## Binary Choice

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## Outline

- Model specification
  - Error term
- 2 Applying the model
- Maximum likelihood estimation
- Estimation output
- Back to the scale

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## Example

#### Data

- Unit of analysis: travelers (simulated observations)
- Choice set: choice of car (C) or transit (T)
- Independent variable: travel time
- Ben-Akiva & Lerman (1985) Discrete Choice Analysis: Theory and Applications to Travel Demand, MIT Press (p.88)

## Example

### Data from 21 decision makers

|    | Time | Time    |        |    | Time | Time    |        |
|----|------|---------|--------|----|------|---------|--------|
| #  | auto | transit | Choice | #  | auto | transit | Choice |
| 1  | 52.9 | 4.4     | Т      | 11 | 99.1 | 8.4     | Т      |
| 2  | 4.1  | 28.5    | Т      | 12 | 18.5 | 84.0    | C      |
| 3  | 4.1  | 86.9    | C      | 13 | 82.0 | 38.0    | C      |
| 4  | 56.2 | 31.6    | Т      | 14 | 8.6  | 1.6     | Т      |
| 5  | 51.8 | 20.2    | Т      | 15 | 22.5 | 74.1    | C      |
| 6  | 0.2  | 91.2    | C      | 16 | 51.4 | 83.8    | C      |
| 7  | 27.6 | 79.7    | C      | 17 | 81.0 | 19.2    | Т      |
| 8  | 89.9 | 2.2     | Т      | 18 | 51.0 | 85.0    | C      |
| 9  | 41.5 | 24.5    | Т      | 19 | 62.2 | 90.1    | C      |
| 10 | 95.0 | 43.5    | Т      | 20 | 95.1 | 22.2    | Т      |
|    |      |         |        | 21 | 41.6 | 91.5    | C      |

## Binary choice model

### Specification of utility functions

$$U_C = \beta_1 T_C + \varepsilon_C$$
  
$$U_T = \beta_1 T_T + \varepsilon_T$$

where  $T_C$  is the travel time by car (min) and  $T_T$  the travel time by transit (min).

### Choice model

$$P(C|\{C,T\}) = P(U_C \ge U_T)$$

$$= P(\beta_1 T_C + \varepsilon_C \ge \beta_1 T_T + \varepsilon_T)$$

$$= P(\beta_1 T_C - \beta_1 T_T \ge \varepsilon_T - \varepsilon_C)$$

$$= P(\varepsilon \le \beta_1 (T_C - T_T))$$

where  $\varepsilon = \varepsilon_T - \varepsilon_C$ .



### Error term

## Three questions about the random variables $\varepsilon_{\mathcal{T}}$ and $\varepsilon_{\mathcal{C}}$

- What's their mean?
- What's their variance?
- What's their distribution?

### Note

For binary choice it is sufficient to make assumptions about  $\varepsilon = \varepsilon_{T} - \varepsilon_{C}$ 

## The mean

### Change of variables

- Define  $E[\varepsilon_C] = \beta_C$  and  $E[\varepsilon_T] = \beta_T$ .
- Define  $\varepsilon_{\mathcal{C}}' = \varepsilon_{\mathcal{C}} \beta_{\mathcal{C}}$  and  $\varepsilon_{\mathcal{T}}' = \varepsilon_{\mathcal{T}} \beta_{\mathcal{T}}$ ,
- so that  $E[\varepsilon_C'] = E[\varepsilon_T'] = 0$ .

### Choice model

$$P(C|\{C,T\}) =$$

$$\begin{array}{lll} \Pr(\beta_{1}(T_{C}-T_{T}) & \geq & \varepsilon_{T}-\varepsilon_{C}) = \\ \Pr(\beta_{1}(T_{C}-T_{T}) & \geq & \varepsilon'_{T}+\beta_{T}-\varepsilon'_{C}-\beta_{C}) = \\ \Pr(\beta_{1}(T_{C}-T_{T})+(\beta_{C}-\beta_{T}) & \geq & \varepsilon'_{T}-\varepsilon'_{C}) = \\ \Pr(\beta_{1}(T_{C}-T_{T})+\beta_{0} & \geq & \varepsilon') \end{array}$$

where  $\beta_0 = \beta_C - \beta_T$  and  $\varepsilon' = \varepsilon'_T - \varepsilon'_C$ .

