Binary choice

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Outline

Simple example

Choice

between *Auto* and *Transit*

Data

#	Time auto	Time transit	Choice	#	Time auto	Time transit	Choice
1	52.9	4.4	T	11	99.1	8.4	T
2	4.1	28.5	T	12	18.5	84.0	C
3	4.1	86.9	C	13	82.0	38.0	C
4	56.2	31.6	T	14	8.6	1.6	T
5	51.8	20.2	T	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	T
8	89.9	2.2	T	18	51.0	85.0	C
9	41.5	24.5	T	19	62.2	90.1	C
10	95.0	43.5	T	20	95.1	22.2	T
				21	41.6	91.5	C

Outline

Binary choice model

Specification of the utilities

$$\begin{aligned} U_C &= \beta_1 T_C + \varepsilon_C \\ U_T &= \beta_1 T_T + \varepsilon_T \end{aligned}$$

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

Choice model

$$\begin{aligned} P(C|\{C,T\}) &= \Pr(U_C \geq U_T) \\ &= \Pr(\beta_1 T_C + \varepsilon_C \geq \beta_1 T_T + \varepsilon_T) \\ &= \Pr(\beta_1 (T_C - T_T) \geq \varepsilon_T - \varepsilon_C) \\ &= \Pr\left(\varepsilon \leq \beta_1 (T_C - T_T)\right) \end{aligned}$$

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

Error term

Three assumptions about the random variables ε_T and ε_C

1. What's their mean?
2. What's their variance?
3. What's their distribution?

Note

- For binary choice, it would be sufficient to make assumptions about $\varepsilon = \varepsilon_T - \varepsilon_C$.
- But we want to generalize later on.

The mean

Change of variables

- Define $\mathrm{E}[\varepsilon_C] = \beta_C$ and $\mathrm{E}[\varepsilon_T] = \beta_T$.
- Define $\varepsilon'_C = \varepsilon_C - \beta_C$ and $\varepsilon'_T = \varepsilon_T - \beta_T$,
- so that $\mathrm{E}[\varepsilon'_C] = \mathrm{E}[\varepsilon'_T] = 0$.

Choice model

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

$$\begin{array}{lcl}
\Pr(\beta_1(T_C - T_T) & \geq & \varepsilon_T - \varepsilon_C) = \\
\Pr(\beta_1(T_C - T_T) & \geq & \varepsilon'_T + \beta_T - \varepsilon'_C - \beta_C) = \\
\Pr(\beta_1(T_C - T_T) + (\beta_C - \beta_T) & \geq & \varepsilon'_T - \varepsilon'_C) = \\
\Pr(\beta_1(T_C - T_T) + \beta_0 & \geq & \varepsilon')
\end{array}$$

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

The mean

Specification

- The means of the error terms can be included as parameters of the deterministic part.
- Only the mean of the difference of the error terms is identified.

Alternative Specific Constant

Equivalent specifications:

$$\begin{array}{rcll} U_C & = & \beta_1 T_C & +\varepsilon_C \\ U_T & = & \beta_1 T_T + \beta_T & +\varepsilon_T \end{array} \quad \text{or} \quad \begin{array}{rcll} U_C & = & \beta_1 T_C + \beta_C & +\varepsilon_C \\ U_T & = & \beta_1 T_T & +\varepsilon_T \end{array}$$

In practice: associate an alternative specific constant with all alternatives but one.

The mean

Note

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

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

The bottom line...

If the deterministic part of the utility functions contains an Alternative Specific Constant (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

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

Link with the variance

$$\begin{aligned} \mathrm{Var}(\alpha U_C) &= \alpha^2 \mathrm{Var}(U_C) \\ \mathrm{Var}(\alpha U_T) &= \alpha^2 \mathrm{Var}(U_T) \end{aligned}$$

Variance is not identified

- As any α 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 decided.

The distribution

Assumption 1

ε_T and ε_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 $N(\mu, \sigma^2)$

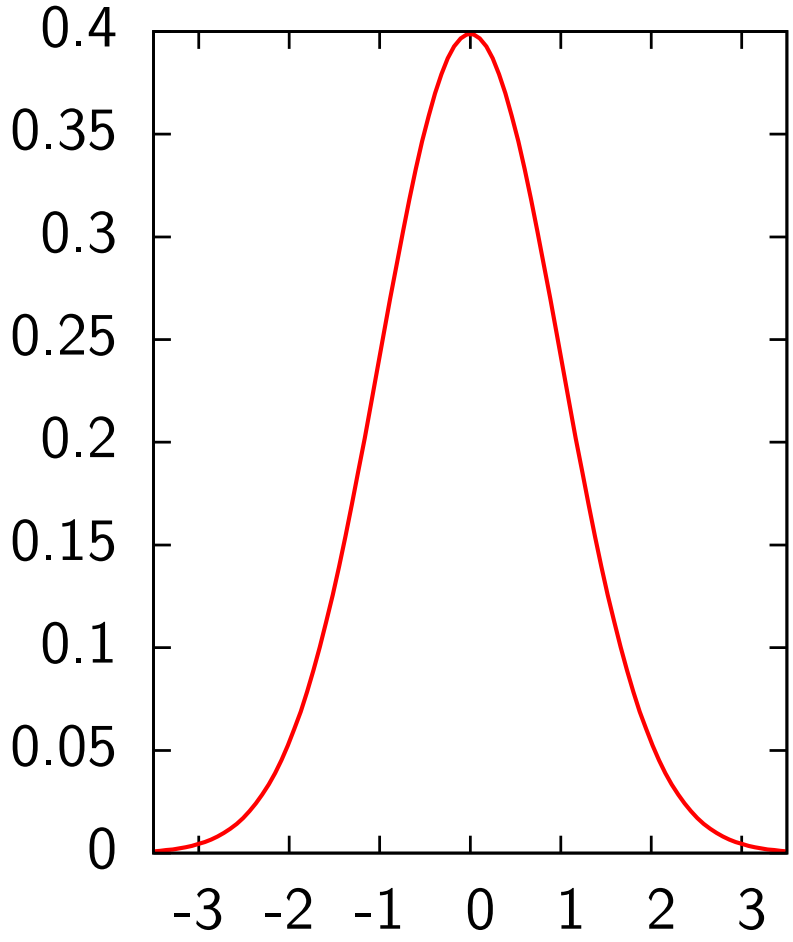
Probability density function (pdf)

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

Cumulative distribution function (CDF)

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

No closed form.



The distribution

$\varepsilon = \varepsilon_T - \varepsilon_C$

- From the properties of the normal distribution, we have

$$\begin{aligned} \varepsilon_C &\sim N(0,1) \\ \varepsilon_T &\sim N(0,1) \\ \varepsilon = \varepsilon_T - \varepsilon_C &\sim N(0,2) \end{aligned}$$

- As the variance is arbitrary, we may also assume

$$\begin{aligned} \varepsilon_C &\sim N(0,0.5) \\ \varepsilon_T &\sim N(0,0.5) \\ \varepsilon = \varepsilon_T - \varepsilon_C &\sim N(0,1) \end{aligned}$$

The binary probit model

Choice model

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

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

The distribution

Assumption 2

ε_T and ε_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: $\text{EV}(\eta, \mu)$.

Assumed distribution

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

The Extreme Value distribution EV(η, μ)

Probability density function (pdf)

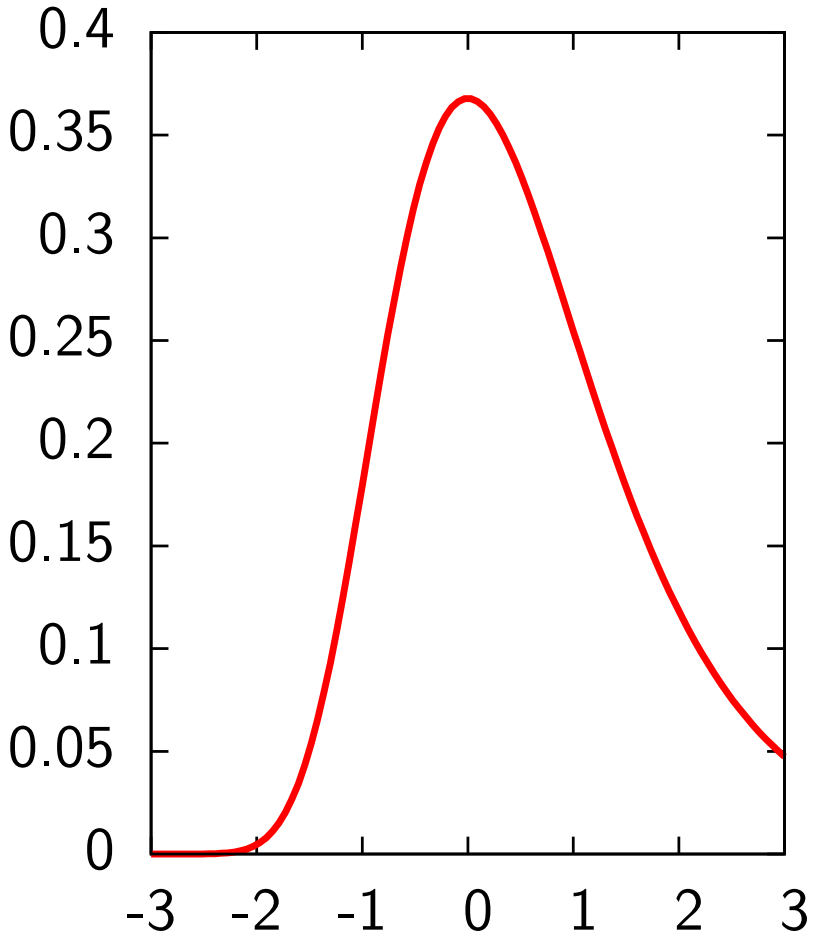
$$f(t) = \mu e^{-\mu(t-\eta)} e^{-e^{-\mu(t-\eta)}}$$

