

# Advances in the initialization of probit model estimation and the {ino} R package

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# What is this talk about?

1 The initialization problem

2 The probit model

3 New initialization idea

4 The {ino} R package

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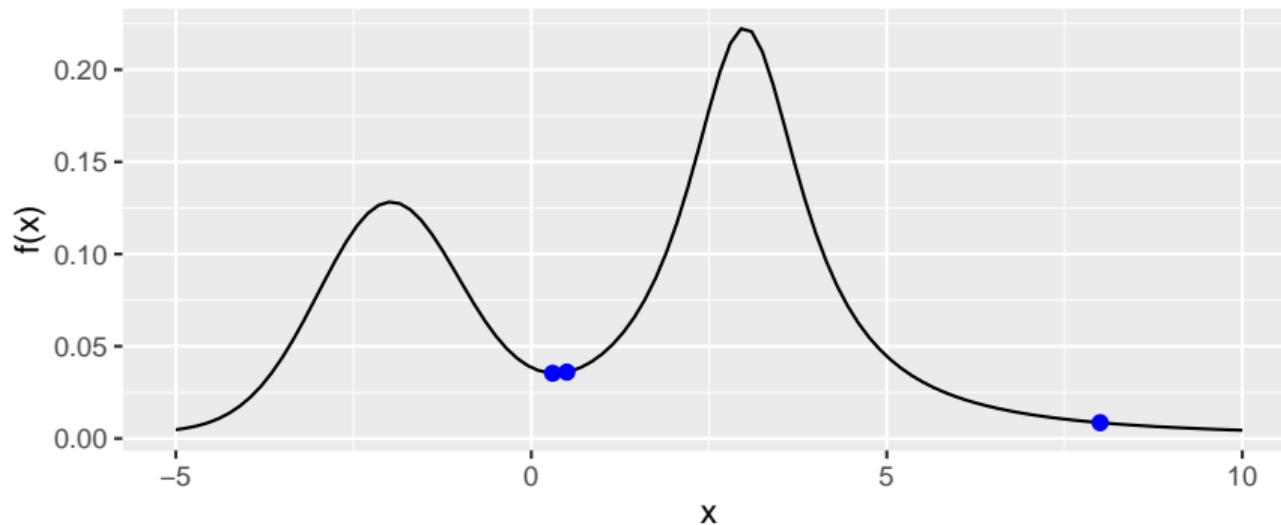
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# Why do we have a problem?

Numerical optimization path

3 different starting points



# We find a local optimum

We find the global optimum



# Convergence takes long

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# Model definition

## Given choice data

- Discrete choice of decider  $n$ :  $y_n \in \{1, \dots, J\}$
- Matrix of (alternative- or decider-specific) covariates of  $n$ :  $X_n \in \mathbb{R}^{J \times P}$

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## Probit model

$$\begin{aligned} U_n &= X_n \beta + \epsilon_n \in \mathbb{R}^J && \text{(Latent utilities)} \\ \epsilon_n &\sim \mathcal{N}_J(0, \Sigma) && \text{(Error term)} \\ y_n &= \arg \max U_n && \text{(Choice link)} \end{aligned}$$

What we want? Estimates  $\hat{\beta}$  (mean sensitivities) and  $\hat{\Sigma}$  (error characterization).

# Model normalization

The probit model (like any utility model) must be normalized:

## Scale normalization

- $U > U' \Leftrightarrow c \cdot U > c \cdot U' \quad \forall c \in \mathbb{R}_+$
- For identification, fix, e.g., one entry of  $\beta$  to 1 (determines  $c$ )

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## Level normalization

- $U > U' \Leftrightarrow U + k > U' + k \quad \forall k \in \mathbb{R}$
- Consider utility differences:  $U > U' \Leftrightarrow (U + k) - (U' + k) > 0$  (cancels  $k$ )
- Note: we loose one dimension ( $J \rightsquigarrow J - 1$ )

# Utility differences

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The difference operator looks like this:

$$\Delta_i = \frac{i-1}{i+1} \begin{pmatrix} 1 & -1 & & \\ & \ddots & -1 & 0 \\ & & 1 & -1 \\ & & & -1 & 1 \\ 0 & -1 & & \ddots & \\ & -1 & & & 1 \end{pmatrix} \in \{-1, 0, 1\}^{(J-1) \times J}$$

