Lectures 15: Confidence interval review and Bootstrap III.

error propagation for nonlinear functions of fit parameters

with material from

The University of Texas at Austin, CS 395T, Spring 2010, Prof. William H. Press previously:

Maximum Likelihood parameter errors?

How accurately are the fitted parameters determined?
As Bayesians, we would **instead** say, what is their posterior distribution?

Taylor series:

$$-\tfrac{1}{2}\chi^2(\mathbf{b}) \approx -\tfrac{1}{2}\chi^2_{\mathrm{min}} - \tfrac{1}{2}(\mathbf{b}-\mathbf{b}_0)^T \left[\frac{1}{2}\frac{\partial^2\chi^2}{\partial\mathbf{b}\partial\mathbf{b}}\right](\mathbf{b}-\mathbf{b}_0)$$

So, while exploring the χ^2 surface to find its minimum, we must also calculate the Hessian (2nd derivative) matrix at the minimum.

Then

$$P(\mathbf{b}|\{y_i\}) \propto \exp\left[-\tfrac{1}{2}(\mathbf{b}-\mathbf{b}_0)^T \mathbf{\Sigma}_b^{-1}(\mathbf{b}-\mathbf{b}_0)\right] P(\mathbf{b})$$

with

$$\mathbf{\Sigma}_b = \left[\frac{1}{2}\frac{\partial^2\chi^2}{\partial\mathbf{b}\partial\mathbf{b}}\right]^{-1}$$

covariance (or "standard error") matrix
of the fitted parameters

Notice that if (i) the Taylor series converges rapidly and (ii) the prior is uniform, then the posterior distribution of the $\mathbf{b}$'s is multivariate Normal, a very useful CLT-ish result!

multivariate normal distribution

Question: What is the generalization of

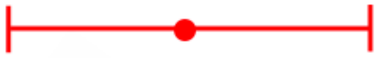
$$\chi^2 = \sum_i \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2, \qquad x_i \sim \mathrm{N}(\mu_i, \sigma_i)$$

to the case where the x_i's are normal, **but not independent**?
I.e., **x** comes from a multivariate Normal distribution?

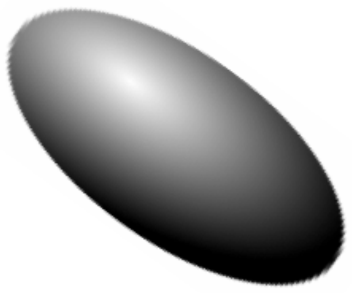
$$N(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{M/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp[-\tfrac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})]$$

The mean and covariance of r.v.'s from this distribution are*

$$\boldsymbol{\mu} = \langle \mathbf{x} \rangle \qquad \boldsymbol{\Sigma} = \left\langle (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T \right\rangle$$



In the one-dimensional case σ is the standard deviation, which can be visualized as "error bars" around the mean.



In more than one dimension Σ can be visualized as an error ellipsoid around the mean in a similar way.

$$1 = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

multivariate normal distribution

Multivariate Normal Distributions

Generalizes Normal (Gaussian) to M-dimensions
Like 1-d Gaussian, completely defined by its mean and (co-)variance
Mean is a M-vector, covariance is a M x M matrix

$$N(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{M/2}\det(\boldsymbol{\Sigma})^{1/2}}\exp[-\tfrac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})]$$

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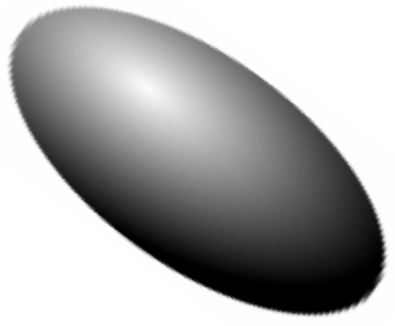

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linear error propagation for arbitrary function of parameters

What is the uncertainty in quantities other than the fitted coefficients:

Method 1: Linearized propagation of errors

$\mathbf{b}_0$ is the MLE parameters estimate

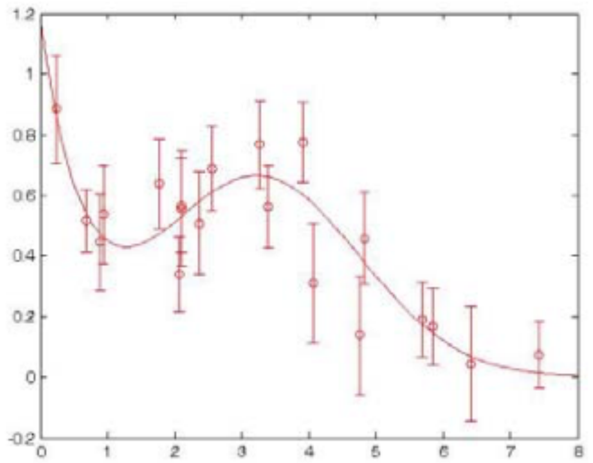
$\mathbf{b}_1 \equiv \mathbf{b} - \mathbf{b}_0$ is the RV as the parameters fluctuate

$$
\begin{aligned}
f \equiv f(\mathbf{b}) &= f(\mathbf{b}_0) + \nabla f \; \mathbf{b}_1 + \cdots \\
\langle f \rangle &\approx \langle f(\mathbf{b}_0) \rangle + \nabla f \; \cancel{\langle \mathbf{b}_1 \rangle} = f(\mathbf{b}_0) \\
\langle f^2 \rangle - \langle f \rangle^2 &\approx 2 f(\mathbf{b}_0)(\nabla f \; \cancel{\langle \mathbf{b}_1 \rangle}) + \left\langle (\nabla f \; \mathbf{b}_1)^2 \right\rangle \\
&= \nabla f \; \left\langle \mathbf{b}_1 \mathbf{b}_1^T \right\rangle \nabla f^{\,T} \\
&= \nabla f \; \mathbf{\Sigma} \, \nabla f^{\,T}
\end{aligned}
$$

linear error propagation for arbitrary function of parameters

In our example, if we are interested in the area of the “hump”,

```
bfit =
    1.1235    1.5210    0.6582    3.2654    1.4832
covar =
    0.1349    0.2224    0.0068   -0.0309    0.0135
    0.2224    0.6918    0.0052   -0.1598    0.1585
    0.0068    0.0052    0.0049    0.0016   -0.0094
   -0.0309   -0.1598    0.0016    0.0746   -0.0444
    0.0135    0.1585   -0.0094   -0.0444    0.0948
```



$$f = b_3 b_5$$

$$\nabla f = (0, 0, b_5, 0, b_3)$$

$$\nabla f\, \mathbf{\Sigma}\, \nabla f^T = b_5^2 \Sigma_{33} + 2 b_3 b_5 \Sigma_{35} + b_3^2 \Sigma_{55} = 0.0336$$