Cumulative distribution function (CDF)

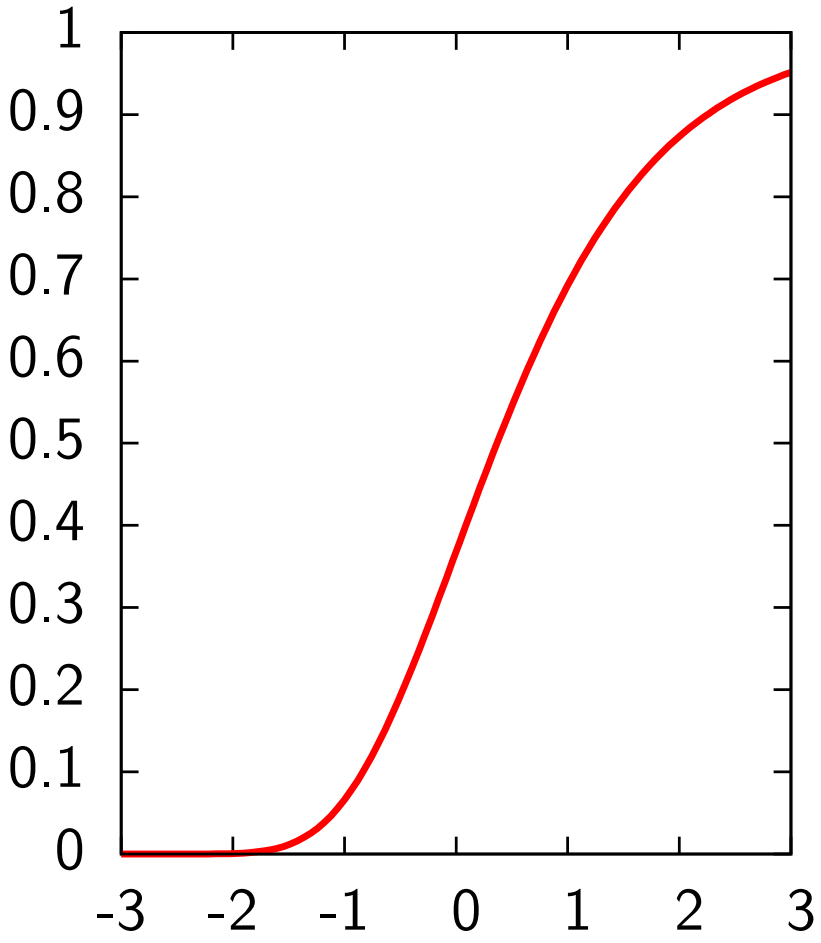
$$\begin{aligned} P(c \geq \varepsilon) = F(c) &= \int_{-\infty}^{c} f(t)dt \\ &= e^{-e^{-\mu(c-\eta)}} \end{aligned}$$

The Extreme Value distribution

pdf EV(0,1)



CDF EV(0,1)



The Extreme Value distribution

Properties

If

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

then

$$\mathrm{E}[\varepsilon] = \eta + \frac{\gamma}{\mu} \quad \text{and} \quad \mathrm{Var}[\varepsilon] = \frac{\pi^2}{6\mu^2}$$

where γ 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

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

The Logistic distribution: Logistic(η,μ)

Probability density function (pdf)

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

Cumulative distribution function (CDF)

$$P(c \geq \varepsilon) = F(c) = \int_{-\infty}^{c} f(t)dt = \frac{1}{1+\exp\left(-\frac{t-\eta}{\mu}\right)}$$

The binary logit model

Choice model

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

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

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

Outline

Back to the example

Choice

between *Auto* and *Transit*

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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*: $y_{\text{auto},1} = 0$, $y_{\text{transit},1} = 1$

Choice

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

First individual

Utility functions

$$\begin{aligned} V_{C1} &= \beta_1 T_{C1} &&= -5.29 \\ V_{T1} &= \beta_1 T_{T1} + \beta_0 &&= 0.06 \end{aligned}$$

Choice model

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

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*: $y_{\text{auto},2} = 0$, $y_{\text{transit},2} = 1$

Choice

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

Second individual

Utility functions

$$\begin{aligned} V_{C2} &= \beta_1 T_{C2} &&= -0.41 \\ V_{T2} &= \beta_1 T_{T2} + \beta_0 &&= -2.35 \end{aligned}$$

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

Likelihood

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

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

Likelihood of the sample

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

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

Likelihood

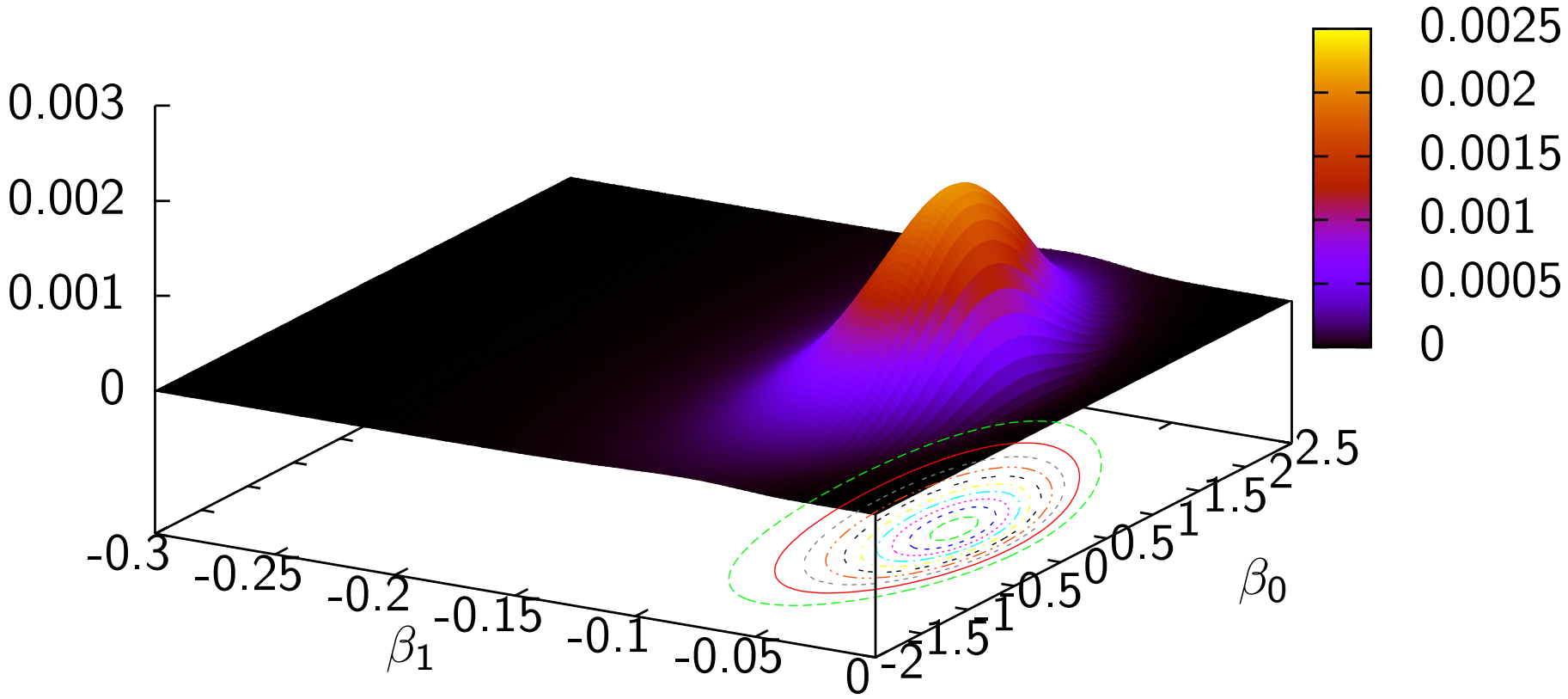
Likelihood

- Probability that the model fits all observations.
- It is a function of the parameters.