# Optimization problem

Probability for choosing alternative  $i$ :

$$P_{ni}(\beta, \Sigma) = \text{Prob}(\Delta_i U_n < 0) = \underbrace{\Phi_{J-1}(-\Delta_i X_n \beta \mid 0, \Delta_i \Sigma \Delta_i')}_{\text{Computation expensive}}$$

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Note: instead of  $\Sigma$ , optimize over  $L$  with  $\Sigma = LL'$ , where  $L$  is the lower-triangular Cholesky root with positive diagonal entries (for uniqueness)

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# Using regression

Let's initialize  $\beta$ .

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Let's initialize  $\beta$ . Idea:

1. Assume that  $\Sigma$  is known (if unknown, set  $\Sigma = I^{J \times J}$ )
2. Consider first-order Taylor approximation of  $P_{n:}$  around 0:

$$P_{n:}(-\Delta_{:,X_n}\beta \mid \Sigma) = P_{n:}(0 \mid \Sigma) + \nabla P_{n:}(0 \mid \Sigma) \cdot (-\Delta_{:,X_n}\beta) + R$$

3. Since  $\mathbb{E}(y_n \mid \Sigma) = P_{n:}(-\Delta_{:,X_n}\beta \mid \Sigma)$ :

$$y_n = P_{n:}(0 \mid \Sigma) + \underbrace{\nabla P_{n:}(0 \mid \Sigma) \cdot (-\Delta_{:,X_n}\beta)}_{\hat{X}_n} + e_n \quad (\text{not a catch-22!})$$

4. Compute OLS estimator  $\hat{\beta}_{OLS}$  (very fast, just matrix product and inverting)

# Using MCMC

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## Trigger warning

Bayes people, please cover your eyes. Abuse of Bayes idea incoming.

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Idea:

1. Assume that  $\beta$  is known (if unknown, set  $\beta = \hat{\beta}_{OLS}$ )
2. Consider posterior of model parameters, including augmented  $(U_n)_n$ :

$$\text{Prob}(\beta, \Sigma, U \mid y) \propto \text{Prob}(\beta, \Sigma) \cdot \text{Prob}(U \mid \beta, \Sigma) \cdot 1\{y_n = \arg \max U_n\}$$

3. Assume conjugate prior and draw from posterior using Gibbs sampling (fairly fast)
4. Find  $\hat{\Sigma}_{MCMC}$  as marginal posterior mode

# Putting it together

Algorithm:

1. Initialize  $\Sigma = \mathbf{1}^{J \times J}$
2. Estimate  $\hat{\beta}_{OLS}$  using OLS
3. Estimate  $\hat{\Sigma}_{MCMC}$  via MCMC
4. Initialize MLE with  $(\hat{\beta}_{OLS}, \hat{\Sigma}_{MCMC})$

Hope:

- with Step 2 and 3, we initialize MLE close at the global optimum
- so that 4 is faster and more likely converges

## Simulation results

Settings:  $N = 200$ ,  $J = 4$ ,  $P = 4$ ,  $X_n \stackrel{iid}{\sim} \mathcal{N}(0, 1)^{J \times P}$

True parameter:  $\beta \sim \mathcal{N}(0, 1)^P$ ,  $\beta_1 = 1$ ,  $\Sigma = LL' \sim \mathcal{W}^{-1}$

Compare: Random initialization versus strategy in terms of computation time (sec) and deviation of MLE from true parameter (ndev)