$$\sqrt{0.0336} = 0.18$$

So $b_3 b_5 = 0.98 \pm 0.18$ ← the one standard deviation (1-σ) error bar

A function of normals is not normal

Sampling the posterior histogram

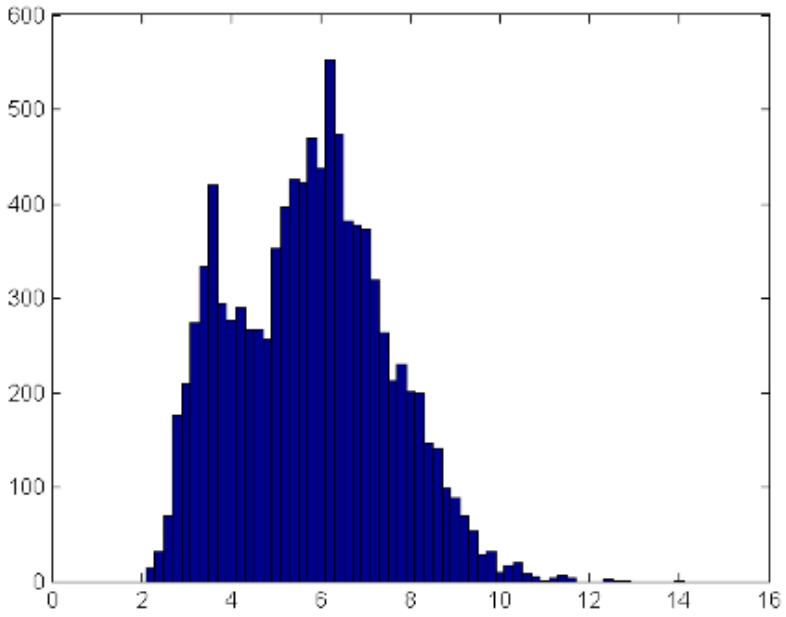
Method 2: Sample from the posterior distribution

1. Generate a large number of (vector) **b**'s

$$\mathbf{b} \sim \mathrm{MVNormal}(\mathbf{b}_0, \boldsymbol{\Sigma}_b)$$

2. Compute your $f(\mathbf{b})$ separately for each **b**

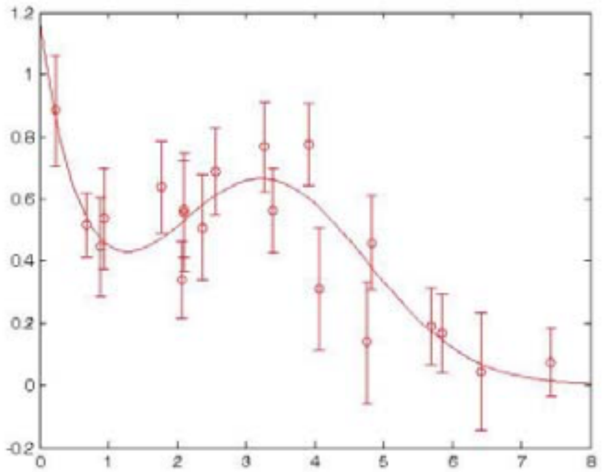
3. Histogram



Note again that **b** is typically (close to) m.v. normal because of the CLT, but your (nonlinear) f may not, in general, be anything even close to normal!

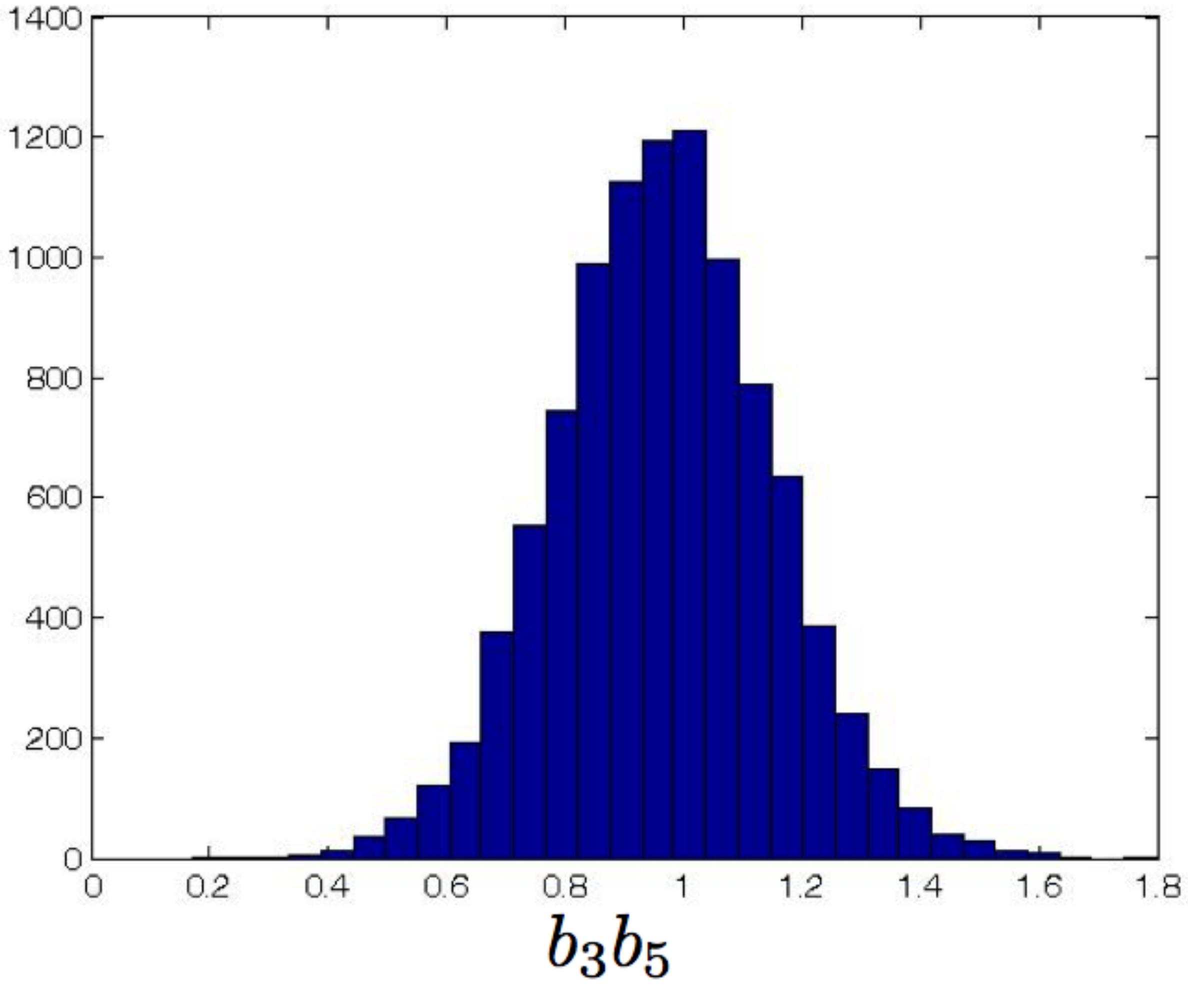
Sampling the posterior histogram

Our example:



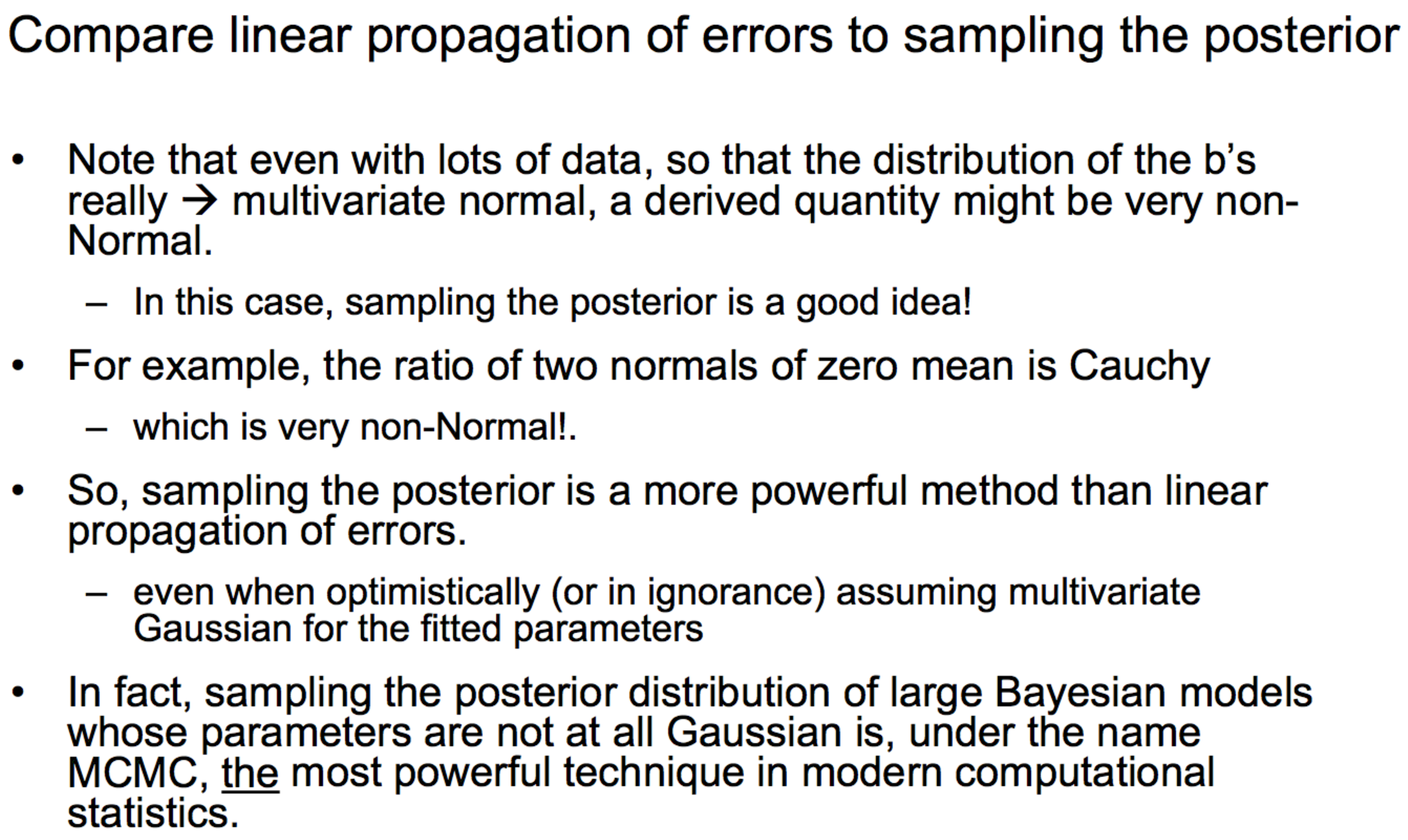
```
bees = mvnrnd(bfit,covar,10000);
humps = bees(:,3).*bees(:,5);
hist(humps,30);
std(humps)
```

```
std = 0.1833
```



Does it matter that I use the full covar, not just the 2x2 piece for parameters 3 and 5?

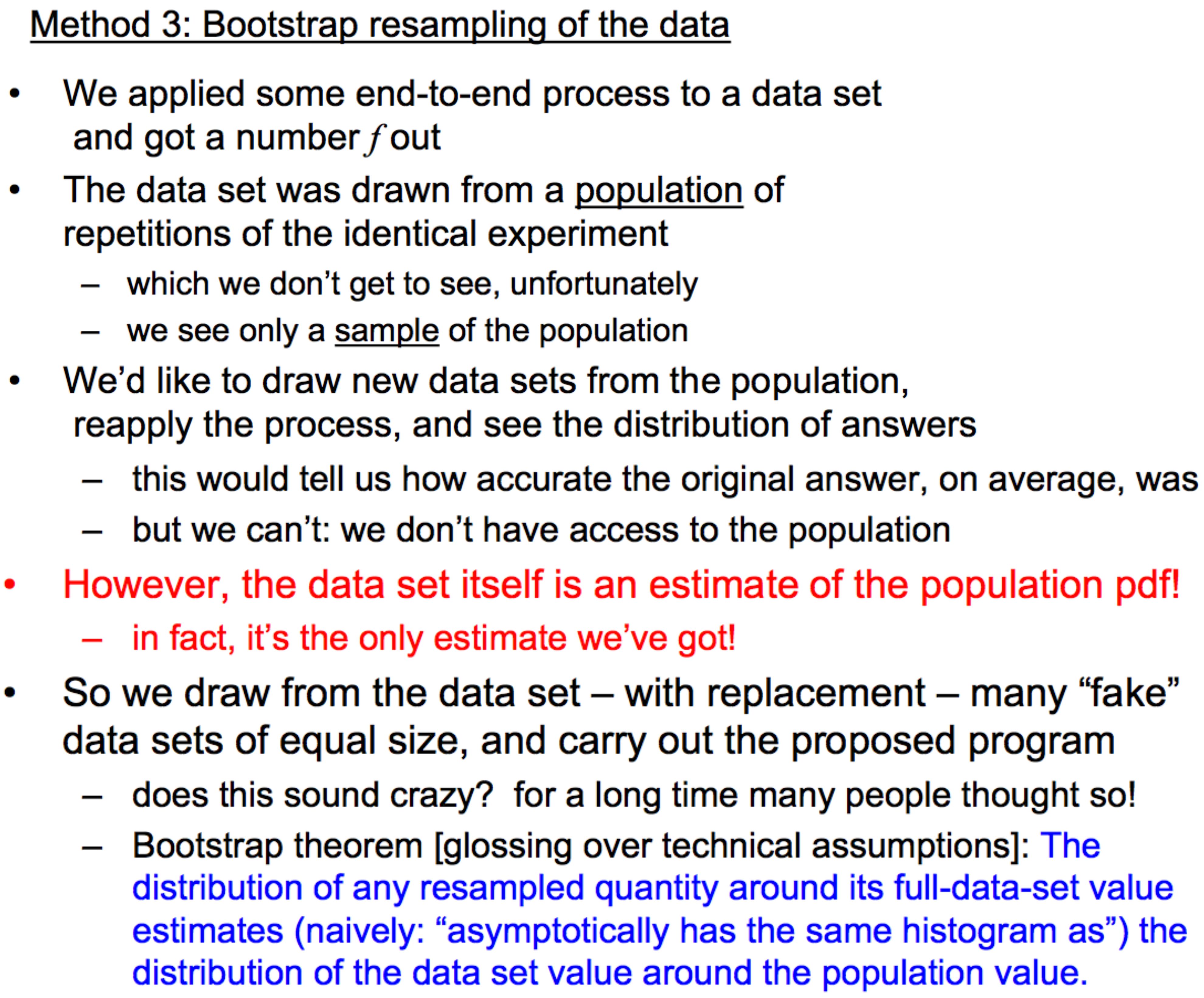
comparison of linear propagation and posterior sampling:



Compare linear propagation of errors to sampling the posterior

- Note that even with lots of data, so that the distribution of the b's really → multivariate normal, a derived quantity might be very non-Normal.
  - In this case, sampling the posterior is a good idea!
- For example, the ratio of two normals of zero mean is Cauchy
  - which is very non-Normal!.
- So, sampling the posterior is a more powerful method than linear propagation of errors.
  - even when optimistically (or in ignorance) assuming multivariate Gaussian for the fitted parameters
- In fact, sampling the posterior distribution of large Bayesian models whose parameters are not at all Gaussian is, under the name MCMC, the most powerful technique in modern computational statistics.

