Bayesian Inference and the Parametric Bootstrap

Bradley Efron

Stanford University

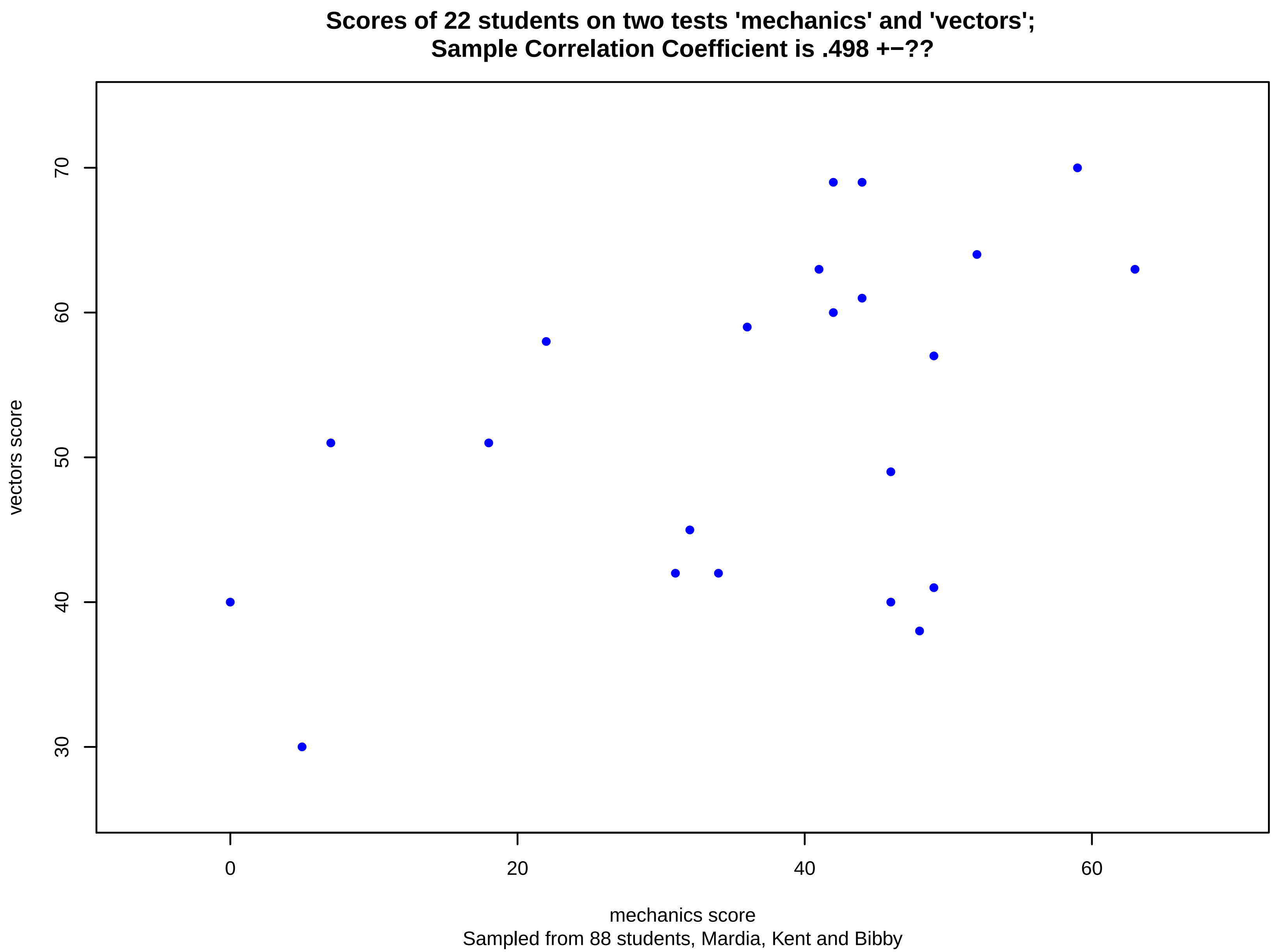
Importance Sampling for Bayes Posterior Distribution

- Newton and Raftery (1994 *JRSS-B*)
  "Nonparametric Bootstrap: good choice"
  (actually used a smoothed nonparametric bootstrap)
- Today Parametric Bootstrap
  - Good computational properties when applicable
  - Connection between Bayes and frequentist inference

Student Score Data

(Mardia, Kent and Bibby)

- $n = 22$ students' scores on two tests: *mechanics*, *vectors*
- Data $\quad \boldsymbol{y} = (y_1, y_2, \ldots, y_{22})$ with $y_i = (\text{mec}_i, \text{vec}_i)$
- *Parameter of interest* $\quad \theta = \text{correlation (mec, vec)}$
- *Sample correlation coefficient* $\quad \hat{\theta} = 0.498 \pm\ ??$


Scores of 22 students on two tests 'mechanics' and 'vectors';
Sample Correlation Coefficient is .498 +−??
vectors score
30
40
50
60
70
0
20
40
60
mechanics score
Sampled from 88 students, Mardia, Kent and Bibby

