Model Selection, Estimation, and Bootstrap Smoothing

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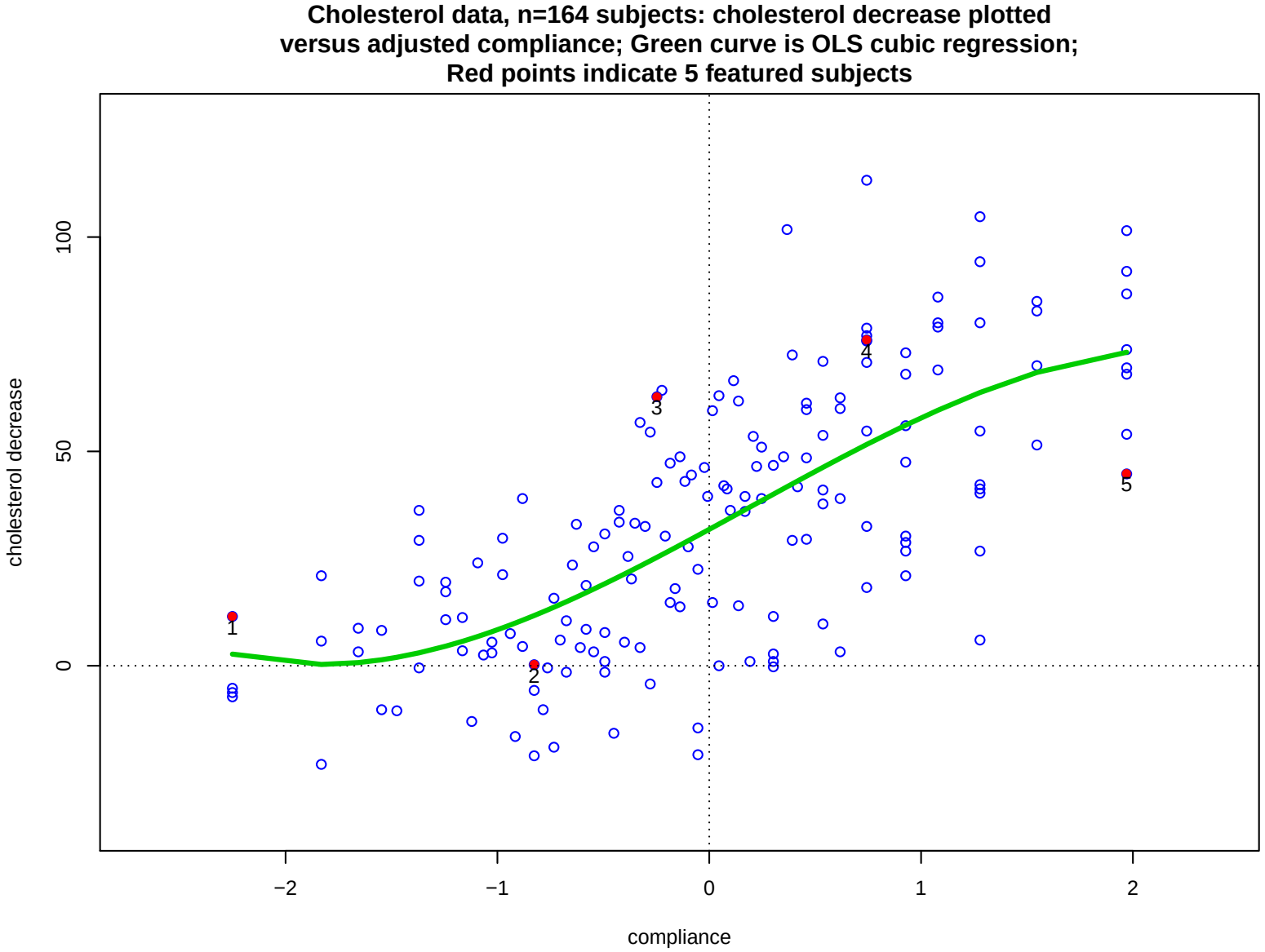
Estimation After Model Selection

- Usually:
  (a) look at data
  (b) choose model (linear, quad, cubic . . . ?)
  (c) fit estimates using chosen model
  (d) analyze as if pre-chosen
- Today: include model selection process in the analysis
- Question:
  Effects on standard errors, confidence intervals, etc.?
- *Two Examples*: nonparametric, parametric

Cholesterol Data

- $n = 164$ men took Cholestyramine for ~ 7 years
- $x =$ *compliance measure* (adjusted: $x \sim \mathcal{N}(0,1)$)
- $y =$ *cholesterol decrease*
- *Regression* y on x?

  [wish to estimate: $\mu_j = E\{y|x_j\},\ j = 1,2,\ldots,n$]


Cholesterol data, n=164 subjects: cholesterol decrease plotted
versus adjusted compliance; Green curve is OLS cubic regression;
Red points indicate 5 featured subjects
cholesterol decrease
100
50
0
−2
−1
0
1
2
compliance
1
2
3
4
5

C_p Selection Criterion

- *Regression Model* $\underset{n\times 1}{\boldsymbol{y}} = \underset{n\times m}{X}\ \underset{m\times 1}{\beta} + \underset{n\times 1}{\boldsymbol{e}} \quad \left[e_i \sim (0, \sigma^2)\right]$
- C_p Criterion $\boxed{\left\|\boldsymbol{y} - X\hat{\beta}\right\|^2 + 2m\sigma^2}$

  $\hat{\beta}$ = OLS estimate, m = "degrees of freedom"
- *Model Selection*: From possible models $X_1, X_2, X_3, \ldots$ choose the one minimizing C_p.
- Then use OLS estimate from chosen model.

C_p for Cholesterol Data

Model	df	$C_p - 80000$	(Boot %)
$\mathcal{M}_1$ (linear)	2	1132	(19%)
$\mathcal{M}_2$ (quad)	3	1412	(12%)
$\mathcal{M}_3$ (cubic)	4	667	(34%)
$\mathcal{M}_4$ (quartic)	5	1591	(8%)
$\mathcal{M}_5$ (quintic)	6	1811	(21%)
$\mathcal{M}_6$ (sextic)	7	2758	(6%)

($\sigma = 22$ from "full model" $\mathcal{M}_6$)