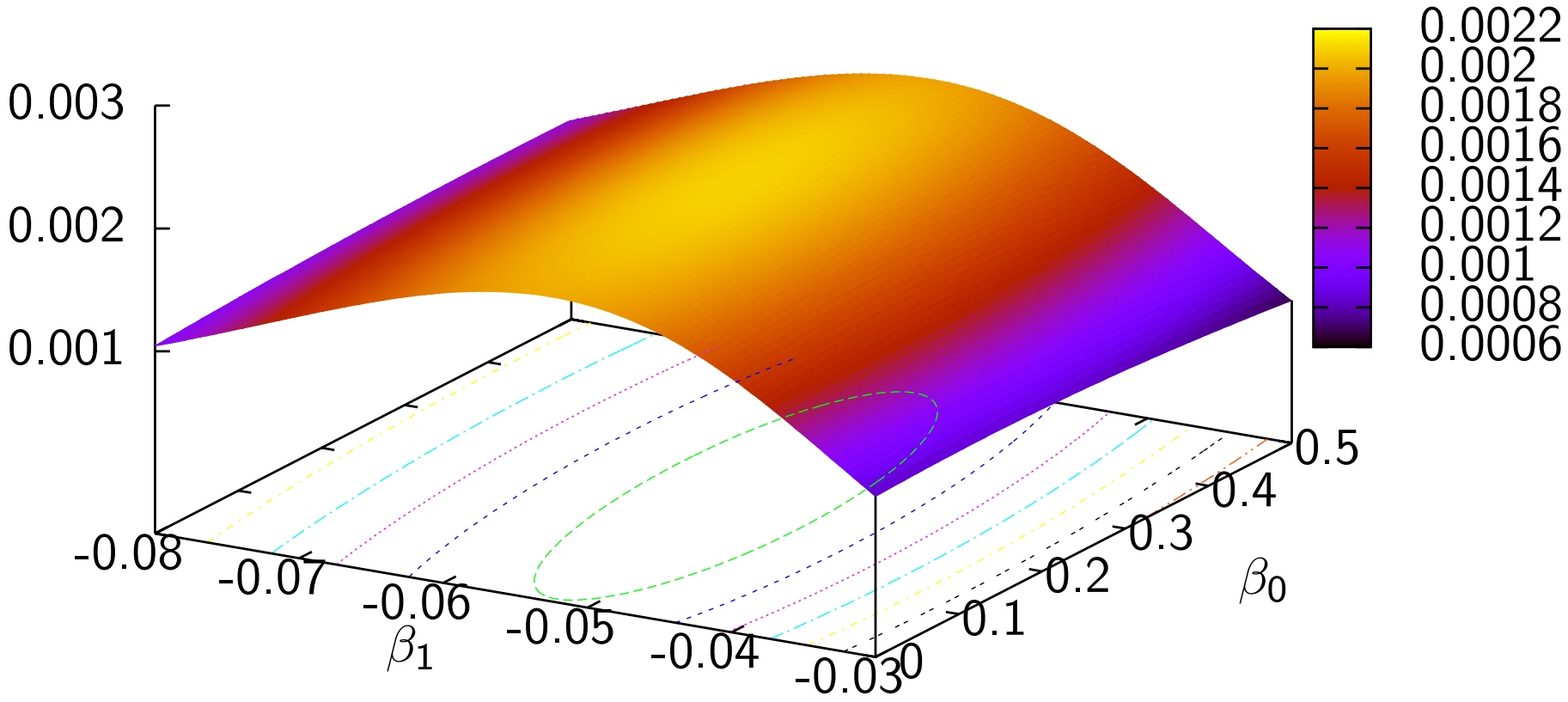
Examples

β_0	β_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)



Outline

Maximum likelihood estimation

Estimators for the parameters

Parameters that achieve the maximum likelihood

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

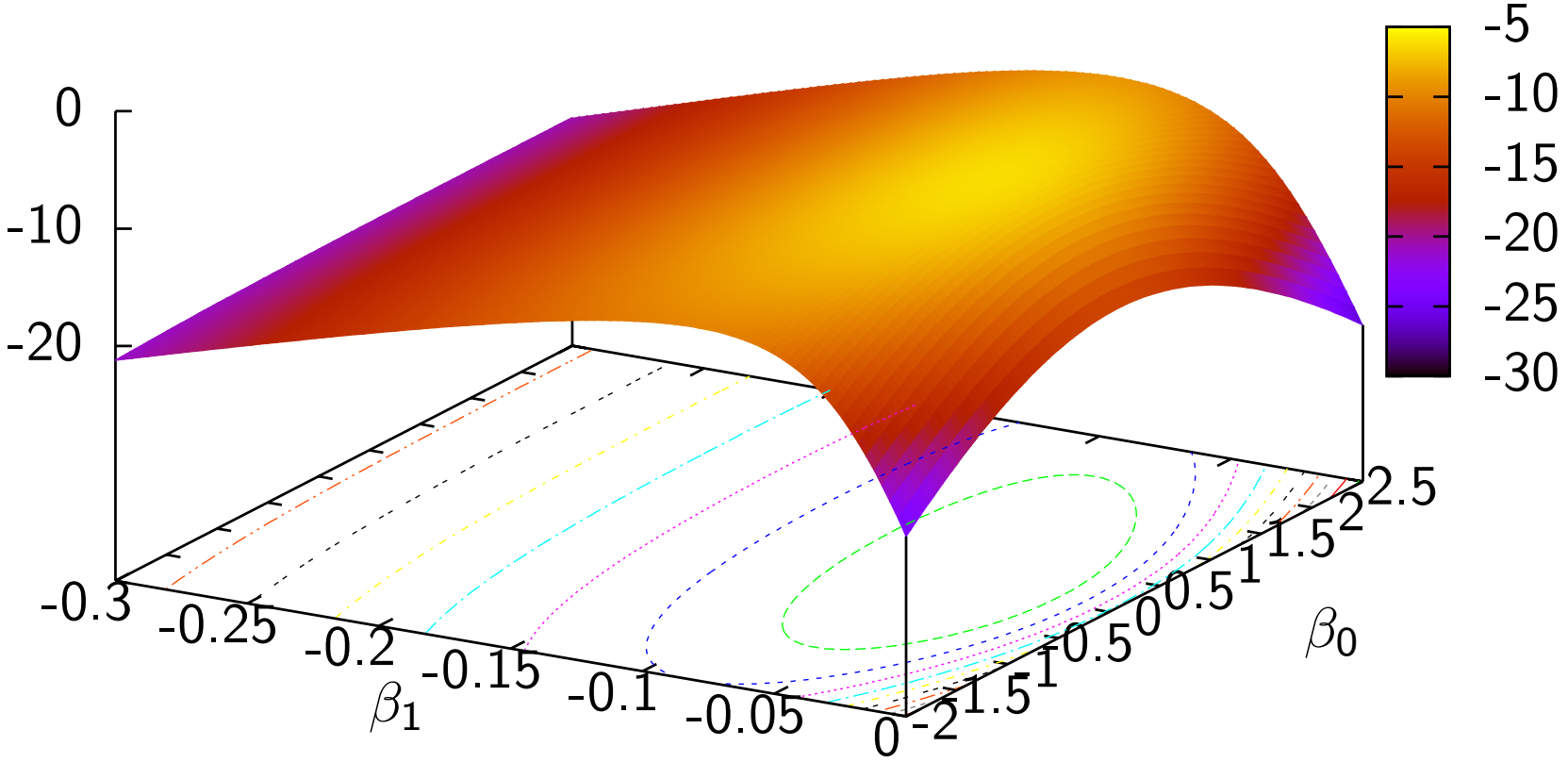
Log likelihood

Alternatively, we prefer to maximize the log likelihood

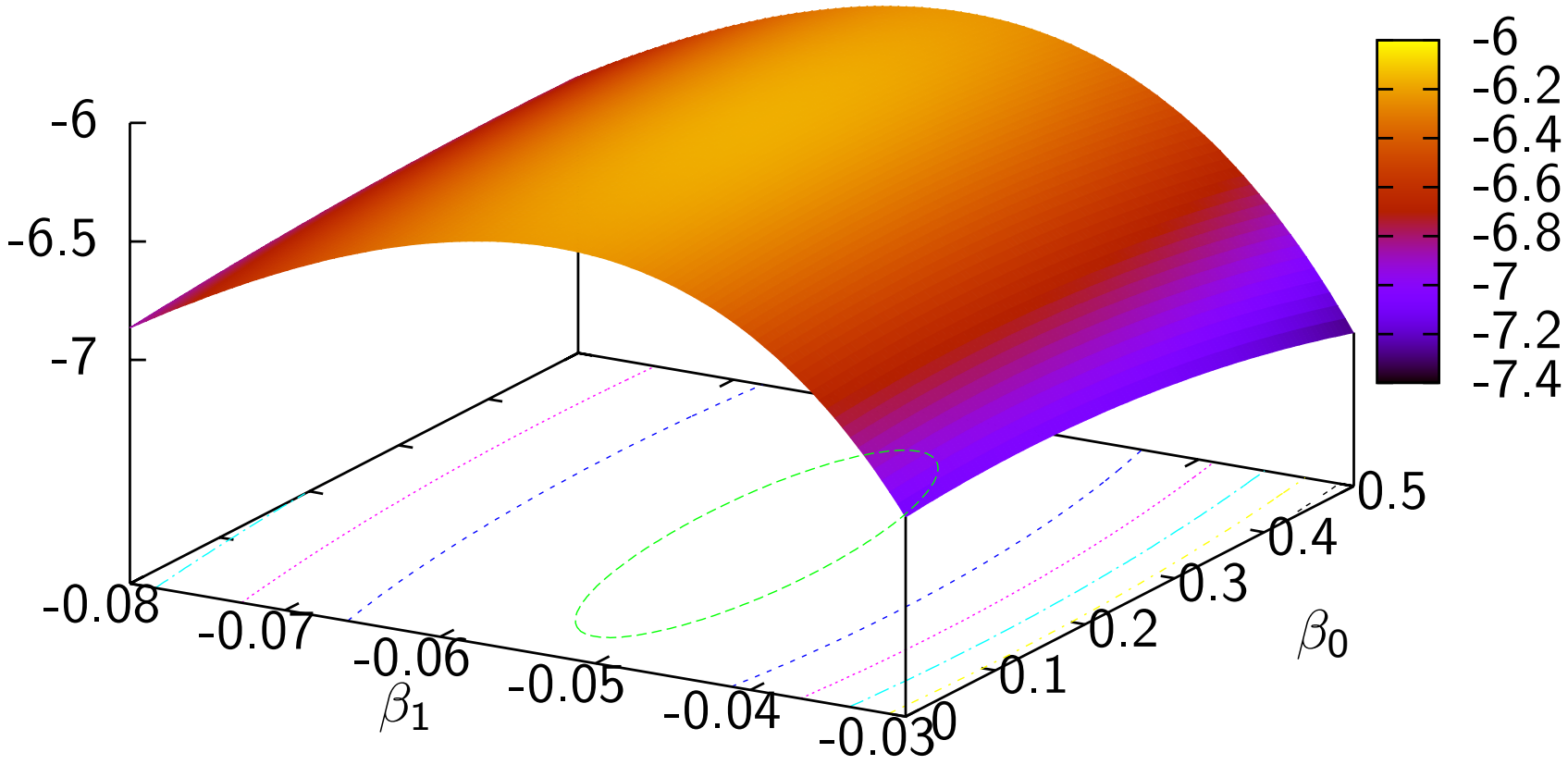
$$\max_{\beta} \ln \prod_{n} \left(P_n(\text{auto})^{y_{\text{auto},n}} P_n(\text{transit})^{y_{\text{transit},n}} \right) =$$