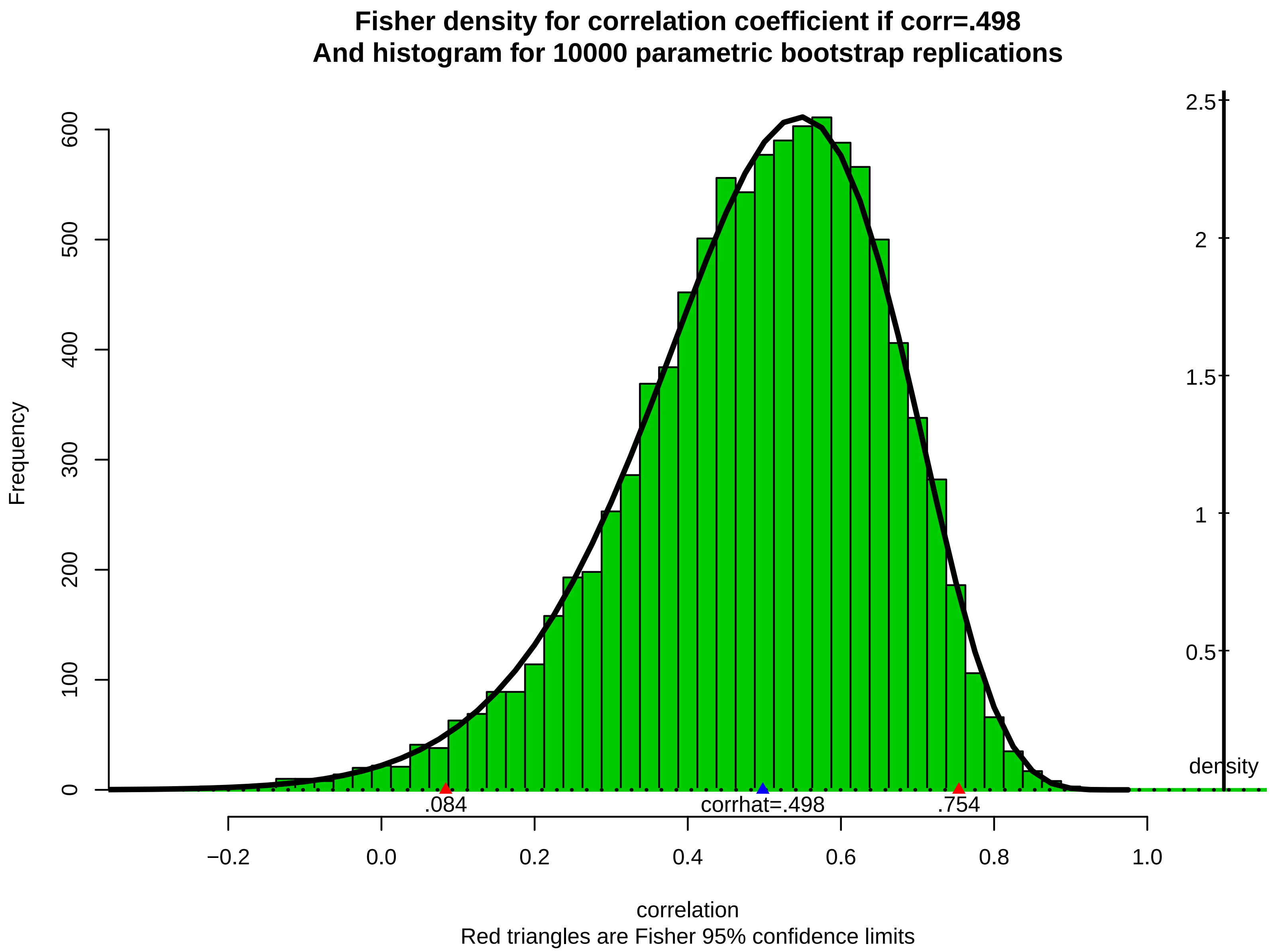
R. A. Fisher (1915)

- Density $f_\theta\left(\hat{\theta}\right)$

$$= \frac{n-2}{\pi}(1-\theta^2)^{(n-1)/2}\left(1-\hat{\theta}^2\right)^{(n-4)/2}\int_0^\infty \left[\cosh(w)-\theta\hat{\theta}\right]^{-(n-1)}\,dw$$

- *Bivariate normal* $\quad y_i \overset{\text{ind}}{\sim} \mathcal{N}_2(\mu, \Sigma) \qquad i = 1, 2, \ldots, n$
- 95% confidence limits (from z transform)

$$\boxed{\theta \in (0.084, 0.754)}$$


Fisher density for correlation coefficient if corr=.498
And histogram for 10000 parametric bootstrap replications
Frequency
0
100
200
300
400
500
600
2.5
2
1.5
1
0.5
density
.084
corrhat=.498
.754
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
correlation
Red triangles are Fisher 95% confidence limits

Parametric Bootstrap Computations

- *Assume* $y_i \overset{\text{ind}}{\sim} \mathcal{N}_2(\mu, \Sigma)$ • *Estimate* $\hat{\mu}$ and $\hat{\Sigma}$ by MLE
- Bootstrap sample $y_i^* \overset{\text{ind}}{\sim} \mathcal{N}_2\left(\hat{\mu}, \hat{\Sigma}\right)$ for $i = 1, 2, \ldots, 22$
- Bootstrap replication $\hat{\theta}^*$ = corr coeff for $\boldsymbol{y}^* = (y_1^*, y_2^*, \ldots, y_{22}^*)$
- Bootstrap standard deviation

$$\mathrm{sd}\left(\hat{\theta}\right) = 0.168 \qquad (B = 10,000)$$

- *Percentile 95% confidence limits* $\boxed{(0.109,\ 0.761)}$

Better Bootstrap Confidence Limits (BCa)

- Idea   Reweighting the B bootstrap replications improves coverage

- Weights involve z_0 (bias correction) and a (acceleration)

- $$W_{\text{BCa}}(\theta) = \frac{\varphi(Z_\theta/(1+aZ_\theta) - z_0)}{(1+aZ_\theta)^2 \varphi(Z_\theta + z_0)} \quad \text{where } Z_\theta = \Phi^{-1} \underbrace{G(\theta)}_{\text{bootstrap cdf}} - z_0$$

- Reweighting the $B = 10{,}000$ bootstraps gave weighted percentiles

$\boxed{(0.075,\ 0.748)}$ Fisher: (0.084, 0.754)

Bayes Posterior Intervals

- *Prior* $\pi(\theta)$
- Posterior expectation for $t(\theta)$:

$$E\left\{t(\theta)|\hat{\theta}\right\} = \int t(\theta)\pi(\theta)f_\theta\left(\hat{\theta}\right)d\theta \Big/ \int \pi(\theta)f_\theta\left(\hat{\theta}\right)d\theta$$

- Conversion factor Ratio of likelihood to bootstrap density:

$$\boxed{R(\theta) = f_\theta\left(\hat{\theta}\right)\Big/ f_{\hat{\theta}}(\theta)} \qquad \left(\text{“}\theta\text{”} = \hat{\theta}^*\right)$$

- Bootstrap integrals

$$E\left\{t(\theta)|\hat{\theta}\right\} = \frac{\int t(\theta)\pi(\theta)R(\theta)f_{\hat{\theta}}(\theta)\,d\theta}{\int \pi(\theta)R(\theta)f_{\hat{\theta}}(\theta)\,d\theta}$$

Bootstrap Estimation of Bayes Expectation $E\{t(\theta)|\hat{\theta}\}$

- Parametric bootstrap replications $f_{\hat{\theta}}(\cdot) \rightarrow \theta_1, \theta_2, \ldots, \theta_i, \ldots, \theta_B$
- $t_i = t(\theta_i), \quad \pi_i = \pi(\theta_i), \quad R_i = R(\theta_i)$:

$$\boxed{\hat{E}\left\{t(\theta)|\hat{\theta}\right\} = \sum_{i=1}^{B} t_i \pi_i R_i \Bigg/ \sum_{i=1}^{B} \pi_i R_i}$$