Nonparametric Bootstrap Analysis

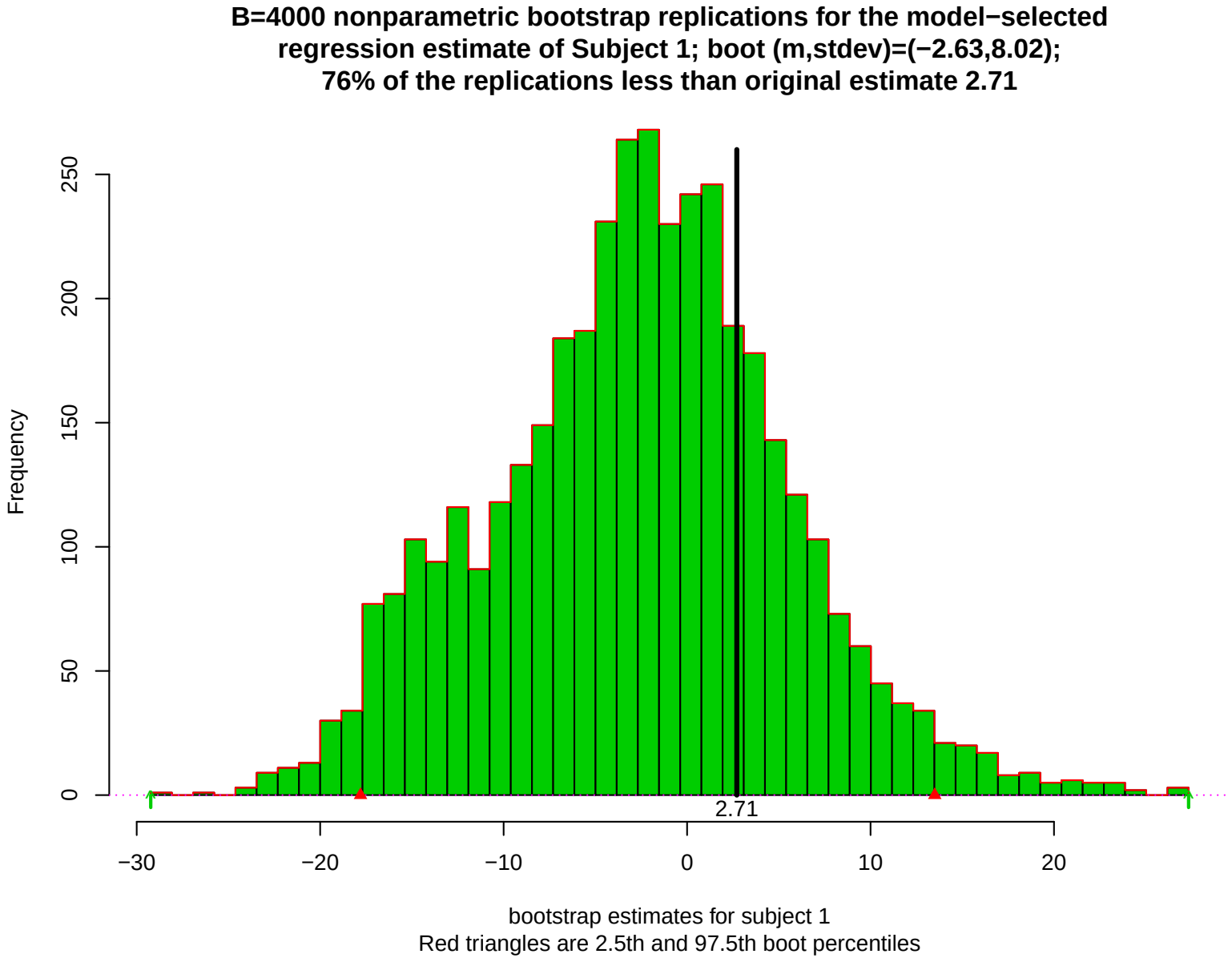
- data $= \{(x_i, y_i),\ i = 1, 2, \ldots, n = 164\}$ gave original estimate

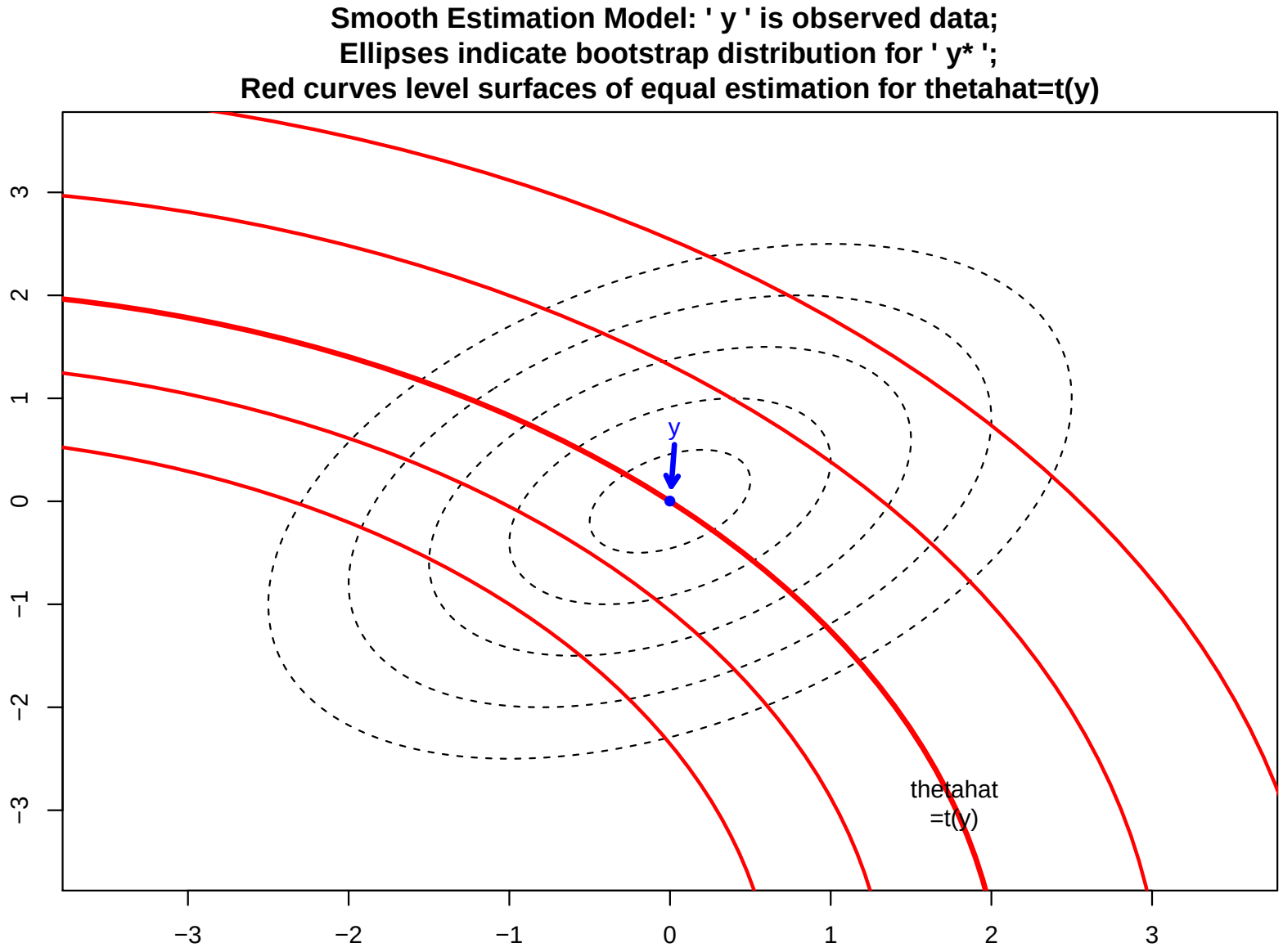
$$\hat{\boldsymbol{\mu}} = X_3 \hat{\beta}_3$$

- *Bootstrap data set* $\text{data}^* = \left\{(x_j, y_j)^*,\ j = 1, 2, \ldots, n\right\}$ where $(x_j, y_j)^*$ drawn randomly and with replacement from data:

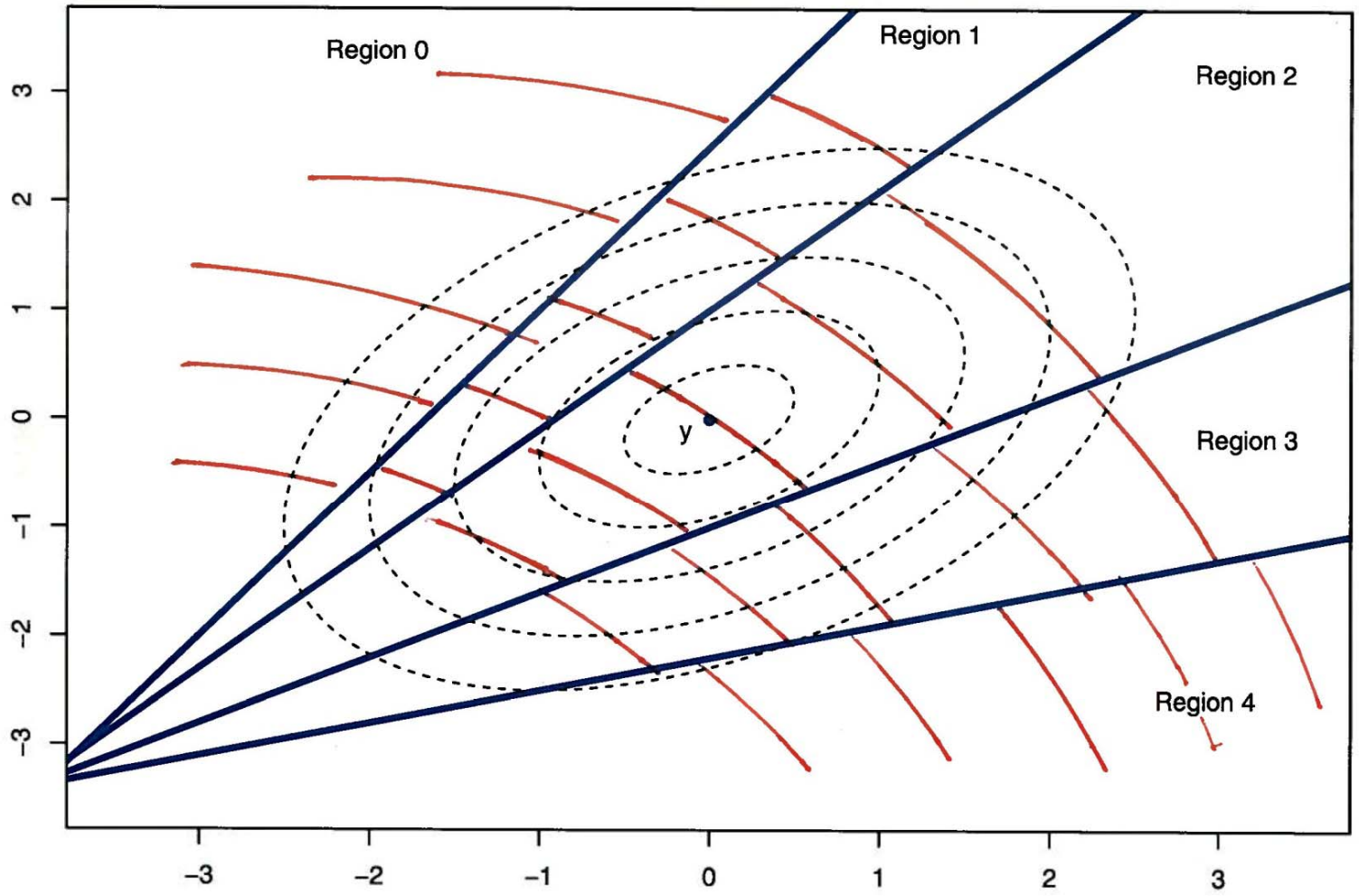
$$\text{data}^* \underset{C_p}{\longrightarrow} m^* \underset{\text{OLS}}{\longrightarrow} \hat{\beta}^*_{m^*} \longrightarrow \hat{\boldsymbol{\mu}}^* = X_{m^*} \hat{\beta}^*_{m^*}$$

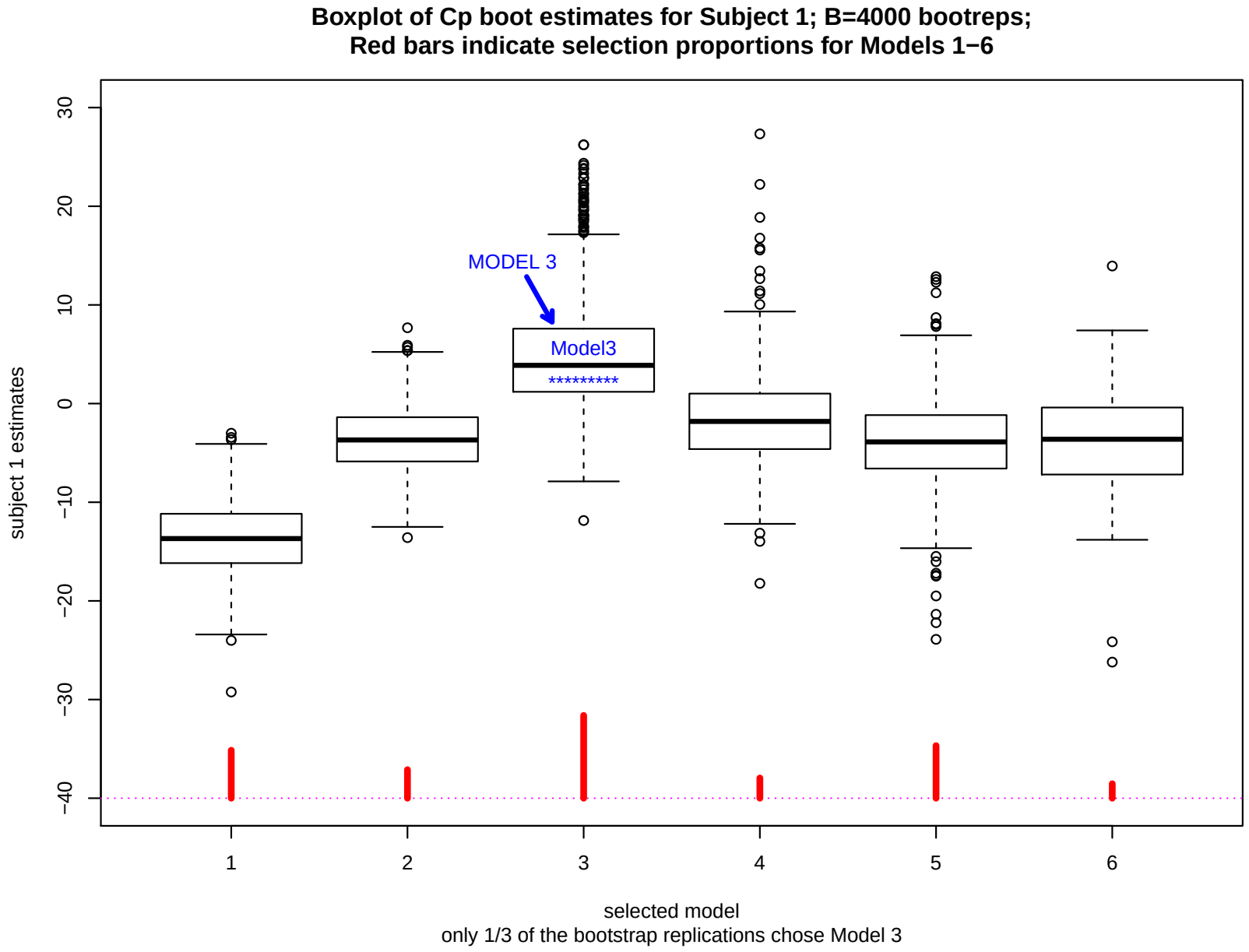
- I did this all $B = 4000$ times.