bootstrap sampling



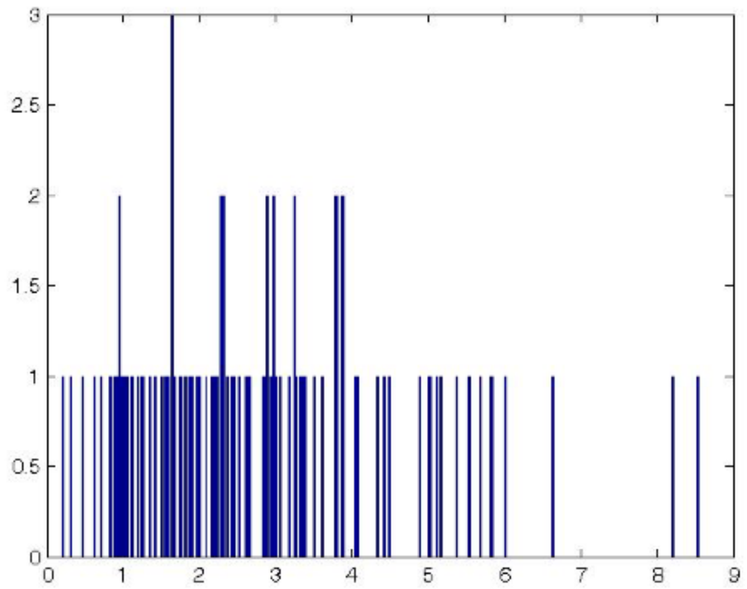
Method 3: Bootstrap resampling of the data

- We applied some end-to-end process to a data set and got a number f out
- The data set was drawn from a population of repetitions of the identical experiment
  - which we don't get to see, unfortunately
  - we see only a sample of the population
- We'd like to draw new data sets from the population, reapply the process, and see the distribution of answers
  - this would tell us how accurate the original answer, on average, was
  - but we can't: we don't have access to the population
- However, the data set itself is an estimate of the population pdf!
  - in fact, it's the only estimate we've got!
- So we draw from the data set – with replacement – many "fake" data sets of equal size, and carry out the proposed program
  - does this sound crazy? for a long time many people thought so!
  - Bootstrap theorem [glossing over technical assumptions]: The distribution of any resampled quantity around its full-data-set value estimates (naively: "asymptotically has the same histogram as") the distribution of the data set value around the population value.

bootstrap sampling

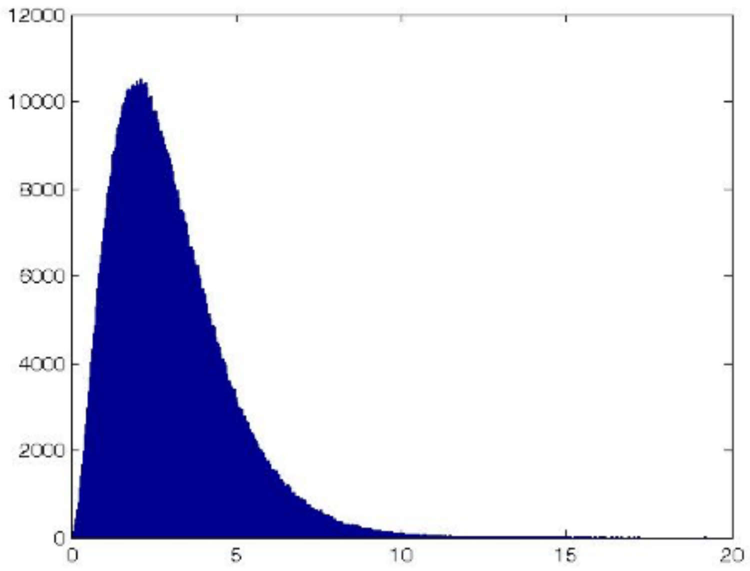
Let’s try a simple example where we can see the “hidden” side of things, too.

Visible side (sample):



These happen to be drawn from a Gamma distribution.

Hidden side (population):



Statistic we are interested in happens to be (it could be anything):

$$\frac{\text{mean of distribution}}{\text{median of distribution}}$$

```
sammedian = median(sample)
sammean = mean(sample)
samstatistic = sammean/sammedian
sammedian =
    2.6505
sammean =
    2.9112
samstatistic =
    1.0984
```

How accurate is this?

```
themedian = median(bigsample)
themean = mean(bigsample)
thestatistic = themean/themedian
themedian =
    2.6730
themean =
    2.9997
thestatistics =
    1.1222
```

bootstrap sampling

Gamma distribution:

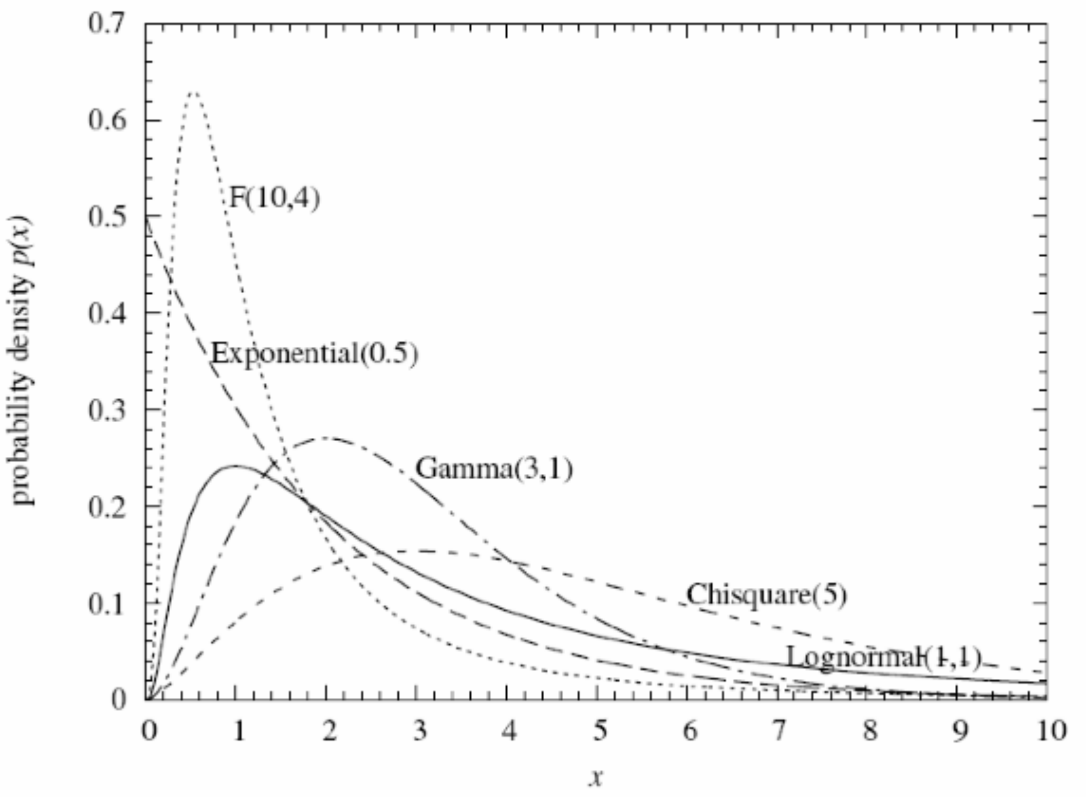
$$x \sim \text{Gamma}(\alpha, \beta), \qquad \alpha > 0,\ \beta > 0$$