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

Maximum likelihood estimation



Maximum likelihood estimation

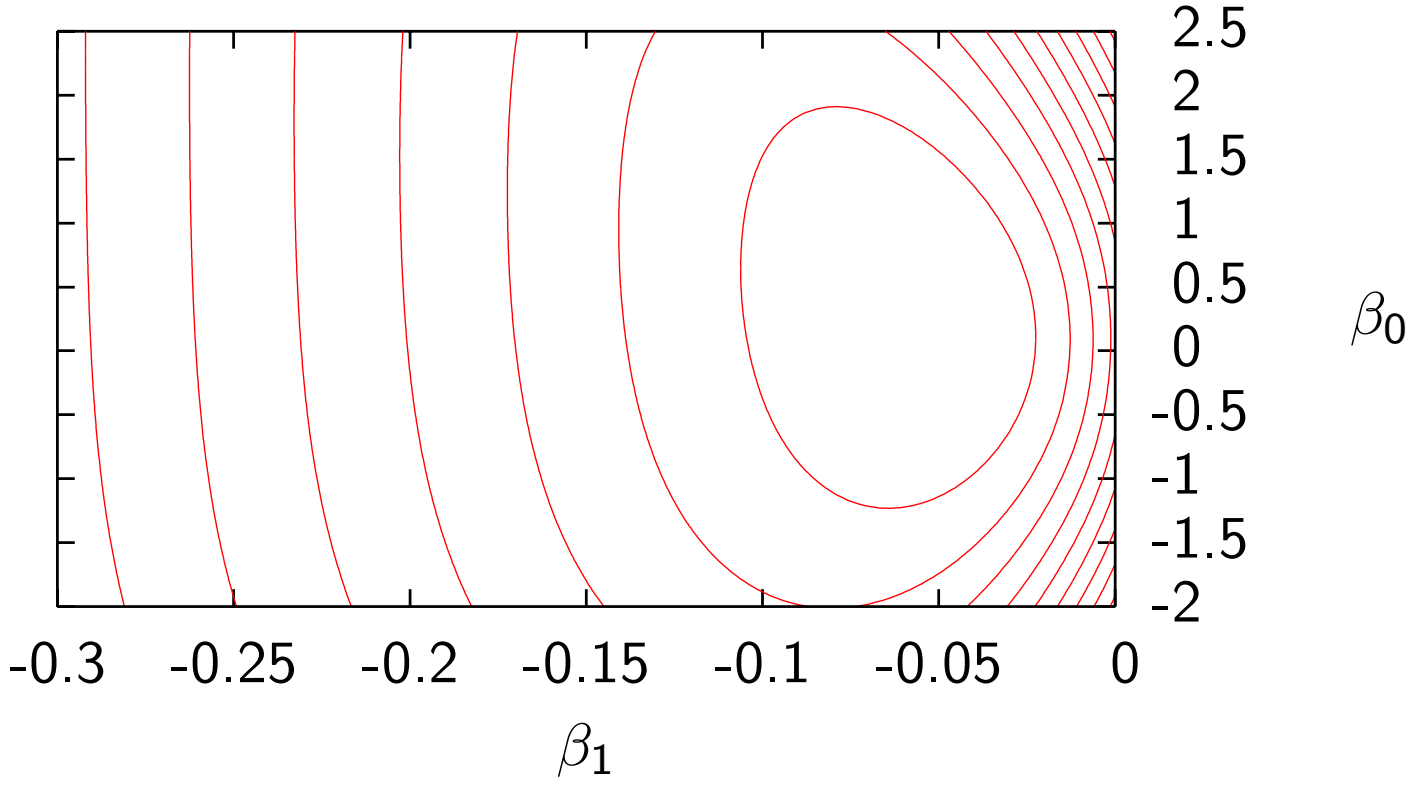


Solving the optimization problem

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

Algorithm CFSQP in Biogeme



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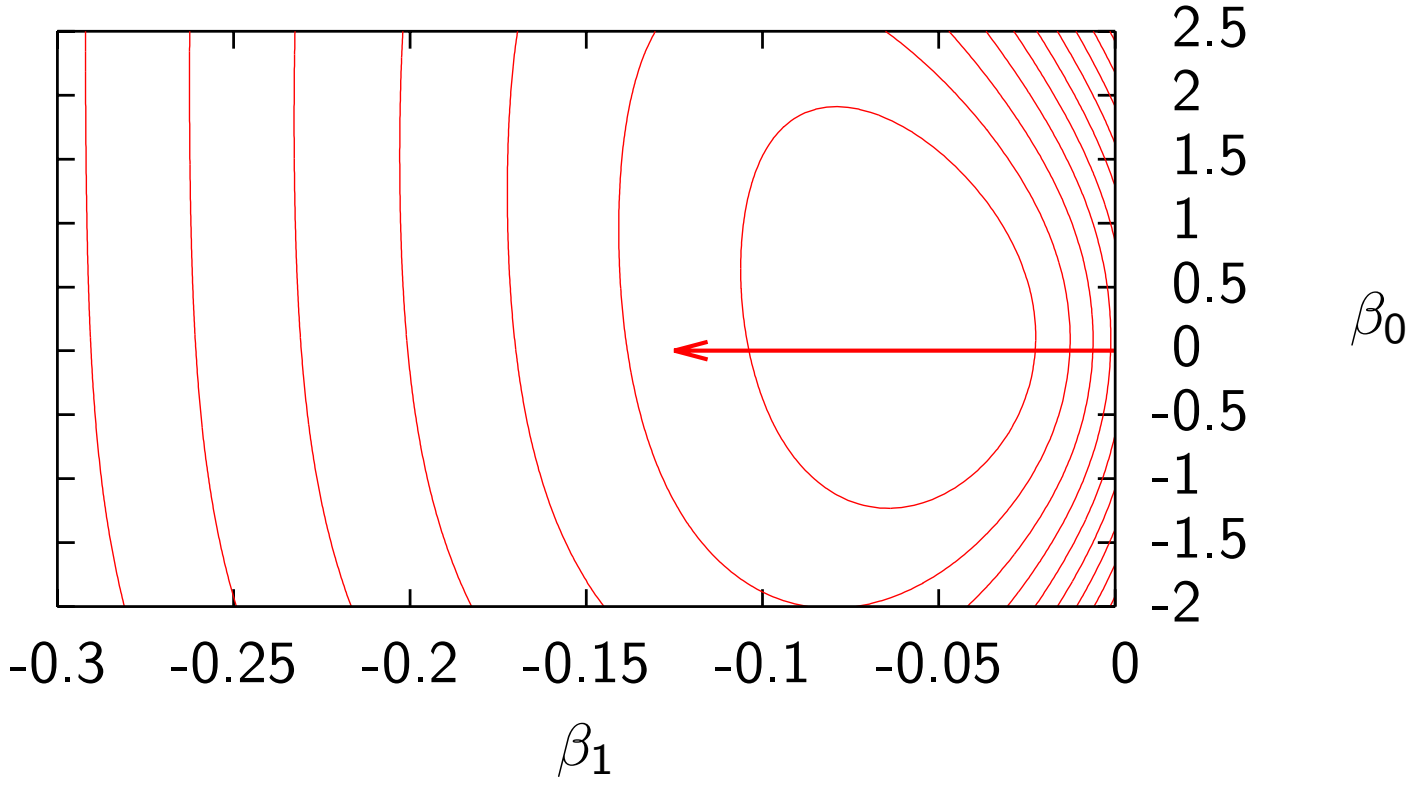