B=4000 nonparametric bootstrap replications for the model−selected
regression estimate of Subject 1; boot (m,stdev)=(−2.63,8.02);
76% of the replications less than original estimate 2.71
Frequency
0
50
100
150
200
250
2.71
−30
−20
−10
0
10
20
bootstrap estimates for subject 1
Red triangles are 2.5th and 97.5th boot percentiles


Smooth Estimation Model: ' y ' is observed data;
Ellipses indicate bootstrap distribution for ' y* ';
Red curves level surfaces of equal estimation for thetahat=t(y)
y
thetahat
=t(y)
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

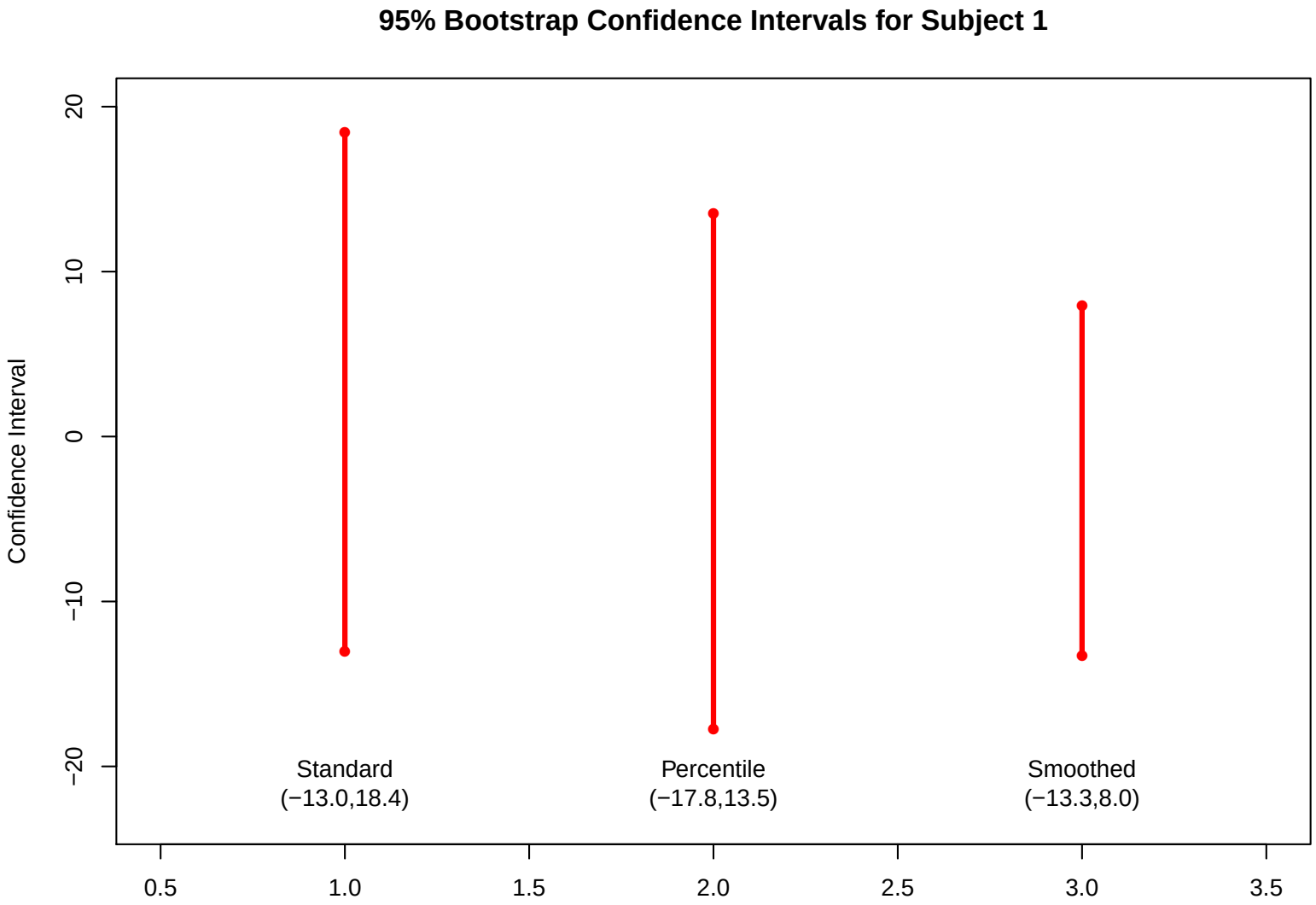
Estimation with model selection: now the curves of equal estimation are discontinuous across the Model region boundaries




Boxplot of Cp boot estimates for Subject 1; B=4000 bootreps;
Red bars indicate selection proportions for Models 1−6
MODEL 3
Model3
****
subject 1 estimates
30
20
10
0
−10
−20
−30
−40
1
2
3
4
5
6
selected model
only 1/3 of the bootstrap replications chose Model 3

Bootstrap Confidence Intervals

- Standard: $\hat{\mu} \pm 1.96\ \widehat{\text{se}}$
- Percentile: $\left[\hat{\mu}^{*(.025)}, \hat{\mu}^{*(.975)}\right]$
- Smoothed Standard: $\tilde{\mu} \pm 1.96\ \widetilde{\text{se}}$
- BCa/ABC: corrects percentiles for bias and changing se


95% Bootstrap Confidence Intervals for Subject 1
Confidence Interval
20
10
0
−10
−20
Standard
(−13.0,18.4)
Percentile
(−17.8,13.5)
Smoothed
(−13.3,8.0)
0.5
1.0
1.5
2.0
2.5
3.0
3.5

Bootstrap Smoothing

- *Idea* Replace original estimator $t(\boldsymbol{y})$ with bootstrap average

$$s(\boldsymbol{y}) = \sum_{i=1}^{B} t\left(\boldsymbol{y}_i^*\right) \Big/ B$$

- Model averaging
- Same as *bagging* ("bootstrap aggregation" Breiman)
- Removes discontinuities
- Reduces variance

Accuracy Theorem

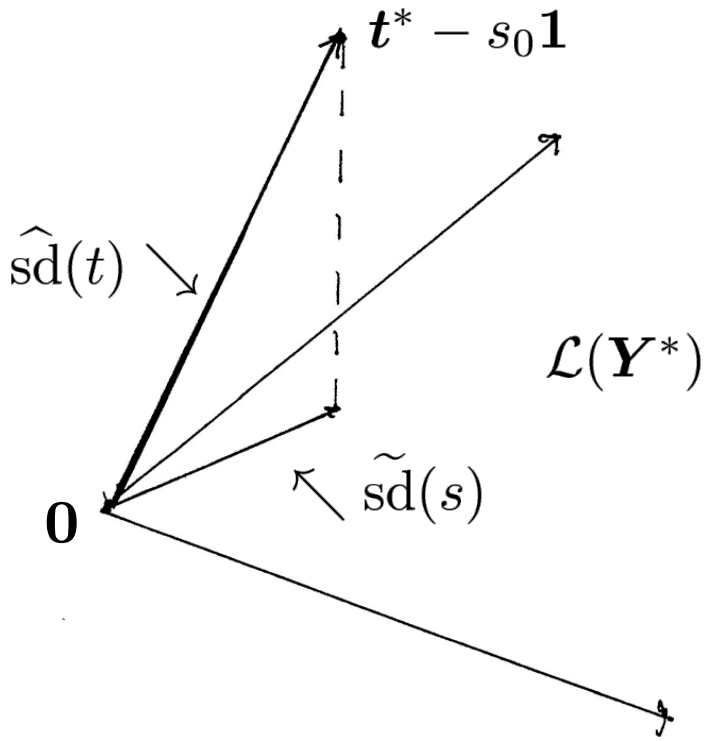
- *Notation* $s_0 = s(\boldsymbol{y}), \quad t_i^* = t(\boldsymbol{y}_i^*),\ i = 1, 2, \ldots B$
- Y_{ij}^* = # of times jth data point appears in ith boot sample
- $\text{cov}_j = \sum_{i=1}^{B} Y_{ij}^* \cdot \left(t_i^* - s_0\right) \Big/ B \quad \left[\text{covariance } Y_{ij}^* \text{ with } t_i^*\right]$

