Lectures 15: Bootstrap II.

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

from Lecture 14: Maximum Likelihood parameter errors?

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

Taylor series:

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

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

Then

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

with

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

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 **b**’s is multivariate Normal, a very useful CLT-ish result!

from Lecture 14:

multivariate normal distribution

Multivariate Normal Distributions

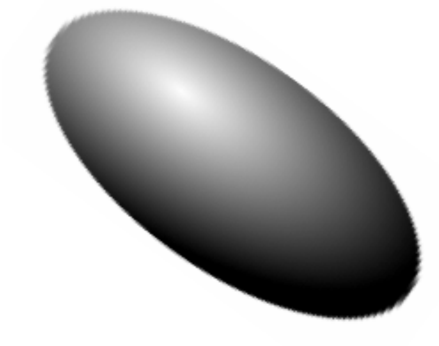
Generalizes Normal (Gaussian) to M-dimensions
Like 1-d Gaussian, completely defined by its mean and (co-)variance
Mean is a M-vector, covariance is a M x M matrix

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

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.

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

from Lecture 14:

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*

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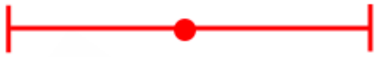

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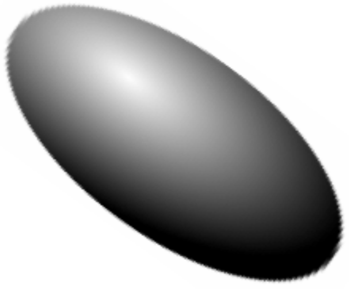

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$$1 = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

from Lecture 14:

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

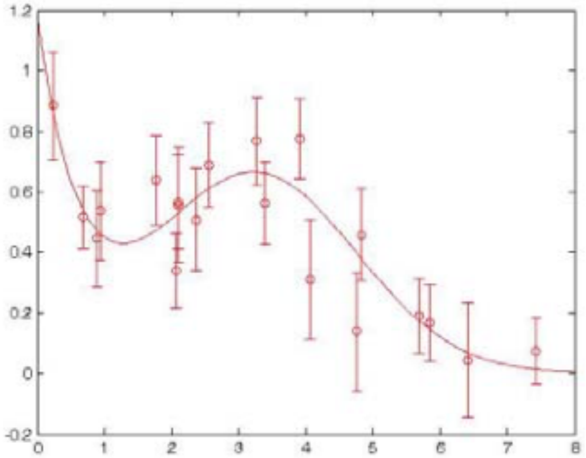
$$
\begin{aligned}
f \equiv f(\mathbf{b}) &= f(\mathbf{b}_0) + \nabla f \; \mathbf{b}_1 + \cdots \\
\langle f \rangle &\approx \langle f(\mathbf{b}_0) \rangle + \nabla f \;\cancel{\langle \mathbf{b}_1 \rangle} = f(\mathbf{b}_0) \\
\langle f^2 \rangle - \langle f \rangle^2 &\approx 2 f(\mathbf{b}_0)(\nabla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

from Lecture 14:

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

from Lecture 14:

Sampling the posterior histogram

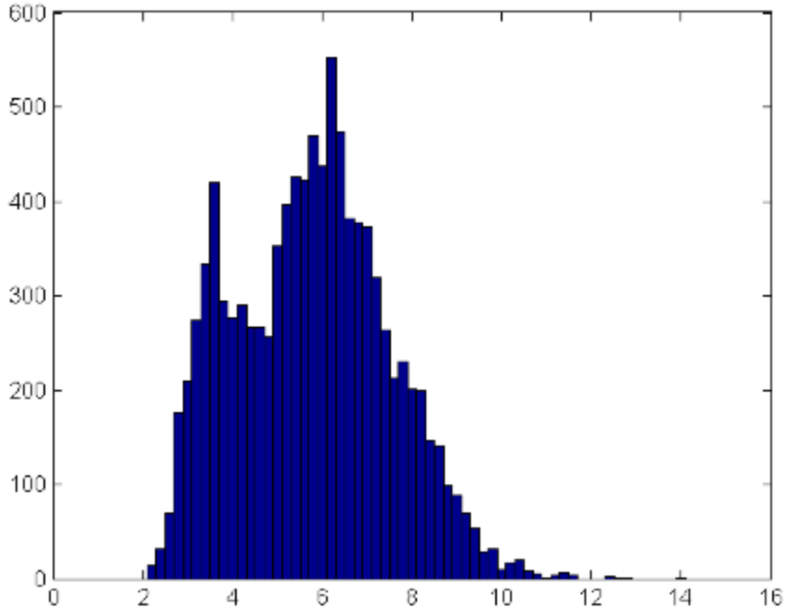
Method 2: Sample from the posterior distribution