- *Reweighting* Weight $\pi_i R_i$ on θ_i
- Importance sampling estimate:

$$\hat{E}\left\{t(\theta)|\hat{\theta}\right\} \rightarrow E\left\{t(\theta)|\hat{\theta}\right\} \qquad \text{as } B \rightarrow \infty$$

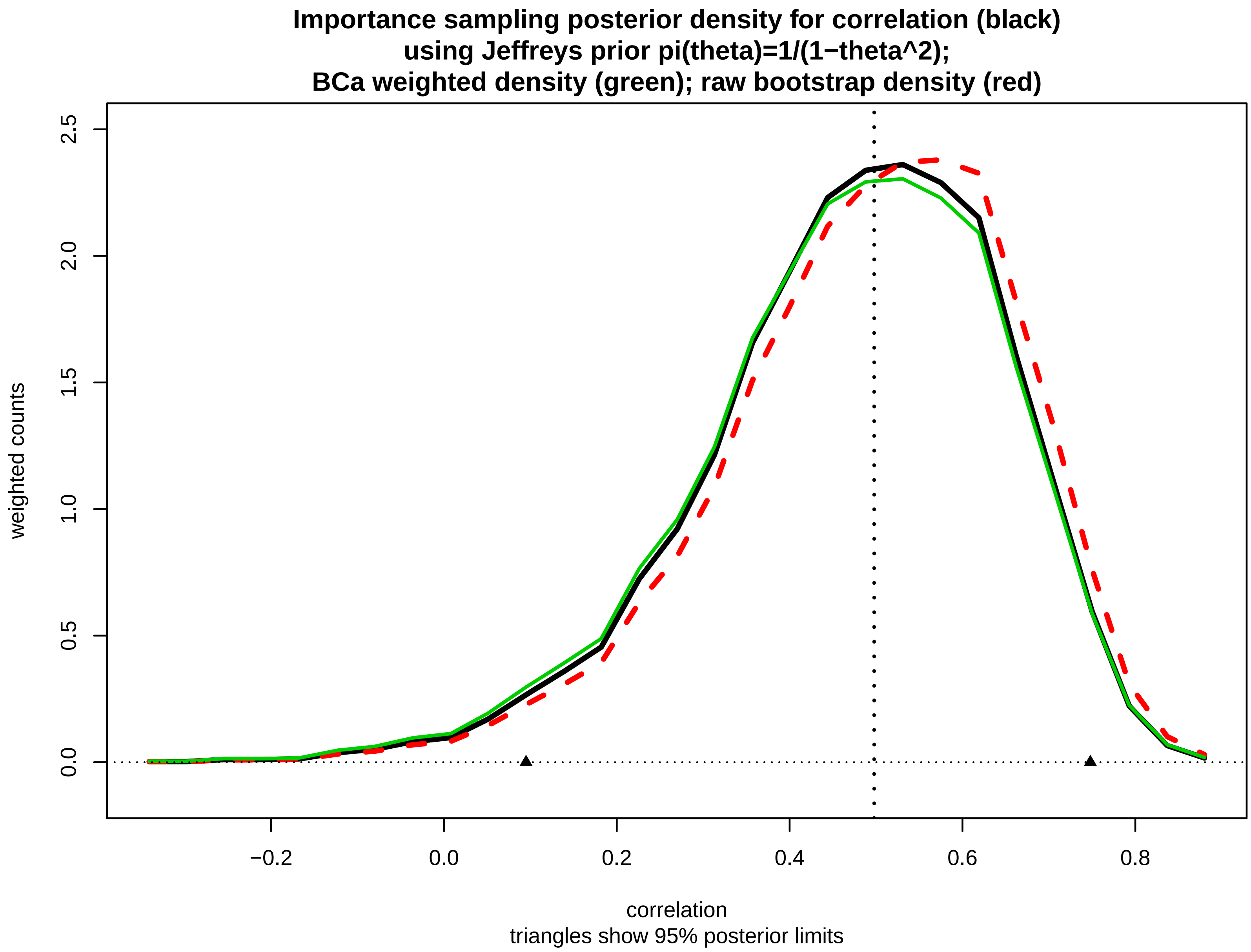
Jeffreys Priors

- Harold Jeffreys (1930s):
  Theory of "uninformative" prior distributions
  ("invariant", "objective", "reference", ...)

- For density family $f_\theta(y)$, $\theta \in \mathcal{R}^p$:

$$\boxed{\pi(\theta) = c|I(\theta)|^{1/2}} \qquad I(\theta) = \text{Fisher info matrix}$$

- *Normal correlation* $\pi(\theta) = 1/(1-\theta^2)$


Importance sampling posterior density for correlation (black)
using Jeffreys prior pi(theta)=1/(1−theta^2);
BCa weighted density (green); raw bootstrap density (red)
weighted counts
0.0
0.5
1.0
1.5
2.0
2.5
−0.2
0.0
0.2
0.4
0.6
0.8
correlation
triangles show 95% posterior limits

Multiparameter Exponential Families $\mathcal{R}^p$

- p-dimensional sufficient statistic $\hat{\beta}$
- p-dimensional parameter vector $\beta = E\left\{\hat{\beta}\right\}$
  (*Poisson*: $e^{-\lambda}\lambda^x/x!$ has $\hat{\beta} = x,\ \beta = \lambda$)
- Hoeffding $\boxed{f_\beta\left(\hat{\beta}\right) = f_{\hat{\beta}}\left(\hat{\beta}\right) e^{-D(\hat{\beta},\beta)/2}}$
- *Deviance* $D(\beta_1, \beta_2) = 2E_{\beta_1} \log\left\{f_{\beta_1}\left(\hat{\beta}\right) \big/ f_{\beta_2}\left(\hat{\beta}\right)\right\}$

Conversion Factor in Exponential Families

- Conversion factor $\quad R(\beta) = f_\beta\left(\hat\beta\right)\Big/f_{\hat\beta}(\beta) \quad$ (with $\hat\beta$ fixed)

$$\boxed{R(\beta) = \nu(\beta)e^{\Delta(\beta)}}$$

where $\Delta(\beta) = \left[D\left(\beta,\hat\beta\right) - D\left(\hat\beta,\beta\right)\right]\Big/2$

- $\nu(\beta) = f_{\hat\beta}\left(\hat\beta\right)\Big/f_\beta(\beta) \doteq 1/\text{Jeffreys prior}$ (Laplace)
- Jeffreys prior $\quad \pi(\beta)R(\beta) \doteq e^{\Delta(\beta)}$