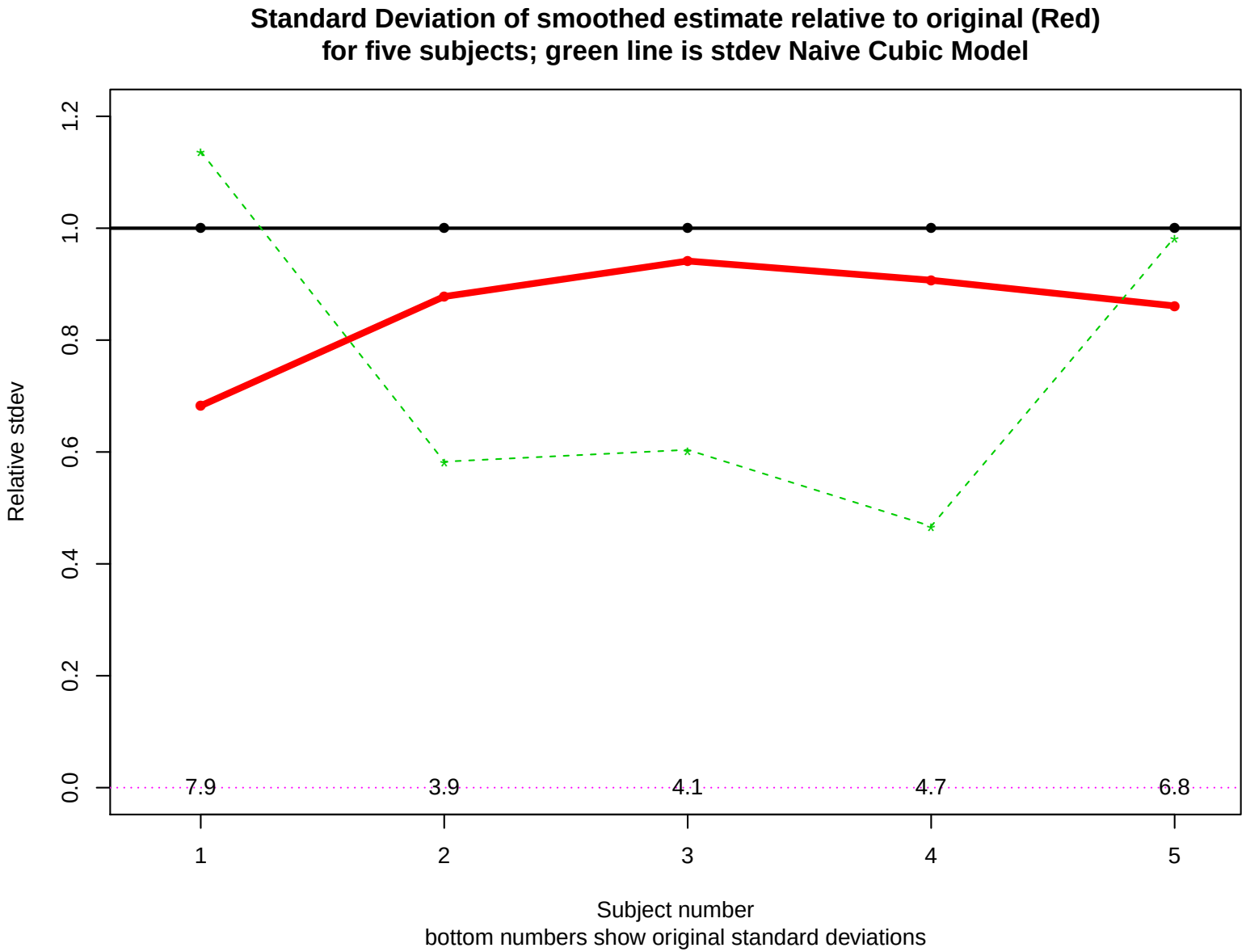
Theorem *The delta method standard deviation estimate for* s_0 *is*

$$\widetilde{\text{sd}} = \left[\sum_{j=1}^{n} \text{cov}_j^2\right]^{1/2},$$

always $\leq \left[\sum_{i=1}^{B} \left(t_i^* - s_0\right)^2 \Big/ B\right]^{1/2}$, *the boot stdev for* $t(\boldsymbol{y})$.

Projection Interpretation




Standard Deviation of smoothed estimate relative to original (Red)
for five subjects; green line is stdev Naive Cubic Model
Relative stdev
0.0
0.2
0.4
0.6
0.8
1.0
1.2
7.9
3.9
4.1
4.7
6.8
1
2
3
4
5
Subject number
bottom numbers show original standard deviations

How Many Bootstrap Replications Are Enough?

- How accurate is $\widetilde{\text{sd}}$? *Jackknife*
- Divide the 4000 bootreps t_i^* into 20 groups of 200 each
- Recompute $\widetilde{\text{sd}}$ with each group removed in turn
- Jackknife gave coef variation $\left(\widetilde{\text{sd}}\right) \doteq 0.02$ for all 164 subjects (could have stopped at $B = 500$)

How Stable Are The Standard Deviations?

- Smoothed standard interval $\tilde{\mu} \pm 1.96\,\widetilde{\mathrm{sd}}$ assumes $\widetilde{\mathrm{sd}}$ "stable"
- "Acceleration" $\tilde{a} = d\widetilde{\mathrm{sd}}/d\tilde{\mu}$,

$$\tilde{a} \doteq \frac{1}{6} \sum \mathrm{cov}_j^3 \Big/ \left(\sum \mathrm{cov}_j^2\right)^{3/2}$$

- $|\tilde{a}| \leq 0.02$ for all 164 subjects

Model Probability Estimates

- 34% of the 4000 bootreps chose the cubic model
- Poor man's Bayes posterior prob for "cubic"
- How accurate is that 34%?
- Apply accuracy theorem to indicator function for choosing "cubic"

