

Inference by Stochastic Optimization: A Free-Lunch Bootstrap

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Introduction: Challenging Inferences

- Extremum estimation: GMM, NLS, MLE, ...
 - where computing the asymptotic variance is not tractable
e.g. rely on transformed/generated data, multi-step estimation, complicated moments/likelihood
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- THIS PAPER: focused on a **Stochastic Newton-Raphson** algorithm, a single run produces
 - a consistent estimator by simple averaging
 - asymptotically valid Bootstrap draws (free-lunch)

The Setup

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for $b = 1, \dots, B$, where $Q_m^{(b)}(\cdot)$ is an m out of n re-sampled objective (or re-weighted/multiplier)

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- **Goal: a 2-in-1 procedure for estimation and inference**

Algorithm: Stochastic Newton-Raphson

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$G_m^{(b)}, H_m^{(b)}$ re-sampled gradient, hessian; $m/n \rightarrow c \in (0, 1]$;
 $\gamma \in (0, 1]$ fixed learning rate

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- iii. $\frac{1}{B} \sum_{b=1}^B \theta^b \simeq \hat{\theta}_n$
- iv. $\text{var}(\theta^b) \simeq \frac{\gamma^2}{1-[1-\gamma]^2} \text{var}(\hat{\theta}_n)$ (the asymptotic variance)

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An Overview of
Derivative-Based Methods

Asymptotic Results

Empirical Illustration

Application:
Sensitivity Analyses

Conclusion

An Overview of Derivative-Based Methods

Gradient Descent and Newton-Raphson Methods

Algorithm: Newton-Raphson

- i. initialize: at θ^0 , given
- ii. for $b = 1, \dots, B$ compute:

$$\theta^b = \theta^{b-1} - \underbrace{\gamma_b}_{\text{learning rate}} \cdot [H_n(\theta^{b-1})]^{-1} G_n(\theta^{b-1})$$

- **Gradient-Descent:** $\theta^b = \theta^{b-1} - \gamma_b \cdot \cancel{[H_n(\theta^{b-1})]^{-1}} G_n(\theta^{b-1})$
 - less costly, slow convergence when $\lambda_{\max}(H_n)/\lambda_{\min}(H_n)$ large

Illustration OLS regression

- OLS regression: $y_i = x_i' \theta + u_i$; $\gamma_b = \gamma$ fixed
- **Newton-Raphson:**

$$\theta^b - \hat{\theta}_n = (1 - \gamma)^b [\theta^0 - \hat{\theta}_n]$$

- for $\gamma_b = 1$ convergence after one iteration

- **Gradient Descent:**

$$\theta^b - \hat{\theta}_n = (I - 2\gamma[\sum_i x_i x_i' / n])^b [\theta^0 - \hat{\theta}_n]$$

- very slow convergence when $\lambda_{\max}(X'X)/\lambda_{\min}(X'X)$ large

Stochastic Gradient Descent

- Full sample G_n, H_n costly to compute for n very large
- **Solution:** use a *minibatch* (small) of subsamples $m \ll n$
- In practice: $m = 1$ is popular

Algorithm: Stochastic Gradient-Descent

- i. initialize: at θ^0 , given
- ii. for $b = 1, \dots, B$ compute:

$$\theta^b = \theta^{b-1} - \gamma_b \cdot G_{\textcolor{red}{m}}^{(b)}(\theta^{b-1})$$

Simple Illustration: OLS estimation ($m = 1$)

- Mini-batch with $m = 1$
- **Stochastic Gradient Descent:**

$$\theta^b - \hat{\theta}_n = (I - 2\gamma_b \underbrace{x_i^{(b)} x_i^{(b)'} }_{\text{noisy}})(\theta^{b-1} - \hat{\theta}_n) - 2\gamma_b \underbrace{x_i^{(b)} \hat{u}_i^{(b)}}_{\text{noisy}}$$

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- For $\theta^b \xrightarrow{P^*} \hat{\theta}_n$ we need $\gamma_b \searrow 0$
 - **fast enough** so that $\mathbb{E}^* \|2\gamma_b [x_i^{(b)} x_i^{(b)'}] \theta^{(b-1)}\|^2 \rightarrow 0$
 - **not too fast** so that $\mathbb{E}^* \|(1 - 2\gamma_b x_i^{(b)} x_i^{(b)'}) (\theta^{b-1} - \hat{\theta}_n)\|^2 \rightarrow 0$ \Rightarrow convergence can be very slow
 - in practice: adaptive methods (adagrad, RMSprop, ...)

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 - in practice: adaptive methods (adagrad, RMSprop, ...)
- **Stochastic Newton-Raphson:** $H_1^{(b)}$ often noisy/near singular
 - e.g. $x_i = (1, x_{i,1})$, $x_{i,1} \sim \text{Bernoulli}(p)$ $\Rightarrow x_i x_i'$ singular wp. 1 for any $p \in [0, 1]$

This Paper: S-NR with larger batches

- Three changes over S-GD:
 - a. re-introduce the Hessian $H_m^{(b)}(\theta^{b-1})$ (NR)
 - b. sample m out of n observations, $m/n \rightarrow c \in (0, 1]$
 - c. fixed learning rate $\gamma_b = \gamma \in (0, 1]$

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$$\theta^b = \theta^{b-1} - \gamma \cdot [H_m^{(b)}(\theta^{b-1})]^{-1} G_m^{(b)}(\theta^{b-1})$$

Simple Illustration: OLS estimation ($m/n \rightarrow c \in (0, 1]$)