### Error term

#### The mean

- ullet The mean of arepsilon can be included as a parameter of the deterministic part of utility
- Only the mean of the difference of the error terms is meaningful

## Alternative Specific Constant (ASC)

$$U_C = \beta_1 T_C + \varepsilon_C \text{ or } U_C = \beta_1 T_C - \beta_0 + \varepsilon_C$$
  
 $U_T = \beta_1 T_T + \beta_0 + \varepsilon_T \text{ or } U_T = \beta_1 T_T + \varepsilon_T$ 

In practice: needs to associate an ASC with all alternatives but one

### The mean

#### Note

Adding the same constant (K) to all utility functions does not affect the choice model

$$Pr(U_C \ge U_T) = Pr(U_C + K \ge U_T + K) \quad \forall K \in \mathbb{R}^n.$$

#### The bottom line...

If the deterministic part of the utility functions contains an ASC for all alternatives but one, the mean of the error terms can be assumed to be zero without loss of generality.

## The variance

### Utility is ordinal

Utilities can be scaled up or down without changing the choice probability

$$\Pr(U_C \ge U_T) = \Pr(\alpha U_C \ge \alpha U_T) \quad \forall \alpha > 0$$

#### Link with the variance

$$Var(\alpha U_C) = \alpha^2 Var(U_C)$$
  
 $Var(\alpha U_T) = \alpha^2 Var(U_T)$ 

### Variance is not identified

- As any  $\alpha$  can be selected arbitrarily, any variance can be assumed.
- No way to identify the variance of the error terms from data.
- The scale has to be arbitrarily defined.

### Error term

#### The variance

Imposing an arbitrary variance amounts to imposing an arbitrary scale to the utility

## The distribution

### Assumption 1

 $\varepsilon_T$  and  $\varepsilon_C$  are the sum of many r.v. capturing unobservable attributes (e.g. mood, experience), measurement and specification errors.

#### Central-limit theorem

The sum of many i.i.d. random variables approximately follows a normal distribution:  $N(\mu, \sigma^2)$ .

### Assumed distribution

$$\varepsilon_C \sim N(0,1), \quad \varepsilon_T \sim N(0,1)$$

### The normal distribution

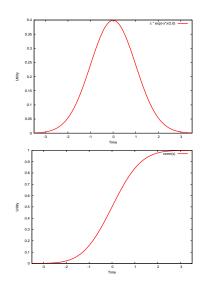
Probability density function (pdf):

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(t-\mu)^2}{2\sigma^2}}$$

Cumulative distribution function (CDF)

$$P(c \ge \varepsilon) = F(c) = \int_{-\infty}^{c} f(t)dt$$

No closed form



## The normal distribution

$$\varepsilon = \varepsilon_T - \varepsilon_C$$

• From the properties of the normal distribution, we have

$$\begin{array}{rcl} \varepsilon_{C} & \sim & \mathcal{N}(0,1) \\ \varepsilon_{T} & \sim & \mathcal{N}(0,1) \\ \varepsilon = \varepsilon_{T} - \varepsilon_{C} & \sim & \mathcal{N}(0,2) \end{array}$$

As the variance is arbitrary, we may also assume

$$arepsilon_{C} \sim N(0, 0.5)$$
 $arepsilon_{T} \sim N(0, 0.5)$ 
 $arepsilon = arepsilon_{T} - arepsilon_{C} \sim N(0, 1)$ 

## The binary probit model

### Choice model

$$P(C|\{C,T\}) = \Pr(\beta_1(T_C - T_T) + \beta_0 \ge \varepsilon) = F_{\varepsilon}(\beta_1(T_C - T_T) + \beta_0)$$

The binary probit model

$$P(C|\{C,T\}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\beta_1(T_C - T_T) - \beta_0} e^{-\frac{1}{2}t^2} dt$$

Not a closed form expression

### Error term

#### The distribution

If the error terms are assumed to follow a normal distribution, the corresponding model is called

Probability Unit Model or Probit Model.

## The distribution

### Assumption 2

 $\varepsilon_T$  and  $\varepsilon_C$  are the maximum of many r.v. capturing unobservable attributes (e.g. mood, experience), measurement and specification errors.

#### Gumbel theorem

The maximum of many i.i.d. random variables approximately follows an Extreme Value distribution:  $EV(\eta, \mu)$ .