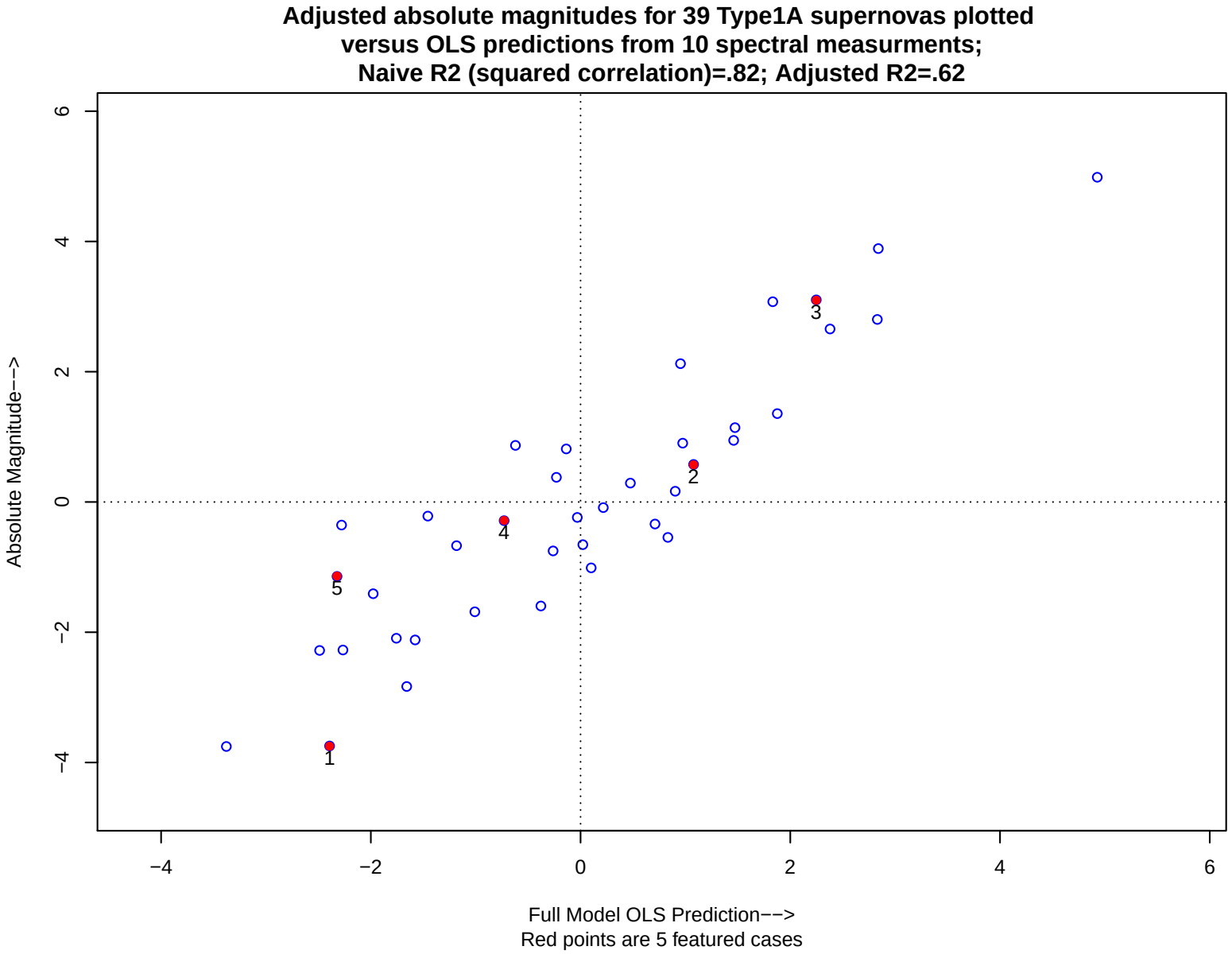
Model	Boot %	± Standard Error
$\mathcal{M}_1$ (linear)	19%	±24
$\mathcal{M}_2$ (quad)	12%	±18
$\mathcal{M}_3$ (cubic)	34%	±24
$\mathcal{M}_4$ (quartic)	8%	±14
$\mathcal{M}_5$ (quintic)	21%	±27
$\mathcal{M}_6$ (sextic)	6%	±6

The Supernova Data

- data $= \{(x_j, y_j),\ j = 1, 2, \ldots, n = 39\}$
- y_j = absolute magnitude of Type Ia supernova
- x_j = vector of 10 spectral energies (350–850nm)
- Full Model $\underset{39\times 10}{\boldsymbol{y} = X}\boldsymbol{\beta} + \boldsymbol{e}$ $\quad \left[\boldsymbol{e}_i \overset{\text{ind}}{\sim} \mathcal{N}(0,1)\right]$

Ordinary Least Squares Prediction

- Full Model $\boldsymbol{y} \sim \mathcal{N}_{39}(X\beta, I)$
- OLS Estimates $\hat{\boldsymbol{\mu}}_{\text{OLS}} = X\hat{\boldsymbol{\beta}}_{\text{OLS}}$ $\left[\arg\min \left\|\boldsymbol{y} - X\beta\right\|^2\right]$
- *Naive* $R^2 = 0.82$ $\left[= \widehat{\text{cor}}\,(\hat{\mu}_{\text{OLS}}, y)^2\right]$
- *Adjusted* $R^2 = 0.69$ $\left[R^2 - \left(1 - R^2\right)\frac{m}{n-m}\right.$ where $m = 10$ the df$\left.\right]$


Adjusted absolute magnitudes for 39 Type1A supernovas plotted
versus OLS predictions from 10 spectral measurments;
Naive R2 (squared correlation)=.82; Adjusted R2=.62
Absolute Magnitude−−>
Full Model OLS Prediction−−>
Red points are 5 featured cases
1
2
3
4
5
−4
−2
0
2
4
6

Lasso Model Selection

- *Lasso* estimate is $\hat{\beta}$ minimizing $\left\|\boldsymbol{y} - X\beta\right\|^2 + \lambda \sum_1^p \left|\beta_k\right|$
- *Shrinks* OLS estimates toward zero (all the way for some)
- Degrees of freedom "m" = number of nonzero $\hat{\beta}_k$'s
- *Model Selection*: Choose λ (or m) to maximize adjusted R^2.
- Then $\hat{\boldsymbol{\mu}} = X\hat{\beta}_m$.

Lasso for the Supernova Data

λ	m (# nonzero $\hat{\beta}_k$'s)	Naive R^2	Adjusted R^2	
63.0	**1**	.17	**.12**	
12.9	**4**	.77	**.72**	
3.56	**7**	.81	**.73**	*(Selected)*
0.50	**9**	.82	**.71**	
0	**10**	.82	**.69**	*(OLS)*

Parametric Bootstrap Smoothing

- *Original Estimates*

$$\boldsymbol{y} \xrightarrow{\text{Lasso}} m,\ \hat{\boldsymbol{\beta}}_m \longrightarrow \hat{\boldsymbol{\mu}} = X\hat{\boldsymbol{\beta}}_m$$

- Full Model Bootstrap $\quad \boldsymbol{y}^* \sim \mathcal{N}_{39}\left(\hat{\boldsymbol{\mu}}_{\text{OLS}}, I\right)$

$$\boldsymbol{y}^* \longrightarrow m^*, \hat{\boldsymbol{\beta}}^*_{m^*} \longrightarrow \hat{\boldsymbol{\mu}}^* = X\hat{\boldsymbol{\beta}}^*_{m^*}$$

- I did this all $B = 4000$ times. $\quad$ • $t^*_{ik} = \hat{\boldsymbol{\mu}}^*_{ik}$

- Smoothed Estimates $\quad s_k = \sum_{i=1}^{4000} t^*_{ik} \Big/ 4000 \qquad [k = 1, 2, \ldots, 39]$