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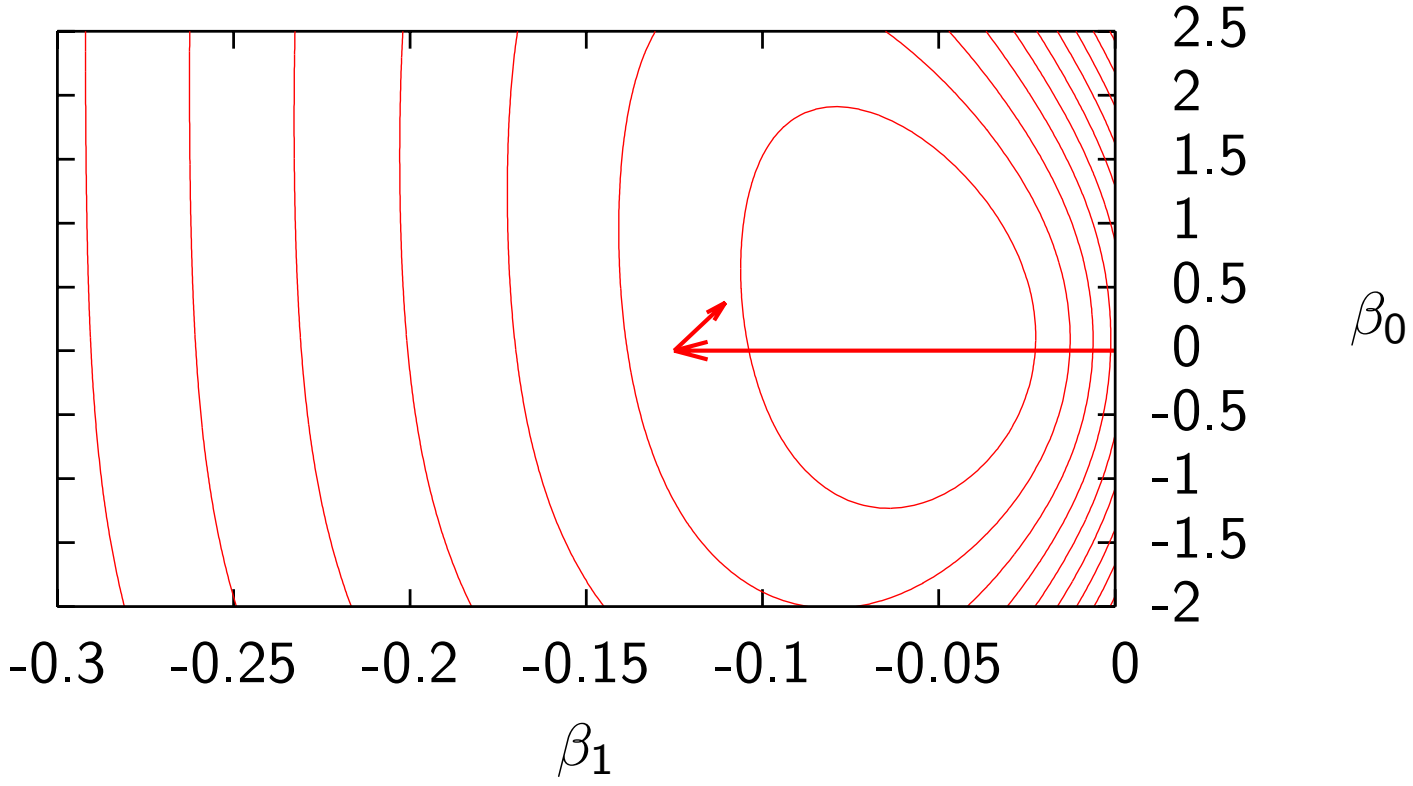

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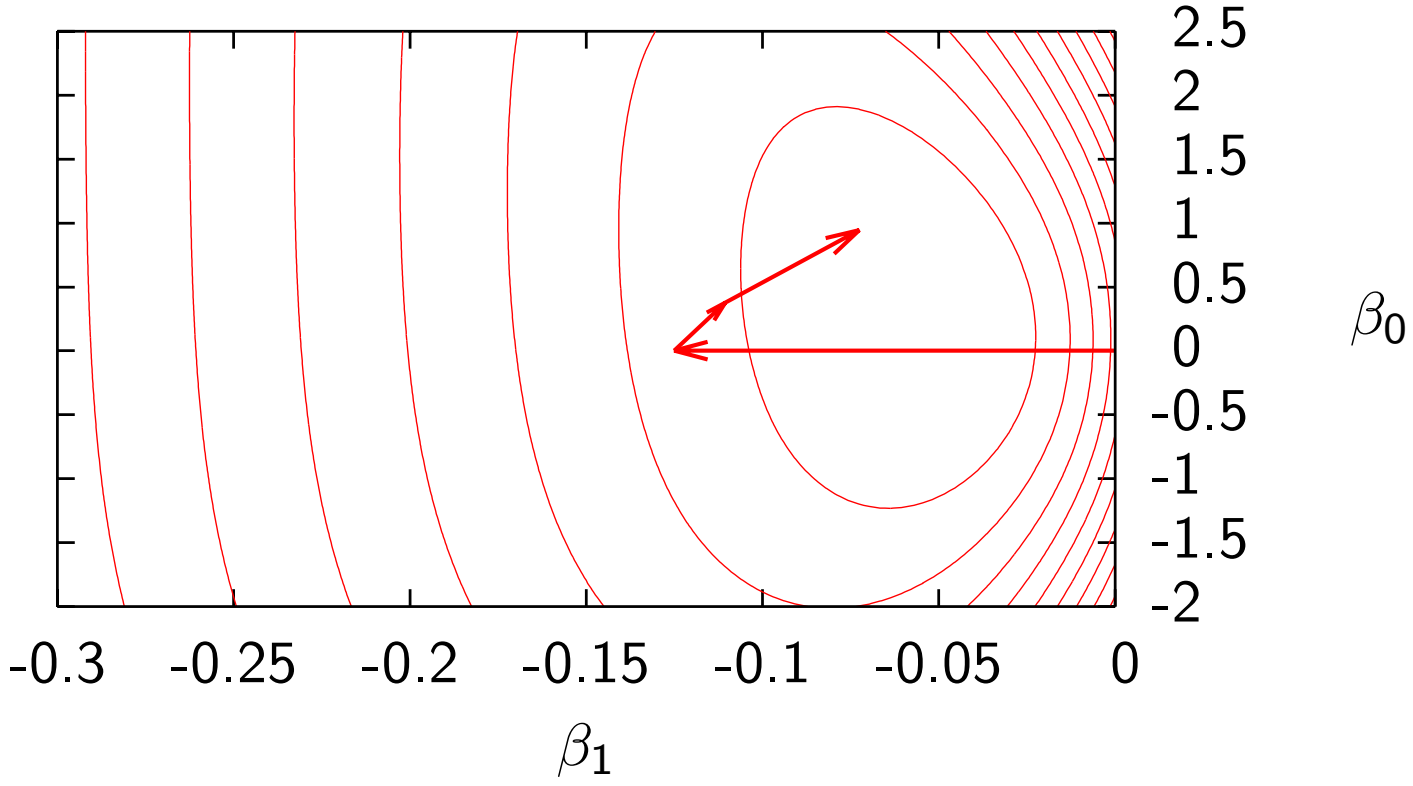