- Stochastic Newton-Raphson:

$$\theta^b - \hat{\theta}_n = \underbrace{(1 - \gamma)(\theta^{b-1} - \hat{\theta}_n)}_{\text{deterministic cv.}} + \underbrace{\gamma(\hat{\theta}_m^{(b)} - \hat{\theta}_n)}_{\text{noise}}$$

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- For $\gamma = 1$, $\theta^b = \hat{\theta}_m^{(b)}$ the bootstrapped estimate
- $\theta^b \not\stackrel{p}{\rightarrow} \hat{\theta}_n$ with γ fixed but
 - $\mathbb{E}^*(\theta^b) \simeq \hat{\theta}_n$ and $\text{var}^*(\theta^b) \simeq \frac{\gamma^2}{1-[1-\gamma]^2} \text{var}^*(\hat{\theta}_m^{(b)})$

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- Now: extend this result to a class of non-linear models

Asymptotic Results

Assumption (Sample Objective Function)

- i. $\|H_n(\theta)^{-1}G_n(\theta)\|_2 \leq \overline{C}\|\theta - \hat{\theta}_n\|_2,$
- ii. $\underline{C}\|\theta - \hat{\theta}_n\|_2^2 \leq \langle \theta - \hat{\theta}_n, H_n(\theta)^{-1}G_n(\theta) \rangle,$
- iii. $\underline{c}_H \leq \lambda_{\min}(H_n(\theta)^{-1}) \leq \lambda_{\max}(H_n(\theta)^{-1}) \leq \overline{C}_H,$
- iv. $\|H_n(\theta) - H_n(\hat{\theta}_n)\|_2 \leq C_{n,1} \times \|\theta - \hat{\theta}_n\|_2,$
- v. $\|\sup_{\theta \in \Theta} G_n(\theta)\|_2 \leq \overline{C}_n$

Remark: conditions i-iii. imply strong convexity

Lemma (Newton-Raphson)

Suppose Assumption 1 holds, then for $\gamma \in (0, 1)$ small enough, $\exists \bar{\gamma} \in (0, 1)$ such that for any θ^0 :

$$\|\theta_{NR}^b - \hat{\theta}_n\|_2 \leq (1 - \bar{\gamma}) \|\theta^{b-1} - \hat{\theta}_n\|_2 \leq (1 - \bar{\gamma})^b \|\theta^0 - \hat{\theta}_n\|_2$$

Assumption (Re-Sampled Objective Function)

Suppose the following holds uniformly over $\theta \in \Theta$:

- i. $\| [H_m^{(b)}(\theta)]^{-1} [G_m^{(b)}(\theta) - G_m^{(b)}(\hat{\theta}_n) - H_m^{(b)}(\theta)(\theta - \hat{\theta}_n)] \|_2 \leq C_{m,1} \times \|\theta - \hat{\theta}_n\|_2^2,$
- ii. $\mathbb{E}^* \left(\sup_{\theta \in \Theta} \| [H_n(\theta)]^{-1} - [H_m^{(b)}(\theta)]^{-1} \|_2^2 \right)^{1/2} \leq C_{m,2} \times m^{-1/2},$
- iii. $\left[\mathbb{E}^* \left(\sup_{\theta \in \Theta} \| H_n(\theta) - H_m^{(b)}(\theta) \|_2^2 \right) \right]^{1/2} \leq C_{m,3} \times m^{-1/2},$
- iv. $\left[\mathbb{E}^* \left(\sup_{\theta \in \Theta} \| G_m^{(b)}(\theta) \|_2^2 \right) \right]^{1/2} \leq \overline{C},$ for
 $G_m^{(b)}(\theta) \stackrel{\text{def}}{=} \sqrt{m} [G_m^{(b)}(\theta) - G_n(\theta)].$

where $C_{m,1/2/3}$ and $(C_n)_{n \geq 1}$ are bounded above, $\overline{C} < +\infty$.

Lemma (Linearization of the S-NR Markov-Chain)

Suppose Assumptions 1-3 hold, then for $\gamma \in (0, 1)$ small enough, $\exists \bar{\gamma} \in (0, 1)$ such that $\forall \theta^0$, uniformly in $b \geq 1$:

$$\begin{aligned} \mathbb{E}^* \left(\left\| \theta_{NR}^b - \hat{\theta}_n + \gamma \sum_{j=0}^{b-1} (1-\gamma)^j \mathbb{Z}_m^{b-j} \right\|_2^2 \right)^{1/2} \\ \lesssim m^{-1} + b\rho^b [d_{0,n} + d_{0,n}^2] \end{aligned}$$

where $\rho = \max(1-\gamma, 1-\bar{\gamma}) \in [0, 1)$; $d_{0,n} = \mathbb{E}^* \left(\|\theta^0 - \hat{\theta}_n\|_2^2 \right)^{1/2}$
and $\mathbb{Z}_m^{b-j} = [H_n(\hat{\theta}_n)]^{-1} G_m^{(b-j)}(\hat{\theta}_n)$

Theorem (Convergence in Distribution)

Suppose Assumptions 1-3 hold, let $\mathbb{Z}_m^b = [H_n(\hat{\theta}_n)]^{-1} G_m^{(b)}(\hat{\theta}_n)$ and $\Sigma_n = \text{var}^(\mathbb{Z}_m^b)$. Suppose*

$0 < \underline{\lambda} \leq \lambda_{\min}(\Sigma_n) \leq \bar{\lambda} \leq \lambda_{\max}(\Sigma_n) < +\infty$, and conditions on the characteristic function of \mathbb{Z}_m^b hold then:

$$\sqrt{m}\Sigma_n^{-1/2}(\theta^b - \hat{\theta}_n) \xrightarrow{d^*} \mathcal{N}\left(0, \frac{\gamma^2}{1 - [1 - \gamma]^2} I\right),$$

as $m, b \rightarrow \infty$; if $\log(m)/b \rightarrow 0$ and $d_{0,n} = O(1)$, $n/m = O(1)$.

