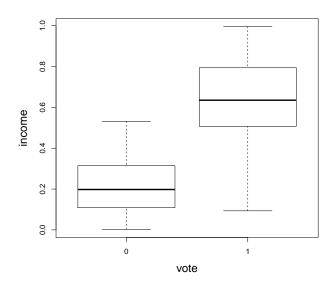


Data: income and voting records of 200 voters

• income: income quantile

vote: whether voted in the last election

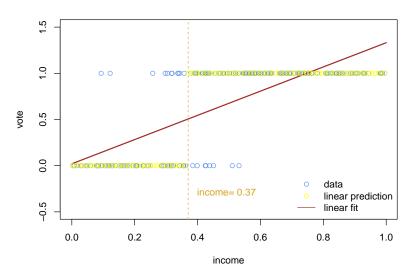




```
require(AER)
attach(read.csv("voting.txt"))
coeftest(lm(vote ~ income))

##
## t test of coefficients:
##
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.020419  0.047237  0.4323  0.666
## income  1.310588  0.083000 15.7902  <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1</pre>
```

To predict vote at income = 0.5:



$$\Pr(y = 1|x) = \sigma(x'\beta) = \frac{\exp(x'\beta)}{1 + \exp(x'\beta)}$$
 (5)

, where $\sigma(z) \equiv (1 + e^{-z})^{-1}$ is called the **logistic function** or **sigmoid** function^{2,3}.

²More precisely, the logistic regression model is a discriminative probabilistic model with p(y|x) as the target function and $\mathcal{H} = \{q(y|x) : q(y=1|x) = \sigma(x'\beta)\}$, i.e.,

$$\Pr\left(y|x\right) = \rho\left(y|x\right) \qquad \text{true distribution}$$

$$\Pr\left(y|x\right) = q\left(y|x\right) = \begin{cases} \sigma\left(x'\beta\right) & y = 1 \\ 1 - \sigma\left(x'\beta\right) & y = 0 \end{cases} \quad \text{hypothesis}$$

³The logistic function defines the CDF of the *standard logistic distribution*:

$$\mathcal{F}(x) = \frac{\exp(x)}{1 + \exp(x)}$$

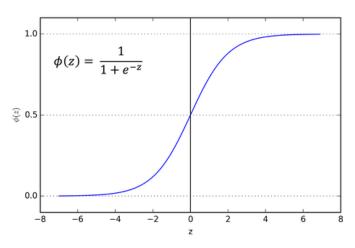
(5)
$$\Rightarrow$$

$$\log \frac{\Pr(y=1|x)}{\Pr(y=0|x)} = x'\beta$$

, i.e., logistic regression assumes that the log odds is a linear function⁴.

⁴If p denotes the probability of "success", then $\frac{p}{1-p}$ is the odds of success.





Sigmoid Function (Logistic CDF)

The logistic regression model can be estimated by maximum likelihood.

Given data
$$\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\},$$

$$\widehat{\beta} = \arg\max_{\beta} \log \mathcal{L}(\beta)$$

, where

$$\log \mathcal{L}(\beta) = \sum_{i=1}^{N} \log \Pr(y_i | x_i; \beta)$$

$$= \sum_{i=1}^{N} \left[y_i \log \sigma \left(x_i' \beta \right) + (1 - y_i) \log \left(1 - \sigma \left(x_i' \beta \right) \right) \right]$$

$$= \sum_{i=1}^{N} \left[y_i x_i' \beta - \log \left(1 + \exp \left(x_i' \beta \right) \right) \right]$$

Equivalently, logistic regression minimizes the cross-entropy training error (also called **deviance**) 5,6 :

$$E_{in}(\beta) = -\frac{1}{N} \sum_{i=1}^{N} \left[y_i \log \sigma \left(x_i' \beta \right) + (1 - y_i) \log \left(1 - \sigma \left(x_i' \beta \right) \right) \right]$$
 (6)

⁵Recall that given true distribution p(y|x) and hypothesis q(y|x), cross-entropy

$$\mathbb{H}\left(p,q\right) = -\sum_{x} p\left(y|x\right) \log q\left(y|x\right)$$

, with the in-sample expression being $-\frac{1}{N}\sum_{i=1}^{N}\log q\left(y_{i}|x_{i}\right)$.

⁶If we let $y \in \{-1, 1\}$, then (6) can be written as

$$E_{in}(\beta) = -\frac{1}{N} \sum_{i=1}^{N} \log \sigma \left(y_i x_i' \beta \right) = \frac{1}{N} \sum_{i=1}^{N} \log \left(1 + \exp \left(-y_i x_i' \beta \right) \right)$$

, where we use the fact that $\sigma(-z) = 1 - \sigma(z)$.

Then, given a new data point x_0 , we predict y_0 to be

$$\widehat{y}_0 = \begin{cases} 1 & \text{if } \widehat{p}\left(y_0 = 1 | x_0\right) = \frac{\exp\left(x_0'\widehat{\beta}\right)}{1 + \exp\left(x_0'\widehat{\beta}\right)} > 0.5\\ 0 & \text{o.w.} \end{cases}$$

Note that this is equivalent to the decision rule:

$$\widehat{y}_0 = \begin{cases} 1 & \text{if } \log \frac{\widehat{p}(y_0 = 1 | x_0)}{\widehat{p}(y_0 = 0 | x_0)} = x_0' \widehat{\beta} > 0 \\ 0 & \text{o.w.} \end{cases}$$

, i.e., logistic regression yields the decision boundary: $\mathbf{x}'\widehat{\boldsymbol{\beta}} = \mathbf{0}.$

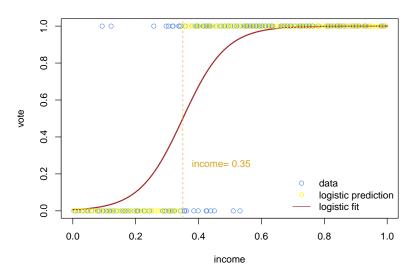
```
logitfit <- glm(vote ~ income, family=binomial)
coeftest(logitfit)

##

## z test of coefficients:
##

## Estimate Std. Error z value Pr(>|z|)
## (Intercept) -5.08565   0.86061 -5.9093 3.435e-09 ***
## income   14.53879   2.24278   6.4825 9.023e-11 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

To predict vote at income = 0.5:

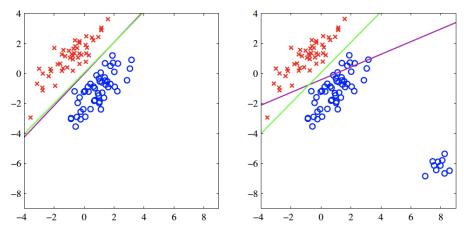


Linear vs. Logistic Regression

- For many binary classification problems, linear regression and logistic regression yield similar results.
- However, linear regression can be less robust due to the error measure it uses, which is based on the squared-error loss⁷.
- When estimating (3) using least squares, the method seeks to find $\widehat{\beta}$ such that each $x_i'\widehat{\beta}$ is as close to y_i as possible, even though all we need is for $\mathcal{I}\left(x_i'\widehat{\beta}-0.5\right)$ to be the same as y_i .
- In particular, the L2 loss penalizes cases in which $y_i=1$ and $x_i'\widehat{\beta}\gg 1$, or $y_i=0$ and $x_i'\widehat{\beta}\ll 0$, even though they lead to correct classification.
- In a sense, the L2 loss penalizes predictions that are "too correct" in that they lie a long way on the correct side of the decision boundary.

 $^{^{7}\}mbox{We}$ will talk about additional problems linear regression has for multiclass classification.

Linear vs. Logistic Regression



Data from two classes are denoted by red crosses and blue circles, with decision boundaries found by least squares (magenta) and logistic regression (green). Least squares can be highly sensitive to outliers, unlike logistic regression.

Five groups of animals were exposed to a dangerous substance in varying concentrations. Let n_i be the number of animals and y_i the number that died in group i.

Concentration	$\log_{10} \mathrm{conc}$	n_i	${y}_i$	p_{i}
1×10^{-5}	-5	6	0	0.000
1×10^{-4}	-4	6	1	0.167
1×10^{-3}	-3	6	4	0.667
1×10^{-2}	-2	6	6	1.000
1×10^{-1}	-1	6	6	1.000

How to model y_i as a function of log conc?

In addition to binary classification, logistic regression is suitable for regression problems where the response variable is the sum of individual binary outcomes.

The model is8:

$$y_i \sim \text{Binomial}(n_i, \pi_i)$$
 (7)
 $\pi_i = \sigma(x_i'\beta)$

$$y_i \sim \mathsf{Binomial}\left(1, \sigma\left(x_i'eta
ight)
ight) = \mathsf{Bernoulli}\left(\sigma\left(x_i'eta
ight)
ight)$$

⁸The logistic model for binary classification can be similarly written as:

The log likelihood function is:

$$\log \mathcal{L}(\beta) = \sum_{i=1}^{N} \log \left(\binom{n_i}{y_i} \left[\pi_i(\beta) \right]^{y_i} \left[1 - \pi_i(\beta) \right]^{n_i - y_i} \right)$$

$$\propto \sum_{i=1}^{N} \left[y_i \log \pi_i(\beta) + (n_i - y_i) \log (1 - \pi_i(\beta)) \right]$$

$$= \sum_{i=1}^{N} \left[y_i \left(x_i' \beta \right) - n_i \log (1 + \exp \left(x_i' \beta \right)) \right]$$

```
## Logistic Regression
require(AER)
y \leftarrow c(0,1,4,6,6)
n \leftarrow c(6,6,6,6,6)
logconc \leftarrow c(-5, -4, -3, -2, -1)
logitfit <- glm(cbind(y,n-y) ~ logconc, family=binomial)</pre>
coeftest(logitfit)
##
## z test of coefficients:
##
##
               Estimate Std. Error z value Pr(>|z|)
   (Intercept) 9.5868 3.7067 2.5864 0.009699 **
            2.8792 1.1023 2.6121 0.008999 **
## logconc
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Let $p_i = y_i / n_i$ be the *observed* proportion that died in group i. Can we run linear regression of p_i on log conc? i.e.,

$$p_i = x_i'\beta + e_i$$

Yes, but the linear model may generate predictions outside the range of $\left[0,1\right]\,\dots$

Better: let

$$z_i \equiv \log \frac{p_i}{1 - p_i}$$

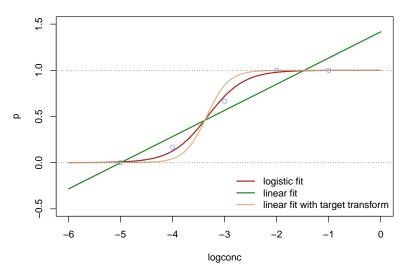
and regress

$$z_i = x_i' \beta + e_i \tag{8}$$

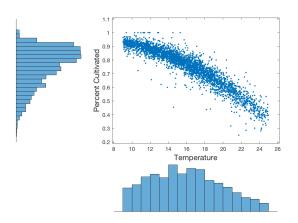
When n_i is large, model (8) \rightarrow the logistic model (7).

```
## Linear Regression: p = x'*beta + e
p <- y/n
lsfit1 <- lm(p ~ logconc)</pre>
coeftest(lsfit1)
##
## t test of coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 1.416667   0.153055   9.2559   0.002668 **
## logconc 0.283333 0.046148 6.1397 0.008690 **
##
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
## Linear regression with target transform:
      z = x'*beta + e, where z = log(p/(1-p))
# Since some p=0 and some p=1, we add a small number eps to p=0,
# and subtract eps from p=1, to avoid log(p/(1-p)) being undefined.
# Note: when n is small, regression results are highly sensitive to eps
eps <- 1e-4
p[p==0] \leftarrow p[p==0] + eps
p[p==1] \leftarrow p[p==1] - eps
z = \log(p/(1-p))
lsfit2 <- lm(z ~ logconc)</pre>
coeftest(lsfit2)
##
## t test of coefficients:
##
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 15.95698 2.47044 6.4592 0.007528 **
## logconc 4.76606 0.74487 6.3986 0.007732 **
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 '
```