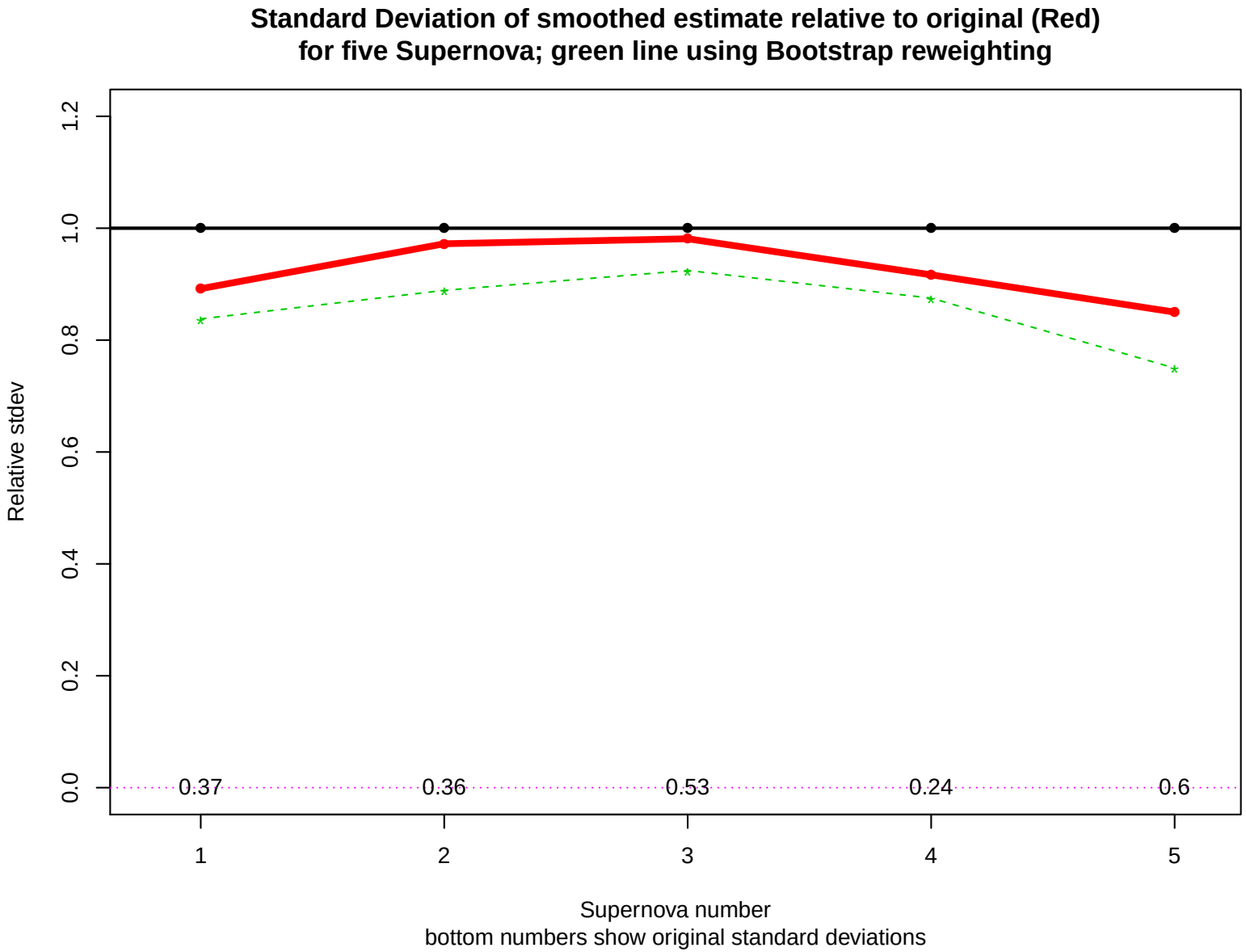
Parametric Accuracy Theorem

Theorem *The delta method standard deviation estimate for* s_k *is*

$$\widehat{\mathrm{sd}}_k = \left[\widehat{\mathbf{cov}}_k' \, \mathcal{G} \, \widehat{\mathbf{cov}}_k\right]^{1/2},$$

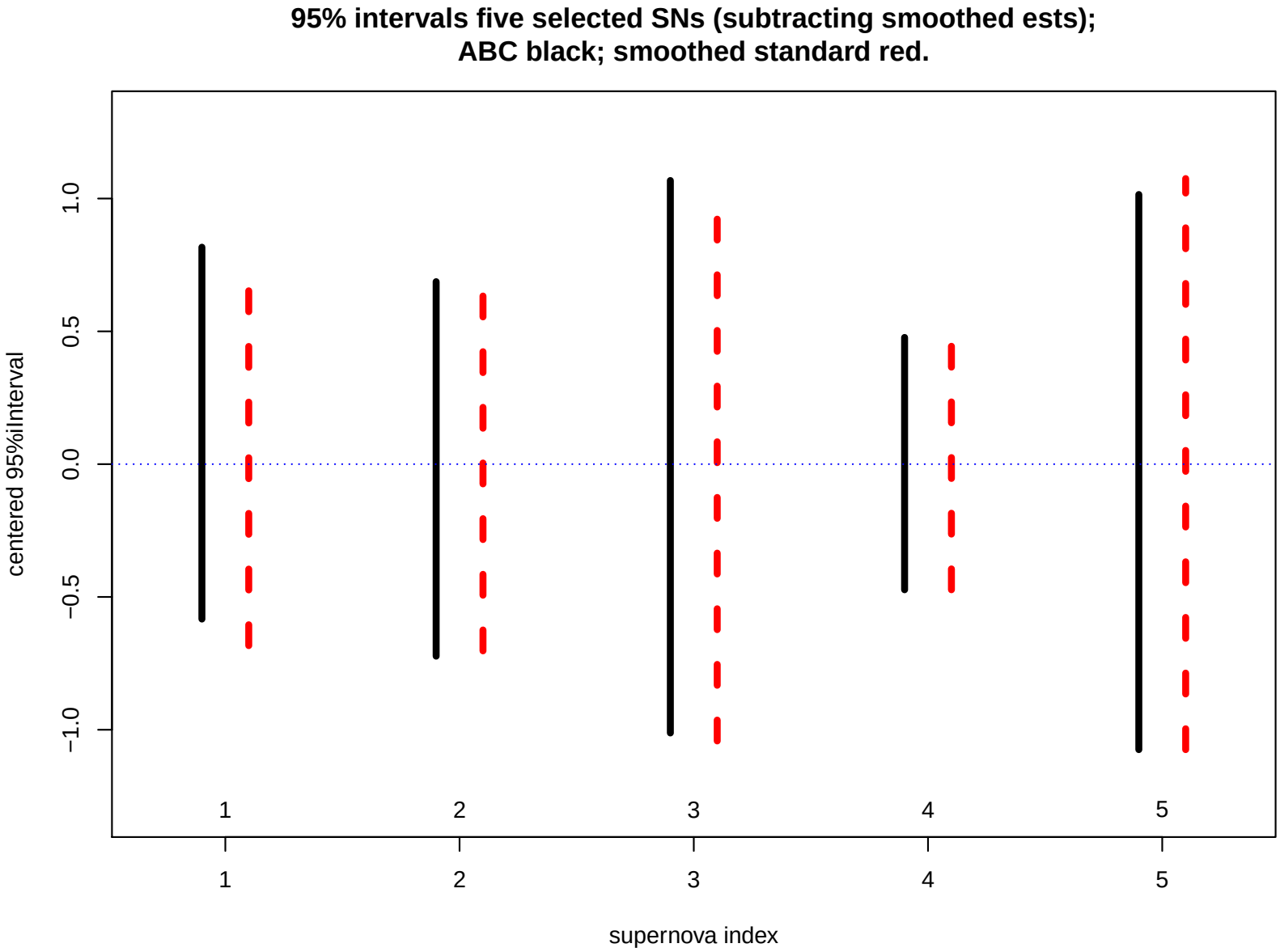
where $\mathcal{G} = X'X$ *and* $\widehat{\mathbf{cov}}_k$ *is bootstrap covariance between* $\hat{\beta}^*_{\mathrm{OLS}}$ *and* t^*_k.