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

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

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

3. Histogram

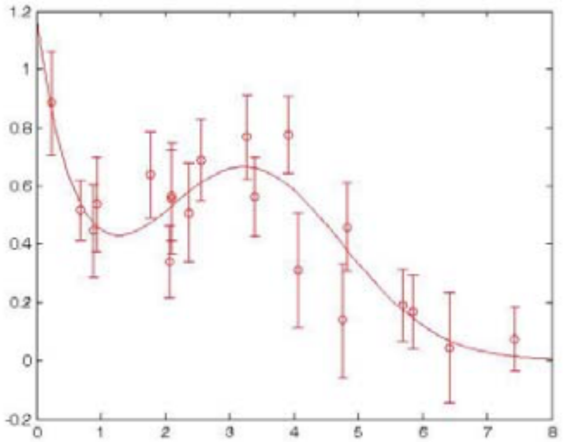


Note again that **b** is typically (close to) m.v. normal because of the CLT, but your (nonlinear) f may not, in general, be anything even close to normal!

from Lecture 14:

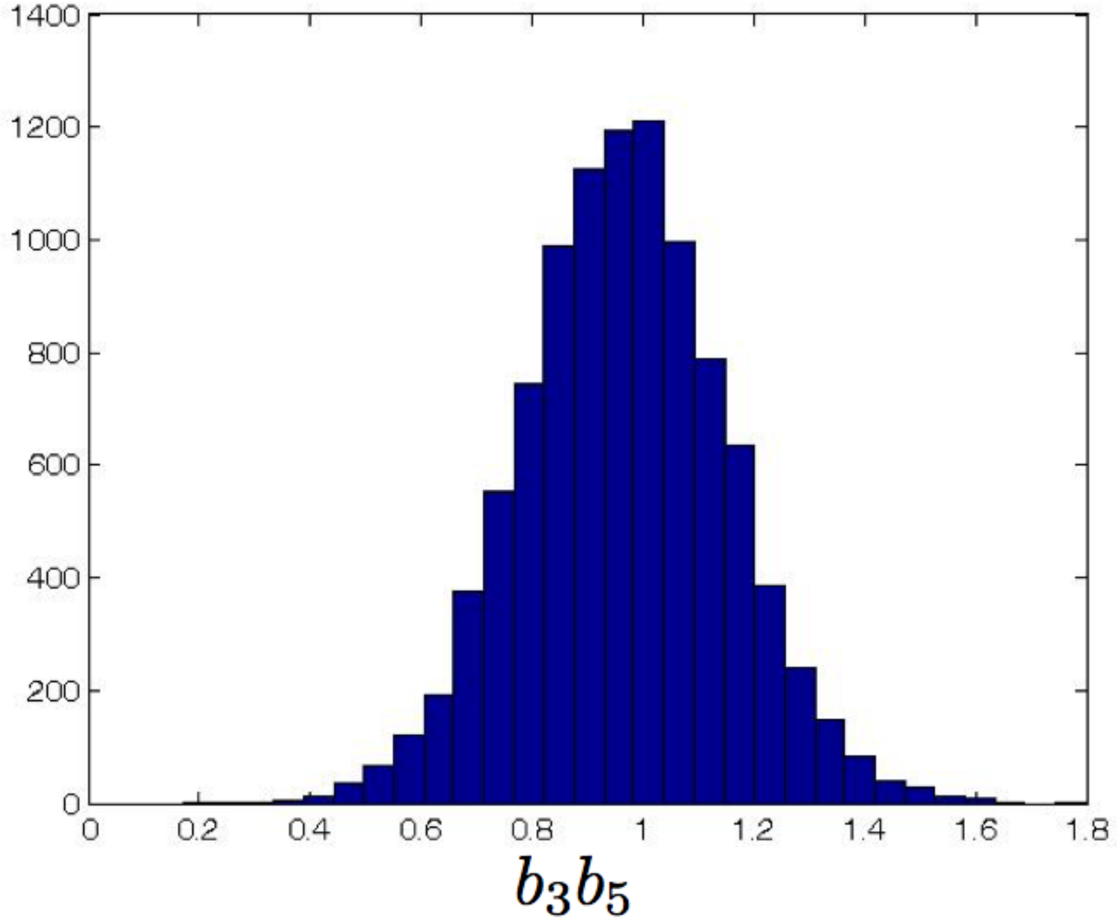
Sampling the posterior histogram

Our example:



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

```
std = 0.1833
```



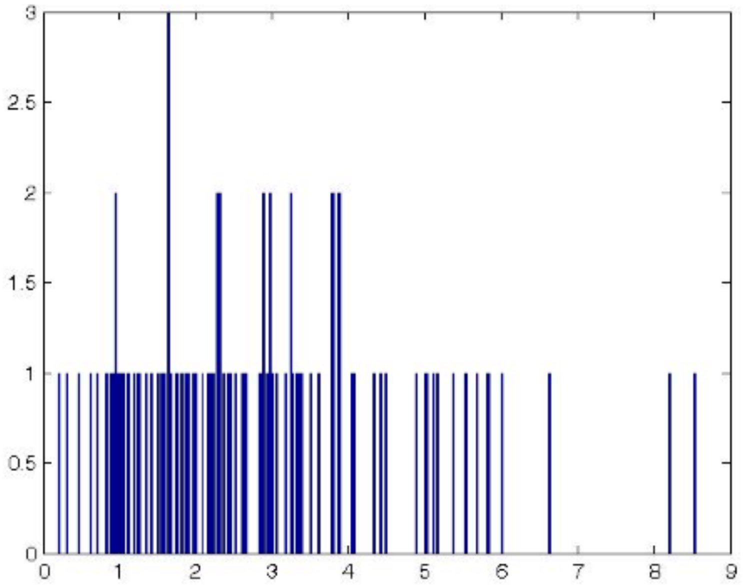
Does it matter that I use the full covar, not just the 2x2 piece for parameters 3 and 5?

from Lecture 14:

bootstrap sampling example 1

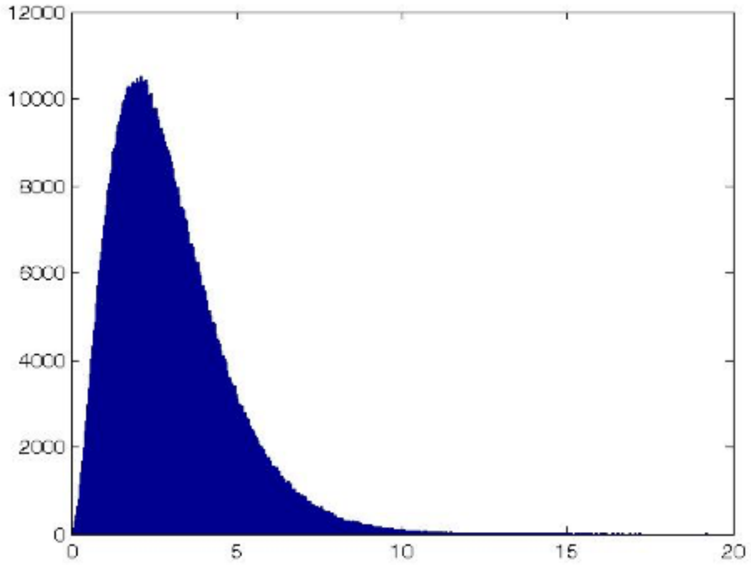
Let’s try a simple example where we can see the “hidden” side of things, too.