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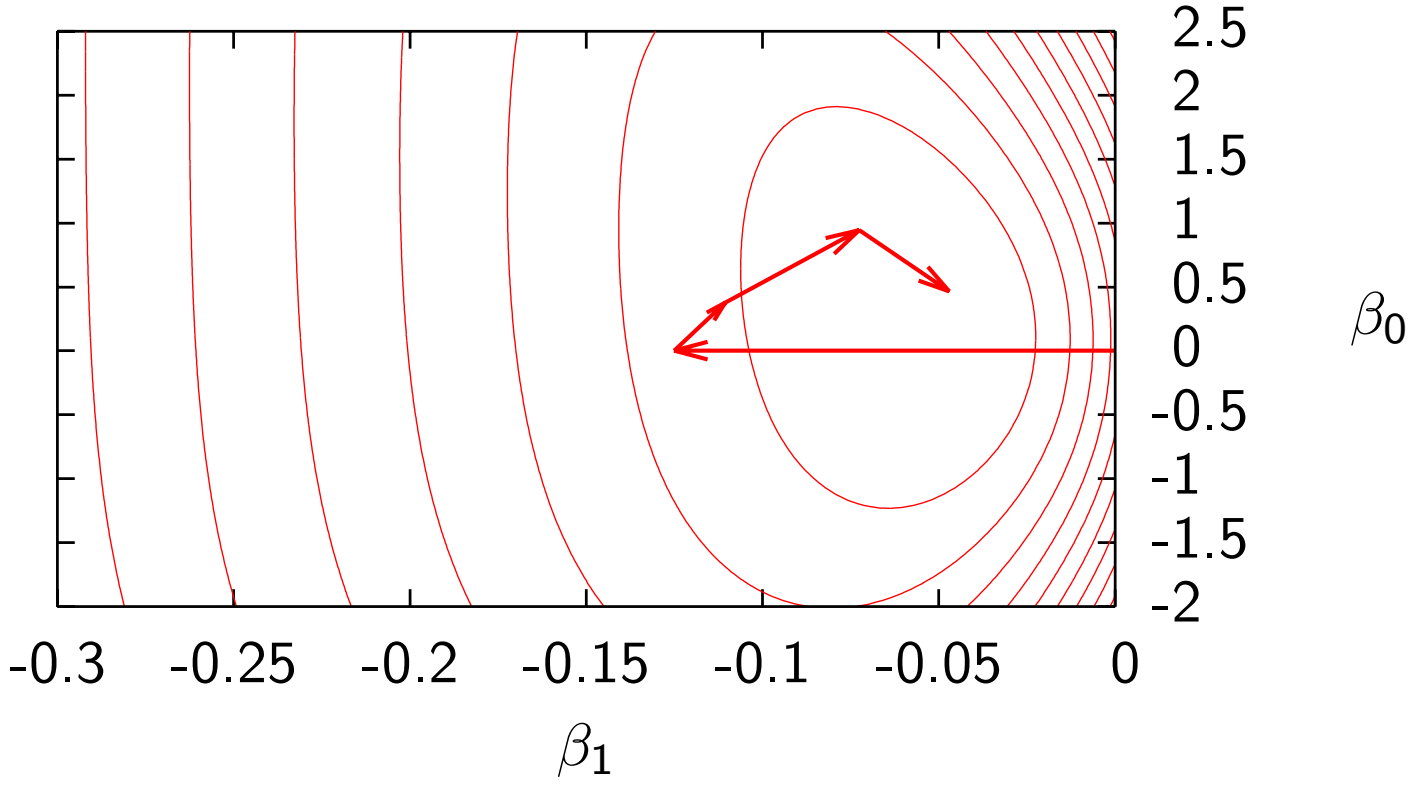

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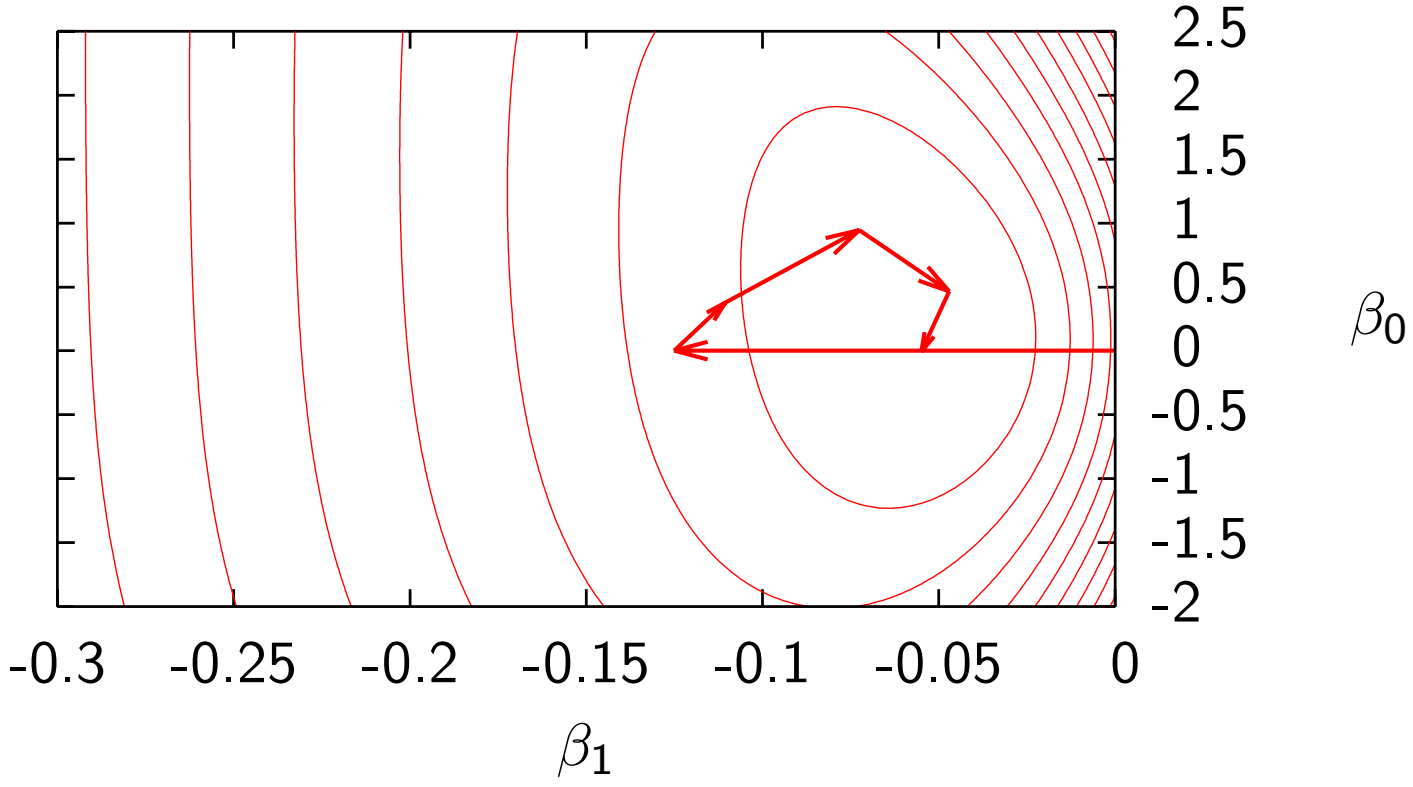

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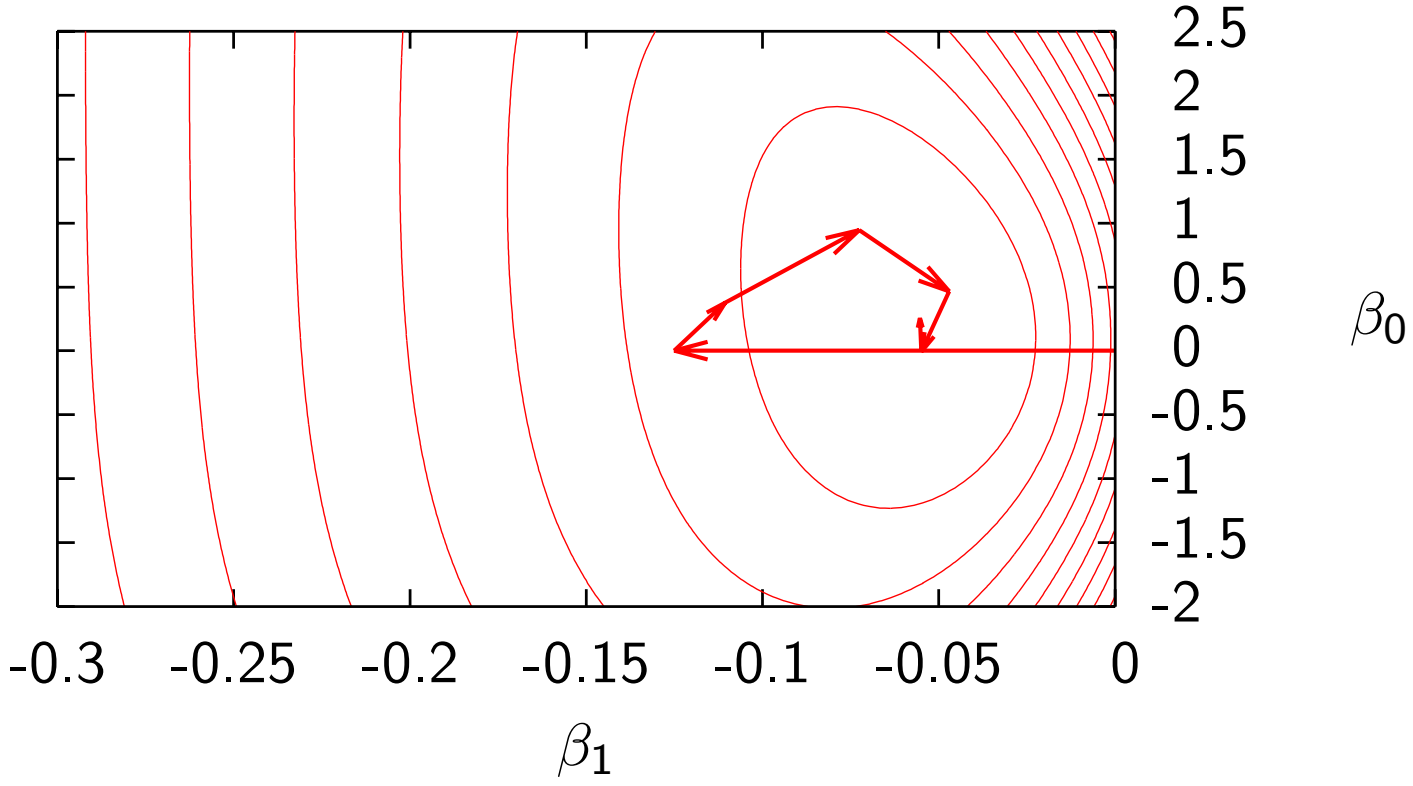