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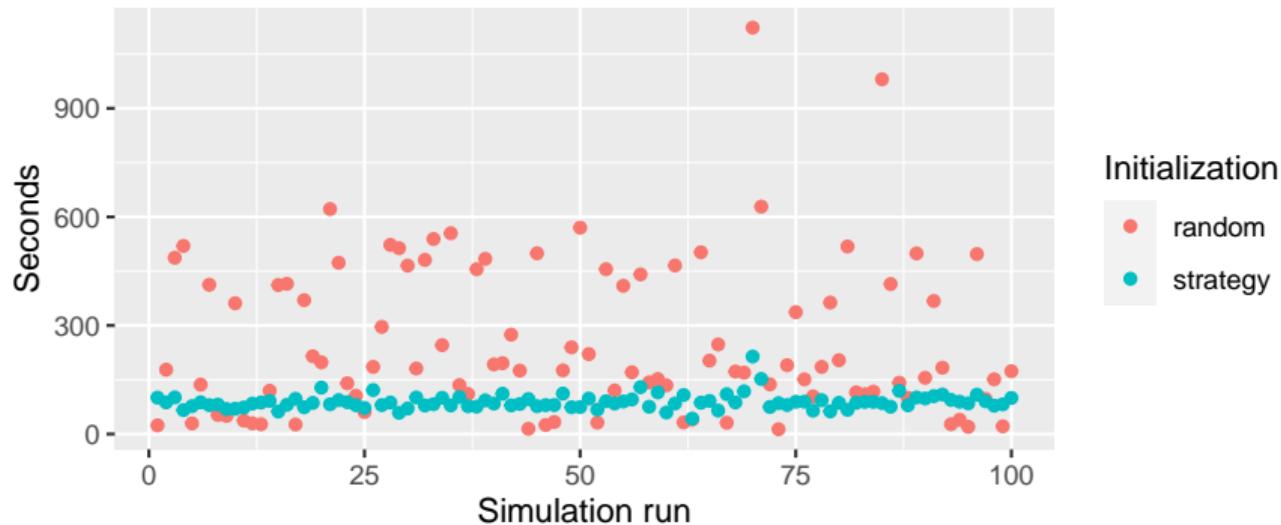
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Table 1: One example run.

	b_1	b_2	b_3	b_4	_1	_2	_3	_4	_5	_6	sec	ndev
true_par	1	0.57	-1.10	1.17	2.46	-0.04	-0.13	2.38	0.10	1.13	0.00	0.00
init_random	1	-0.10	1.15	-0.91	0.23	-0.17	-0.91	0.78	-0.27	0.95	0.00	0.43
est_random	1	0.69	-1.14	1.36	2.10	-1.25	-0.32	1.48	0.38	0.92	487.14	0.16
init_strategy	1	0.87	-1.28	1.25	1.99	-1.22	-0.36	0.72	-0.52	0.66	1.20	0.23
est_strategy	1	0.69	-1.14	1.36	2.10	-1.25	-0.32	1.48	0.38	0.92	101.37	0.16