### Assumed distribution

$$\varepsilon_C \sim \mathsf{EV}(0,1), \quad \varepsilon_T \sim \mathsf{EV}(0,1).$$

## The Extreme Value distribution $EV(\eta, \mu)$

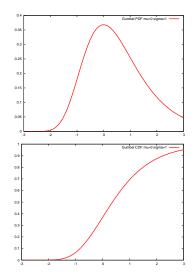
Probability density function (pdf)

$$f(t) = \mu e^{-\mu(t-\eta)} e^{-e^{-\mu(t-\eta)}}$$

Cumulative distribution function (CDF)

$$P(c \ge \varepsilon) = F(c) = \int_{-\infty}^{c} f(t)dt$$
  
=  $e^{-e^{-\mu(c-\eta)}}$ 

## The Extreme Value distribution



## The Extreme Value distribution

### **Properties**

lf

$$\varepsilon \sim \mathsf{EV}(\eta, \mu)$$

then

$$\mathsf{E}[arepsilon] = \eta + rac{\gamma}{\mu} \quad \mathsf{and} \quad \mathsf{Var}[arepsilon] = rac{\pi^2}{6\mu^2}$$

where  $\gamma$  is Euler's constant.

### Euler's constant

$$\gamma = \lim_{k \to \infty} \sum_{i=1}^{k} \frac{1}{i} - \ln k = -\int_{0}^{\infty} e^{-x} \ln x dx \approx 0.5772$$



### The distribution

$$\varepsilon = \varepsilon_T - \varepsilon_C$$

From the properties of the extreme value distribution, we have

$$\varepsilon_C \sim \text{EV}(0,1)$$
  
 $\varepsilon_T \sim \text{EV}(0,1)$   
 $\varepsilon \sim \text{Logistic}(0,1)$ 

## The Logistic distribution: Logistic $(\eta, \mu)$

Probability density function (pdf)

$$f(t) = \frac{\mu e^{-\mu(t-\eta)}}{(1 + e^{-\mu(t-\eta)})^2}$$

Cumulative distribution function (CDF)

$$P(c \ge \varepsilon) = F(c) = \int_{-\infty}^{c} f(t)dt = \frac{1}{1 + e^{-\mu(c-\eta)}}$$

with  $\mu > 0$ .

## The binary logit model

#### Choice model

$$P(C|\{C,T\}) = \Pr(\beta_1(T_C - T_T) + \beta_0 \ge \varepsilon) = F_{\varepsilon}(\beta_1(T_C - T_T) + \beta_0)$$

The binary logit model

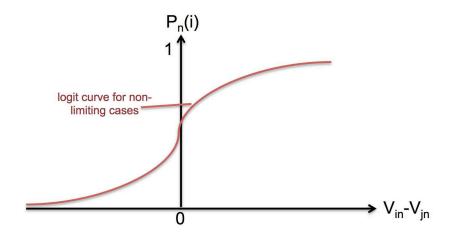
$$P(C|\{C,T\}) = \frac{1}{1 + e^{-(\beta_1(T_C - T_T) + \beta_0)}} = \frac{e^{\beta_1 T_C + \beta_0}}{e^{\beta_1 T_C + \beta_0} + e^{\beta_1 T_T}}$$

The binary logit model

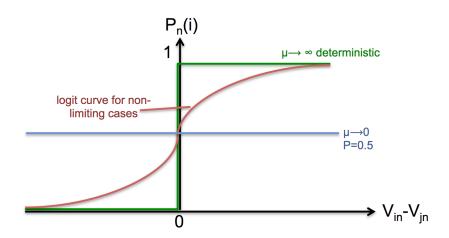
$$P(C|\{C,T\}) = \frac{e^{V_C}}{e^{V_C} + e^{V_T}}$$



## Logit curve



## Logit curve: limiting cases



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- Back to the scale

## Back to the example

### Remember the data from our 21 decision makers?

|    | Time | Time    |        |    | Time | Time    |        |
|----|------|---------|--------|----|------|---------|--------|
| #  | auto | transit | Choice | #  | auto | transit | Choice |
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## First individual

#### **Parameters**

Let's assume that  $\beta_0=0.5$  and  $\beta_1=-0.1$ 

### **Variables**

Let's consider the first observation:

- $T_{C1} = 52.9$
- $T_{T1} = 4.4$
- Choice = transit:  $y_{auto,1} = 0$ ,  $y_{transit,1} = 1$

### Choice

What's the probability given by the model that this individual indeed chooses *transit*?