Data on 3144 counties, including agricultural land (fields) available in each county, the number of fields that are being cultivated, and the annual average temperature of each county.



```
cropland <- read.csv("cropland.txt")</pre>
attach(cropland)
head(cropland)
##
     temperature fields cultivated percentCultivated
        13.18475
                    63
                               49
                                           0.7777778
## 1
## 2
       12.35680
                   165
                              147
                                           0.8909091
## 3
    17.57882
                    38
                               30
                                          0.7894737
     20.86867 152
                               95
                                          0.6250000
## 4
## 5 13.88084
                   88
                               69
                                          0.7840909
       17.18088
                                          0.7382199
## 6
                    191
                              141
```

```
## Logistic Regression
require (AER)
logitfit <- glm(cbind(cultivated, fields-cultivated) ~ temperature,</pre>
             family=binomial)
coeftest(logitfit)
##
## z test of coefficients:
##
             Estimate Std. Error z value Pr(>|z|)
##
  (Intercept) 4.266957 0.017392 245.34 < 2.2e-16 ***
##
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
## Linear Regression
lsfit <- lm(percentCultivated ~ temperature)
coeftest(lsfit)

##

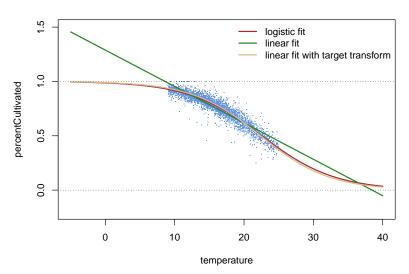
## t test of coefficients:
##

## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 1.28838143 0.00383395 336.05 < 2.2e-16 ***
## temperature -0.03349385 0.00023385 -143.23 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1</pre>
```

Cropland

```
## Linear Regression with target transform
p <- percentCultivated</pre>
eps <- 1e-4
p[p==1] = p[p==1] - eps
lsfit2 <- lm(log(p/(1-p)) ~ temperature)
coeftest(lsfit2)
##
## t test of coefficients:
##
##
                Estimate Std. Error t value Pr(>|t|)
   (Intercept) 4.5086192 0.0430642 104.695 < 2.2e-16 ***
## temperature -0.2012857  0.0026266 -76.632 < 2.2e-16 ***
##
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Cropland



Classification Error

A binary classifier can make two types of errors:

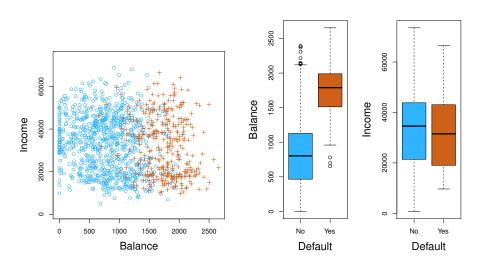
- False positive rate (FPR): $Pr(\hat{y} = 1 | y = 0)$
- False negative rate (FNR): $Pr(\hat{y} = 0 | y = 1)$

The **sensitivity** of the classifier is $\Pr(\hat{y} = 1 | y = 1)$ and the **specificity** of the classifier is $\Pr(\hat{y} = 0 | y = 0)$.

Classification Error

		Predicted class		
		– or Null	+ or Non-null	Total
True	- or Null	True Neg. (TN)	False Pos. (FP)	N
class	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

Name	Definition	Synonyms
False Pos. rate	FP/N	Type I error, 1—Specificity
True Pos. rate	TP/P	1—Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P^*	Precision, 1—false discovery proportion
Neg. Pred. value	TN/N*	



```
require(ISLR) # contains the data set 'Default'
attach(Default)
Default <- Default[,-2]
head(Default)
    default balance income
##
         No 729,5265 44361,625
## 1
## 2
         No 817.1804 12106.135
         No 1073.5492 31767.139
## 3
## 4
         No 529.2506 35704.494
## 5
         No 785.6559 38463.496
## 6
         No
             919.5885 7491.559
```

```
require (AER)
logitfit <- glm(default ~., data=Default, family=binomial)</pre>
coeftest(logitfit)
##
## z test of coefficients:
##
##
                 Estimate Std. Error z value Pr(>|z|)
   (Intercept) -1.1540e+01 4.3476e-01 -26.5447 < 2.2e-16 ***
  balance 5.6471e-03 2.2737e-04 24.8363 < 2.2e-16 ***
## income 2.0809e-05 4.9852e-06 4.1742 2.991e-05 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
cutoff <- .5
logit.p <- logitfit$fit</pre>
logit.y <- as.factor(logit.p > cutoff)
levels(logit.y) <- c("No","Yes")</pre>
t <- table(logit.y,default,dnn=c("predicted default","true default"))
t
##
                    true default
## predicted default No Yes
                 No 9629 225
##
                 Yes 38 108
##
prop.table(t,2)
##
                    true default
## predicted default
                               No
                                          Yes
                 No 0.996069101 0.675675676
##
                 Yes 0.003930899 0.324324324
##
```

• Overall training error rate: (225 + 38)/10,000 = 2.63%

• FPR: 0.39%. Specificity: 99.61%

• FNR: 67.57%. Sensitivity: 32.43%

- Note that only 333/10,000 = 3.33% individuals defaulted in the data. Hence a simple but useless *null* classifier that always predicts "No" will result in an error rate of 3.33%.
- From the perspective of a credit card company that is trying to identify high-risk individuals, the FNR – not the overall error rate – is what's important.
 - Incorrectly classifying an individual who will not default, though still to be avoided, is less problematic.



- In binary classification, the Bayes classifier assigns $\widehat{y}=1$ if $p\left(y=1|x\right)>0.5$ here 0.5 is used as a threshold in order to classify $\widehat{y}=1$ based on $p\left(y=1|x\right)$.
- Recall that we can use different loss functions to control which type of error we want to minimize: the overall error rate, FPR, or FNR. This is equivalent to changing the threshold for classifying $\hat{y}=1$.
- If we are more concerned about FNR, then we can lower this threshold. For example, if we use 0.1 as the threshold, then we assign $\hat{y}=1$ if $p(y=1|x)>0.1^{10}$.

 $^{^{9}}$ other than the 0-1 loss which gives us the Bayes classifier.

¹⁰This is equivalent to using the loss function: $\ell(y, \hat{y}) = 9$ if $(y, \hat{y}) = (1, 0)$, $\ell(y, \hat{y}) = 1$ if $(y, \hat{y}) = (0, 1)$, and $\ell(y, \hat{y}) = 0$ otherwise.

```
cutoff <- .1
logit.y <- as.factor(logit.p > cutoff)
levels(logit.y) <- c("No","Yes")</pre>
t <- table(logit.y,default,dnn=c("predicted default","true default"))
t
##
                   true default
## predicted default No Yes
##
                No 9105 90
##
                Yes 562 243
prop.table(t,2)
##
                   true default
## predicted default
                            No Yes
##
                No 0.94186407 0.27027027
##
                Yes 0.05813593 0.72972973
```

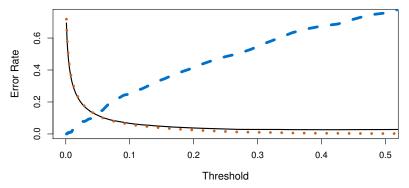
- Overall training error rate: (90 + 562)/10,000 = 6.52%
- FPR: 5.81%. Specificity: 94.19%
- FNR: 27.03%. Sensitivity: 72.97%

```
cutoff <- .01
logit.y <- as.factor(logit.p > cutoff)
levels(logit.y) <- c("No","Yes")</pre>
t <- table(logit.y,default,dnn=c("predicted default","true default"))
t
##
                   true default
## predicted default No Yes
##
                No 7134 10
##
                Yes 2533 323
prop.table(t,2)
##
                   true default
## predicted default
                            No
                               Yes
##
                No 0.73797455 0.03003003
##
                Yes 0.26202545 0.96996997
```

• Overall training error rate: (10 + 2533)/10,000 = 25.43%

• FPR: 26.20%. Specificity: 74.80%

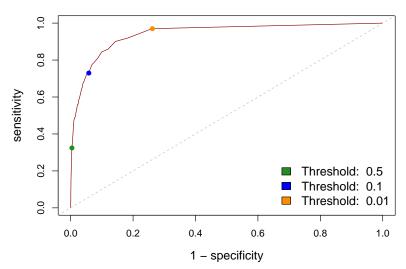
• FNR: 3.00%. Sensitivity: 97.00%



Black solid line: overall error rate; Orange dotted line: FPR; Blue dashed line: FNR.

The ROC Curve

- The **ROC curve** displays sensitivity (1–FNR) vs 1–specificity (FPR) for *all* possible thresholds.
- The overall performance of a classifier, summarized over all possible thresholds, is given by the **area under the curve (AUC)**.
- An ideal ROC curve hugs the top left corner (high sensitivity, high specificity): the larger the AUC the better the classifier.
- ROC curves are useful for comparing different classifiers.

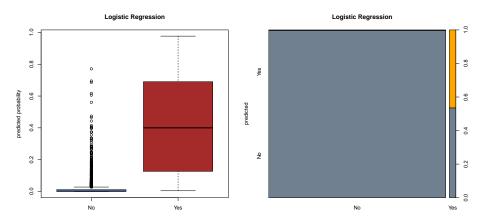


- The error rates we have calculated so far are training errors.
- Now let's split our sample into a training data set and a test data set.
- We are going to fit our models on the *training data* and test their performance on the *test data*.

```
test <- sample(1:nrow(Default),2000) # sample 2000 random indices 
 TR.X \leftarrow Default[-test,-1] #training X 
 TE.X \leftarrow Default[test,-1] #test X 
 TR.y \leftarrow default[-test] #training y 
 TE.y \leftarrow default[test] #test y
```

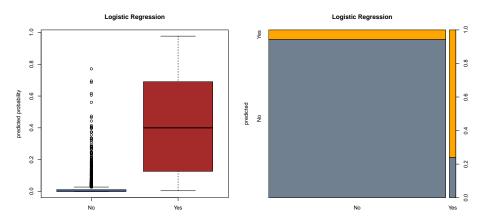
```
cutoff <- .5 # threshold
logitfit <- glm(TR.y ~., data=TR.X, family=binomial)
logit.p <- predict(logitfit,TE.X,type="response")
logit.pred <- as.factor(logit.p > cutoff)
levels(logit.pred) <- c("No","Yes")
table(logit.pred,TE.y,dnn=c("predicted default","true default"))

## true default
## predicted default No Yes
## No 1923 38
## Yes 6 33</pre>
```



```
cutoff <- .1 # threshold
logitfit <- glm(TR.y ~., data=TR.X, family=binomial)
logit.p <- predict(logitfit,TE.X,type="response")
logit.pred <- as.factor(logit.p > cutoff)
levels(logit.pred) <- c("No","Yes")
table(logit.pred,TE.y,dnn=c("predicted default","true default"))

## true default
## predicted default No Yes
## No 1819 17
## Yes 110 54</pre>
```



Similarity-Based Methods

- One way to classify data is to assign a new input the class of the most similar input(s) in the data. This is called the nearest neighbor method.
- The nearest neighbor method is a **similarity-based method**. These methods are *model free* and hence *nonparametric*.
 - ▶ If everyone around you is a republican, you are probably a republican.

- Given an input x, the **K-nearest neighbors** (**KNN**) classifier finds the K points that are closest in distance to x^{11} , denoted by $\mathcal{N}_K(x) = \left\{x_{(1)}, \dots, x_{(K)}\right\}$, and then classify using **majority vote**: let y be the most common class among $\left\{y_{(1)}, \dots, y_{(K)}\right\}^{12}$.
- Equivalently, the KNN classifier can be thought of as first estimating

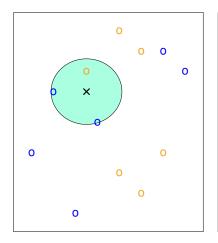
$$\widehat{p}(y = j|x) = \frac{1}{K} \sum_{i \in \mathcal{N}_K(x)} \mathcal{I}(y_i = j)$$

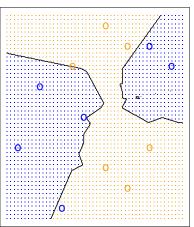
, where $y \in \{1, \dots, J\}$, and then applying the Bayes classifier.

¹¹To do this, we need a **distance measure**, or **similarity measure**. For real-valued inputs, the common choice is to use the Euclidean distance: d(x, x') = ||x - x'||.

¹²Ties are broken at random.

KNN



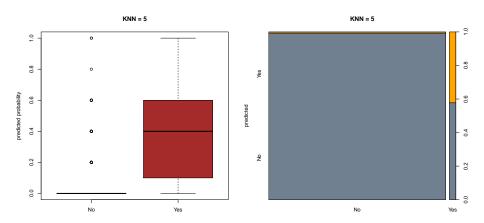


KNN in two dimensions (K = 3)

```
## KNN
# To perform KNN classification, we first standardize the x variables
# so that all variables have mean zero and standard deviation one.
s.balance <- scale(balance)
s.income <- scale(income)
SX <- data.frame(s.balance,s.income) #standardized x variables
TR.SX <- SX[-test,]
TE.SX <- SX[test,]</pre>
```

```
require(class)
K <- 5 #K value
knn.pred <- knn(TR.SX,TE.SX,TR.y,k=K,prob=TRUE)
table(knn.pred,TE.y,dnn=c("predicted default","true default"))