Example: Multivariate Normal

- $y_i \overset{\text{ind}}{\sim} \mathcal{N}_d(\mu, \Sigma)$ for $i = 1, 2, \ldots, n$

- $\Delta =$

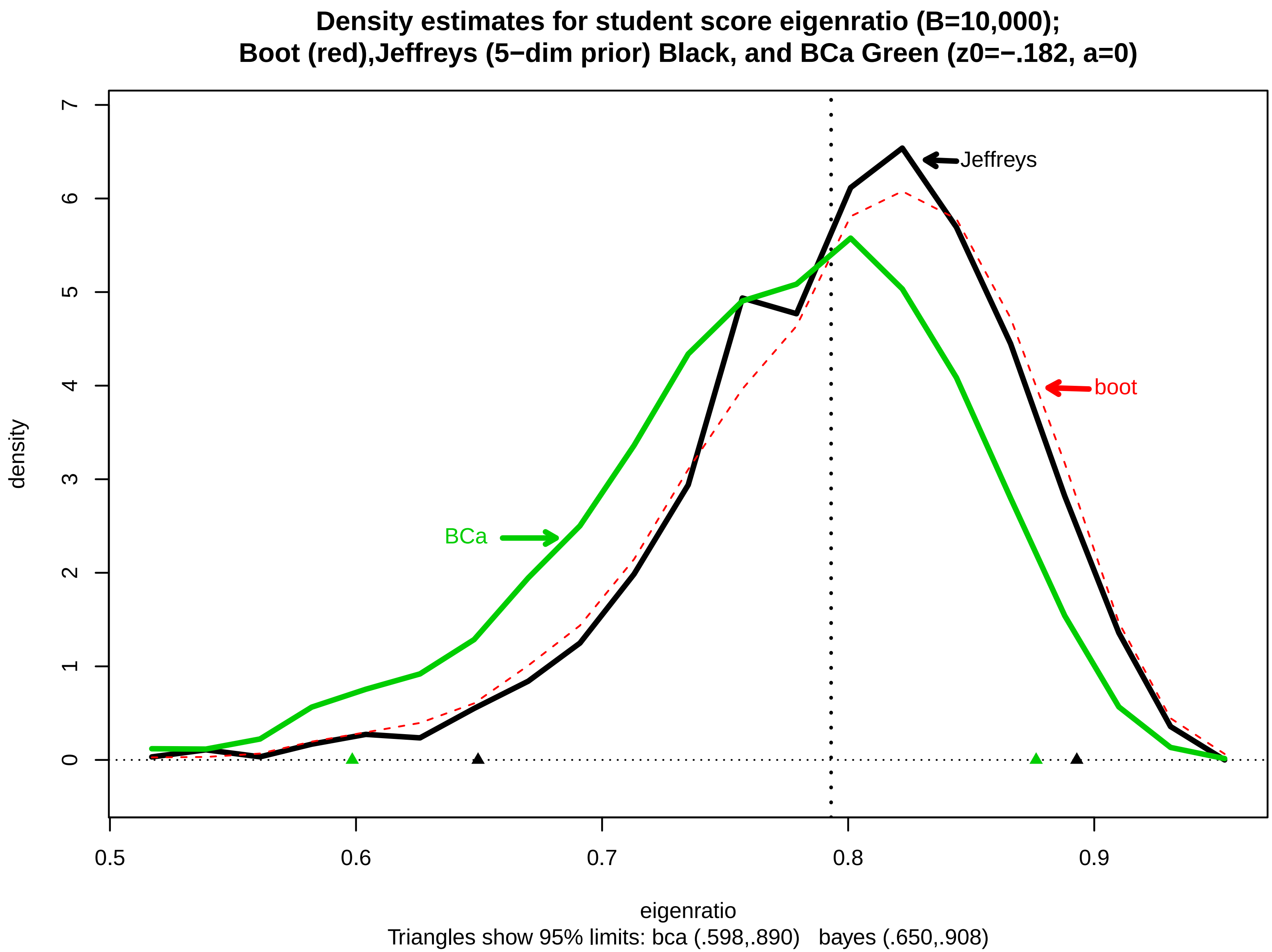
$$n\left\{(\mu - \hat{\mu})' \frac{\hat{\Sigma}^{-1} - \Sigma^{-1}}{2} (\mu - \hat{\mu}) + \frac{1}{2} \operatorname{tr}\left(\Sigma \hat{\Sigma}^{-1} - \hat{\Sigma} \Sigma^{-1}\right) + \log \frac{|\hat{\Sigma}|}{|\Sigma|}\right\}$$

- "eigenratio" (student score data)