## First individual

### Utility functions

$$V_{C1} = \beta_1 T_{C1} = -5.29$$
  
 $V_{T1} = \beta_1 T_{T1} + \beta_0 = 0.06$ 

#### Choice model

$$P_1(\mathsf{transit}) = \frac{e^{V_{T1}}}{e^{V_{T1}} + e^{V_{C1}}} = \frac{e^{0.06}}{e^{0.06} + e^{-5.29}} \cong 1$$

### Comments

- The model fits the observation very well.
- Consistent with the assumption that travel time is the only explanatory variable.



## Second individual

#### **Parameters**

Let's assume that  $\beta_0 = 0.5$  and  $\beta_1 = -0.1$ 

### **Variables**

- $T_{C2} = 4.1$
- $T_{T2} = 28.5$
- Choice = transit:  $y_{auto,2} = 0$ ,  $y_{transit,2} = 1$

### Choice

What's the probability given by the model that this individual indeed chooses *transit*?

## Second individual

### Utility functions

$$V_{C2} = \beta_1 T_{C2} = -0.41$$
  
 $V_{T2} = \beta_1 T_{T2} + \beta_0 = -2.35$ 

#### Choice model

$$P_2(\text{transit}) = \frac{e^{V_{T2}}}{e^{V_{T2}} + e^{V_{C2}}} = \frac{e^{-2.35}}{e^{-2.35} + e^{-0.41}} \cong 0.13$$

### Comment

- The model fits the observation poorly.
- But the assumption is that travel time is the only explanatory variable.
- Still, the probability is not small.



## Back to the example

#### Two observations

The probability that the model reproduces both observations is

$$P_1(\text{transit})P_2(\text{transit}) = 0.13$$

#### All observations

The probability that the model reproduces all observations is

$$P_1(\text{transit})P_2(\text{transit})\dots P_{21}(\text{auto}) = 4.62 \ 10^{-4}$$

In general

$$\mathcal{L}^* = \prod_n (P_n(\mathsf{auto})^{y_{\mathsf{auto},n}} P_n(\mathsf{transit})^{y_{\mathsf{transit},n}})$$

where  $y_{j,n}$  is 1 if individual n has chosen alternative j, 0 otherwise

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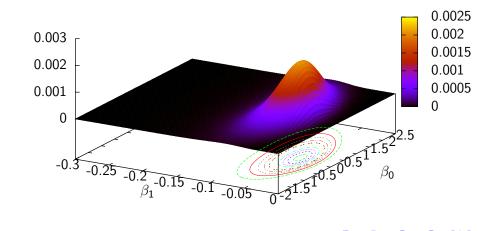
## Back to the example

- $\mathcal{L}^*$  is called the likelihood of the sample for a given model.
- Probability that the model fits all observations
- It is a function of the parameters

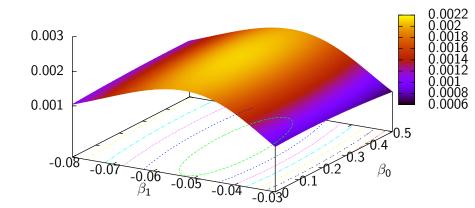
Examples for some values of  $\beta_0$  and  $\beta_1$ 

| $\beta_{0}$ | $\beta_1$ | $\mathcal{L}^*$   |
|-------------|-----------|-------------------|
| 0           | 0         | $4.57 \ 10^{-07}$ |
| 0           | -1        | $1.97 \ 10^{-30}$ |
| 0           | -0.1      | $4.1 \ 10^{-04}$  |
| 0.5         | -0.1      | $4.62 \ 10^{-04}$ |

## Likelihood function



## Likelihood function (zoom)



### Maximum likelihood estimation

#### Estimators for the parameters

Parameters that achieve the maximum likelihood

$$\max_{\beta} \prod_{n} (P_n(\mathsf{auto}; \beta)^{y_{\mathsf{auto},n}} P_n(\mathsf{transit}; \beta)^{y_{\mathsf{transit},n}})$$

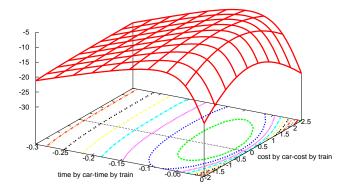
#### Log likelihood

Alternatively, we prefer to maximize the log likelihood

$$\max_{\beta} \ln \prod_{n} (P_n(\mathsf{auto})^{y_{\mathsf{auto},n}} P_n(\mathsf{transit})^{y_{\mathsf{transit},n}}) =$$

$$\max_{\beta} \sum_{n} \ln (y_{\text{auto},n} P_n(\text{auto}) + y_{\text{transit},n} P_n(\text{transit}))$$