$$p(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}, \qquad x > 0$$

$$\text{Mean}\{\text{Gamma}(\alpha, \beta)\} = \alpha/\beta$$

$$\text{Var}\{\text{Gamma}(\alpha, \beta)\} = \alpha/\beta^2$$

When $\alpha \geq 1$ there is a single mode at $x = (\alpha - 1)/\beta$



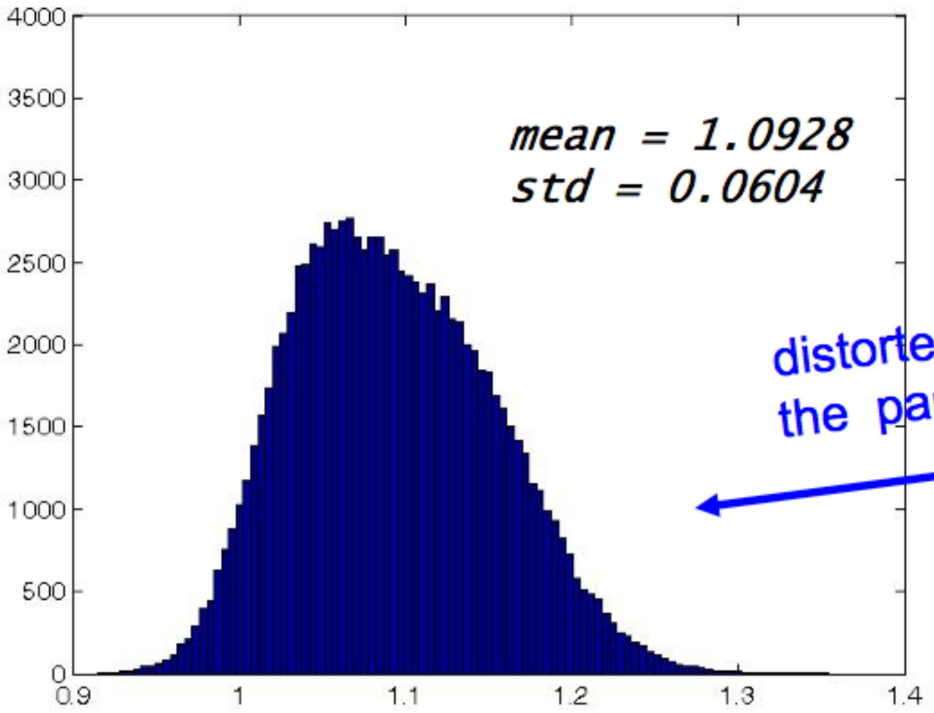
bootstrap sampling

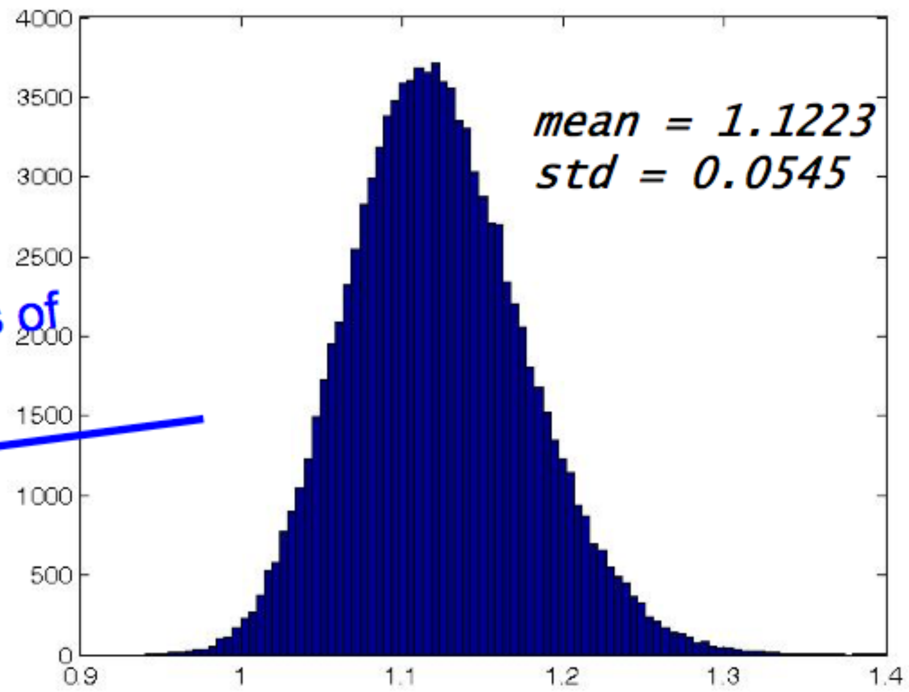
To estimate the accuracy of our statistic, we bootstrap

```
ndata = 100;
nboot = 100000;
vals = zeros(nboot,1);
for j=1:nboot,
   choose = randsample(ndata,ndata,true);
   vals(j) = mean(sample(choose))
          /median(sample(choose));
end
hist(vals,100)
```

new sample of integers in 1:ndata, with replacement

```
ndata = 100;
nboot = 100000;
vals = zeros(nboot,1);
for j=1:nboot,
   sam = randg(3,[ndata 1]);
   vals(j) = mean(sam)/median(sam);
end
hist(vals,100)
```





distorted by peculiarities of the particular data set

Things to notice:

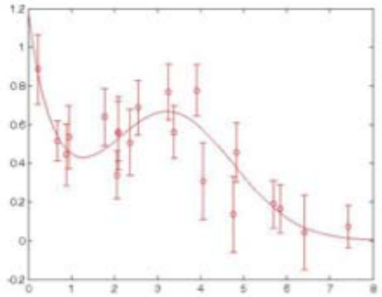
The mean of resamplings does <u>not</u> improve the original estimate! (Same data!)

The distribution around the mean is not <u>identical</u> to that of the population. But it is <u>close</u> and would become identical asymptotically for large *ndata* (not *nboot*!).

bootstrap sampling

```
ndata = 20;
nboot = 1000;
vals = zeros(nboot,1);
ymodel = @(x,b) b(1)*exp(-b(2)*x)+b(3)*exp(-(1/2)*((x-b(4))/b(5)).^2);
for j=1:nboot,
   samp = randsample(ndata,ndata,true);
   xx = x(samp);
   yy = y(samp);
   ssig = sig(samp);
   chisqfun = @(b) sum(((ymodel(xx,b)-yy)./ssig).^2);
   bguess = [1 2 .7 3.14 1.5];
   options = optimset('MaxFunEvals',10000,'MaxIter',
          10000,'TolFun',0.001);
   [b fval flag] = fminsearch(chisqfun,bguess,options);
   if (flag == 1), vals(j) = b(3)*b(5);
   else vals(j) = 100; end
end
hist(vals(vals < 2),30);
std(vals(vals < 2))
```