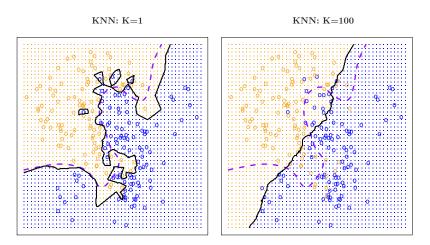
## true default
## predicted default No Yes
## No 1916 41
## Yes 13 30</pre>
```



KNN

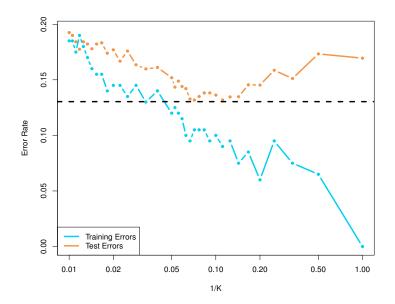
In choosing K, we face the bias-variance tradeoff:

- With K = 1, the KNN training error rate is 0. Bias is low and variance is high.
- As K grows, the method becomes less flexible and produces a decision boundary that is closer to linear, with lower variance and higher bias.



Black curve: KNN decision boundary. Purple curve: Bayes decision boundary (decision boundary based on the Bayes classifier and the true p(y|x))

KNN



Parametric vs. Nonparametric Methods

- KNN is a nonparametric (model-free) method. In general, these
 methods can work well for prediction in a wide variety of situations,
 since they don't make any real assumptions.
- The downside is that they are essentially a black box and lack interpretability. They are also more computationally expensive since they typically need to store the entire data and use them whenever predicting on a new point.
 - ▶ In contrast, parametric methods summarize the data with a fixed set of parameters, which are sufficient for prediction.
- In addition, KNN suffers from the curse of dimensionality: given N, when p is large¹³, data become relatively sparse. In high dimensions, the neighborhood represented by the K nearest points may not be local.

 $^{^{13}}p$ being the dimension of the input space.

Multiclass Classification

For multiclass problems, let $y \in \{1, ..., J\}$.

The Bayes classifier is:

$$\widehat{y}(x) = \underset{c \in \{1,...,J\}}{\operatorname{arg max}} \{\widehat{p}(y = c|x)\}$$

Linear Regression

$$\Pr\left(y=j|x\right)=x'\beta_{j}\tag{9}$$

Given data $\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\}$, let's define $y_i^j = \mathcal{I}(y_i = j)$. Then (9) implies the following J regression equations:

$$y_i^j = x_i' \beta_j + e_j, \quad j = 1, \dots, J$$
 (10)

, where each y_i^j is a binary variable.

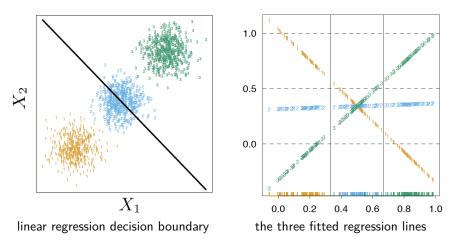
Estimating (10) gives us $\{\widehat{\beta}_j\}_{j=1}^J$. Then, given a new data point x_0 , we predict y_0 to be:

$$y_0 = \arg\max_{j} \left\{ x_0' \widehat{\beta}_j \right\} \tag{11}$$

Linear Regression

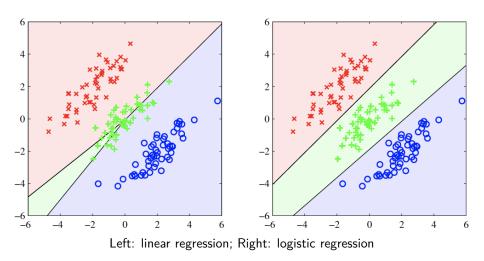
- In addition to a lack of robustness, the linear regression approach can have serious problems dealing with multiclass problems $(J \ge 3)$.
- Because of the rigid nature of the linear regression model, classes can be masked by others particularly when J is large and p is small.

Linear Regression



For this particular 3-class problem, linear regression misses the middle class completely. This problem is called **masking**. Projecting onto the line joining the three class centroids shows why this happened.

Linear Regression



Multinomial Logistic Regression

$$\Pr\left(y = j | x\right) = \frac{\exp\left(x'\beta_j\right)}{\sum_{\ell=1}^{J} \exp\left(x'\beta_\ell\right)} \tag{12}$$

 $(12) \Rightarrow$

$$\ln \frac{\Pr(y = j|x)}{\Pr(y = k|x)} = x'(\beta_j - \beta_k)$$

• The function $\sigma_j(z) \equiv \frac{\exp(z_j)}{\sum_{\ell=1}^J \exp(z_\ell)}$ is called the **softmax function**¹⁴ – a generalization of the sigmoid.

 $^{^{14}}z = (z_1, \ldots, z_J).$

Multinomial Logistic Regression

Note that since $\sum_{j=1}^{J} \Pr(y=j|x)=1$, we only need to estimate $\Pr(y=j|x)$ for J-1 classes of y. Therefore, we can choose one class of y, say y=1, to be the **reference level** and *normalize* β_1 to 0.

This implies

$$\begin{split} \Pr\left(y=1|x\right) &= \frac{1}{1+\sum_{\ell=2}^{J} \exp\left(x'\beta_{\ell}\right)} \\ \Pr\left(y=j|x\right) &= \frac{\exp\left(x'\beta_{j}\right)}{1+\sum_{\ell=2}^{J} \exp\left(x'\beta_{\ell}\right)}, \qquad j=2,\ldots,J \end{split}$$

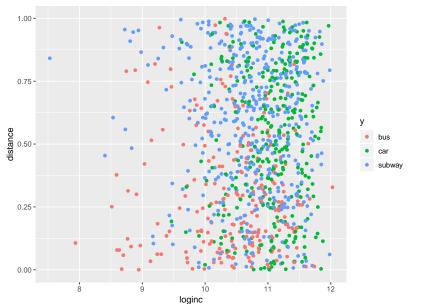
, and

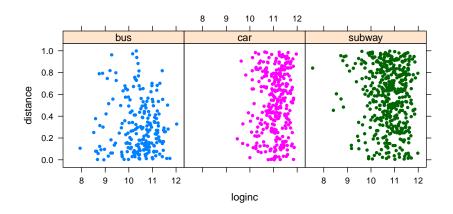
$$\ln \frac{\Pr(y = j|x)}{\Pr(y = 1|x)} = x'\beta_j$$

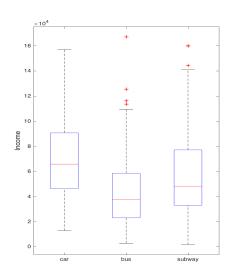
, i.e., $\exp(x'\beta_i)$ becomes the probability of y=j relative to y=1.

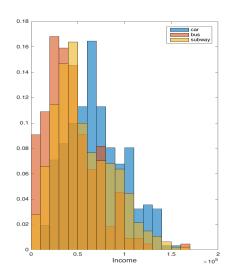
Modes of transportation: $\{bus, car, subway\}$ Individual variables: log (annual) income, distance to work (from 0 to 1)

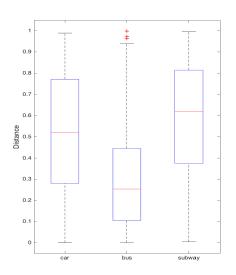
```
prop.table(table(y))
## y
     bus car subway
##
## 0.22 0.31 0.47
income <- exp(loginc)</pre>
cbind(mean(income[y=="bus"]),mean(income[y=="car"]),
mean(income[y=="subway"]))
## [,1] [,2] [,3]
## [1,] 42792 70006.83 56048.95
cbind(mean(distance[y=="bus"]),mean(distance[y=="car"]),
mean(distance[y=="subway"]))
##
            [,1] [,2] [,3]
## [1,] 0.3032989 0.5149095 0.580446
```

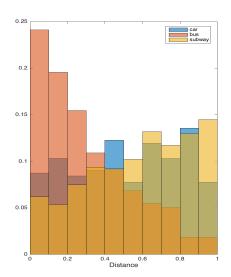












```
require(nnet)
logitfit <- multinom(y ~ loginc + distance)</pre>
require(AER)
coeftest(logitfit)
##
## z test of coefficients:
##
                     Estimate Std. Error z value Pr(>|z|)
##
                                1.85544 -10.0294 < 2.2e-16 ***
## car:(Intercept) -18.60894
                1.64705 0.16969 9.7061 < 2.2e-16 ***
## car:loginc
## car:distance 2.93996
                                0.37602 7.8187 5.339e-15 ***
## subway:(Intercept) -8.55927
                                1.45952 -5.8645 4.506e-09 ***
  subway:loginc
                0.72359
                                0.13545 5.3421 9.189e-08 ***
  subway:distance 3.75524
                                0.35014 10.7248 < 2.2e-16 ***
##
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Estimation results: (reference level: bus)

$$\log \frac{\widehat{p}\left(\operatorname{car}|x\right)}{\widehat{p}\left(\operatorname{bus}|x\right)} = -18.61 + 1.65 \times \operatorname{loginc} + 2.94 \times \operatorname{distance} \qquad (13)$$

$$= x'\widehat{\beta}_{\operatorname{car}}$$

$$\log \frac{\widehat{p}\left(\operatorname{subway}|x\right)}{\widehat{p}\left(\operatorname{bus}|x\right)} = -8.56 + 0.72 \times \operatorname{loginc} + 3.76 \times \operatorname{distance}$$

$$= x'\widehat{\beta}_{\operatorname{subway}}$$

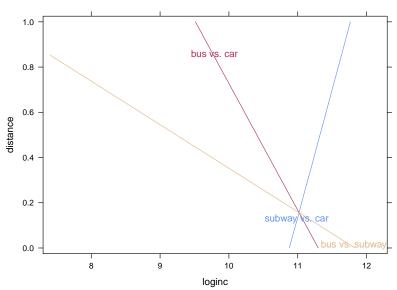
, where x=[1,loginc,distance]', $\widehat{\beta}_{\text{car}}=[-18.61,1.65,2.94]'$, and $\widehat{\beta}_{\text{subway}}=[-8.56,0.72,3.76]'$.

$$(13) \Rightarrow \hat{p} (\text{bus}|x) = \frac{1}{1 + \exp\left(x'\hat{\beta}_{\text{car}}\right) + \exp\left(x'\hat{\beta}_{\text{subway}}\right)}$$

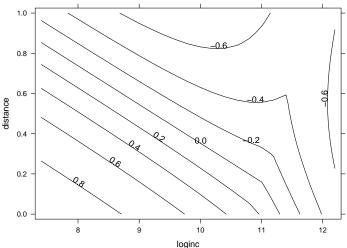
$$\hat{p} (\text{car}|x) = \frac{\exp\left(x'\hat{\beta}_{\text{car}}\right)}{1 + \exp\left(x'\hat{\beta}_{\text{car}}\right) + \exp\left(x'\hat{\beta}_{\text{subway}}\right)}$$

$$\hat{p} (\text{subway}|x) = \frac{\exp\left(x'\hat{\beta}_{\text{subway}}\right)}{1 + \exp\left(x'\hat{\beta}_{\text{car}}\right) + \exp\left(x'\hat{\beta}_{\text{subway}}\right)}$$

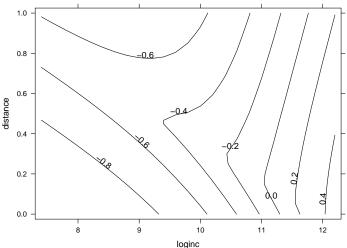
- ullet Decision boundary between bus and car: $x'\widehat{eta}_{\mathsf{car}}=0$
- Decision boundary between bus and subway: $x'\widehat{\beta}_{\text{subway}}=0$
- ullet Decision boundary between car and subway: $x'\left(\widehat{eta}_{ extsf{subway}}-\widehat{eta}_{ extsf{car}}
 ight)=0$



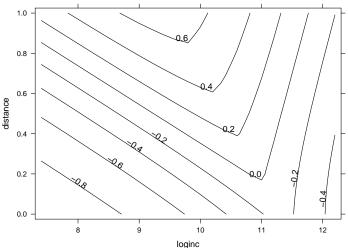
Contour plot of $-\max\left(x'\widehat{\beta}_{\mathsf{car}}, x'\widehat{\beta}_{\mathsf{subway}}\right)$:



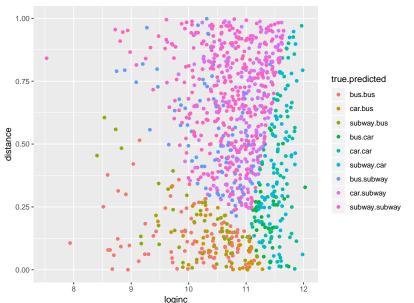
Contour plot of $x'\widehat{\beta}_{car} - \max(0, x'\widehat{\beta}_{subway})$:

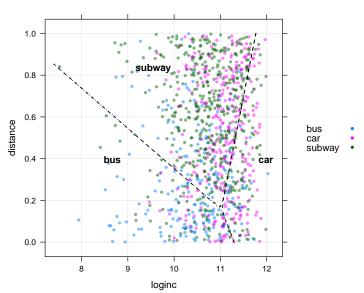


Contour plot of $x'\widehat{\beta}_{subway} - \max(0, x'\widehat{\beta}_{car})$:



```
logit.yhat <- predict(logitfit)</pre>
t <- table(logit.yhat,y,dnn=c("predicted","true"))
t
##
           true
## predicted bus car subway
##
     bus 101 41 55
     car 33 78 72
##
     subway 86 191 343
##
1 - sum(diag(t))/sum(t) # training error rate
## [1] 0.478
```





Now suppose there is no subway, what will be the share of bus and car as mode of transportation among the commuters?