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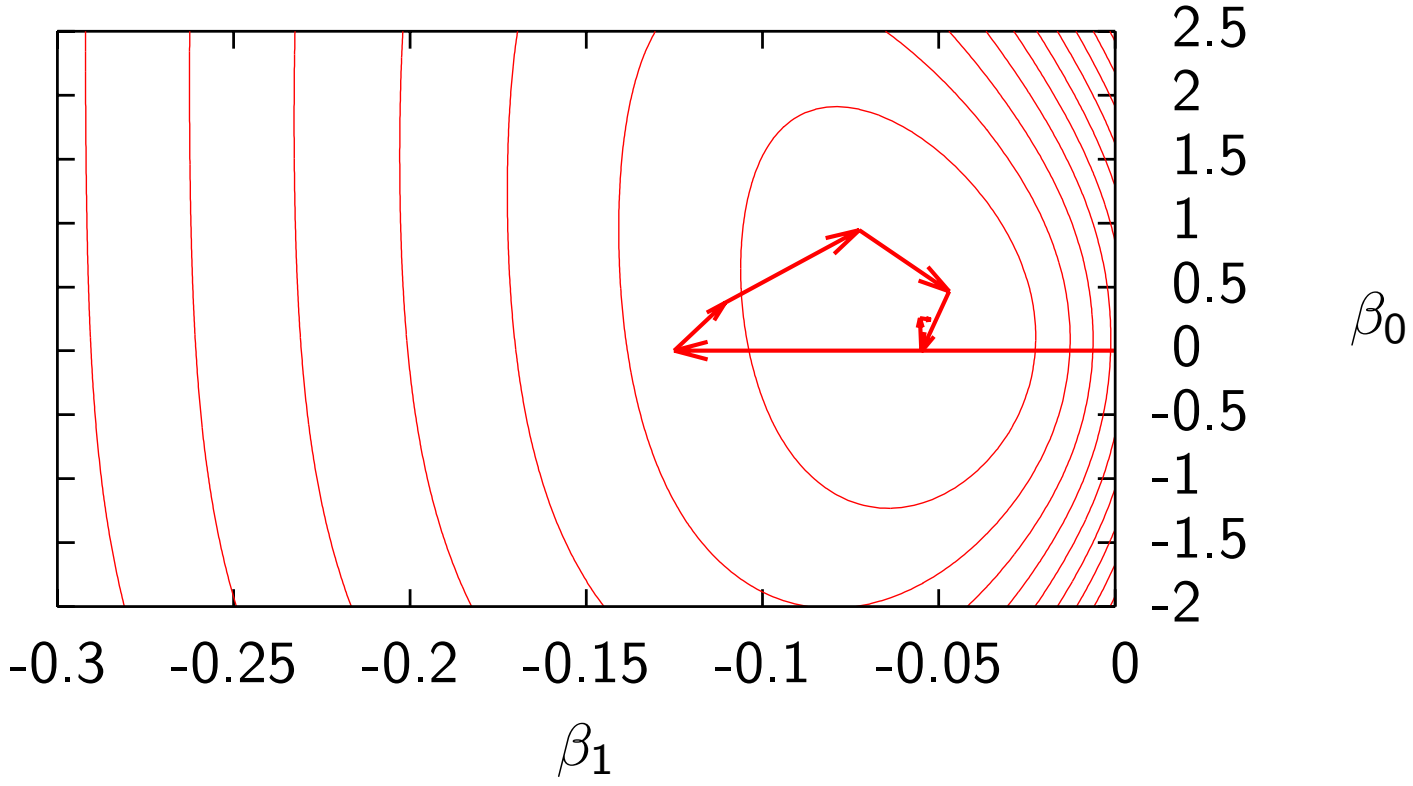


Nonlinear optimization

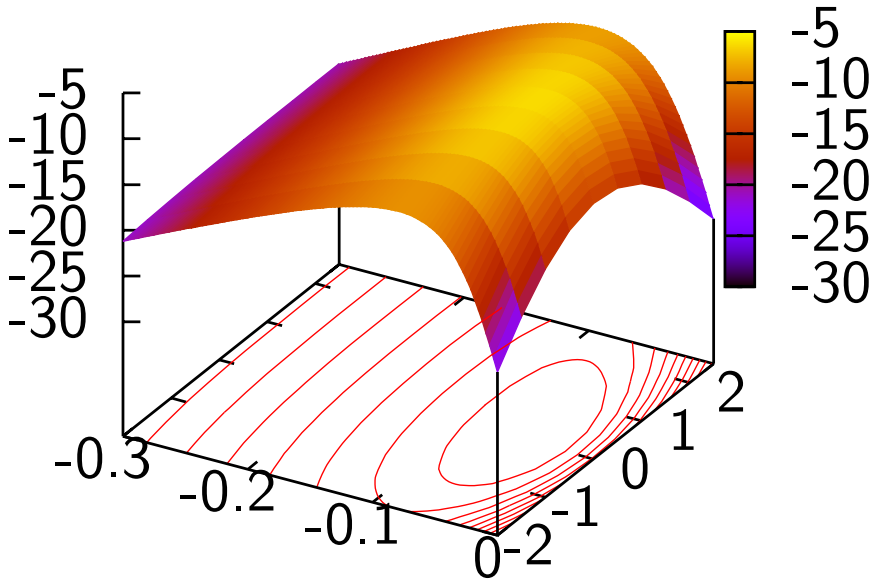
Things to be aware of...

- Iterative methods terminate when a given stopping criterion is verified, based on the fact that, if β^* is the optimum,

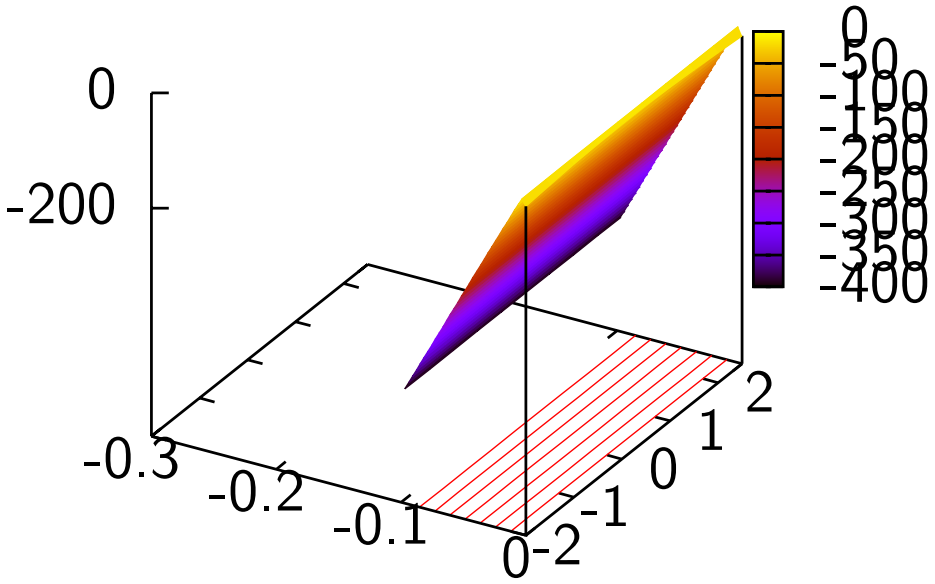
$$\nabla \mathcal{L}(\beta^*) = 0$$

- Stopping criteria usually vary across optimization packages, which may produce slightly different solutions
  They are usually using a parameter defining the required precision
- Most methods are sensitive to the conditioning of the problem.
- A well-conditioned problem is a problem for which all parameters have almost the same magnitude

Nonlinear optimization

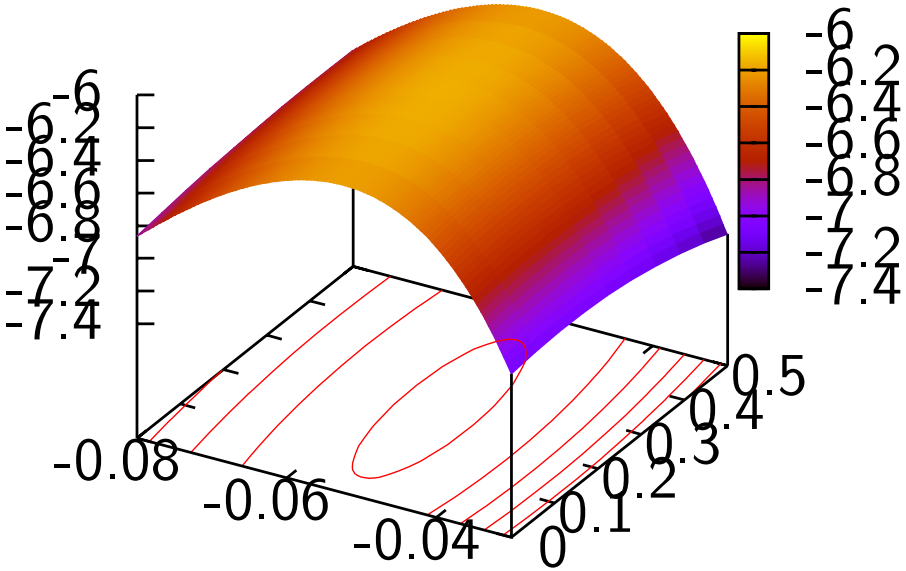


Time in min.