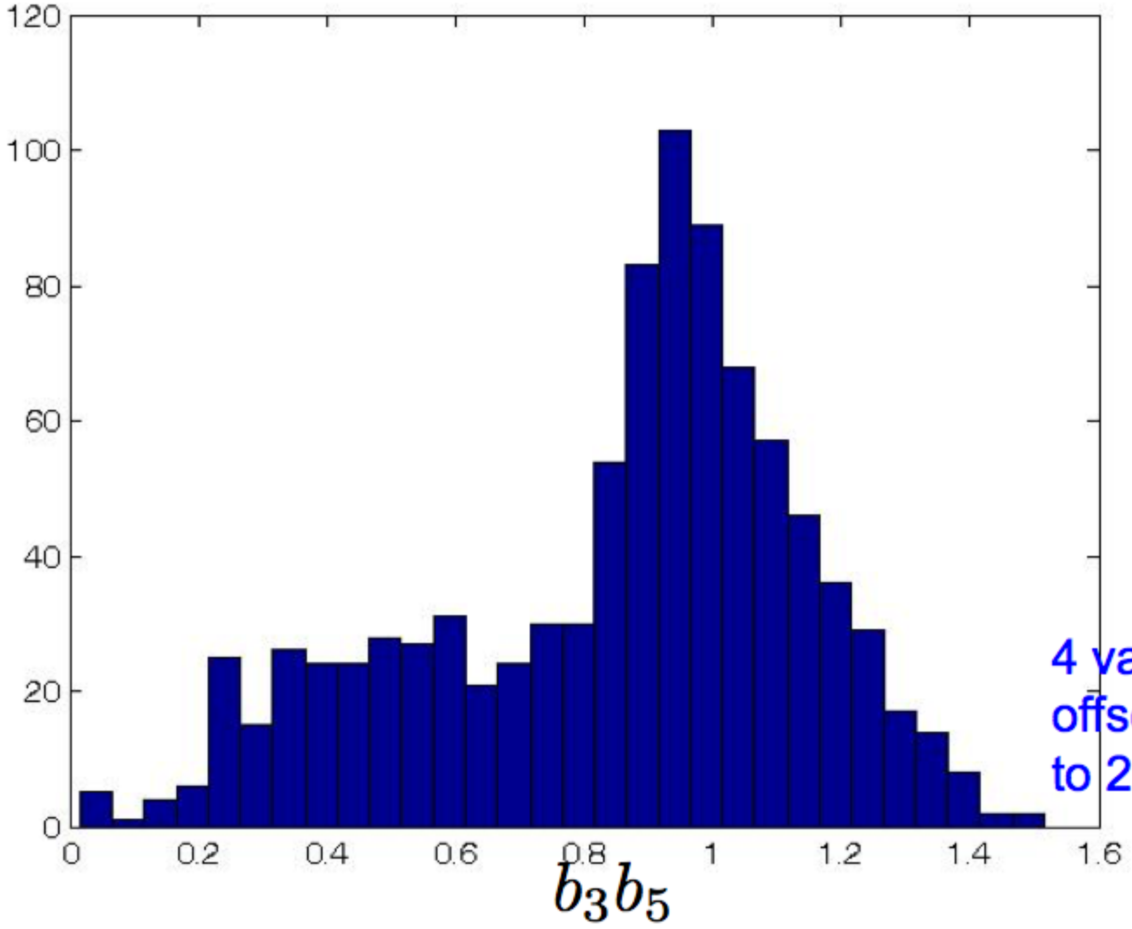
new sample of integers in 1:ndata, with replaceme



here is the embedded “whole statistical analysis of a data set” inside the bootstrap loop

```
      0.2924
```

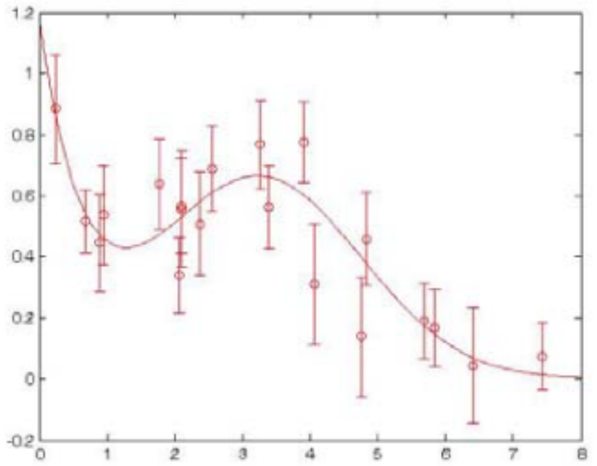
So we get the peak around 1, as before, but a much broader distribution.

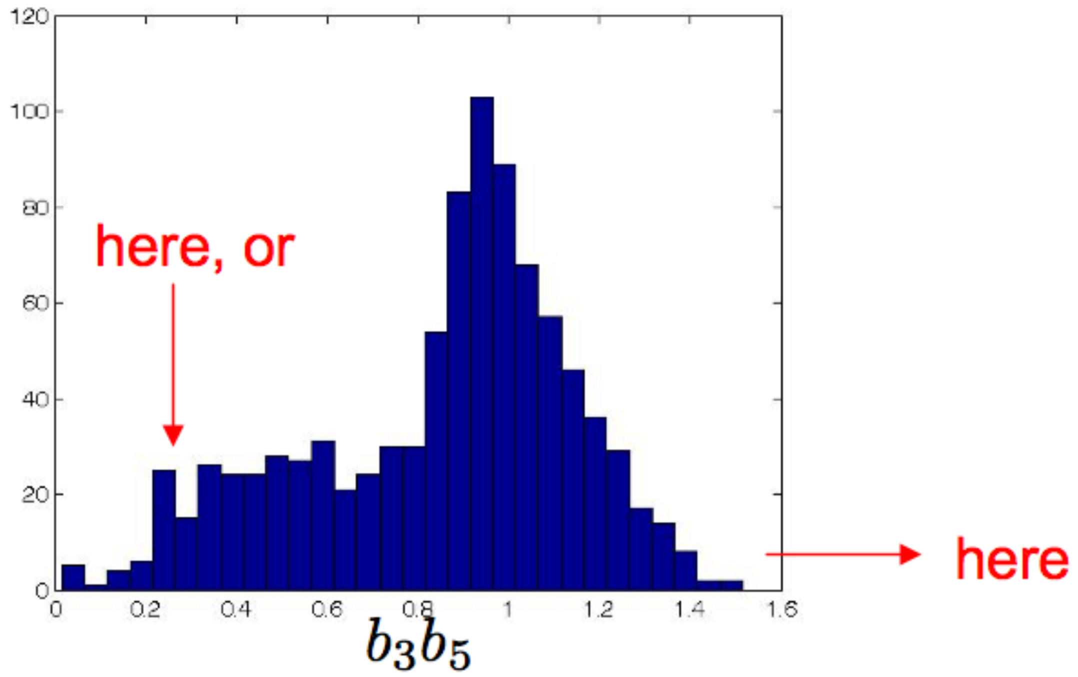


4 values offscale (up to 27!)