- $\theta = \dfrac{\lambda_1}{\lambda_1 + \lambda_2}$

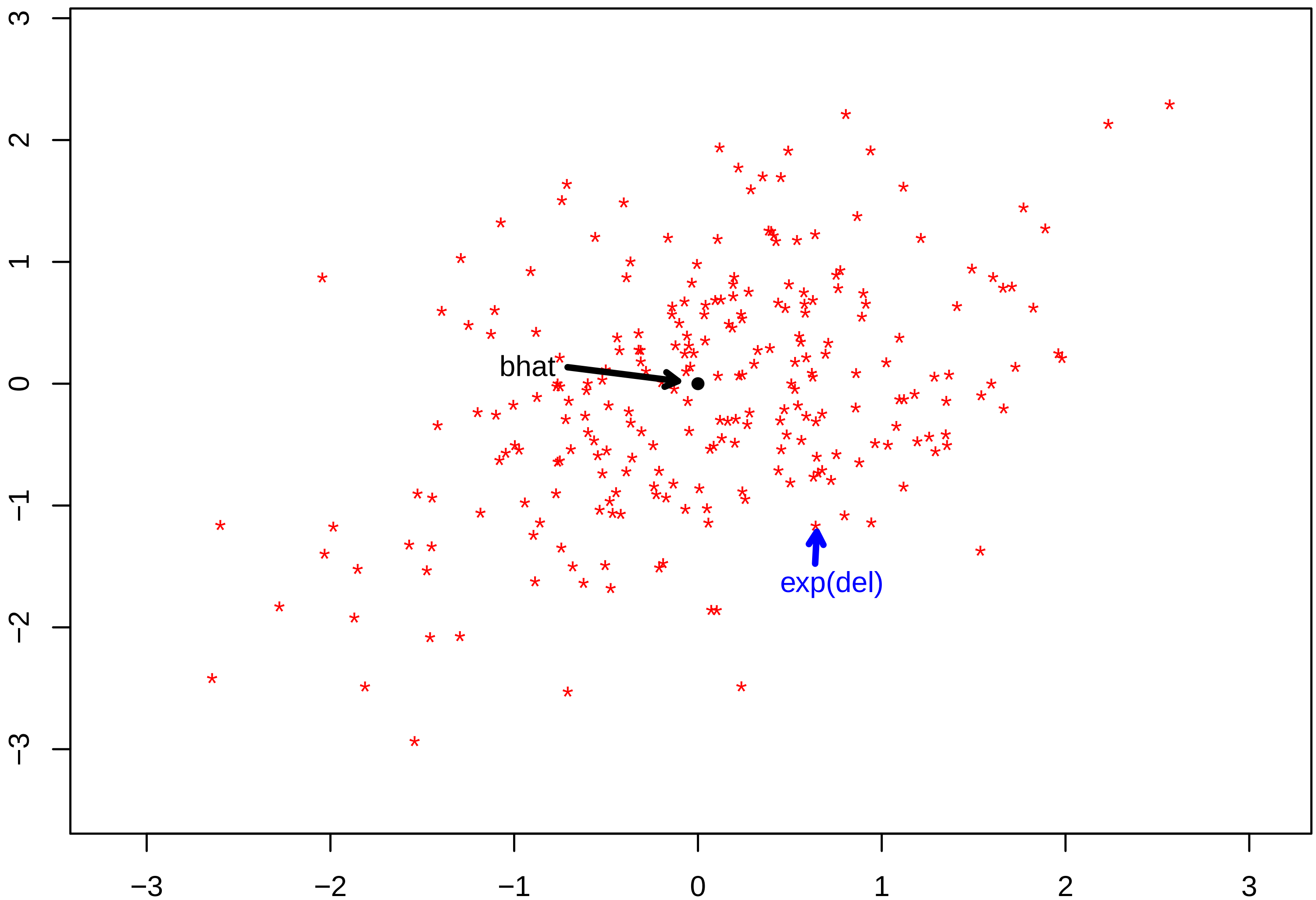
- $\hat{\theta} = \dfrac{\hat{\lambda}_1}{\hat{\lambda}_1 + \hat{\lambda}_2} = 0.793 \pm\ ??$

- Bootstrap $\quad y_i^* \overset{\text{ind}}{\sim} \mathcal{N}_d\left(\hat{\mu}, \hat{\Sigma}\right) \quad i = 1, 2, \ldots, n \to \theta_1, \theta_2, \ldots, \theta_B$



Density estimates for student score eigenratio (B=10,000);
Boot (red),Jeffreys (5−dim prior) Black, and BCa Green (z0=−.182, a=0)
Jeffreys
boot
BCa
density
0
1
2
3
4
5
6
7
0.5
0.6
0.7
0.8
0.9
eigenratio
Triangles show 95% limits: bca (.598,.890) bayes (.650,.908)

Reweighting the parametric bootstrap points



Prostate Cancer Study

(Singh et al, 2002)

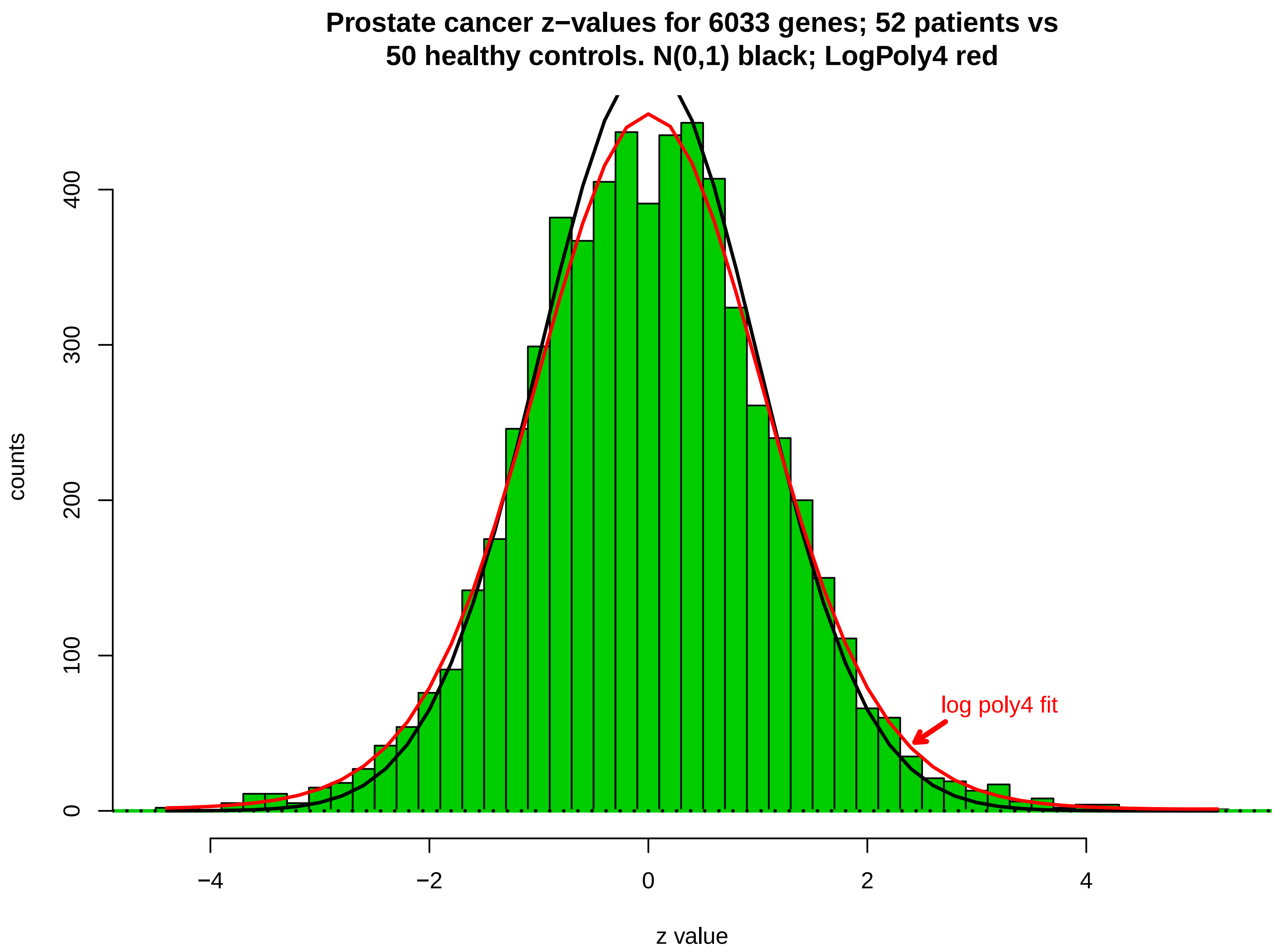
- *Microarray study*

  102 men: 52 prostate cancer, 50 healthy controls

- 6033 genes z_i test statistic for H_{0i}: "no difference"

$$\boxed{H_{0i} : z_i \sim \mathcal{N}(0, 1)}$$

- *Goal* Identify genes involved in prostate cancer


Prostate cancer z−values for 6033 genes; 52 patients vs 50 healthy controls. N(0,1) black; LogPoly4 red
counts
0
100
200
300
400
log poly4 fit
−4
−2
0
2
4
z value