From (13), we know that:

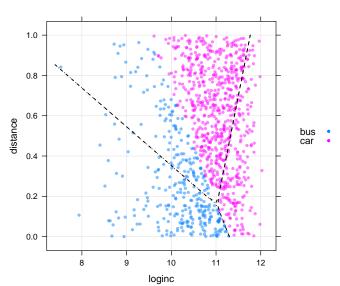
$$\log rac{\widehat{p}\left(\mathsf{car}|x
ight)}{\widehat{p}\left(\mathsf{bus}|x
ight)} = -18.61 + 1.65 imes \mathsf{loginc} + 2.94 imes \mathsf{distance}$$

The decision boundary between bus and car does *not* change whether there is subway or not.

```
require(ramify)
logit.phat <- predict(logitfit,type="probs")
counterfactual.p <- logit.phat[,c(1,2)] # no subway
counterfactual.p <- counterfactual.p/rowSums(counterfactual.p)
counterfactual.y <- as.factor(argmax(counterfactual.p))
levels(counterfactual.y) <- c("bus","car")
table(counterfactual.y,logit.yhat)

## logit.yhat
## counterfactual.y bus car subway
## bus 197 0 116
## car 0 183 504</pre>
```

Counterfactual Prediction



Calculating Market Share

Assume the observed data $\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\}$ is a random sample drawn from the underlying population. Then the "market share" of alternative j – the share of individuals in the population that choose j – is

$$\Pr(y_i = j) = \int \Pr(y_i = j | x_i) f(x_i) dx_i$$

$$\approx \frac{1}{N} \sum_{i=1}^{N} \Pr(y_i = j | x_i)$$

, i.e., we can average individual conditional choice probabilities to get an estimate of the market share of each alternative in the population.

```
# note: average choice probabilities estimated by logistic regression
# on the training data always match the observed shares of choices
# (if intercepts are included in the model)
marketShare.subway = colMeans(logit.phat)
marketShare.subway
        bus
                 car subwav
##
## 0.2199985 0.3100005 0.4700010
marketShare.nosubway = colMeans(counterfactual.p)
marketShare.nosubway
        bus car
##
## 0.3822821 0.6177179
```

predicted share	with subway	without subway
bus	22%	38%
car	31%	62%

Is this reasonable? Many people use subway not because of income or distance considerations, but because they cannot drive or they strongly prefer public transportation. For these people, if there is no subway, they would mostly switch to bus rather than car...

For the multinomial logistic regression model,

$$\log \frac{\Pr(y = j|x)}{\Pr(y = k|x)} = x'(\beta_j - \beta_k)$$

for any two classes j and k.

The probability of y = j relative to y = k depends only on $x'\beta_j$ and $x'\beta_k$ – in particular, it is *not* affected by the existence and the properties of other classes.

This is called the **independence of irrelevant alternatives** (**IIA**) property.

As an illustration of the IIA property (and why it can be undesirable in some cases), consider a more extreme example of the transportation problem:

Blue bus, Red bus

A route is currently served by a blue bus. People traveling along this route can either take the blue bus or drive themselves.

Suppose we observe each traveler's transportation choice, but do not observe any other characteristics. Our logistic regression model is then simply:

$$\log \frac{\Pr(\mathsf{blue}\;\mathsf{bus}|x)}{\Pr(\mathsf{car}|x)} = \beta_0 \tag{15}$$

, where x=1. If currently 40% of the travelers take the blue bus, while 60% drive, then $\widehat{\beta}_0 = \log\left(\frac{2}{3}\right)$.

Blue bus, Red bus (cont.)

Note that (15) predicts the relative share of blue bus riders to car drivers to be 2:3 regardless of what other transportation options are available.

What if the government now decides to introduce a red bus to this route, which is identical to the blue bus except the color of the paint?

Suppose people do not care about color, so that $\frac{Pr(\text{red bus})}{Pr(\text{blue bus})}=1$, then the model would predict the rider shares to be

 $\begin{array}{l} \mathsf{Pr}\,(\mathsf{blue}\;\mathsf{bus}) : \mathsf{Pr}\,(\mathsf{red}\;\mathsf{bus}) : \mathsf{Pr}\,(\mathsf{car}) = 2 : 2 : 3 \\ \Rightarrow \mathsf{Pr}\,(\mathsf{blue}\;\mathsf{bus}) = \mathsf{Pr}\,(\mathsf{red}\;\mathsf{bus}) = 28.57\%, \mathsf{Pr}\,(\mathsf{car}) = 42.86\% \;. \end{array}$

This is clearly unreasonable, since we should expect $Pr(blue\ bus) = Pr(red\ bus) = 20\%, Pr(car) = 60\%$, i.e., the bus riders would be split between the blue bus and the red bus, while the car drivers continue to drive.

The problem is due to *unobserved* variables. Suppose the true model is:

$$\Pr\left(y = j | x, z\right) = \frac{\exp\left(x'\beta_j + z'\gamma_j\right)}{\sum_{\ell} \exp\left(x'\beta_\ell + z'\gamma_\ell\right)}$$

, where z is unobserved 15. Then

$$\Pr(y = j|x) = \int \frac{\exp(x'\beta_j + z\gamma_j)}{\sum_{\ell} \exp(x'\beta_\ell + z\gamma_\ell)} f(z) dz$$

In this case, $\log \frac{\Pr(y=j|x)}{\Pr(y=k|x)}$ is in general no longer a function of $x'\beta_j$ and $x'\beta_k$ only, hence the IIA no longer holds.

¹⁵e.g., preference for public transportation.

Multinomial Logistic Regression

As in the binary case, multinomial logistic regression can be used for problems where the response variable is the sum of individual discrete outcomes.

The model is:

$$y_i \sim \mathsf{Multinomial}\left(n_i, \pi_i\right)$$
 (16)

, where $\pi_i = (\pi_{i1}, \dots, \pi_{iJ}), \; \sum_{j=1}^J \pi_{ij} = 1$, and

$$\pi_{ij} = \frac{\exp\left(x_i'\beta_j\right)}{\sum_{\ell=1}^{J} \exp\left(x_i'\beta_\ell\right)}$$

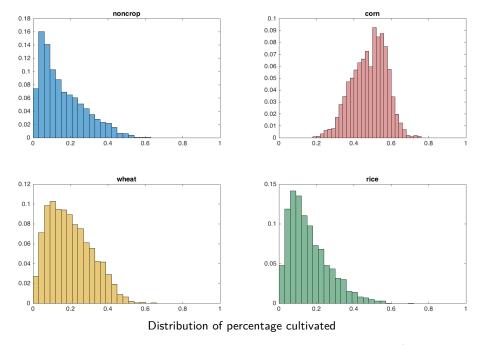
• When $n_i = 1$, (16) becomes the multinomial logistic model for multiclass classification.

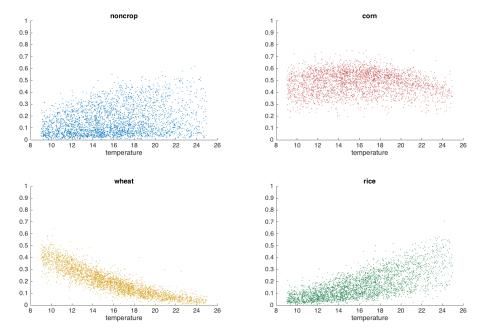
Crop Choice

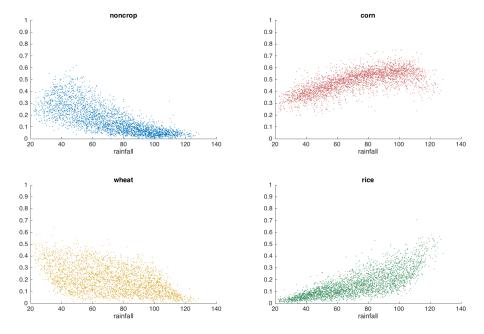
```
Crops: {corn, wheat, rice}
```

3144 counties, data on each county include number of agricultural land (fields) available, number of fields that are being cultivated for each crop, average temperature, and average monthly rainfall.

```
cropchoice <- read.csv("cropchoice.txt")</pre>
attach(cropchoice)
head(cropchoice,5)
    temperature rainfall fields noncrop corn wheat rice
##
## 1
        13.18475 75.26666
                               63
                                            31
                                                  17
        12.35680 102.37572
## 2
                              165
                                           100
                                                  30
                                                       28
       17.57882 101.61363
                                            26 3 8
## 3
                               38
                                        1
                                            78
                                                  12
                                                       17
##
       20.86867 64.35788
                              152
                                       45
        13.88084 107.54101
                               88
                                                  15
                                                       15
##
  5
                                            54
```







Crop Choice

```
require(nnet)
crops <- cbind(noncrop,corn,wheat,rice)</pre>
logitfit <- multinom(crops ~ temperature + rainfall)</pre>
require (AER)
coeftest(logitfit)
##
   z test of coefficients:
##
##
                        Estimate
                                  Std. Error z value Pr(>|z|)
                    0.63814409
                                  0.02120175 30.099 < 2.2e-16 ***
   corn: (Intercept)
## corn:temperature -0.12877826
                                  0.00128084 -100.542 < 2.2e-16 ***
## corn:rainfall
                  0.03864995
                                  0.00022141 174.564 < 2.2e-16 ***
## wheat:(Intercept) 2.57310771
                                  0.02427508 105.998 < 2.2e-16 ***
   wheat:temperature -0.25688133
                                  0.00156614 -164.022 < 2.2e-16 ***
   wheat:rainfall
                      0.02567228
                                  0.00025031
                                              102.563 < 2.2e-16 ***
## rice:(Intercept)
                    -3.26197982
                                  0.02843702 -114.709 < 2.2e-16 ***
                                  0.00155758 -14.393 < 2.2e-16 ***
## rice:temperature
                    -0.02241833
## rice:rainfall
                      0.05132472
                                  0.00026986 \quad 190.187 < 2.2e-16 ***
## ---
                  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
                                                                    © Jiaming Mao
```

Can we run linear regression instead?

Yes. Let y_{ij} be the number of fields used for crop j in county i, with j=1 denoting no cultivated crops. Let n_i be the number of fields in county i. Let $p_{ij}=y_{ij}/n_i$ and $z_{ij}=\log p_{ij}-\log p_{i1}$. Then we can estimate the following J-1 linear regression equations:

$$z_i = x_i' \beta_j + e_j, \quad j = 2, ..., J$$
 (17)

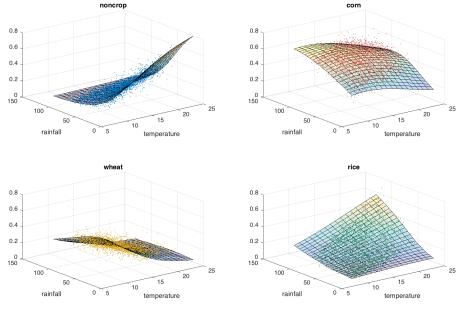
, where $x_i = [1, temperature_i, rainfall_i]$.