bootstrap sampling

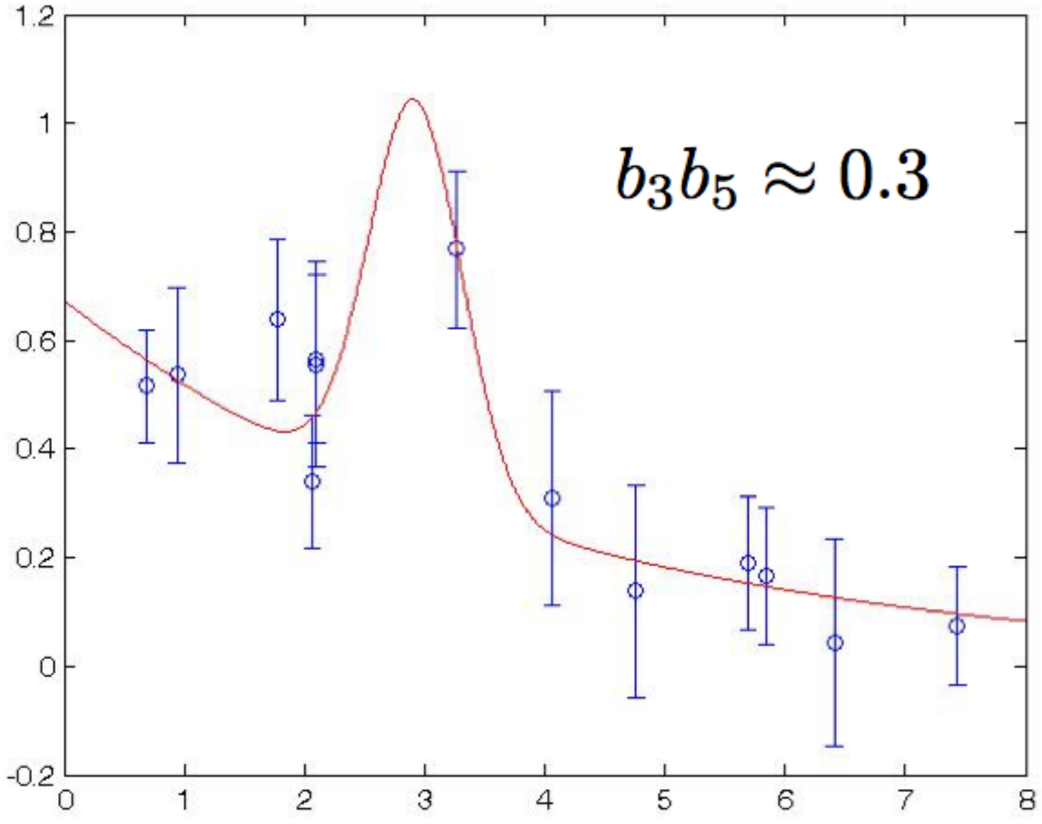
Can you guess what the extreme bootstrap cases look like, compared to the full data?