Poisson Regression Models

- *Histogram* $y_j = \#\{z_i \in \text{bin}_j\}$
- $x_j = \text{midpoint bin}_j, \;\; j = 1, 2, \ldots, J$
- Poisson model $y_j \overset{\text{ind}}{\sim} \text{Poi}(\mu_j)$
  with $\log(\mu_j) = \text{poly}(x_j, \text{degree} = m)$
- Exponential family degree $p = m + 1$
- Let $\eta_j = \log(\mu_j)$

$$\boxed{\Delta = (\boldsymbol{\eta} - \hat{\boldsymbol{\eta}})' \, (\boldsymbol{\mu} + \hat{\boldsymbol{\mu}}) - 2\left(\sum \mu_j - \sum \hat{\mu}_j\right)}$$

Parametric False Discovery Rate Estimates

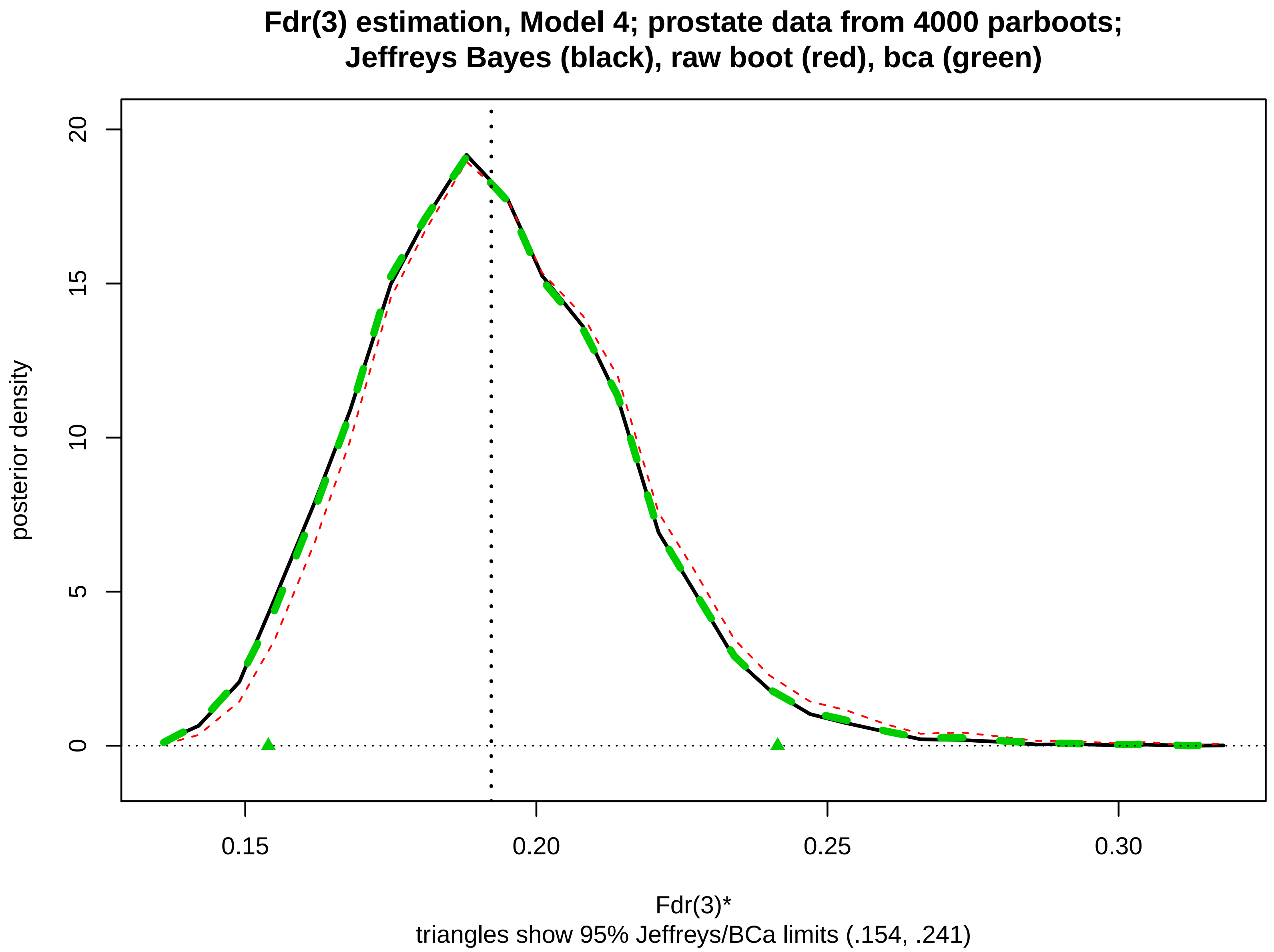
- `glm(y~poly(x,4),Poisson)` $\longrightarrow \left\{\hat{\mu}_j\right\}$ ("log poly 4")