### Maximum likelihood estimation



## Solving the optimization problem

#### Unconstrained nonlinear optimization

- Iterative methods
- Designed to identify a local maximum
- When the function is concave, a local maximum is also a global maximum
- For binary logit, the log-likelihood is concave
- Use the derivatives of the objective function

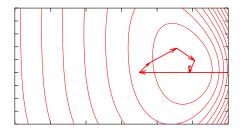
Example: package CFSQP used in BIOGEME

### Example of algorithm

### Tests with CFSQP package within BIOGEME

| Prec.   | $eta_{f 0}^*$ | $eta_1^*$   | $\mathcal{L}^*(eta^*)$ | $\  abla \mathcal{L}^*(eta^*)\ $ |  |  |  |
|---------|---------------|-------------|------------------------|----------------------------------|--|--|--|
| 1.0     | +0.0000e+00   | +1.4901e-08 | -14.56                 | 456.05                           |  |  |  |
| 1.0e-01 | +2.5810e-01   | -5.5361e-02 | -6.172                 | 4.9646                           |  |  |  |
| 1.0e-02 | +2.4274e-01   | -5.2330e-02 | -6.167                 | 1.9711                           |  |  |  |
| 1.0e-03 | +2.3732e-01   | -5.3146e-02 | -6.166                 | 0.089982                         |  |  |  |
| 1.0e-04 | +2.3758e-01   | -5.3110e-02 | -6.166                 | 0.0015384                        |  |  |  |
| 1.0e-05 | +2.3757e-01   | -5.3110e-02 | -6.166                 | 0.0015384                        |  |  |  |

# Example of algorithm: CFSQP



### Nonlinear optimization

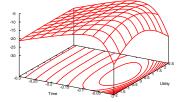
#### Things to be aware of...

• Iterative methods terminate when a given stopping criterion is verified, based on the fact that, if  $\beta^*$  is the optimum,

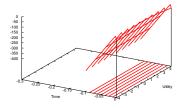
$$\nabla \mathcal{L}(\beta^*) = 0$$

- Stopping criteria vary across optimization packages (based on required precision) → slightly different solutions
- Most methods are sensitive to the conditioning of the problem
- $\bullet$  A well-conditioned problem  $\to$  all parameters have almost the same magnitude

### Nonlinear optimization



Time in min.



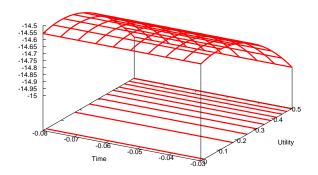
Time in sec.

### Nonlinear optimization

#### Things to be aware of...

- Convergence may be very slow or even fail if likelihood function is flat
- It happens when the model is not identifiable
- Structural flaw in the model (e.g. full set of alternative specific constants)
- Lack of variability in the data (all prices are the same across the sample)

## Nonlinear programming



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## Output of the estimation

### Solution of $\max_{\beta \in \mathbb{R}^K} \mathcal{L}(\beta)$

- β\*
- L(β\*)

### Case study

- $\beta_0^* = 0.2376$
- $\beta_1^* = -0.0531$
- $\mathcal{L}(\beta_0^*, \beta_1^*) = -6.166$

### Second derivatives

Information about the quality of the estimators.

Let

$$\nabla^{2}\mathcal{L}(\beta^{*}) = \begin{pmatrix} \frac{\partial^{2}\mathcal{L}}{\partial\beta_{1}^{2}} & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{1}\partial\beta_{2}} & \cdots & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{1}\partial\beta_{K}} \\ \frac{\partial^{2}\mathcal{L}}{\partial\beta_{2}\partial\beta_{1}} & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{2}^{2}} & \cdots & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{2}\partial\beta_{K}} \end{pmatrix}$$

$$\vdots & \vdots & \vdots & \vdots \\ \frac{\partial^{2}\mathcal{L}}{\partial\beta_{K}\partial\beta_{1}} & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{K}\partial\beta_{2}} & \cdots & \frac{\partial^{2}\mathcal{L}}{\partial\beta_{K}^{2}} \end{pmatrix}$$

 $-\nabla^2 \mathcal{L}(\beta^*)^{-1}$  is a consistent estimator of the variance-covariance matrix of the estimates