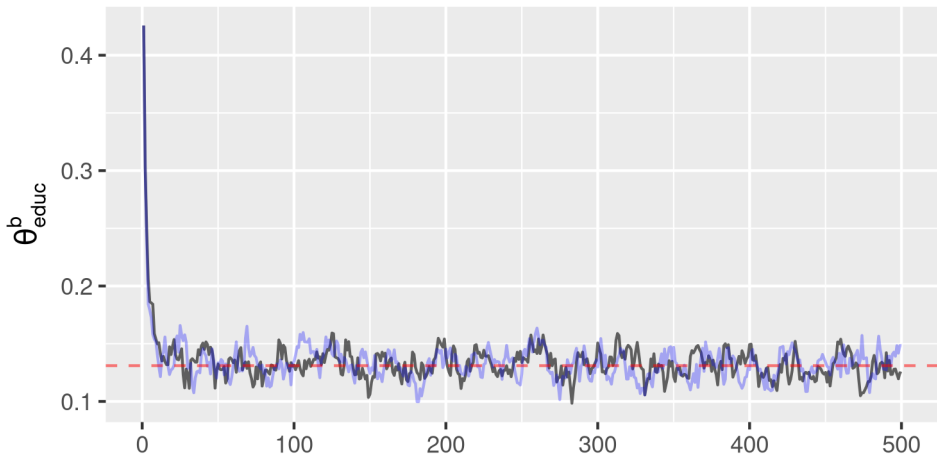
Empirical Illustration

Simple Example: Mroz (1987) Probit model

- Probit model: $\mathbb{P}(y_i = 1|x_i) = \Phi(x_i'\theta)$
- Sample of $n = 753$ observations, $m = n$, $\gamma = 0.3$
- $SNR_{np/m}$: iid re-sampling and multiplier Bootstrap
- Compare $\hat{\theta}_{n,MLE}$, asym. & boot. standard errors with SNR

	nwifeinc	educ	exper	exper2	age	kidslt6	kidsge6	constant
$\hat{\theta}_{n,MLE}$	-0.012	0.131	0.123	-0.002	-0.053	-0.868	0.036	0.270
Asym.	(0.005)	(0.025)	(0.019)	(0.001)	(0.008)	(0.119)	(0.043)	(0.509)
$\bar{\theta}_{n,boot}$	-0.012	0.134	0.124	-0.002	-0.054	-0.883	0.036	0.275
Boot.	(0.005)	(0.027)	(0.020)	(0.001)	(0.009)	(0.122)	(0.046)	(0.524)
SNR_{np}	-0.012	0.133	0.123	-0.002	-0.053	-0.873	0.038	0.263
	(0.005)	(0.026)	(0.019)	(0.001)	(0.010)	(0.119)	(0.046)	(0.510)
SNR_m	-0.012	0.132	0.123	-0.002	-0.053	-0.872	0.036	0.267
	(0.006)	(0.026)	(0.020)	(0.001)	(0.008)	(0.119)	(0.046)	(0.512)

Simple Example: Mroz (1987) Probit model



red: $\hat{\theta}_n$; black/blue: SNR with iid/multiplier Bootstrap

Application: Sensitivity Analyses

- **Influential observations:**

a subset $\mathcal{I} \subset \{1, \dots, n\}$ of the data which impacts the conclusions significantly

- e.g. leads to very different point estimates or standard errors
 - outliers
 - leverage points
 - ...
- Idea: under H_0 (no influential observations) removing \mathcal{I} during the iterations should not significantly affect the Markov-Chain
- Under H_1 (influential observations) should lead to a structural break in the levels/variance

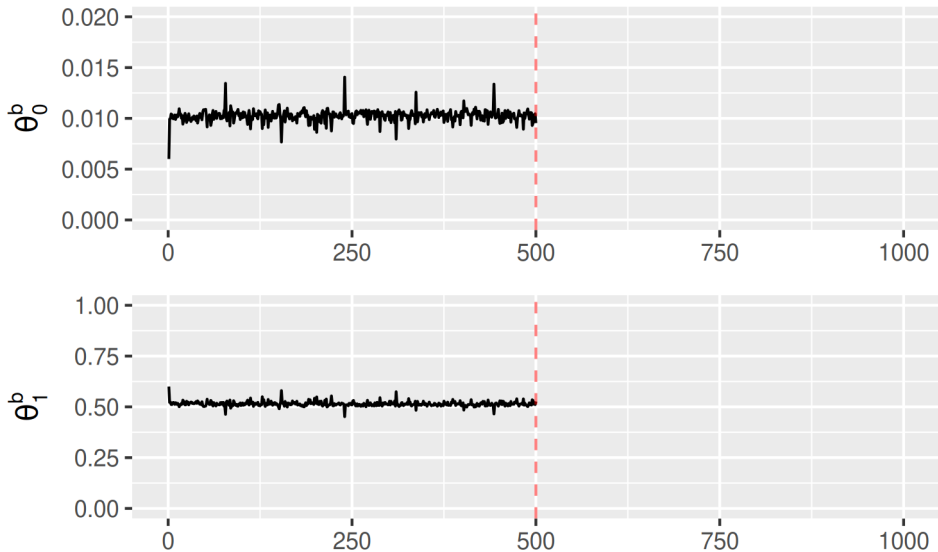
Simple Example: IBES

- Institutional Brokers' Estimate System (IBES)
- Large database of analyst earnings estimates vs. realized
- Predictive regression:

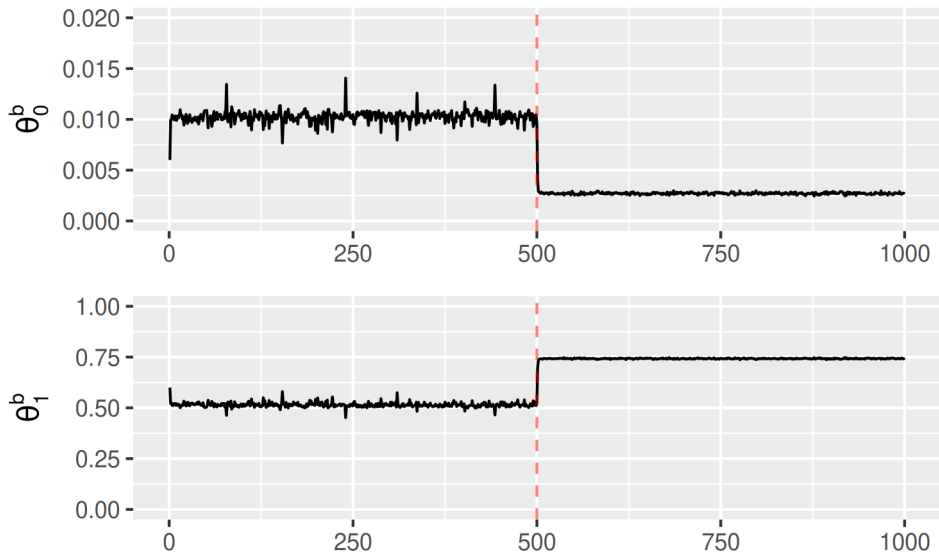
$$y_i^{\text{actual}} = \theta_0 + \theta_1 y_i^{\text{medest}} + e_i$$

- medest = median estimate
- Rational expectations: $\theta_0 \simeq 0, \theta_1 \simeq 1$
- Experiment: remove the 2% most influential obs. & compare
- $n = 9,278$ firms, $t = 01/1985 - 12/2017$
- $\gamma = 0.8$; $m = 6,000$ (re-sample firms)

Simple Example: IBES - Full Sample



Simple Example: IBES - Without Outliers



Main Example: PSID Income Dynamics

- Panel Study of Income Dynamics (PSID)
- Moffitt and Zhang (2018) earnings volatility
- 3,508 males (36,403 person-year obs.)
- Model permanent and transitory components:

$$y_{iat} = \alpha_t \mu_{ia} + \beta_t \nu_{ia}$$

$$\mu_{ia} = \mu_{i0} + \sum_{s=1}^a \omega_{is}$$

$$\nu_{ia} = \varepsilon_{ia} + \sum_{s=1}^{a-1} \psi_{a,a-s} \varepsilon_{is}, \quad a \geq 2$$

- $a = \text{age} \in [24, 54]$

- De-trend the data using OLS with polynomial regressors
- Aggregate residual autocovariances by age-group
- Match sample with model-based autocovariance matrix
- **Warning:**
 - original paper estimates 11 variance parameters
 - we only estimate 4 because of **identification issues**

$$\text{var}(\mu_{i,0}) : \nu_0$$

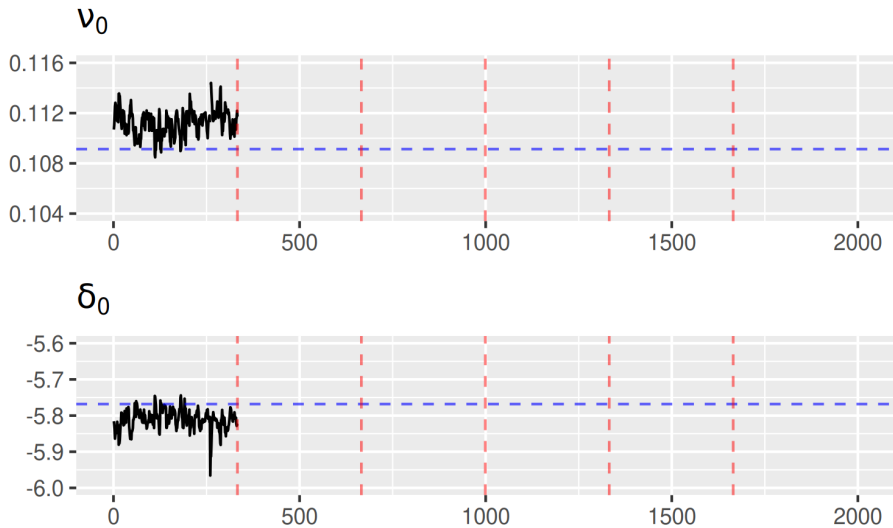
$$\text{var}(\omega_{ir}) : \delta_0, \delta_1$$