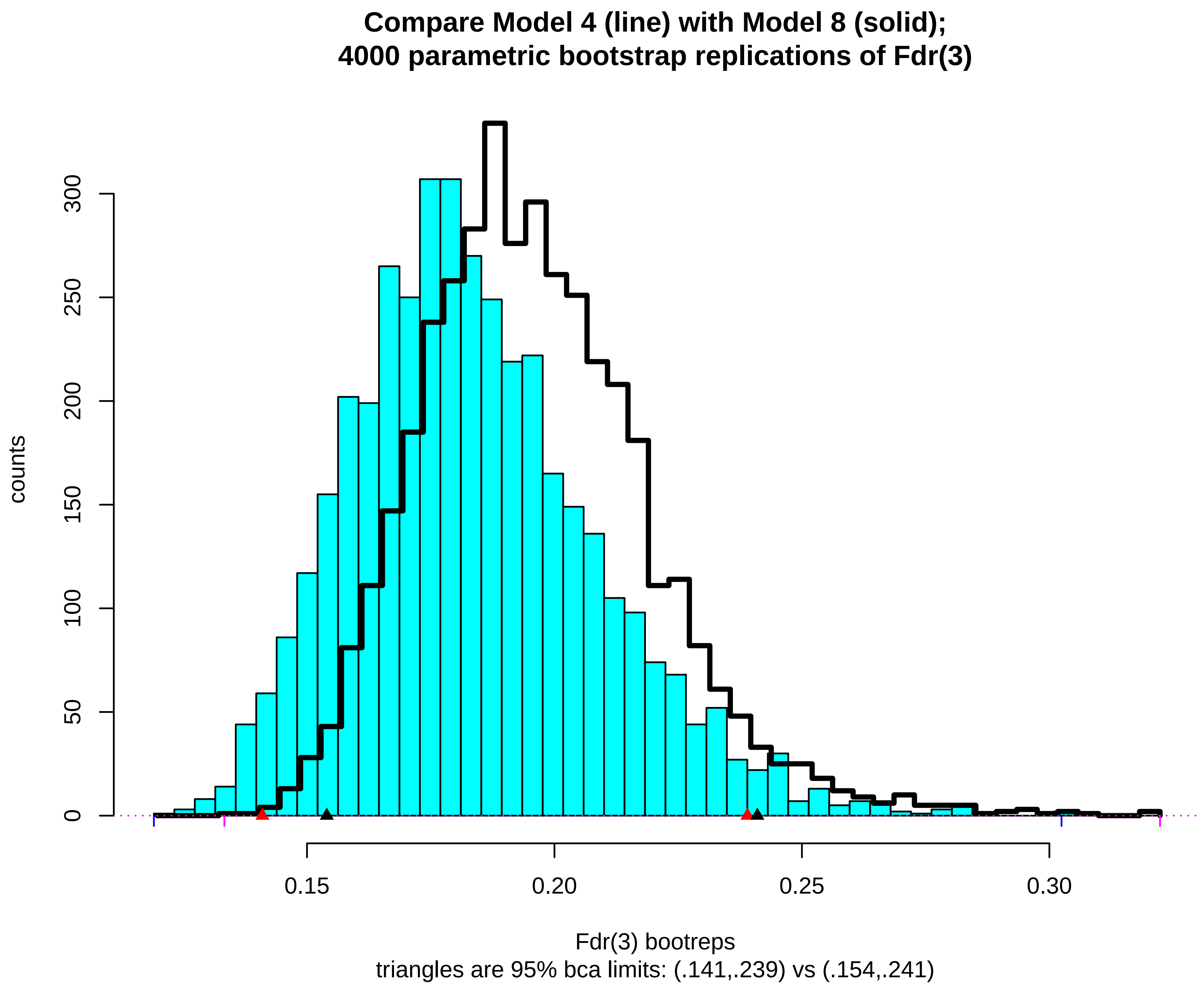
- $\theta = \boxed{\widehat{\mathrm{Fdr}}(3) = [1-\Phi(3)] \Big/ \left[1-\hat{F}(3)\right]} \approx \Pr\{\text{null}|z \geq 3\}$

  ($\hat{F}$ is smoothed CDF estimate)

- Model 4: $\widehat{\mathrm{Fdr}}(3) = 0.192 \pm$??

- Parametric bootstrap $y_j^* \overset{\text{ind}}{\sim} \text{Poi}\left(\hat{\mu}_j\right) \rightarrow \left\{\hat{\mu}_j^*\right\} \longrightarrow \widehat{\mathrm{Fdr}}(3)^*$


Fdr(3) estimation, Model 4; prostate data from 4000 parboots;
Jeffreys Bayes (black), raw boot (red), bca (green)
posterior density
0
5
10
15
20
0.15
0.20
0.25
0.30
Fdr(3)*
triangles show 95% Jeffreys/BCa limits (.154, .241)


Compare Model 4 (line) with Model 8 (solid);
4000 parametric bootstrap replications of Fdr(3)
counts
0
50
100
150
200
250
300
0.15
0.20
0.25
0.30
Fdr(3) bootreps
triangles are 95% bca limits: (.141,.239) vs (.154,.241)

Model Selection: AIC = Deviance + 2 · df

Model	AIC	boot counts	Bayes counts†	
M2	142.6	0	0.0	
M3	143.1	0	0.0	
M4	**73.3**	1266	1458	(36%)
M5	74.3	415	462	(12%)
M6	75.8	215	197	(5%)
M7	77.8	54	67	(2%)
M8	75.6	2050	1816	(45%)

† Model 8, Jeffreys prior

Internal Accuracy of Bayes Estimates

- B for computing $\hat{E}\left\{t(\beta)|\hat{\beta}\right\} = \sum_{1}^{B} t_i \pi_i R_i \Big/ \sum_{1}^{B} \pi_i R_i$?

- Define $r_i = \pi_i R_i$ and $s_i = t_i \pi_i R_i$
- $\hat{c}_{ss} = \sum_{1}^{B} (s_i - \bar{s})^2 / B$, etc.

$$\boxed{\mathrm{CV}\left\{\hat{E}\right\}^2 = \frac{1}{B}\left(\frac{\hat{c}_{ss}}{\bar{s}^2} - 2\frac{\hat{c}_{sr}}{\bar{s}\bar{r}} + \frac{\hat{c}_{rr}}{\bar{r}^2}\right)}$$

- *Example* $\quad t = \mathrm{Fdr}(3)$

  4000 parametric bootreps, Jeffreys Bayes

- Model 4 $\quad \hat{E} = 0.193 \quad \widehat{\mathrm{CV}} = \mathbf{0.0019}$

- Model 8 $\quad \hat{E} = 0.179 \quad \widehat{\mathrm{CV}} = \mathbf{0.0025}$

Sampling Variability of Bayes Estimates

- *How much* would $\hat{E}\left\{t(\beta)|\hat{\beta}\right\}$ vary for new $\hat{\beta}$'s?
  (i.e., frequentist properties of Bayes estimates)
- Need to bootstrap the parametric bootstrap calculations for $\hat{E}\left\{t(\beta)|\hat{\beta}\right\}$
- Shortcut "Bootstrap after bootstrap"