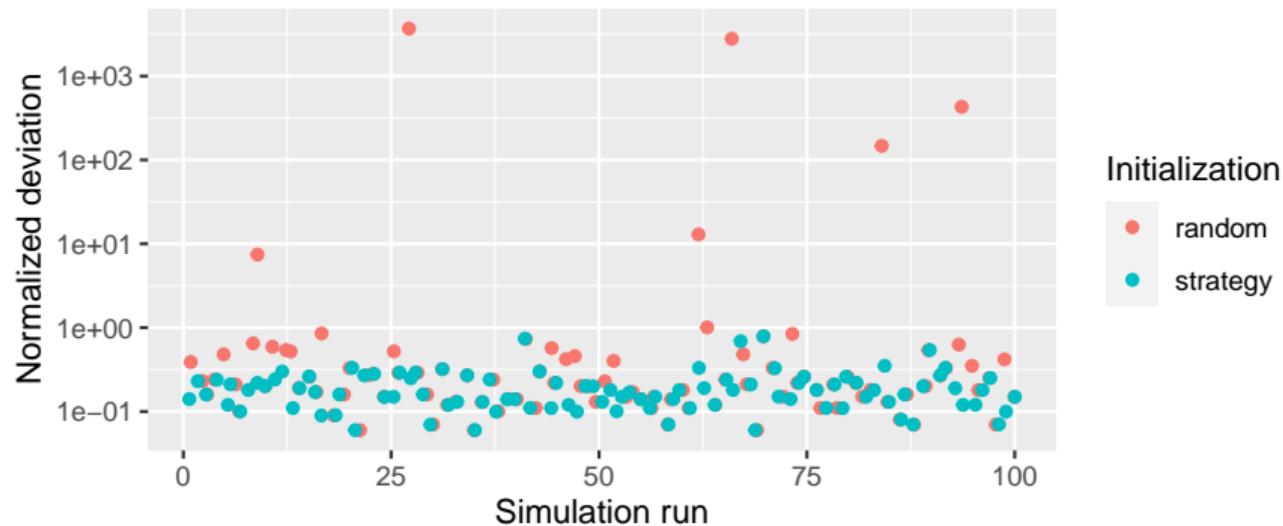
# Simulation results

Improvement of computation time  
Strategy yields faster MLE in 79 of 100 cases



# Simulation results

Improvement of convergence to global optimum  
Strategy has same or smaller deviation in 98 of 100 cases



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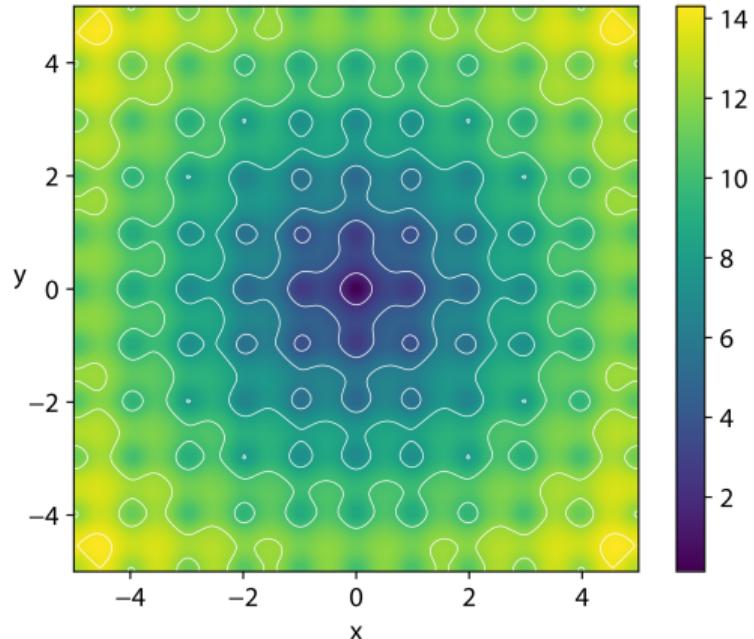
# Purpose

- Joint work with Marius
- Implements strategies for the initialization of numerical optimization:
  - effect of random initialization versus fixed initialization
  - effect of standardizing covariates
  - effect of subsetting covariates
  - effect of alternating optimization
  - comparing optimizer
  - number of identified optima
- Available on CRAN

```
> library("ino")
```

# Setup

```
> x <- setup_ino(  
+   f = f_ackley,  
+   npar = 2,  
+   global = c(0,0),  
+   opt = set_optimizer_nlm()  
+ )  
  
## Function to be optimized  
## f: f_ackley  
## npar: 2  
##  
## Numerical optimizer  
## 'stats::nlm': <optimizer 'stats::nlm'>  
##  
## Optimization runs  
## Records: 0
```



# Random initialization

```
> random_INITIALIZATION(x) %>% get_vars(vars = ".estimate")
```

```
## [1] 2.82139e-07 -1.75042e-07
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```
> x <- random_initialization(  
+   x, runs = 100, ncores = 3,  
+   sampler = function() stats::rnorm(npar(x))  
+ )
```

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> random_initialization(x) %>% get_vars(vars = ".estimate")
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```

```
> overview_optima(x, digits = 2)
```

```
##   optimum frequency  
## 1      0        44  
## 2    2.58       36  
## 3    3.57       12  
## 4    5.38        6  
## 5    6.56        1  
## 6    7.96        1
```

# Thanks for listening!

Key message:

- MLE for probit model is sensitive to initial values
- Regression + MCMC reduce computation time
- {ino} provides universal initialization strategies

Open questions:

- Consistency of strategy?
- How to initialize parameters of mixing distribution?

Please let me know:

- How is initialization an issue for you?
- Thoughts on {ino}?
- Other ideas for initialization?



[loelschlaeger.de/talks](http://loelschlaeger.de/talks)



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