$$\text{var}(\varepsilon_{ir}) : \gamma_0, \gamma_1, k$$

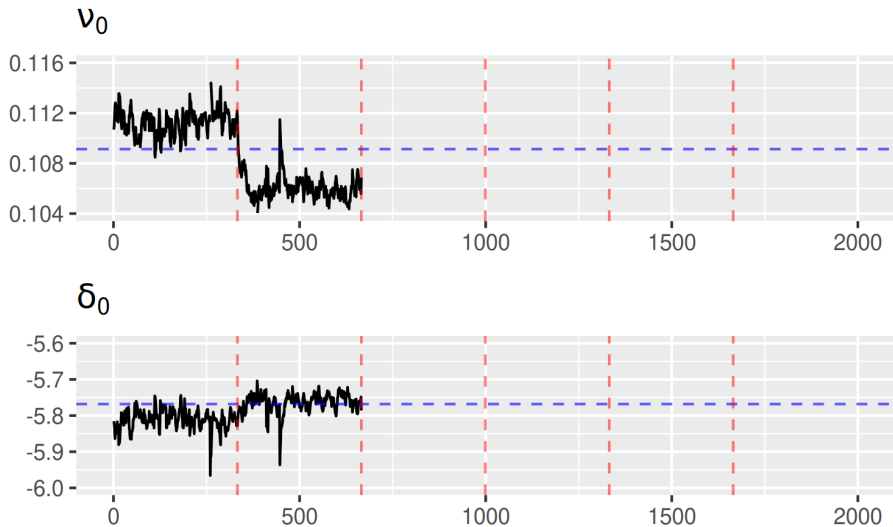
$$\psi_{a,a-r} : \pi, \cancel{\chi_1}, \cancel{\eta_1}, \cancel{\eta_2}, \cancel{\eta_3}$$

- **Goal:** Are the results sensitive to particular age groups?

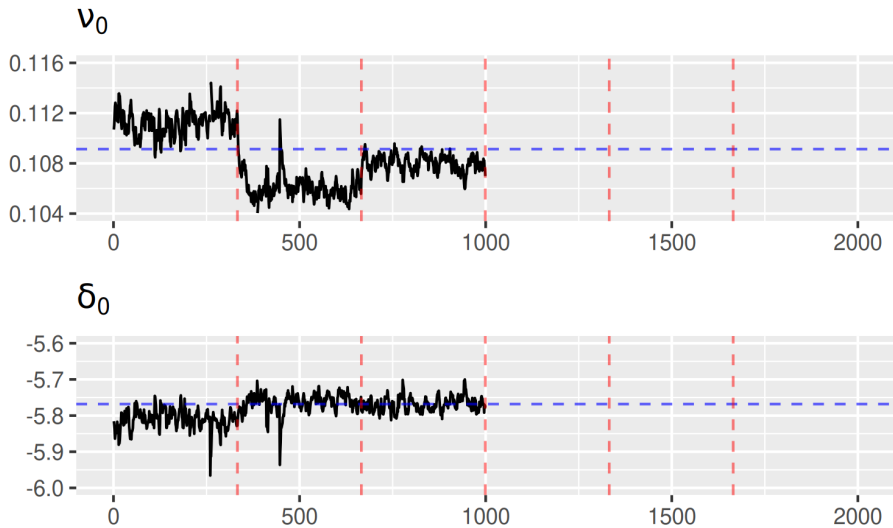
Influence: estimates without 24-28 age group



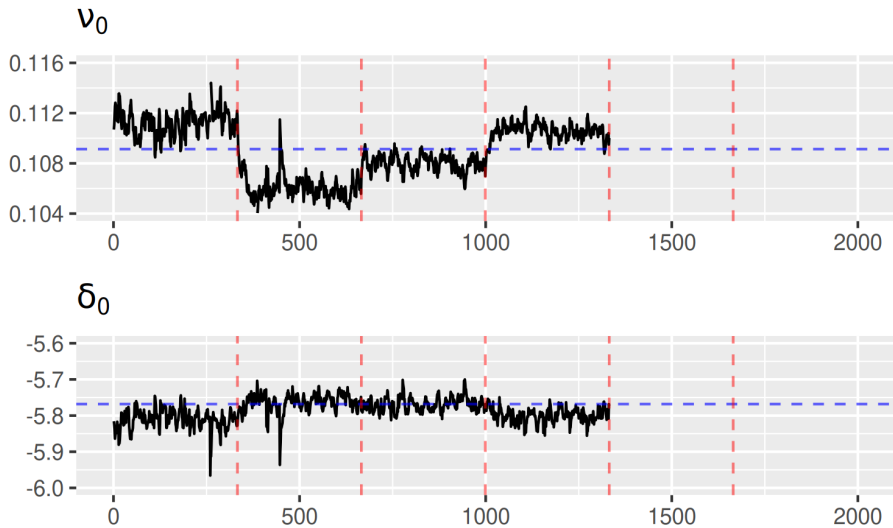
Influence: estimates without 29-33 age group



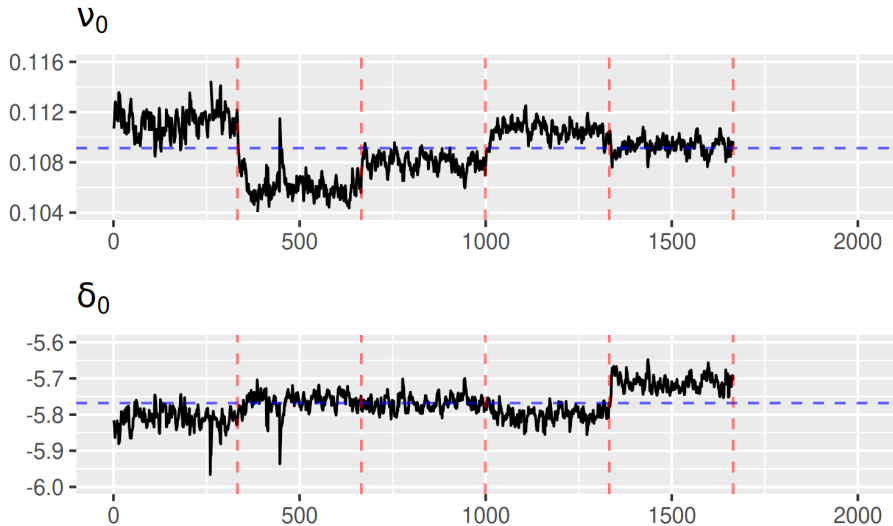
Influence: estimates without 34-38 age group