- Always less than the bootstrap estimate of stdev for t_k
- Projection into $\mathcal{L}\left(\hat{\beta}^*_{\mathrm{OLS}}\right)$
- Exponential families


Standard Deviation of smoothed estimate relative to original (Red)
for five Supernova; green line using Bootstrap reweighting
Relative stdev
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.37
0.36
0.53
0.24
0.6
1
2
3
4
5
Supernova number
bottom numbers show original standard deviations

Better Confidence Intervals

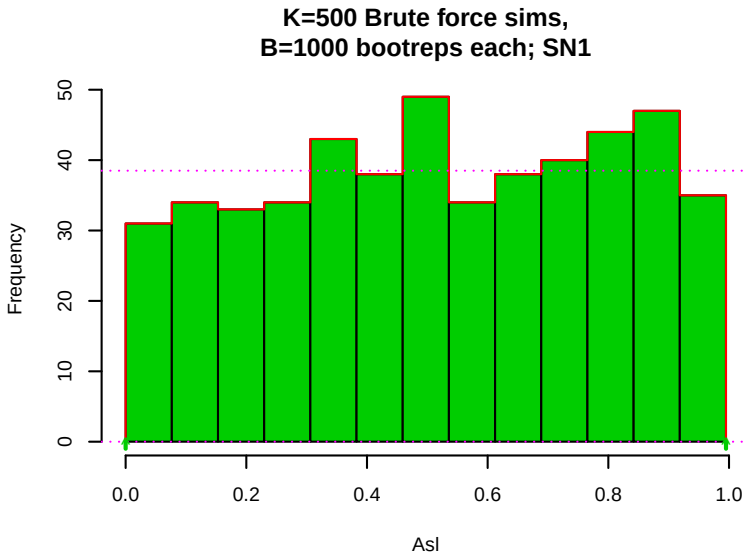
- Smoothed standard intervals and percentile intervals have coverage errors of order $O\left(1/\sqrt{n}\right)$.
- "ABC" intervals have errors $O(1/n)$: corrects for bias and "acceleration" (change in stdev as estimate varies).
- Uses local reweighting for 2nd order correction

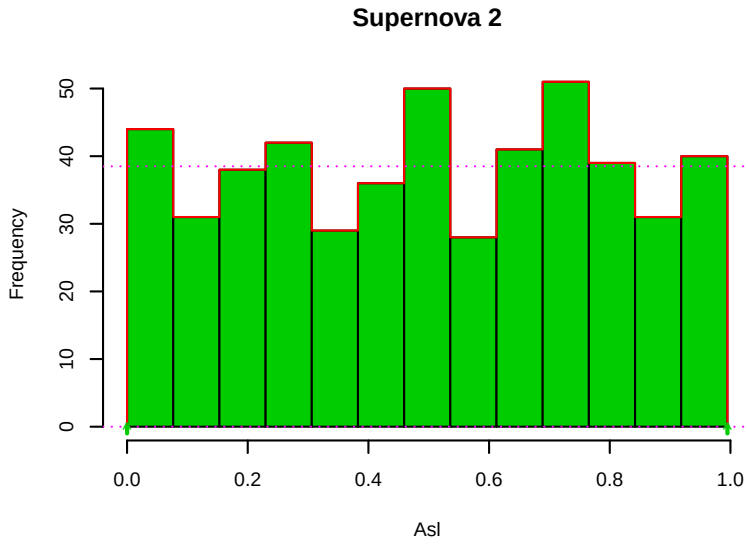

95% intervals five selected SNs (subtracting smoothed ests);
ABC black; smoothed standard red.
centered 95%iInterval
1.0
0.5
0.0
−0.5
−1.0
1
2
3
4
5
supernova index

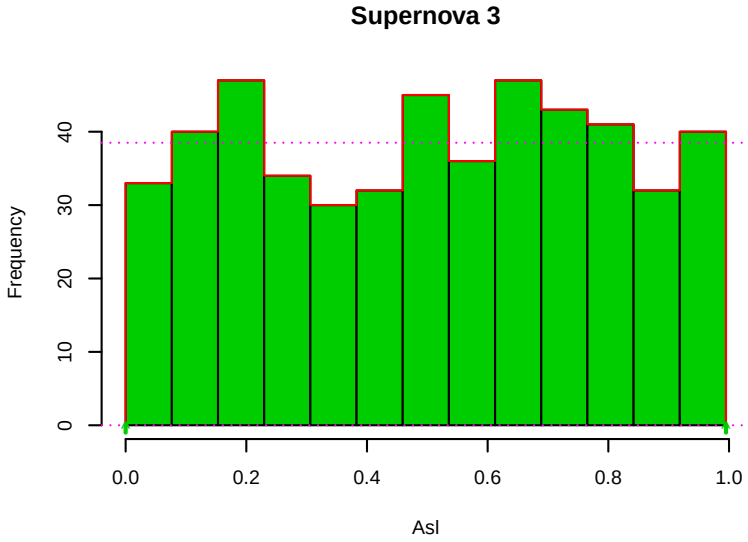
Brute Force Simulation

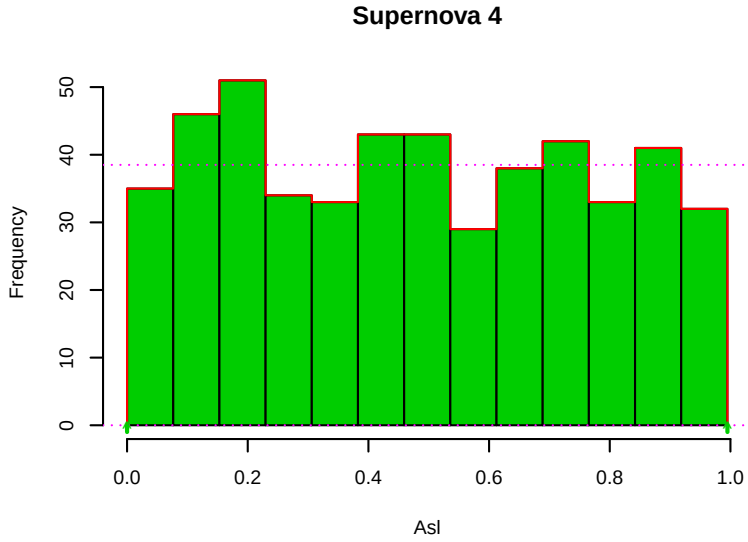
- Sample 500 times: $\boldsymbol{y}^* \sim \mathcal{N}(\hat{\mu}_{\text{OLS}}, I)$; gives $\hat{\mu}^*_{\text{OLS}}$
- Resample $B = 1000$ times: $\boldsymbol{y}^{**} \sim \mathcal{N}(\hat{\mu}^*_{\text{OLS}}, I)$
- Use ABC to get $\widetilde{\text{sd}}$, $\widetilde{\text{bias}}$, $\widetilde{\text{acceleration}}$
- Calculate ABC coverage of one-sided interval $(-\infty, s_k)$

  [s_k the original smoothed estimate]
- Should be uniform $[0, 1]$


K=500 Brute force sims,
B=1000 bootreps each; SN1
Frequency
0
10
20
30
40
50
0.0
0.2
0.4
0.6
0.8
1.0
Asl


Supernova 2
Frequency
0
10
20
30
40
50
0.0
0.2
0.4
0.6
0.8
1.0
Asl


Supernova 3
Frequency
0
10
20
30
40
0.0
0.2
0.4
0.6
0.8
1.0
Asl


Supernova 4
Frequency
0
10
20
30
40
50
0.0
0.2
0.4
0.6
0.8
1.0
Asl

References

Berk, R., Brown, L., Buja, A., Zhang, K. and Zhao, L. (2012). Valid post-selection inference. Submitted *Ann. Statist.* `http://stat.wharton.upenn.edu/~zhangk/PoSI-submit.pdf`; **conservative frequentist intervals à la Tukey, Scheffé**.

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