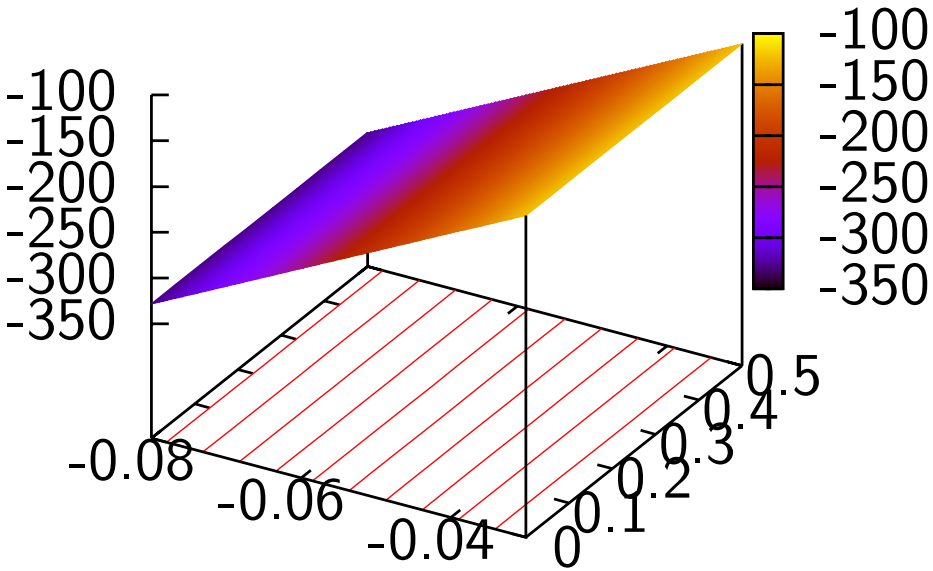


Time in sec.

Nonlinear optimization



Time in min.



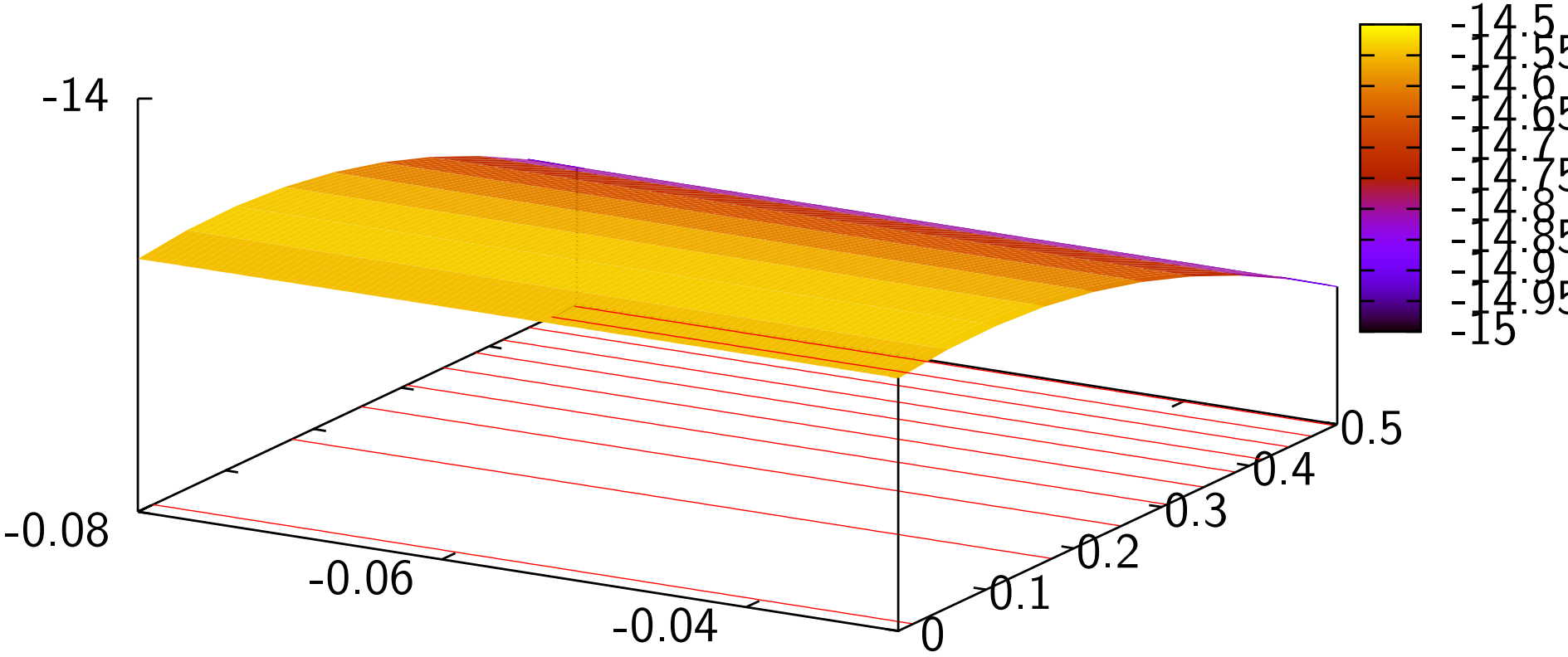
Time in sec.

Nonlinear optimization

Things to be aware of...

- Convergence may be very slow or even fail if the 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 optimization



Outline

Output of the estimation

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

- β^*
- $\mathcal{L}(\beta^*)$

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

$$\nabla^2 \mathcal{L}(\beta^*) = \begin{pmatrix} \frac{\partial^2 \mathcal{L}}{\partial \beta_1^2} & \frac{\partial^2 \mathcal{L}}{\partial \beta_1 \partial \beta_2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial \beta_1 \partial \beta_K} \\ \frac{\partial^2 \mathcal{L}}{\partial \beta_2 \partial \beta_1} & \frac{\partial^2 \mathcal{L}}{\partial \beta_2^2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial \beta_2 \partial \beta_K} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 \mathcal{L}}{\partial \beta_K \partial \beta_1} & \frac{\partial^2 \mathcal{L}}{\partial \beta_K \partial \beta_2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial \beta_K^2} \end{pmatrix}$$

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

Statistics

Statistics on the parameters

Parameter	Value	Std Err.	t-test
β_0	0.2376	0.7505	0.32
β_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_0: the two models are equivalent
- Under H_0, $-2(\mathcal{L}(0) - \mathcal{L}(\beta^*))$ is asymptotically distributed as χ^2 with K degrees of freedom.
- Similar to the F test in regression models

Rho (bar) squared

ρ^2

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

Similar to the R^2 in regression models

$\bar{\rho}^2$

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

Outline

Back to the scale

Comparing models

- Arbitrary scale may be problematic when comparing models
- Binary probit: $\sigma^2 = \text{Var}(\varepsilon_i - \varepsilon_j) = 1$
- Binary logit: $\text{Var}(\varepsilon_i - \varepsilon_j) = \pi^2/(3\mu) = \pi^2/3$
- $\text{Var}(\alpha U) = \alpha^2 \text{ Var } (U)$.
- 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	
β_0	0.064	0.238	0.117
β_1	-0.030	-0.053	-0.054

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

Outline

Maximum likelihood for binary logit

- Let $\mathcal{C}_n = \{i, j\}$
- 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

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

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

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

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

Maximum likelihood for binary logit

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\partial \mathcal{L}}{\partial V_{in}} \frac{\partial V_{in}}{\partial \theta} + \frac{\partial \mathcal{L}}{\partial V_{jn}} \frac{\partial V_{jn}}{\partial \theta}$$

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial V_{in}} &= \sum_{n=1}^{N} \left(y_{in} \frac{\partial \ln P_n(i)}{\partial V_{in}} + y_{jn} \frac{\partial \ln P_n(j)}{\partial V_{in}} \right) \\
&= \sum_{n=1}^{N} \left(y_{in} P_n(j) - y_{jn} P_n(i) \right) \\
&= \sum_{n=1}^{N} \left(y_{in}(1 - P_n(i)) - (1 - y_{in}) P_n(i) \right) \\
&= \sum_{n=1}^{N} \left(y_{in} - P_n(i) \right) \\
&= -\sum_{n=1}^{N} \left(y_{jn} - P_n(j) \right)
\end{aligned}$$

Maximum likelihood for binary logit

$$\frac{\partial \mathcal{L}}{\partial \theta} = \sum_{n=1}^{N} (y_{in} - P_n(i)) \frac{\partial V_{in}}{\partial \theta} + (y_{jn} - P_n(j)) \frac{\partial V_{jn}}{\partial \theta}$$

$$= \sum_{n=1}^{N} (y_{in} - P_n(i)) (\frac{\partial V_{in}}{\partial \theta} - \frac{\partial V_{jn}}{\partial \theta})$$

If $V_{in} = \sum_k \theta_k x_{ink}$, then

$$\frac{\partial \mathcal{L}}{\partial \theta_k} = \sum_{n=1}^{N} (y_{in} - P_n(i))(x_{ink} - x_{jnk})$$