When n_i is large, (17) \rightarrow the multinomial logistic model (16).

```
p <- crops/fields
eps <- 1e-4
p[p==0] = p[p==0] + eps
z.corn = log(p[,2]) - log(p[,1])
lsfit.corn <- lm(z.corn ~ temperature + rainfall)</pre>
coeftest(lsfit.corn)
##
## t test of coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
##
   (Intercept) 0.64378418 0.06253041 10.296 < 2.2e-16 ***
## temperature -0.14078836  0.00371590 -37.888 < 2.2e-16 ***
## rainfall 0.04268634 0.00059017 72.329 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
z.wheat = log(p[,3]) - log(p[,1])
lsfit.wheat <- lm(z.wheat ~ temperature + rainfall)</pre>
coeftest(lsfit.wheat)
##
## t test of coefficients:
##
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept) 2.85626917 0.07518212 37.991 < 2.2e-16 ***
## temperature -0.28943989  0.00446774 -64.784 < 2.2e-16 ***
## rainfall 0.02933530 0.00070958 41.342 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
z.rice = log(p[,4]) - log(p[,1])
lsfit.rice <- lm(z.rice ~ temperature + rainfall)</pre>
coeftest(lsfit.rice)
##
## t test of coefficients:
##
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept) -3.68724544 0.07945515 -46.4066 < 2.2e-16 ***
## temperature -0.02622848  0.00472166  -5.5549  3.009e-08 ***
## rainfall 0.05834856 0.00074991 77.8074 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```



Multinomial Logistic Fit

Discrete Choice Models

- In the econometrics literature, the response variables in classification problems are often individual choices.
 - Here "individuals" can refer to people, firms, governments any unit of decision making.
- Discrete choice models are a class of econometric models of how individuals make choices.
 - ► These models can be considered structural models of decision making based on utility maximization.

- Individual i faces a choice among J alternatives.
- ullet The utility associated with alternative j is U_{ij} .
- The individual chooses the alternative that generates the highest utility, i.e., let $y_i \in \{1,\ldots,J\}$ denote the choice the individual makes, then

$$y_i = \underset{j \in \{1,...,J\}}{\text{arg max}} \{U_{ij}\}$$
 (18)

We do not observe U_{ij}^{16} . Instead, we observe (x_{ij}, y_i) , where x_{ij} are characteristics associated with individual i and alternative j.

In general, x_{ij} may contain two types of variables: s_i and z_{ij}

- s_i : individual-specific variables (e.g., income)
- z_{ij} : alternative-specific variables (e.g., price)¹⁷

 $^{^{16}}U_{ij}$ is called a **latent variable**.

¹⁷If z_{ij} is the same for all i, then we can denote it by z_i .

Since we observe x_{ij} but not U_{ij} , we can write:

$$U_{ij} = f_j(x_{ij}) + e_{ij} (19)$$

, where e_{ij} captures unobserved factors¹⁸ that influence U_{ij}^{19} .

Let $e_i \equiv [e_{i1}, \dots, e_{iJ}]'$. We assume

$$e_i \sim^{i.i.d.} \mathcal{F}_e(.)$$

Different specifications of $f_j(x_{ij})$ and $\mathcal{F}_e(.)$ lead to different discrete choice models.

¹⁹One can think of $f_j(x_{ij})$ as the **systematic** component of a decision maker's utility and e_{ij} as the **idiosyncratic** or **stochastic** component.



¹⁸Unobserved to *us* not to individual *i*

Let
$$x_{i} = \{x_{ij}\}_{j=1}^{J}$$
. (18) and (19) \Rightarrow

$$\Pr(y_{i} = j | x_{i}) = \Pr(U_{ij} > U_{i\ell} \ \forall \ell \neq j | x_{i})$$

$$= \Pr(f_{j}(x_{i}) + e_{ij} > f_{\ell}(x_{i}) + e_{i\ell} \ \forall \ell \neq j | x_{i})$$

$$= \int \mathcal{I}(e_{i\ell} - e_{ij} < f_{j}(x_{i}) - f_{\ell}(x_{i}) \ \forall \ell \neq j) \, d\mathcal{F}_{e}(e_{i})$$

, i.e., once we place assumptions on $f_j(x_{ij})$ and $\mathcal{F}_e(.)$, we can calculate $\Pr(y_i = j | x_i)$, which is called the **conditional choice probability (CCP)** in discrete choice models²⁰.

²⁰The random utility framework assumes that the individual knows her U_{ij} , so that her decision is *deterministic*. However, since we do not observe U_{ij} , we can only calculate the probability of her choosing each alternative conditional on the variables we observe.

Discrete choice models derived from the random utility framework has the following features:

- The absolute level of utility is irrelevant. Only differences in utility matter.
- 2 The overall scale of utility is irrelevant.

Only Differences in Utility Matter

The absolute level of utility is irrelevant. If a constant is added to the utility of all alternatives, then the alternative with the highest utility does not change.

The following models are equivalent:

Model 1:
$$U_{ij} = f_j(x_{ij}) + e_{ij}$$

Model 2: $U_{ij} = \alpha + f_j(x_{ij}) + e_{ij}$

, where α is any constant.

Only Differences in Utility Matter

Example

Consider a binary choice problem: $y \in \{A, B\}$. The following models are equivalent:

Model 1

$$U_{iA} = \mu_A + e_{iA}, \ e_{iA} \sim \mathcal{N}\left(0, \sigma_A^2\right)$$

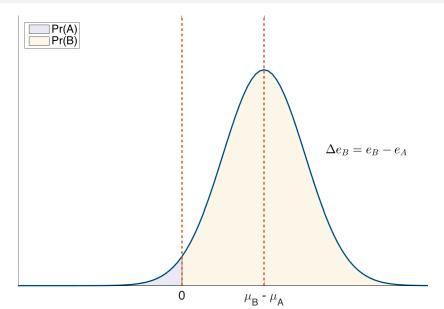
 $U_{iB} = \mu_B + e_{iB}, \ e_{iB} \sim \mathcal{N}\left(0, \sigma_B^2\right)$

Model 2

$$\begin{aligned} &U_{iA} = 0 \\ &U_{iB} = \Delta \mu_B + \Delta e_{iB}, \ \Delta e_{iB} \sim \mathcal{N} \left(0, \sigma_A^2 + \sigma_B^2 \right) \end{aligned}$$

, where $\Delta \mu_B = \mu_B - \mu_A$ and $\Delta e_{iB} = e_{iB} - e_{iA}$.

Only Differences in Utility Matter



The overall scale of utility is irrelevant. Multiplying the utility of all alternatives does not change individual choice: the alternative with the highest utility is the same irrespective of how utility is scaled.

The following models are equivalent:

Model 1:
$$U_{ij} = f_j(x_{ij}) + e_{ij}$$

Model 2:
$$U_{ij} = \lambda f_j(x_{ij}) + \lambda e_{ij}$$

, where λ is any positive constant.

Example (cont.)

The following models are equivalent to Model 1 and Model 2:

Model 3

$$U_{iA} = \widetilde{\mu}_A + \widetilde{e}_{iA}, \quad \widetilde{e}_{iA} \sim \mathcal{N}\left(0, \frac{\sigma_A^2}{\sigma_A^2 + \sigma_B^2}\right)$$

$$U_{iB} = \widetilde{\mu}_B + \widetilde{e}_{iB}, \quad \widetilde{e}_{iB} \sim \mathcal{N}\left(0, \frac{\sigma_A^2}{\sigma_A^2 + \sigma_B^2}\right)$$

, where
$$\widetilde{\mu}_j=\lambda\mu_j,\widetilde{e}_{ij}=\lambda e_{ij},$$
 and $\lambda=1\left/\sqrt{\sigma_A^2+\sigma_B^2}\right.$

Example (cont.)

Model 4

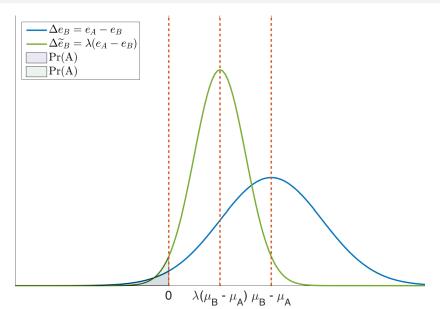
$$U_{iA} = 0$$

$$U_{iB} = \Delta \widetilde{\mu}_B + \Delta \widetilde{e}_{iB}, \ \Delta \widetilde{e}_{iB} \sim \mathcal{N}(0, 1)$$

, where $\Delta \widetilde{\mu}_B = \widetilde{\mu}_B - \widetilde{\mu}_A$ and $\Delta \widetilde{e}_{iB} = \widetilde{e}_{iB} - \widetilde{e}_{iA}$.

Therefore, in Model 1, the parameters $\mu_A, \mu_B, \sigma_A, \sigma_B$ are not separately *identifiable*, because an infinite number of models (corresponding to different values of α and γ) are *consistent* with the same choice behavior.

To estimate the model, we need to *normalize* the level and scale of utility. What we can estimate as a result is $\Delta \widetilde{\mu}_B = \lambda \left(\mu_B - \mu_A \right)$ – the *scaled* difference between μ_A and μ_B .



For
$$j = 1, \ldots, J$$
,

$$U_{ij} = x'_{ij}\beta_j + e_{ij}$$

, and

$$e_i = \left[egin{array}{c} e_{i1} \ dots \ e_{iJ} \end{array}
ight] \sim \mathcal{N}\left(0,\Sigma
ight)$$

For binary discrete choice problems, let $y \in \{A, B\}$. We have:

$$U_{iA} = x'_{iA}\beta_A + e_{iA}$$

$$U_{iB} = x'_{iB}\beta_B + e_{iB}$$
(20)

, and

$$e_{i} = \begin{bmatrix} e_{iA} \\ e_{iB} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} \sigma_{A}^{2} & \sigma_{AB} \\ . & \sigma_{B}^{2} \end{bmatrix} \right)$$
(21)

Note that $(21) \Rightarrow$

$$e_{iA}-e_{iB}\sim\mathcal{N}\left(0,\sigma_{A}^{2}+\sigma_{B}^{2}-2\sigma_{AB}
ight)$$

Normalizing (20) \Rightarrow

$$U_{iA} = 0$$

$$U_{iB} = x'_{iB}\widetilde{\beta}_B - x'_{iA}\widetilde{\beta}_A + \Delta \widetilde{e}_{iB}$$

, where, let $\lambda=1\left/\sqrt{\sigma_A^2+\sigma_B^2-2\sigma_{AB}}\right$, then $\widetilde{\beta}_A=\lambda\beta_A,\widetilde{\beta}_B=\lambda\beta_B$, and $\Delta\widetilde{e}_{iB}=\lambda\left(e_{iB}-e_{iA}\right)\sim\mathcal{N}\left(0,1\right)$.

Example 1

$$U_{iA} = \alpha_A + z'_A \delta_A + e_{iA}$$

$$U_{iB} = \alpha_B + z'_B \delta_B + e_{iB}$$

Here $z'_j\delta_j$ and α_j are both constants and hence cannot be separately identified.

As long as there is an intercept term, alternative-specific variables z_{ij}
must vary with i in order to be identified.

Example 2

$$U_{iA} = \alpha_A + s_i' \gamma + e_{iA}$$

$$U_{iB} = \alpha_B + s_i' \gamma + e_{iB}$$
(22)

$$(22) \Rightarrow$$

$$U_{iB} - U_{iA} = (\alpha_B - \alpha_A) + (e_{iB} - e_{iA})$$

Since only difference in utility matters, γ cannot be identified.

• The coefficients of individual-specific variables must be alternative-specific in order to be identified.

Example 3

$$U_{iA} = \alpha_A + s_i' \gamma_A + e_{iA}$$

$$U_{iB} = \alpha_B + s_i' \gamma_B + e_{iB}$$
(23)

 $(23) \Rightarrow$

$$U_{iB} - U_{iA} = (\alpha_B - \alpha_A) + s_i'(\gamma_B - \gamma_A) + (e_{iB} - e_{iA})$$

- α_A and α_B cannot be separately identified.
- γ_A and γ_B cannot be separately identified.

Example 3 (cont.)

Normalization of the model:

normalize level

$$U_{iA} = 0$$

 $U_{iB} = \Delta \alpha_B + s'_i \Delta \gamma_B + \Delta e_{iB}$

, where
$$\Delta \alpha_B = \alpha_B - \alpha_A$$
, $\Delta \gamma_B = \gamma_B - \gamma_A$, and $\Delta e_{iB} = e_{iB} - e_{iA}$.

normalize scale

$$U_{iA} = 0$$

 $U_{iB} = \Delta \widetilde{\alpha}_B + s_i' \Delta \widetilde{\gamma}_B + \Delta \widetilde{e}_{iB}$

, where we divide $\Delta \alpha_B, \Delta \lambda_B$, and Δe_{iB} by $\sqrt{\sigma_A^2 + \sigma_B^2 - 2\sigma_{AB}}$.

Example 4

$$U_{iA} = \alpha_A + s_i' \gamma_A + z_{iA}' \delta + e_{iA}$$

$$U_{iB} = \alpha_B + s_i' \gamma_B + z_{iB}' \delta + e_{iB}$$
(24)

$$U_{iA} = \alpha_A + s'_i \gamma_A + z'_{iA} \delta_A + e_{iA}$$

$$U_{iB} = \alpha_B + s'_i \gamma_B + z'_{iB} \delta_B + e_{iB}$$
(25)

Here we can specify either $z'_{ij}\delta$ or $z'_{ij}\delta_j$.

 Alternative-specific variables can have either alternative-specific coefficients or generic coefficients that do not change with alternatives.

Example 4 (cont.)

Normalizing $(24) \Rightarrow^a$

$$U_{iA} = 0$$

$$U_{iB} = \Delta \widetilde{\alpha}_B + s_i' \Delta \widetilde{\gamma}_B + (z_{iB} - z_{iA})' \widetilde{\delta} + \Delta \widetilde{e}_{iB}$$

Normalizing $(25) \Rightarrow$

$$U_{iA} = 0$$

$$U_{iB} = \Delta \widetilde{\alpha}_B + s_i' \Delta \widetilde{\gamma}_B + \left(z_{iB}' \widetilde{\delta}_B - z_{iA}' \widetilde{\delta}_A \right) + \Delta \widetilde{e}_{iB}$$

 a For both, $\Delta \widetilde{\alpha}_B, \Delta \widetilde{\gamma}_B, \Delta \widetilde{e}_{iB}$ are defined as before.

$$\widetilde{\delta}=\lambda\delta, \widetilde{\delta}_A=\lambda\delta_A, \widetilde{\delta}_B=\lambda\delta_B, \text{ and } \lambda=1\left/\sqrt{\sigma_A^2+\sigma_B^2-2\sigma_{AB}}\right.$$

Simulation 1:

$$U_{iA} = 5 - 10s_i + e_{iA}$$

$$U_{iB} = -5 + 10s_i + e_{iB}$$

$$e_i = \begin{bmatrix} e_{iA} \\ e_{iB} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix} \right)$$
(26)

Normalizing $(26) \Rightarrow$

$$U_{iA} = 0$$

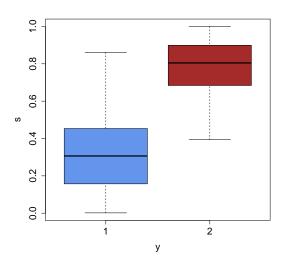
$$U_{iB} = -\frac{12}{\sqrt{5}} + \frac{20}{\sqrt{5}}s_i + \epsilon_{iB}$$

$$= -5.37 + 8.94s_i + \epsilon_{iB}$$

, where $\epsilon_{iB} = \left(e_{iB} - e_{iA}\right) / \sqrt{5} \sim \mathcal{N}\left(0,1\right)$.