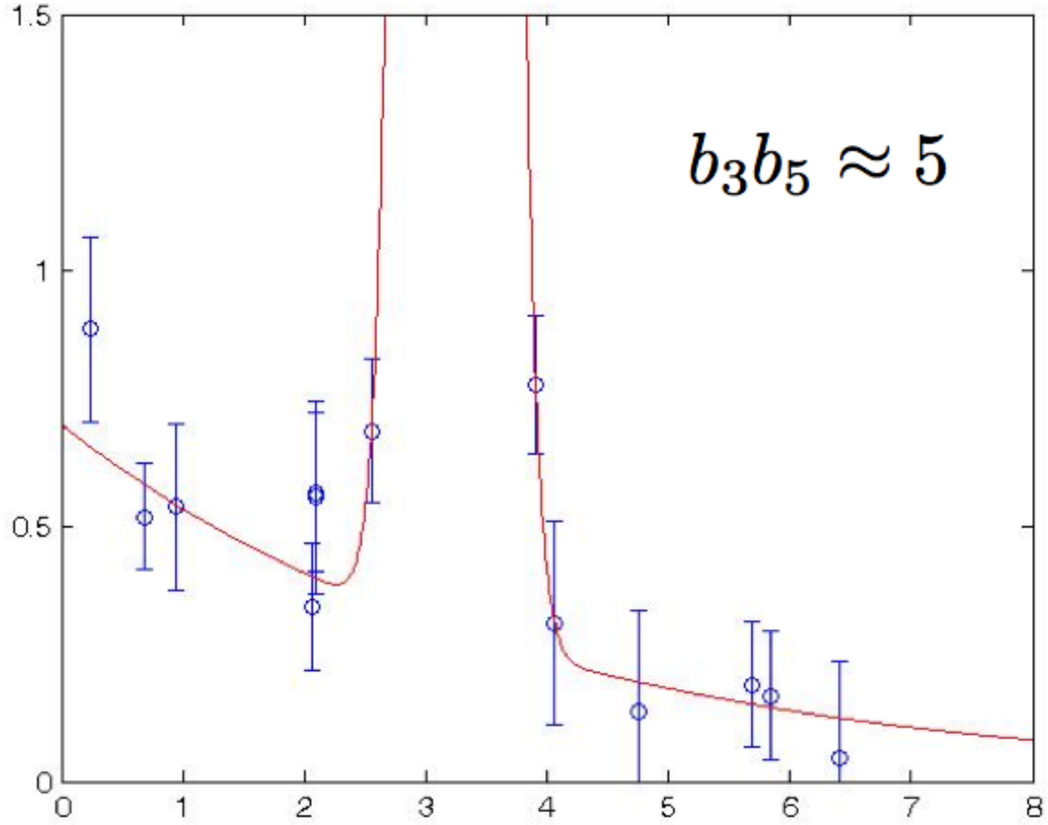




here, or

here

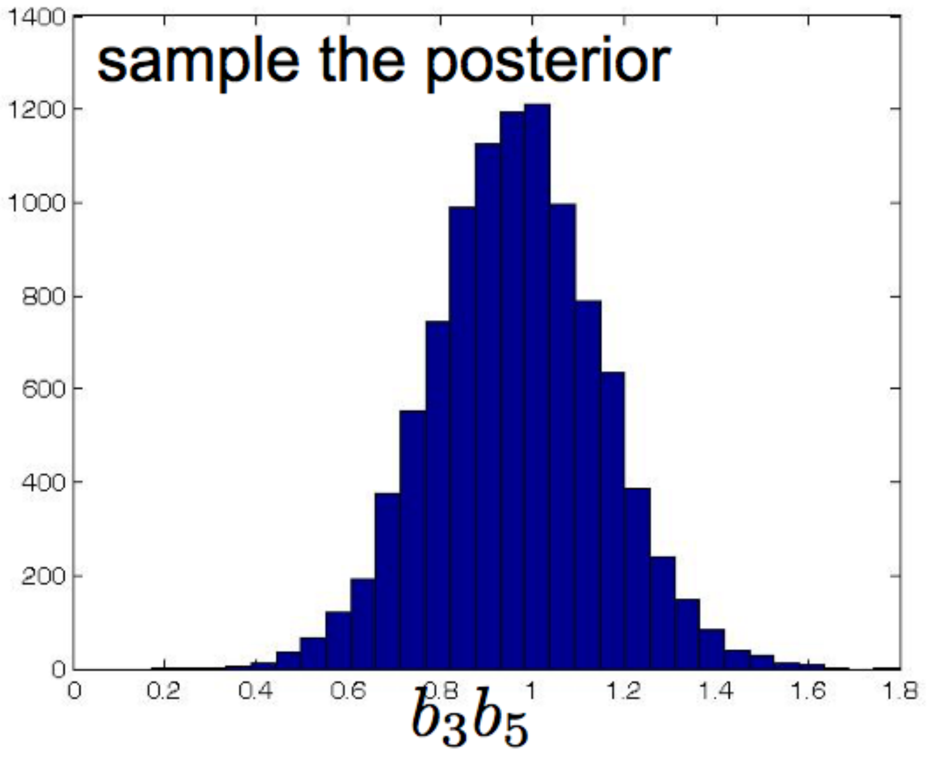


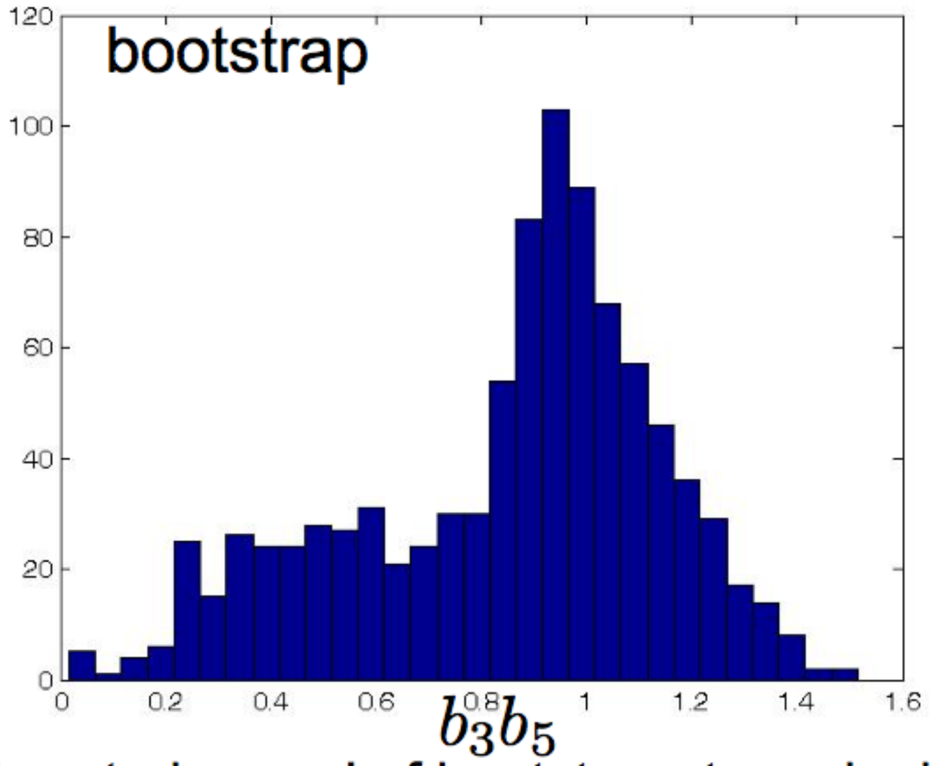


frequentist is concerned about error estimate

bootstrap sampling

We previously compared bootstrap-from-sample to bootstrap-from-population.
More relevant, let's compare boostrap-from-sample to sample-the-posterior:





- We could increase number of samples of posterior, and of bootstrap, to make both curves very smooth.
  - the histograms would not converge to each other!
- We could increase the size of the underlying data sample
  - from 20 (x,y) values to infinity (x,y) values
  - the histograms would converge to each other (modulo technical assumptions)
- For finite size samples, each technique is a valid answer to a different question
  - Frequentist: Imagining repetitions of the experiment, what would be the range of values obtained?
    - And. conservatively, I shouldn't expect my experiment to be better than that, should I?
  - Bayesian: For exactly the data that I see, what is the probability distribution of the parameters?
    - Because maybe I got lucky and my data set really nails the parameters!

bootstrap sampling

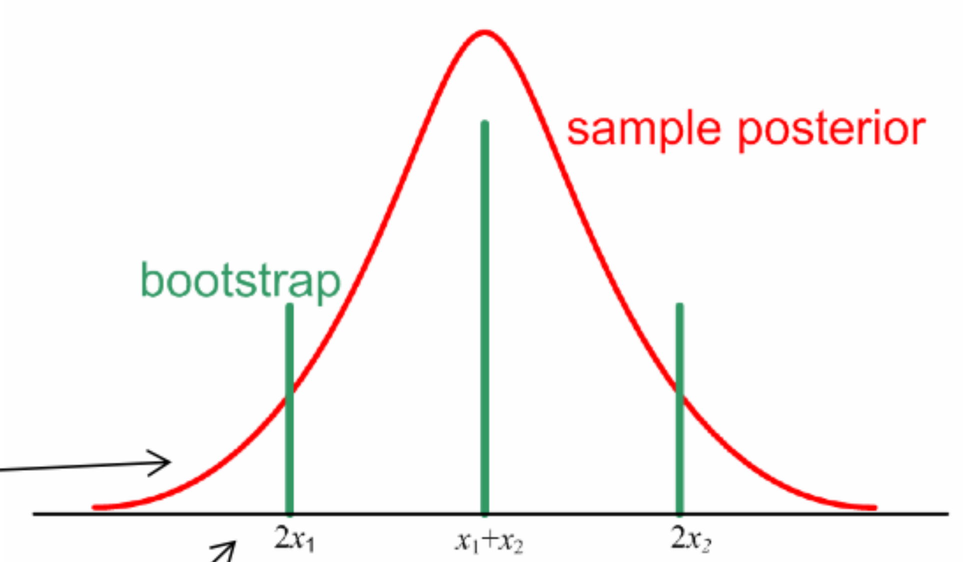
Note that sampling the posterior "honors" the stated measurement errors. Bootstrap doesn't. That can be good!

Suppose (very toy example) the "statistic" is

$$s = x_1 + x_2$$

then the posterior probability is

$$P(s) \propto \exp\left[-\frac{1}{2}\frac{(s - x_1 - x_2)^2}{\sigma_1^2 + \sigma_2^2}\right]$$

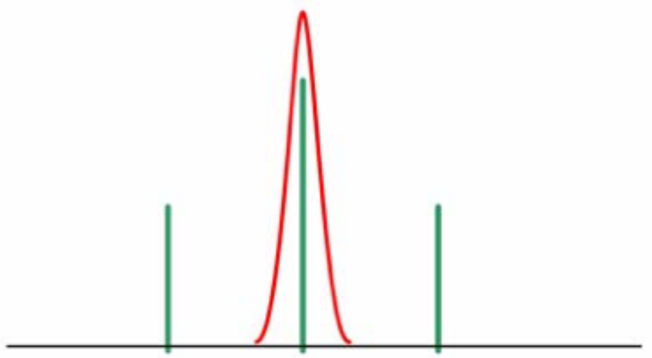


Note that this depends on the σ's!

The bootstrap (here noticeably discrete) doesn't depend on the σ's. In some sense it estimates them, too.

So, if the errors were badly underestimated, sampling the posterior would give too small an uncertainty, while bootstrap would still give a valid estimate.

If the errors are right, both estimates are valid. Notice that the model need not be correct. Both procedures give estimates of the statistical uncertainty of parameters of even a wrong (badly fitting) model. *But for a wrong model, your interpretation of the parameters may not mean anything!*



bootstrap sampling

Compare and contrast bootstrap resampling and sampling from the posterior

Both have same goal: Estimate the accuracy of fitted parameters.

- Bootstrap is frequentist in outlook
  - draw from "the population"
  - even if we have only an estimate of it (the data set)
- Easy to code but computationally intensive
  - great for getting your bearings
  - must repeat your basic fitting calculation over all the data100 or 1000 times
- Applies to both model fitting and descriptive statistics
- Fails completely for some statistics
  - e.g. (extreme example) "harmonic mean of distance between consecutive points"
  - how can you be sure that your statistic is OK (without proving theorems)?
- Doesn't generalize much
  - take it or leave it!
- It is not always obvious what you should resample over
  - things that are independent draws from a population

- Sampling from the posterior is Bayesian in outlook
  - there is only one data set and it is never varied
  - what varies from sample to sample is the goodness of fit of the parameters
  - we don't just sit on the (frequentist's) MLE, we explore around
- In general harder to implement
  - we haven't learned how yet, except in the simple case of an assumed multivariate normal posterior
  - will come back to this later, when we do Markov Chain Monte Carlo (MCMC)
  - may or may not be computationally intensive (depending on whether there are shortcuts possible in computing the posterior)
- Rich set of variations and generalizations are possible