### **Statistics**

#### Statistics on the parameters

| Parameter | Value   | Std Err. | <i>t</i> -test |
|-----------|---------|----------|----------------|
| $\beta_0$ | 0.2376  | 0.7505   | 0.32           |
| $eta_{1}$ | -0.0531 | 0.0206   | -2.57          |

### Summary statistics

- $\mathcal{L}(\beta^*) = -6.166$
- $\mathcal{L}(0) = -14.556$
- $-2(\mathcal{L}(0) \mathcal{L}(\beta^*)) = 16.780$
- $\rho^2 = 0.576, \ \bar{\rho}^2 = 0.439$

## Null log likelihood

### $\mathcal{L}(0)$

sample log likelihood with a trivial model where all parameters are zero, that is a model always predicting

$$P(1|\{1,2\}) = P(2|\{1,2\}) = \frac{1}{2}$$

Purely a function of sample size

$$\mathcal{L}(0) = \log(\frac{1}{2^N}) = -N\log(2)$$

### Likelihood ratio

$$-2(\mathcal{L}(0) - \mathcal{L}(\beta^*))$$

$$\log\left(\frac{\mathcal{L}(0)}{\mathcal{L}(\beta^*)}\right) = \log(\mathcal{L}(0)) - \log(\mathcal{L}(\beta^*)) = \mathcal{L}(0) - \mathcal{L}(\beta^*)$$

#### Likelihood ratio test

- H<sub>0</sub>: the two models are equivalent
- Under  $H_0$ ,  $-2(\mathcal{L}(0) \mathcal{L}(\beta^*))$  is asymptotically distributed as  $\chi^2$  with K degrees of freedom.
- Similar to the F test in regression models

## Rho (bar) squared

 $\rho^2$ 

$$\rho^2 = 1 - \frac{\mathcal{L}(\beta^*)}{\mathcal{L}(0)}$$

Similar to the  $R^2$  in regression models

 $\bar{\rho}^2$ 

$$ar{
ho}^2 = 1 - rac{\mathcal{L}(eta^*) - K}{\mathcal{L}(0)}$$

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# Comparing models

- Arbitrary scale may be problematic when comparing models
- Binary probit:  $\sigma^2 = \text{Var}(\varepsilon_i \varepsilon_j) = 1$
- Binary logit:  $Var(\varepsilon_i \varepsilon_j) = \pi^2/(3\mu) = \pi^2/3$
- $Var(\alpha U) = \alpha^2 Var(U)$ .
- Scaled logit coeff. are  $\pi/\sqrt{3}$  larger than scaled probit coeff.

# Comparing models

#### Estimation results

|               | Probit | Logit  | Probit * $\pi/\sqrt{3}$ |
|---------------|--------|--------|-------------------------|
| $\mathcal{L}$ | -6.165 | -6.166 |                         |
| $\beta_{0}$   | 0.064  | 0.238  | 0.117                   |
| $\beta_1$     | -0.030 | -0.053 | -0.054                  |

Note:  $\pi/\sqrt{3} \approx 1.814$ 

# Appendix

# Maximum likelihood for binary logit

- Let  $C_n = \{i, j\}$
- Let  $y_{in} = 1$  if i is chosen by n, 0 otherwise
- Let  $y_{jn} = 1$  if j is chosen by n, 0 otherwise
- Obviously,  $y_{in} = 1 y_{jn}$
- Log-likelihood of the sample

$$\sum_{n=1}^{N} \left( y_{in} \ln \frac{e^{V_{in}}}{e^{V_{in}} + e^{V_{jn}}} + y_{jn} \ln \frac{e^{V_{jn}}}{e^{V_{in}} + e^{V_{jn}}} \right)$$

## Maximum likelihood for binary logit

$$P_{n}(i) = \frac{e^{V_{in}}}{e^{V_{in}} + e^{V_{jn}}}$$

$$\ln P_{n}(i) = V_{in} - \ln(e^{V_{in}} + e^{V_{jn}})$$

$$\frac{\partial \ln P_{n}(i)}{\partial V_{in}} = 1 - \frac{e^{V_{in}}}{e^{V_{in}} + e^{V_{jn}}} = 1 - P_{n}(i) = P_{n}(j)$$

$$\frac{\partial \ln P_{n}(i)}{\partial V_{jn}} = -\frac{e^{V_{jn}}}{e^{V_{in}} + e^{V_{jn}}} = -P_{n}(j)$$