```
require(ramify)
n = 1e3
s = runif(n)
e1 <- rnorm(n,mean=1,sd=1)
e2 <- rnorm(n,mean=-1,sd=2)
u1 <- 5 - 10*s + e1
u2 <- -5 + 10*s + e2
U <- cbind(u1,u2)
y <- as.factor(argmax(U))
mydata <- data.frame(s,y)</pre>
```

```
head(mydata,5)
##
## 1 0.1680415 1
## 2 0.8075164 2
## 3 0.3849424 1
## 4 0.3277343 1
## 5 0.6021007 2
prop.table(table(y))
## y
## 0.586 0.414
```



Simulation 2:

$$U_{iA} = 5 - 10s_i + e_{iA}$$

$$U_{iB} = -5 + 10s_i + e_{iB}$$

$$e_i = \begin{bmatrix} e_{iA} \\ e_{iB} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 4 \end{bmatrix} \right)$$
(27)

, where we let $\rho\left(e_{iA},e_{iB}\right)=0.5$, so that $\sigma_{AB}=\rho\sigma_{A}\sigma_{B}=1$.

Normalizing $(27) \Rightarrow$

$$U_{iA} = 0$$

$$U_{iB} = -\frac{12}{\sqrt{3}} + \frac{20}{\sqrt{3}}s_i + \epsilon_{iB}$$

$$= -6.93 + 11.55s_i + \epsilon_{iB}$$

, where $\epsilon_{\emph{iB}} = \left(e_{\emph{iB}} - e_{\emph{iA}}\right)\!/\sqrt{3} \sim \mathcal{N}\left(0,1\right)\!.$

```
n = 1e3
s = runif(n)
## generating e
require (MASS)
mu \leftarrow c(1,-1) \# mean
sig \leftarrow c(1,2) \# s.t.d. of each dimension
rho <- .5 # correlation
Sigma <- matrix(c(sig[1]^2,rho*sig[1]*sig[2], # covariance matrix
                   rho*sig[1]*sig[2],sig[2]^2),2,2)
e <- mvrnorm(n,mu,Sigma)
## generating y
e1 <- e[,1]
e2 \leftarrow e[,2]
u1 <- 5 - 10*s + e1
112 < -5 + 10*s + e2
y <- as.factor(argmax(cbind(u1,u2)))
```

```
head(e,4)
            [,1] [,2]
##
## [1,] -0.5750613 -5.1608065
## [2,] 0.1128529 -3.4697423
## [3,] 1.9516721 -1.1075891
## [4,] 0.6012319 -0.4711042
colMeans(e)
## [1] 0.9808862 -1.0736455
var(e)
## [,1] [,2]
## [1,] 1.0208563 0.9980833
## [2,] 0.9980833 3.7899603
```

Simulation 3:

$$U_{iA} = 5 - 10s_i - 0.1z_{iA} + e_{iA}$$

$$U_{iB} = -5 + 10s_i - 0.1z_{iB} + e_{iB}$$

$$e_i = \begin{bmatrix} e_{iA} \\ e_{iB} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix} \right)$$
(28)

Normalizing $(28) \Rightarrow$

$$U_{iA} = 0$$

$$U_{iB} = -\frac{12}{\sqrt{5}} + \frac{20}{\sqrt{5}} s_i - \frac{0.1}{\sqrt{5}} (z_{iB} - z_{iA}) + \epsilon_{iB}$$

$$= -5.37 + 8.94 s_i - 0.045 (z_{iB} - z_{iA}) + \epsilon_{iB}$$

, where $\epsilon_{iB} = \sim \mathcal{N}\left(0,1\right)$.

```
n = 1e3
s = runif(n)
z1 <- 100*runif(n)
z2 <- 50*runif(n)
e1 <- rnorm(n,mean=1,sd=1)
e2 <- rnorm(n,mean=-1,sd=2)
u1 <- 5 - 10*s -0.1*z1 + e1
u2 <- -5 + 10*s -0.1*z2 + e2
y <- as.factor(argmax(cbind(u1,u2)))
mydata <- data.frame(s,z1,z2,y)</pre>
```

```
probitfit <- glm(y ~ s + z1 + z2, family=binomial(link="probit"))</pre>
coeftest(probitfit)
##
## z test of coefficients:
##
##
              Estimate Std. Error z value Pr(>|z|)
## (Intercept) -5.571587  0.431299 -12.9182 < 2.2e-16 ***
          9.401062  0.621498  15.1265 < 2.2e-16 ***
## s
## z1 0.044736 0.003975 11.2544 < 2.2e-16 ***
## z2 -0.046307 0.005858 -7.9049 2.682e-15 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Can we estimate the model with a *generic* coefficient for z_{ij} that does not change with j? Yes!

```
dz = z2 - z1
probitfit <- glm(y ~ s + dz, family=binomial(link="probit"))</pre>
coeftest(probitfit)
##
## z test of coefficients:
##
              Estimate Std. Error z value Pr(>|z|)
##
## (Intercept) -5.623073   0.388506 -14.474 < 2.2e-16 ***
## s
    9.407041 0.621340 15.140 < 2.2e-16 ***
## dz -0.045071 0.003779 -11.927 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Now consider J = 3.

$$U_{ij} = x'_{ij}\beta_j + e_{ij}$$

, and

$$e_i = \left[\begin{array}{c} e_{i1} \\ e_{i2} \\ e_{i3} \end{array} \right] \sim \mathcal{N} \left(0, \left[\begin{array}{ccc} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ . & \sigma_2^2 & \sigma_{23} \\ . & . & \sigma_3^2 \end{array} \right] \right)$$

Normalizing level \Rightarrow

$$U_{i1} = 0$$

 $U_{i2} = (x'_{i2}\beta_2 - x'_{i1}\beta_1) + \Delta e_{i2}$
 $U_{i3} = (x'_{i3}\beta_3 - x'_{i1}\beta_1) + \Delta e_{i3}$

, where $\Delta e_{ij} = e_{ij} - e_{i1}$, and 21

$$\begin{bmatrix} \Delta e_{i2} \\ \Delta e_{i3} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} \sigma_1^2 + \sigma_2^2 - 2\sigma_{12} & \sigma_1^2 + \sigma_{23} - \sigma_{12} - \sigma_{13} \\ & & \sigma_1^2 + \sigma_3^2 - 2\sigma_{13} \end{bmatrix} \right)$$

21

$$Cov(\Delta e_{i2}, \Delta e_{i3}) = Cov(e_{i2} - e_{i1}, e_{i3} - e_{i1})$$

= $\sigma_{23} - \sigma_{21} - \sigma_{13} + \sigma_1^2$

Normalizing scale \Rightarrow

$$\begin{aligned} &U_{i1} = 0 \\ &U_{i2} = \left(x'_{i2}\widetilde{\beta}_2 - x'_{i1}\widetilde{\beta}_1\right) + \Delta \widetilde{e}_{i2} \\ &U_{i3} = \left(x'_{i3}\widetilde{\beta}_3 - x'_{i1}\widetilde{\beta}_1\right) + \Delta \widetilde{e}_{i3} \end{aligned}$$

, where
$$\widetilde{eta}_j=\lambdaeta_j$$
, $\Delta\widetilde{e}_{ij}=\lambda\Delta e_{ij}$, $\lambda=1\left/\sqrt{\sigma_1^2+\sigma_2^2-2\sigma_{12}}\right.$, and

$$\left[\begin{array}{c} \Delta \widetilde{e}_{i2} \\ \Delta \widetilde{e}_{i3} \end{array}\right] \sim \mathcal{N} \left(0, \left[\begin{array}{cc} 1 & \frac{\sigma_1^2 + \sigma_{23} - \sigma_{12} - \sigma_{13}}{\sigma_1^2 + \sigma_2^2 - 2\sigma_{12}} \\ & \frac{\sigma_1^2 + \sigma_3^2 - 2\sigma_{13}}{\sigma_1^2 + \sigma_2^2 - 2\sigma_{12}} \end{array}\right]\right)$$

Thus, before normalization, the covariance matrix of the error term has 6 parameters:

$$\Sigma = \left[\begin{array}{ccc} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ . & \sigma_2^2 & \sigma_{23} \\ . & . & \sigma_3^2 \end{array} \right]$$

After normalization,

$$\widetilde{\Sigma} = \left[egin{array}{cc} 1 & \omega_{12} \ . & \omega_{22} \end{array}
ight]$$

, where
$$\omega_{12}=rac{\sigma_1^2+\sigma_{23}-\sigma_{12}-\sigma_{13}}{\sigma_1^2+\sigma_2^2-2\sigma_{12}}, \omega_{22}=rac{\sigma_1^2+\sigma_3^2-2\sigma_{13}}{\sigma_1^2+\sigma_2^2-2\sigma_{12}}.$$

The number of covariance parameters to estimate decreases from 6 to 2 after normalization.

In general, a model with J alternatives has at most $\frac{1}{2}J(J-1)-1$ covariance parameters after normalization.

Brands: {Heinz, Hunt's, Del Monte, Store Brand}

Variables: the price of each brand, the income of the buyer (in \$1000), the brand purchased

```
ketchup = read.csv("Ketchup.csv")
head(ketchup,2)
##
    choice price.heinz price.hunts price.delmonte price.stb income
                 1.46
                             1.43
                                           1.45 0.99 44.49198
## 1
       stb
                             1.39
                                           1.49 0.89 59.26444
##
     heinz
                 0.99
prop.table(table(ketchup$choice))
##
  delmonte
          heinz
                      hunts
                                 stb
   0.05375 0.51125 0.21375 0.22125
##
```

Model 1:

$$U_{ij} = \alpha_j + \delta \operatorname{price}_{ij} + \gamma_j \operatorname{income}_i + e_{ij}$$

$$e_i \sim \mathcal{N}(0, \Sigma)$$
(29)

```
require(mlogit)
ketchup.long <- mlogit.data(ketchup, shape="wide",</pre>
                        varying=2:5, choice="choice")
head(ketchup.long,8)
##
            choice income
                             alt price chid
## 1.delmonte FALSE 44.49198 delmonte 1.45
## 1.heinz FALSE 44.49198 heinz 1.46
## 1.hunts FALSE 44.49198 hunts 1.43
## 1.stb TRUE 44.49198
                              stb 0.99
## 2.delmonte FALSE 59.26444 delmonte 1.49
## 2.heinz TRUE 59.26444
                            heinz 0.99
## 2.hunts FALSE 59.26444 hunts 1.39
                              stb 0.89
## 2.stb FALSE 59.26444
```

```
# mlogit(y \sim z|s|w,...)
# - s: individual-specific vars
# - z: alternative-specific vars with generic coeffs
# - w: alternative-specific vars with alternative-specific coeffs
probitfit1 <- mlogit(choice ~ price|income, ketchup.long,</pre>
                     reflevel="stb", probit=TRUE)
require(AER)
coeftest(probitfit1)[1:7,]
##
                           Estimate Std. Error t value Pr(>|t|)
## delmonte:(intercept)
                        -1.13931111 1.16876911 -0.9747957 3.299608e-01
## heinz:(intercept)
                        -7.05610040 1.81280583 -3.8923641 1.076714e-04
  hunts:(intercept)
                      -4.32246680 1.33056061 -3.2486057 1.208861e-03
                        -3.07882503 0.61797639 -4.9821078 7.733865e-07
## price
## delmonte:income
                         0.03465121 0.02801584 1.2368435 2.165137e-01
  heinz:income
                         0.18002372 0.04398663 4.0926917 4.703326e-05
                         0.11979359 0.03371002 3.5536490 4.025408e-04
## hunts:income
```

So the estimated covariance matrix is ...