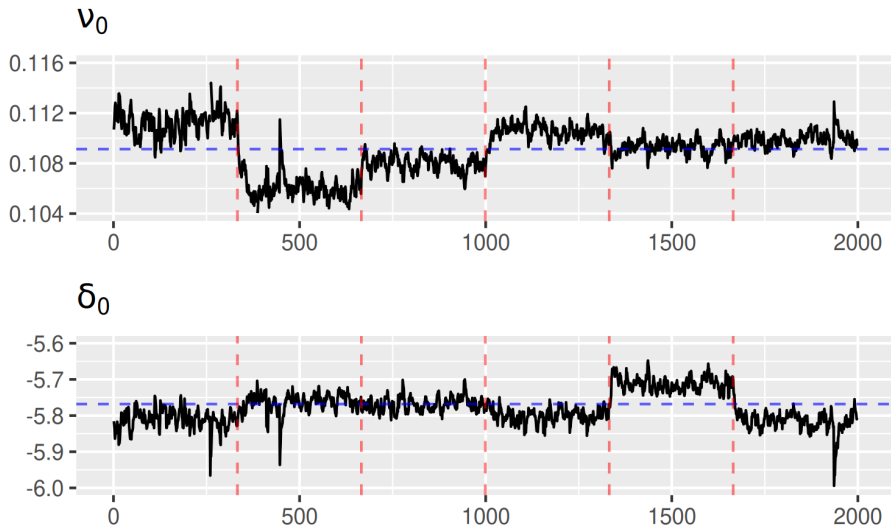
Influence: estimates without 39-43 age group



Influence: estimates without 44-48 age group

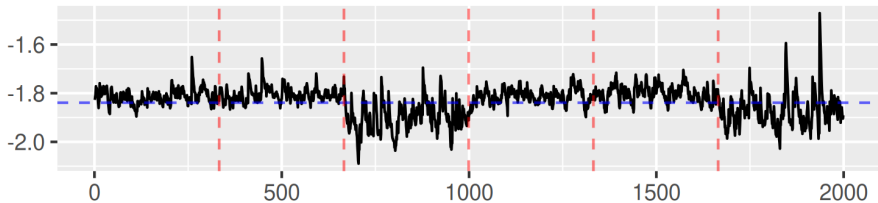


Influence: estimates without 49-54 age group

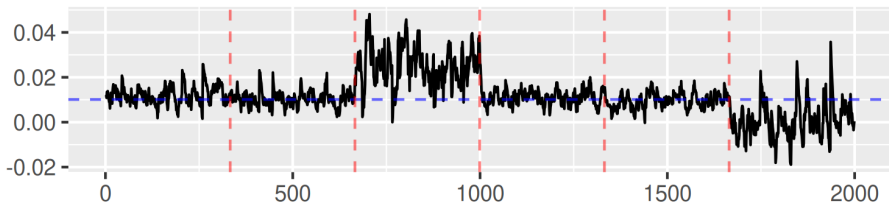


Influence of individual age-groups

Y_0



Y_1



Trimming

Conclusion

- SNR: simultaneous estimation and Bootstrapping
- Appealing for two-step estimators with complicated variance
- Potential avenues of research:
 - Stochastic quasi-Newton Methods (S-BFGS)
computationally very attractive
 - Alternative sampling schemes
look for theoretical guarantees in non-convex settings

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- **Computationally Attractive Bootstrap:**

Davidson and MacKinnon (1999); Andrews (2002); Kline and Santos (2012); Armstrong et al. (2014); Honoré and Hu (2017),...

k-step re-sampling at a converged estimate of $\hat{\theta}_n$

- **Stochastic Derivative-Based Optimization:**

Robbins and Monro (1951); Dvoretzky (1956); Ruppert (1988); Polyak and Juditsky (1992), [...], Bach and Moulines (2011); Moritz et al. (2016); Mandt et al. (2017),...

interested in optimization on very large or online data sets

- **Stochastic Optimization and Inference:**

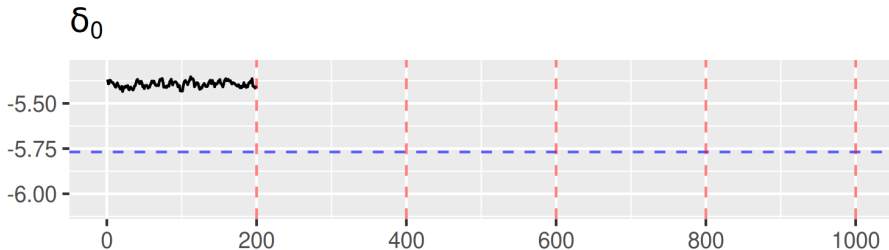
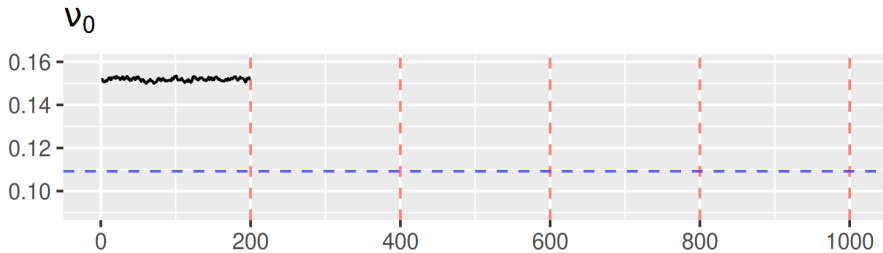
Chernozhukov and Hong (2003),...