Bootstrap-after-Bootstrap Calculations

- $f_{\hat{\beta}}(\cdot) \longrightarrow \beta_1, \beta_2, \ldots, \beta_i, \ldots, \beta_B,$
  the original bootstrap reps under $\hat{\beta}$
- Want bootreps under some other value $\hat{\gamma}$
- Idea Reweight the originals
- Weight $Q_{\hat{\gamma}}(\beta) = f_\beta(\hat{\gamma}) \,/\, f_\beta\left(\hat{\beta}\right)$:

$$\boxed{\hat{E}\{t|\hat{\gamma}\} = \sum_1^B t_i \pi_i R_i Q_{\hat{\gamma}}(\beta_i) \bigg/ \sum_1^B \pi_i R_i Q_{\hat{\gamma}}(\beta_i)}$$

Bootstrap-after-Bootstrap Standard Errors

- BAB

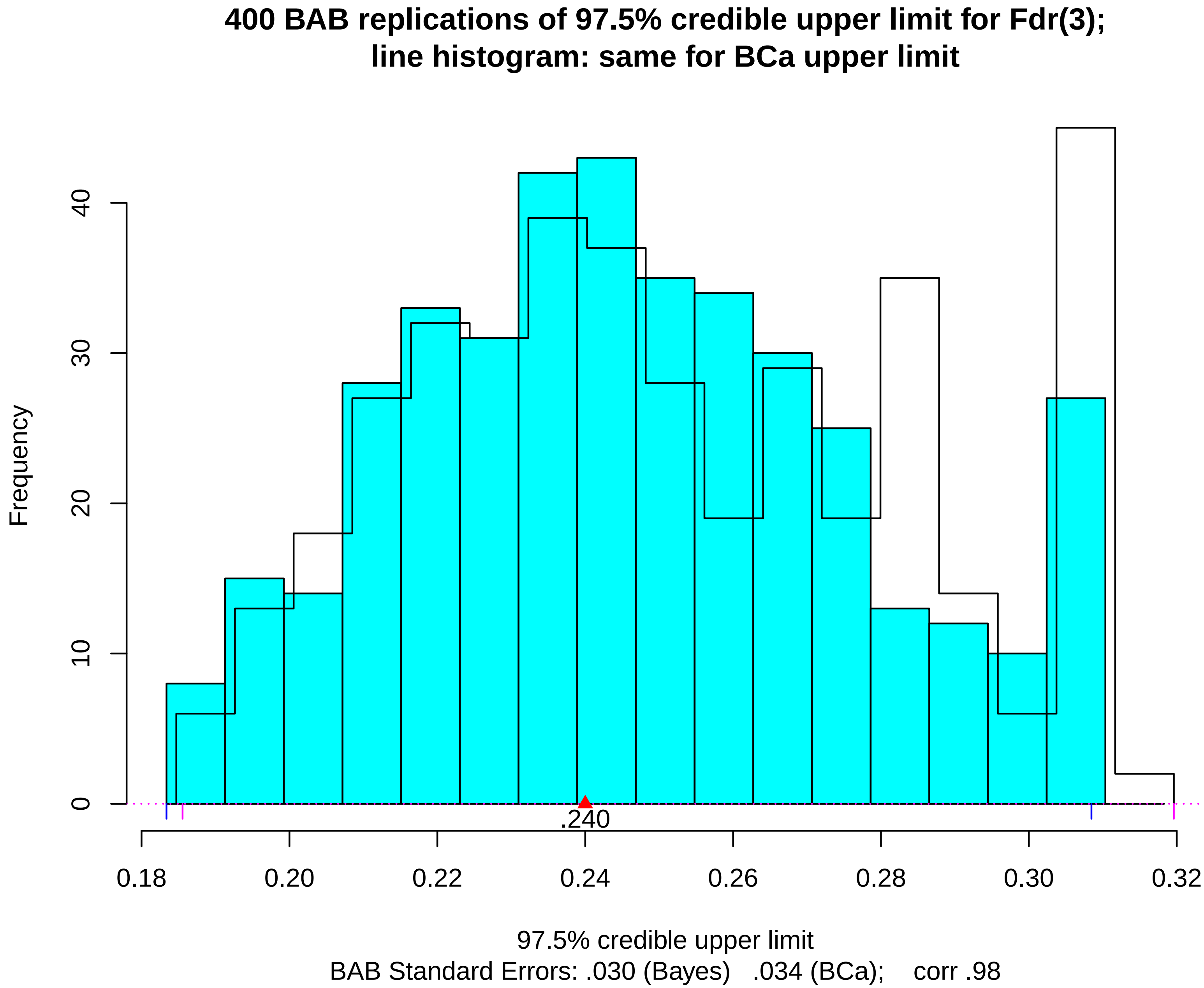
(1) $$f_{\hat{\beta}}(\cdot) \rightarrow \gamma_1, \gamma_2, \ldots, \gamma_k$$

(2) $$\hat{E}_k = \hat{E}\left\{t|\hat{\gamma}_k\right\}$$

(3) $$\text{se}\left\{\hat{E}\right\} = \left[\sum\left(\hat{E}_k - \hat{E}.\right)^2 \big/ K\right]^{1/2}$$

- *Example* Model 4

  97.5% credible limit for $\mathrm{Fdr}(3) = 0.241 \pm$??


400 BAB replications of 97.5% credible upper limit for Fdr(3);
line histogram: same for BCa upper limit
Frequency
0
10
20
30
40
.240
0.18
0.20
0.22
0.24
0.26
0.28
0.30
0.32
97.5% credible upper limit
BAB Standard Errors: .030 (Bayes) .034 (BCa); corr .98

BAB SDs for Bayes Model Selection Proportions

Model	Bayes post. prob.	BAB SD
M4	36%	± 20%
M5	12%	± 14%
M6	5%	± 8%
M7	2%	± 6%
M8	45%	± 27%

- *Model averaging?*

A Few Conclusions . . .

- Parametric bootstrap closely related to objective Bayes.

  (That's why it's a good importance sampling choice.)

- When it applies, parboot approach has both computational and interpretational advantages over MCMC/Gibbs.

- Objective Bayes analyses should be checked frequentistically.

References

- **Bootstrap** DiCiccio and Efron: 1996 *Statist. Sci.* 189–228
- **Bayes and Bootstrap** Newton and Raftery 1994 *JRSS-B* 3–48 (see Discussion!)
- **Objective Priors** Berger and Bernardo 1989 *JASA* 200–207; Ghosh 2011 *Statist. Sci.* 187–202
- **Exponential Families** Efron 2010 *Large-Scale Inference*, Appendix 1
- **MCMC and Bootstrap** 2011: `http://stat.stanford.edu/~brad/papers/`