```
probitfit1$omega$stb #covariance matrix using "stb" as reference

## delmonte heinz hunts
## delmonte 1.0000000 -0.1258684 -0.7047540
## heinz -0.1258684 1.6093156 0.9262337
## hunts -0.7047540 0.9262337 1.8786636
```

$$(\widehat{U}_{i,stb}=0)$$

$$\begin{split} \widehat{U}_{i,\text{delmonte}} &= -1.14 - 3.08 \times \text{price}_{i,\text{delmonte}} + 0.035 \times \text{income}_i + \epsilon_{i,\text{delmonte}} \\ \widehat{U}_{i,\text{heinz}} &= -7.06 - 3.08 \times \text{price}_{i,\text{heinz}} + 0.18 \times \text{income}_i + \epsilon_{i,\text{heinz}} \\ \widehat{U}_{i,\text{hunts}} &= -4.32 - 3.08 \times \text{price}_{i,\text{hunts}} + 0.12 \times \text{income}_i + \epsilon_{i,\text{hunts}} \end{split}$$

, where

$$\begin{bmatrix} \epsilon_{i, \text{delmonte}} \\ \epsilon_{i, \text{heinz}} \\ \epsilon_{i, \text{hunts}} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} 1 & -0.13 & -0.70 \\ . & 1.61 & 0.93 \\ . & . & 1.88 \end{bmatrix} \right)$$



Model 2:

$$U_{ij} = \alpha_j + \delta_j \operatorname{price}_{ij} + \gamma_j \operatorname{income}_i + e_{ij}$$

$$e_i \sim \mathcal{N}(0, \Sigma)$$
(30)

```
coeftest(probitfit2)[1:10,]
```

```
##
                          Estimate Std. Error t value
                                                         Pr(>|t.|)
  delmonte:(intercept)
                       -2.93786780 2.48851715 -1.180570 2.381313e-01
  heinz:(intercept)
                       -9.79073108 4.40531214 -2.222483 2.653490e-02
  hunts:(intercept)
                       -5.50096028 2.64999192 -2.075840 3.823372e-02
  delmonte:income
                        0.04822031 0.03350156 1.439345 1.504514e-01
                        0.25532406 0.13070045 1.953506 5.111457e-02
  heinz:income
  hunts:income
                        0.16927598 0.08526977 1.985182 4.747189e-02
  stb:price
                       -4.10482188 1.79833571 -2.282567 2.272253e-02
  delmonte:price
                       -2.85282115 0.64411156 -4.429079 1.080621e-05
  heinz:price
                       -4.37328318 2.49407340 -1.753470 7.991161e-02
                       -4.71107228 2.57769096 -1.827633 6.798415e-02
## hunts:price
```

```
coeftest(probitfit2)[11:15,]
##
                   Estimate Std. Error
                                        t value Pr(>|t|)
  delmonte.heinz -0.1424442 0.6506784 -0.2189165 0.82677203
  delmonte.hunts -1.0566066 0.8770324 -1.2047520 0.22866213
## heinz.heinz 1.7969567 0.9806295 1.8324522 0.06726274
## heinz.hunts 0.9872264 0.7128141 1.3849704 0.16645499
## hunts.hunts 1.4535726 0.9021936
                                      1.6111537 0.10754821
probitfit2$omega$stb
##
             delmonte
                          heinz
                                    hunts
## delmonte 1.0000000 -0.1424442 -1.056607
           -0.1424442 3.2493438 1.924511
## heinz
## hunts -1.0566066 1.9245106 4.203907
```

$$\begin{split} \widehat{U}_{i,\text{stb}} &= -4.1 \times \text{price}_{i,\text{stb}} \\ \widehat{U}_{i,\text{delmonte}} &= -2.94 - 2.85 \times \text{price}_{i,\text{delmonte}} + 0.048 \times \text{income}_i + \epsilon_{i,\text{delmonte}} \\ \widehat{U}_{i,\text{heinz}} &= -9.79 - 4.37 \times \text{price}_{i,\text{heinz}} + 0.255 \times \text{income}_i + \epsilon_{i,\text{heinz}} \\ \widehat{U}_{i,\text{hunts}} &= -5.50 - 4.71 \times \text{price}_{i,\text{hunts}} + 0.169 \times \text{income}_i + \epsilon_{i,\text{hunts}} \end{split}$$

, where

$$\begin{bmatrix} \epsilon_{i, \text{delmonte}} \\ \epsilon_{i, \text{heinz}} \\ \epsilon_{i, \text{hunts}} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} 1 & -0.14 & -1.06 \\ . & 3.25 & 1.92 \\ . & . & 4.20 \end{bmatrix} \right)$$



Now let's assume the following model:

$$U_{ij} = x'_{ij}\beta_j + e_{ij} \tag{31}$$

, and

$$e_{ij} \sim^{i.i.d.} \text{Gumbel}(0, \sigma)$$

Extreme Value Distribution

The Gumbel distribution, also called the Type I extreme value distribution, has the following CDF:

$$\mathcal{F}\left(e;\mu,\sigma
ight) = \exp\left\{-\exp\left(-rac{e-\mu}{\sigma}
ight)
ight\}$$

- ullet μ is the location parameter.
- \bullet σ is the scale parameter

For $e \sim \text{Gumbel}(\mu, \sigma)$,

$$E\left(e\right) = \mu + \sigma\gamma_{e}$$
 $Var\left(e\right) = \frac{\pi^{2}}{6}\sigma^{2}$

, where $\gamma_e \approx 0.577$ is the Euler constant.

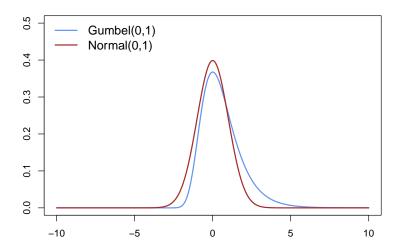
Extreme Value Distribution

• The difference between two extreme value random variables is distributed as a logistic distribution. Let $e_1, e_2 \sim \text{Gumbel}(0,1)$ and let $\Delta e = e_2 - e_1$. Then the CDF of Δe is:

$$\mathcal{F}\left(\Delta e
ight) = rac{\exp\left(\Delta e
ight)}{1+\exp\left(\Delta e
ight)}$$

- In practice, assuming $e_{ij} \sim^{i.i.d.}$ Gumbel is nearly the same as assuming $e_{ij} \sim^{i.i.d.}$ Normal.
 - ► The extreme value distribution has fatter tails than the normal, but the difference is small empirically.

Extreme Value Distribution



We can always normalize the scale of (31) so that $\sigma = 1$:

$$U_{ij} = x'_{ij}\beta_j + e_{ij}$$

, where

$$e_{ij} \sim^{i.i.d.} \mathsf{Gumbel}(0,1)$$

Let $x_i = \{x_{ij}\}_{j=1}^J$ and $V_{ij} = x'_{ij}\beta_j$. We have:

$$\begin{aligned} \Pr(y_{i} = j | x_{i}) &= \Pr(V_{ij} + e_{ij} > V_{i\ell} + e_{i\ell} \ \forall \ell \neq j | x_{i}) \\ &= \Pr(e_{i\ell} < V_{ij} - V_{i\ell} + e_{ij} \ \forall \ell \neq j | x_{i}) \\ &= \int \left[\prod_{\ell \neq j} e^{-e^{-\left(V_{ij} - V_{i\ell} + e_{ij}\right)}\right] e^{-e_{ij}} e^{-e^{-e_{ij}}} de_{ij} \\ &= \frac{\exp(V_{ij})}{\sum_{\ell=1}^{J} \exp(V_{i\ell})} \end{aligned}$$

• Under the assumption of $e_{ij} \sim^{i.i.d.}$ Gumbel (0, 1), the random utility framework gives rise to the logistic model.

Let $\overline{U}_i = E(U_i|x_i)$ be the expected utility of individual i^{22} .

$$\overline{U}_{i} = E[U_{i}|x_{i}]$$

$$= E\left[\max_{j} \{U_{ij}\} \middle| x_{i}\right]$$

$$= \log\left[\sum_{j=1}^{J} \exp(V_{ij})\right]$$

²²Technically, $\overline{U}_i = \log \left[\sum_{j=1}^J \exp \left(V_{ij} \right) \right] + C$, where C is any constant. This is because we can add any C to $\left(U_{i1}, \ldots, U_{iJ} \right)$ and the model would be the same. Therefore, we will not be able to learn the *level* of utilities associated with different alternatives, only the *difference* between them.

For binary problems, the probit model, after normalization, is

$$U_{iA} = x'_{iA}\beta_A$$
$$U_{iB} = x'_{iB}\beta_B + e_{iB}$$

, where $e_{iB} \sim \mathcal{N}\left(0,1\right)$.

Therefore, the probit and the logistic model are basically the same for binary problems.

• For multinomial problems, the two types of models are different as probit allows e_i to have an arbitrary covariance structure.

Income and Voting

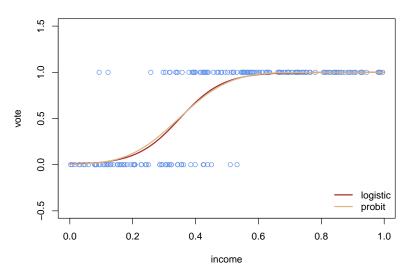
```
probitfit <- glm(vote ~ income, family=binomial(link="probit"))
coeftest(probitfit)

##

## z test of coefficients:
##

## Estimate Std. Error z value Pr(>|z|)
## (Intercept) -2.75277    0.41935 -6.5644 5.225e-11 ***
## income    7.93916    1.07686    7.3725 1.675e-13 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Income and Voting



Marginal Effects

$$U_{ij} = \alpha_j + \gamma_j s_i + \delta z_{ij} + e_{ij}, \quad e_{ij} \sim^{i.i.d.} \text{Gumbel}(0,1)$$
 (32)

 \Rightarrow ²³

$$\frac{\partial \Pr(y_{i} = j | x_{i})}{\partial s_{i}} = \frac{\partial \left[e^{V_{ij}} / \sum_{\ell} e^{V_{i\ell}}\right]}{\partial s_{i}}$$

$$= \Pr(y_{i} = j | x_{i}) \left(\gamma_{j} - \sum_{\ell} \gamma_{\ell} \Pr(y_{i} = \ell | x_{i})\right)$$

$$\frac{\partial \Pr(y_{i} = j | x_{i})}{\partial z_{ij}} = \delta \Pr(y_{i} = j | x_{i}) (1 - \Pr(y_{i} = j | x_{i}))$$

²³If δ is alternative-specific, i.e. δ_j , then $\partial \Pr(y_i = j | x_i) / \partial z_{ij} = \delta_j \Pr(y_i = j | x_i) (1 - \Pr(y_i = j | x_i))$.

Marginal Effects

- For alternative-specific variables, the sign of the coefficient is the sign of the marginal effect: $\gamma > 0 \iff \partial \Pr(y_i = j | x_i) / \partial z_{ij} > 0$.
- For individual-specific variables, the sign of the coefficient is not necessarily the sign of the marginal effect: $\gamma_j > 0$ does not imply $\partial \Pr(y_i = j | x_i) / \partial s_i > 0$.

Choice Probability Elasticity

Let \mathcal{E}_i^J be the **own-elasticity** of the change in $\Pr(y_i = j | x_i)$ given a change in z_{ij} . (32) \Rightarrow

$$\mathcal{E}_{i}^{jj} = \frac{\partial \Pr(y_{i} = j | x_{i})}{\partial z_{ij}} \frac{z_{ij}}{\Pr(y_{i} = j | x_{i})}$$

$$= \delta z_{ij} \left[1 - \Pr(y_{i} = j | x_{i}) \right]$$
(33)

Similarly, we can calculate the **cross-elasticity** of $\Pr(y_i = j | x_i)$ given a change in $z_{ik}, k \neq j$:

$$\mathcal{E}_{i}^{jk} = \frac{\partial \Pr(y_{i} = j | x_{i})}{\partial z_{ik}} \frac{z_{ik}}{\Pr(y_{i} = j | x_{i})}$$

$$= -\delta z_{ik} \Pr(y_{i} = k | x_{i})$$
(34)

Choice Probability Elasticity

- Note that (34) does *not* depend on j a percentage change in z_{ik} results in the *same* percentage change in all $Pr(y_i = j | x_i)$, $j \neq k$.
- For example, consider the car market. Suppose the choice set is $\{\text{Honda, Toyota, Tesla}\}$. Let $z_{ij}=p_{ij}$ be the price of each car to each consumer. Then (34) says that, for each consumer, a 1% decrease in the price of Honda will result in the same percentage decrease in the probability of buying Toyota and the probability of buying Tesla.
- This property, which is called *proportional substitution*, is a manifestation of the IIA property of the logistic model.