MCMC similar to Simulated Annealing with a fixed temperature; (quasi)-posterior distribution asymptotically valid for inference

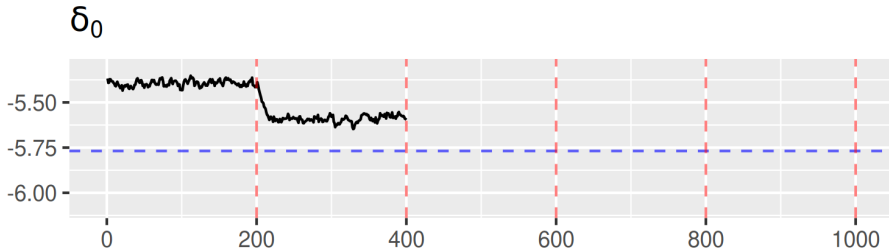
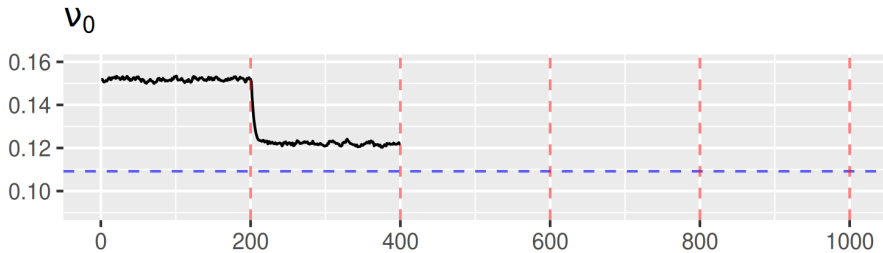
PSID Income Dynamics and Outlier Trimming

- Common empirical practice: remove extreme observations
- Here: the authors of the original paper trimmed the top and bottom 1% observations in each age-time group
 - are the results sensitive to the level of trimming?
- We look at a range of trimming levels: 0, 0.5, 1, 1.5 and 2%

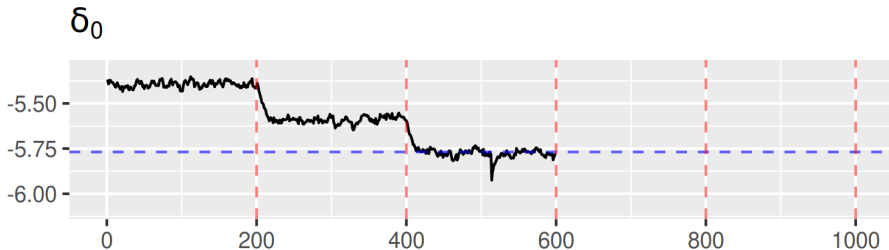
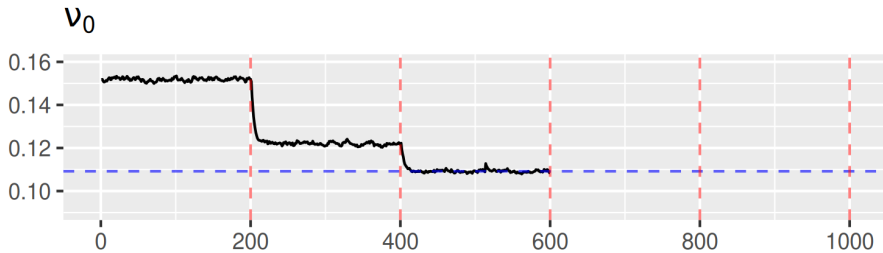
Influence of trimming: no trimming



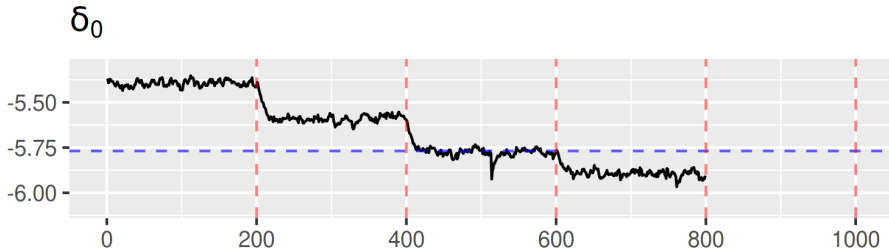
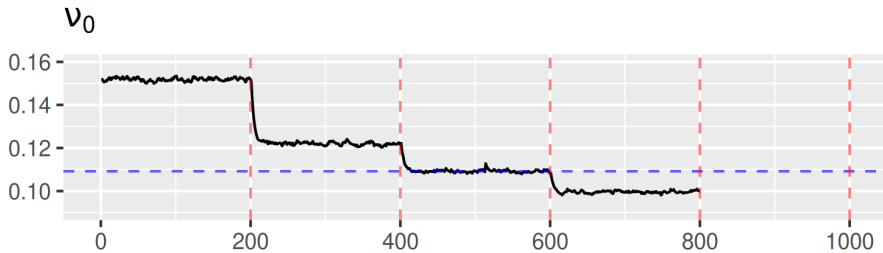
Influence of trimming: trim 0.5%