Independence of Irrelevant Alternatives (IIA)

- The IIA property is the result of assuming that errors are independent of each other.
 - Hence IIA holds not only for logistic models with i.i.d. extreme value distributed errors, but holds in general for discrete choice models with independently distributed errors.
- Multinomial probit models, by allowing for correlated errors, do not have the IIA property.

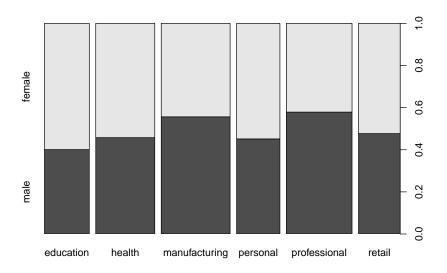
Independence of Irrelevant Alternatives (IIA)

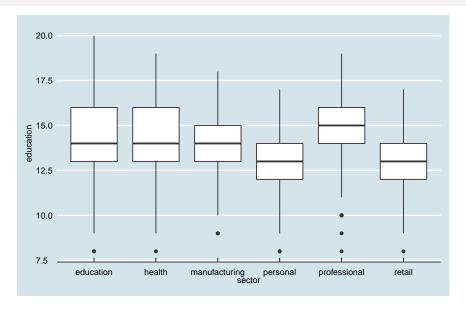
- Note that the IIA property should be a desirable property for well-specified models.
- Under independence, the error for one alternative provides no information about the error for another alternative. This should be the property of a well-specified model such that the unobserved portion of utility is essentially "white noise."
- When a model omits important unobserved variables that explain individual choice patterns, however, the errors can become correlated over alternatives.
- In this sense, the ultimate goal of the researcher is to represent utility so well that the assumption of error independence is appropriate.
- In the absence of that, a discrete choice model that allows for correlated errors, such as the multinomial probit, can be used.

- Sector of employment: Manufacturing, Retail, Education, Health, Personal Service, Professional Service
- Individual variables: sex, education (years of schooling), wage

```
emp <- read.csv("employment.csv")</pre>
emp$sex <- factor(emp$sex,labels=c("male","female"))</pre>
head(emp,4)
##
      sex education
                                   sector
                     wage
  1 female
                                 personal
              15 32241.35
  2 female 16 70051.50
                                education
      male
              13 35248.51 manufacturing
             12 15535.13
                                   health
## 4 female
```

```
require(descr)
freq(emp$sector,plot=FALSE)
## emp$sector
##
                Frequency Percent
                     277 13.85
## education
## health
                     365 18.25
## manufacturing 426 21.30
## personal
                     268 13.40
## professional 406 20.30
## retail
                  258 12.90
## Total
                    2000 100.00
aggregate(wage~sector,emp,mean)
##
           sector wage
## 1 education 57134.48
           health 50039.96
  3 manufacturing 43630.54
## 4
         personal 36799.96
    professional 85319.71
## 5
## 6
           retail 25460.33
```





Model:

$$U_{ij} = \alpha_j + \beta w_{ij} + e_{ij}$$

$$e_{ij} \sim \text{Gumbel } (0, 1)$$
(35)

Let y_i be the observed sector of employment of individual i. To estimate the model, we need to construct *counterfactual wages* w_{ij} for each individual i and sector $j \neq y_i$.

We can predict counterfactual wages by running the following regressions for each sector j:

$$\log w_{ij} = \omega_{0j} + \omega_{1j} \text{Education}_i + \omega_{2j} \text{Female}_i$$

$$+ \omega_{3j} \text{Education}_i \times \text{Female}_i + \xi_{ij}$$
(36)

, where Female $_i$ is an indicator variable.

 $(36) \Rightarrow \widehat{w}_{ii}$. We then estimate:

$$U_{ij} = \alpha_j + \beta \widehat{w}_{ij} + e_{ij}$$

 $e_{ij} \sim \text{Gumbel}(0,1)$

Constructed data set with counterfactual wages:

```
head(emp,4)
##
           sector wage.education wage.health wage.manufacturing
                                 45757.89
                                                  37138.46
## 1
         personal
                     36373.753
        education 60971.110 69129.87
                                               50215.49
## 2
                                                  33982.85
    manufacturing 15656.873
                                 21219.96
## 4
          health
                      7722.895
                                 13269.87
                                                  15023.89
    wage.personal wage.professional wage.retail
##
        45022.19
                         54747.97
                                    32333.67
## 1
## 2
         50944.08
                       83152.41 40173.16
## 3
        37336.32
                        33341.71 24485.34
         31076.01
                         15625.99 16858.23
## 4
```

```
## Estimating the discrete choice model
require (AER)
emp.long <- mlogit.data(emp,shape="wide",varying=2:7,choice="sector")</pre>
modelfit <- mlogit(sector ~ wage, emp.long)</pre>
coeftest(modelfit)
##
## t test of coefficients:
##
##
                                Estimate Std. Error t value Pr(>|t|)
## health:(intercept)
                              8.7959e-02 8.1429e-02 1.0802 0.28019
  manufacturing:(intercept) 1.7359e-01 8.2219e-02 2.1113 0.03487 *
## personal:(intercept)
                             -3.8266e-01 9.5724e-02 -3.9975 6.634e-05 ***
                                          9.7211e-02 -4.0489 5.342e-05 ***
## professional:(intercept)
                             -3.9360e-01
## retail:(intercept)
                         5.5781e-02 8.8256e-02 0.6320
                                                               0.52743
                              3.7627e-05 2.6104e-06 14.4142 < 2.2e-16 ***
## wage
##
                  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
```

Welfare Analysis

The expected utility of individual *i* is:

$$\overline{U}_{i} = \log \left[\sum_{j} \exp \left(\alpha_{j} + \beta w_{ij} \right) \right]$$
(37)

Let $\overline{U}_i^{\$}$ denote the utility of the individual *in monetary terms*. Since in model (35), each dollar in wage adds β to utility, each unit of utility is equivalent to $1/\beta$ dollars. The expected utility of individual i in monetary terms is thus²⁴:

$$\overline{U}_{i}^{\$} = \frac{1}{\beta} \log \left[\sum_{j} \exp\left(\alpha_{j} + \beta w_{ij}\right) \right]$$
 (38)

²⁴More precisely, we can add any constant C to (37) and (38).

Welfare Analysis

```
## Calculating expected utilities
J = 6 # number of sectors
N <- nrow(emp) # mumber of individuals
b <- coef(modelfit)["wage"]
X <- model.matrix(modelfit)
V <- X %*% coef(modelfit)
V <- matrix(V,N,J,byrow=TRUE)
U = log(rowSums(exp(V)))/b
summary(U)
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 52366 68246 84799 94882 101307 564822</pre>
```

Suppose trade liberalization causes a 20% decrease in the wages of manufacturing workers.

- How does the employment pattern change after trade liberalization?
- What are its welfare consequences?

```
emp2 <- emp
emp2$wage.manufacturing <- emp$wage.manufacturing*0.8
emp2.long <- mlogit.data(emp2,shape="wide",varying=2:7,choice="sector")</pre>
colMeans(predict(modelfit,emp2.long))
       education
                        health manufacturing
                                                  personal professional
##
                     0.1937193
                                   0.1657904
                                                 0.1406273
                                                               0.2176602
##
      0.1464848
##
          retail
      0.1357180
##
```

Employment Share Before and After Trade Liberalization

Employment Share	Before	After	
Manufacturing	21.35	16.63	
Retail	12.75	13.41	
Education	14.10	14.91	
Health	18.40	19.52	
Personal Service	12.85	13.49	
Professional Service	20.55	22.05	

```
## Change in expected utilities
dU = U2 - U
summary(dU)
##
       Min. 1st Qu. Median Mean 3rd Qu. Max.
## -4026.199 -2377.896 -1161.950 -1587.433 -755.802 -0.146
emp = data.frame(emp0,U,U2,dU)
# by gender
aggregate(dU ~ sex,emp,mean)
                  dU
## sex
## 1 male -2342.3223
## 2 female -841.5479
```

```
# by education
aggregate(dU ~ education,emp,mean)
      education
                         dU
##
## 1
                -199.81766
              9 -268.37735
## 2
## 3
             10 -424.76973
## 4
             11 -587.90009
## 5
             12 -818.89454
             13 -1228.86410
## 6
             14 -1643.87818
##
## 8
             15 -2208.52149
             16 -2637.40772
##
## 10
             17 -2069.31717
             18 -939.75103
## 11
## 12
             19 -143.24862
             20 -2.87952
## 13
```

Ketchup

Let's take model (29) and compare logistic vs. probit counterfactual predictions:

```
logitfit <- mlogit(choice ~ price|income, ketchup.long, reflevel="stb")</pre>
coeftest(logitfit)
##
## t test of coefficients:
##
##
                         Estimate Std. Error t value Pr(>|t|)
                        -3.831626
                                              -3.2773 0.001094 **
## delmonte:(intercept)
                                    1.169149
## heinz:(intercept)
                       -10.888985
                                    0.946463 -11.5049 < 2.2e-16 ***
## hunts:(intercept)
                        -6,305256
                                    0.871547 -7.2346 1.103e-12 ***
## price
                        -4.418198
                                    0.329590 -13.4051 < 2.2e-16 ***
## delmonte:income
                         0.107143
                                    0.025841 4.1462 3.745e-05 ***
                         0.276613
                                    0.020943 13.2078 < 2.2e-16 ***
## heinz:income
## hunts:income
                         0.180305
                                    0.019794 9.1091 < 2.2e-16 ***
## ---
                  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
```

Counterfactual Experiment: 20% price increase for Heinz

```
newdata <- ketchup.long
idx <- index(newdata)$alt == "heinz"
newdata[idx, "price"] <- newdata[idx, "price"] *1.2 # 20% price increase
# logistic prediction
logit.phat.new <- predict(logitfit,newdata)</pre>
logit.share.new <- colMeans(logit.phat.new)</pre>
logit.share.new
##
          stb delmonte heinz
                                          hunts
## 0.25132916 0.06914047 0.37982532 0.29970505
# probit prediction
probit.phat.new <- predict(probitfit1,newdata)</pre>
probit.share.new <- colMeans(probit.phat.new)</pre>
probit.share.new
##
          stb delmonte
                              heinz
                                          hunts
## 0.22741067 0.07871089 0.37283446 0.32164539
```

Counterfactual Experiment: 20% price increase for Heinz

market share	Heinz	Hunts Del Monte		Store Brand	
	51.13%	21.38%	5.38%	22.13%	
After Heinz price increase:					
logistic	37.98%	29.97%	6.91%	25.13%	
probit	37.28%	32.16%	7.87%	22.74%	

Mode of Transportation

```
## Probit Regression
transport.long <- mlogit.data(transport, shape="wide", choice="y")
probitfit <- mlogit(y ~ 0|loginc+distance, transport.long, probit=TRUE)</pre>
coeftest(probitfit)
##
## t test of coefficients:
##
                    Estimate Std. Error t value Pr(>|t|)
##
## car:(intercept) -8.925928 1.389554 -6.4236 2.062e-10 ***
  subway:(intercept) -1.454769 1.609180 -0.9040
                                                0.3662
## car:loginc
                 subway:loginc 0.118611 0.133202 0.8905 0.3734
## car:distance
                   0.557613 0.532888 1.0464 0.2956
  subway:distance 0.698667 0.772920 0.9039 0.3663
## car.subway
               -0.013351 0.153096 -0.0872
                                                0.9305
## subway.subway 0.315844
                            0.364598 0.8663
                                                0.3865
##
                0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '@ Jaming Mao
## Signif. codes:
```

Mode of Transportation

```
probitfit$omega
## $bus
##
                     subway
                 car
## car 1.00000000 -0.01335131
## subway -0.01335131 0.09993555
##
## $car
##
              bus
                    subway
## bus 1.000000 1.013351
  subway 1.013351 1.126638
##
  $subway
##
             bus
                       car
## bus 0.09993555 0.1132869
## car 0.11328686 1.1266382
```

Counterfactual Experiment: No Subway

```
# To predict choice probabilities without one alternative,
# one trick is to make the xij associated with that alternative
# extremely large or small so that its predicted prob is always 0
newdata <- transport.long
idx <- index(newdata)$alt == "subway"
newdata[idx, "loginc"] <- -1e10
newdata[idx, "distance"] <- -1e10
probit.phat.new <- predict(probitfit,newdata)
probit.share.new <- colMeans(probit.phat.new)</pre>
```

```
## bus car subway
## 0.6047072 0.3952928 0.0000000
```

Counterfactual Experiment: No Subway

Observed Market Share

bus	car	subway	
22%	31%	47%	

Predicted Market Share without Subway

	bus	car	
logistic	38%	62%	
probit	60%	40%	

Acknowledgement

Part of this lecture is adapted from the following sources:

- Bishop, C. M. (2011). Pattern Recognition and Machine Learning.
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