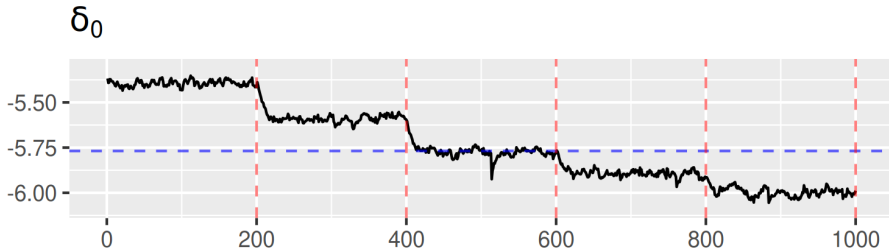
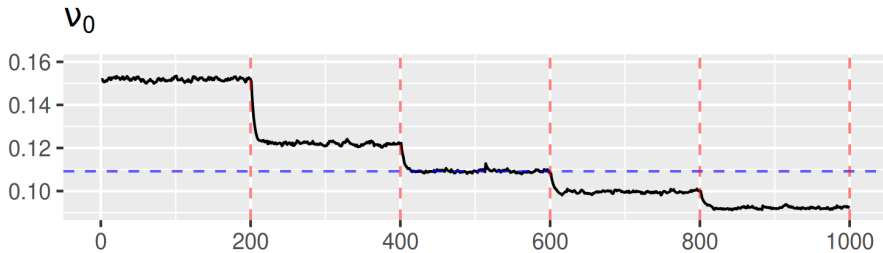
Influence of trimming: trim 1% (baseline)



Influence of trimming: trim 1.5%

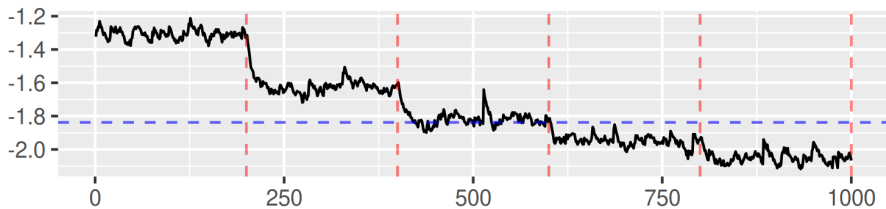


Influence of trimming: trim 2%

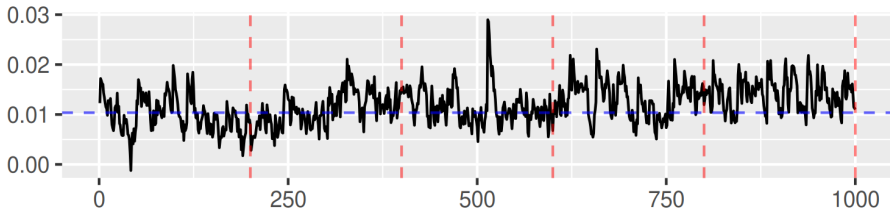


Influence of trimming

Y_0



Y_1



Age Groups

Simple Illustration: OLS estimation by Newton-Raphson

- OLS regression: $y_i = x_i'\theta + u_i$
- Sample objective: $Q_n(\theta) = \sum_{i=1}^n (y_i - x_i'\theta)^2/n$,
 $G_n(\theta) = -2 \sum_i x_i (y_i - x_i'\theta)/n$, $H_n(\theta) = -2 \sum_i x_i x_i'/n$
- **Newton-Raphson Iterations:**

$$\begin{aligned}\theta^b &= \theta^{b-1} + \gamma_b \left(\sum_i x_i x_i' \right)^{-1} \left[\sum_i (x_i y_i - \theta^{b-1} x_i x_i') \right] \\ &= (1 - \gamma_b) \theta^{b-1} + \gamma_b \hat{\theta}_n\end{aligned}$$

- For $\gamma_b = 1$ convergence after one iteration
- For $\gamma_b = \gamma \in (0, 1]$ fixed, the error $\theta^b - \hat{\theta}_n$ is:

$$\theta^b - \hat{\theta}_n = (1 - \gamma)^b [\theta^0 - \hat{\theta}_n]$$

Simple Illustration: OLS estimation by Gradient-Descent

- **Gradient Descent Iterations:**

$$\begin{aligned}\theta^b &= \theta^{b-1} + 2\gamma_b \sum_i x_i [y_i - x_i' \theta^{b-1}] / n \\ &= (I - 2\gamma_b \sum_i x_i x_i' / n) \theta^{b-1} + 2\gamma_b [\sum_i x_i x_i' / n] \hat{\theta}_n\end{aligned}$$

- Re-write the error $\theta^b - \hat{\theta}_n$ as:

$$\theta^b - \hat{\theta}_n = (I - 2\gamma_b [\sum_i x_i x_i' / n]) (\theta^{b-1} - \hat{\theta}_n)$$

- For $\gamma_b = \gamma \leq \lambda_{\max}(\sum_i x_i x_i' / n) / 2$ fixed, the error $\theta^b - \hat{\theta}_n$ is:

$$\theta^b - \hat{\theta}_n = (I - 2\gamma [\sum_i x_i x_i' / n])^b [\theta^0 - \hat{\theta}_n]$$

- Convergence after one iteration in one direction if
 $\gamma = \lambda_{\max}(\sum_i x_i x_i' / n) / 2$

Issues with Mini-Batch Stochastic Newton-Raphson

- Deterministic case: $\theta_{NR}^b \rightarrow \hat{\theta}_n$ faster than $\theta_{GD}^b \rightarrow \hat{\theta}_n$
- Why is S-GD more popular than S-NR?
 - need to compute $[H_1^{(b)}(\theta)]^{-1}$ **often (near)-singular**
 - e.g. $x_i = (1, x_{i,1})$, $x_{i,1} \sim \text{Bernoulli}(p)$
 $\Rightarrow x_i x_i'$ singular wp. 1 for any $p \in [0, 1]$

\Rightarrow mini-batch S-NR can be infeasible/unstable

- some solutions:
 - use more observations for H (Byrd et al., 2016; Li et al., 2018)
 - use accumulated gradient for scaling: adagrad, RMSprop, . . .