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
```

from Lecture 14:

bootstrap sampling example 1

Gamma distribution:

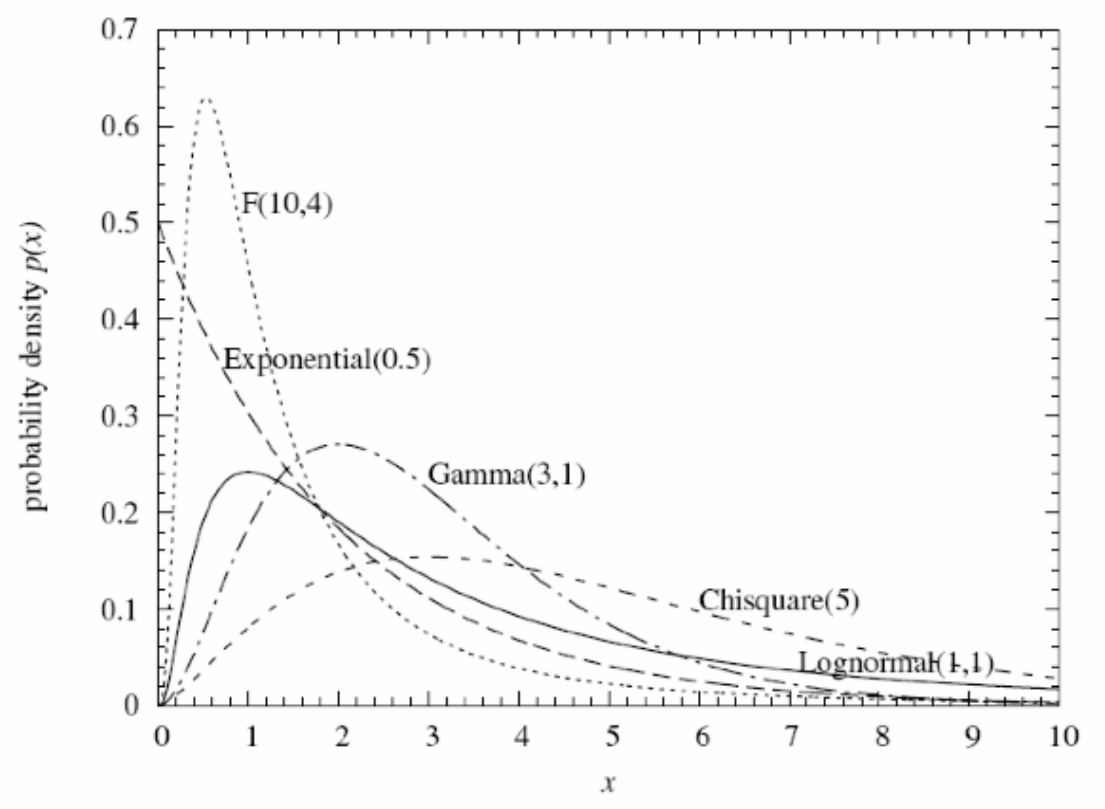
$$x \sim \mathrm{Gamma}(\alpha, \beta), \qquad \alpha > 0,\ \beta > 0$$

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

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

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

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



from Lecture 14:

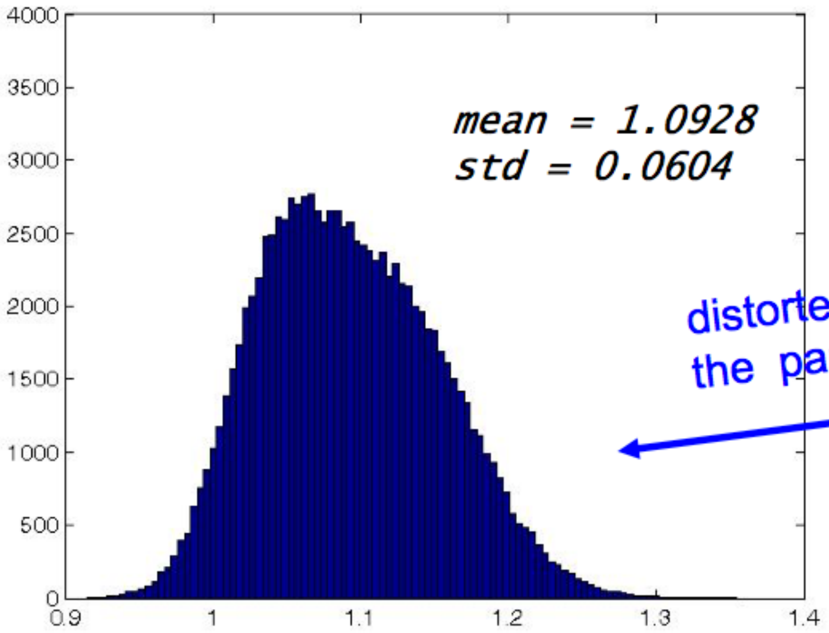
bootstrap sampling example 1

To estimate the accuracy of our statistic, we bootstrap

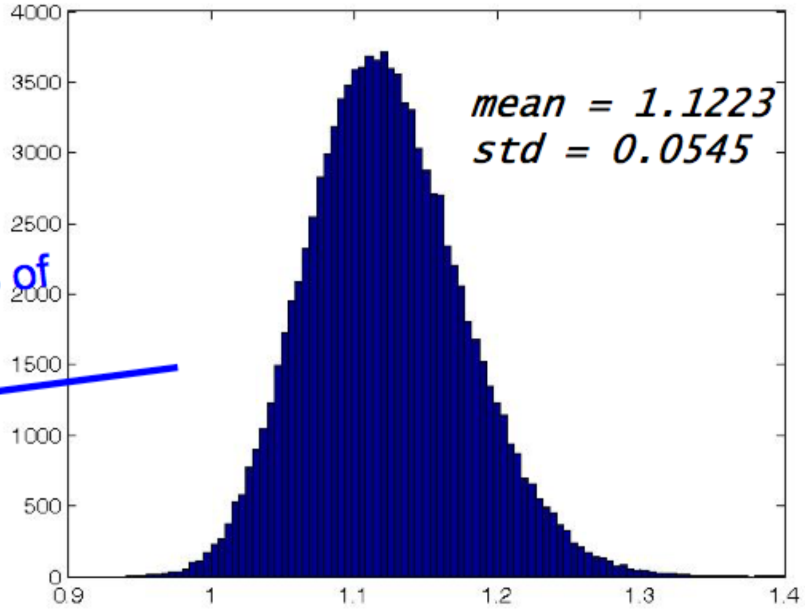
```
ndata = 100;
nboot = 100000;
vals = zeros(nboot,1);
for j=1:nboot,
    choose = randsample(ndata,ndata,true);
    vals(j) = mean(sample(choose))
             /median(sample(choose));
end
hist(vals,100)
```

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:

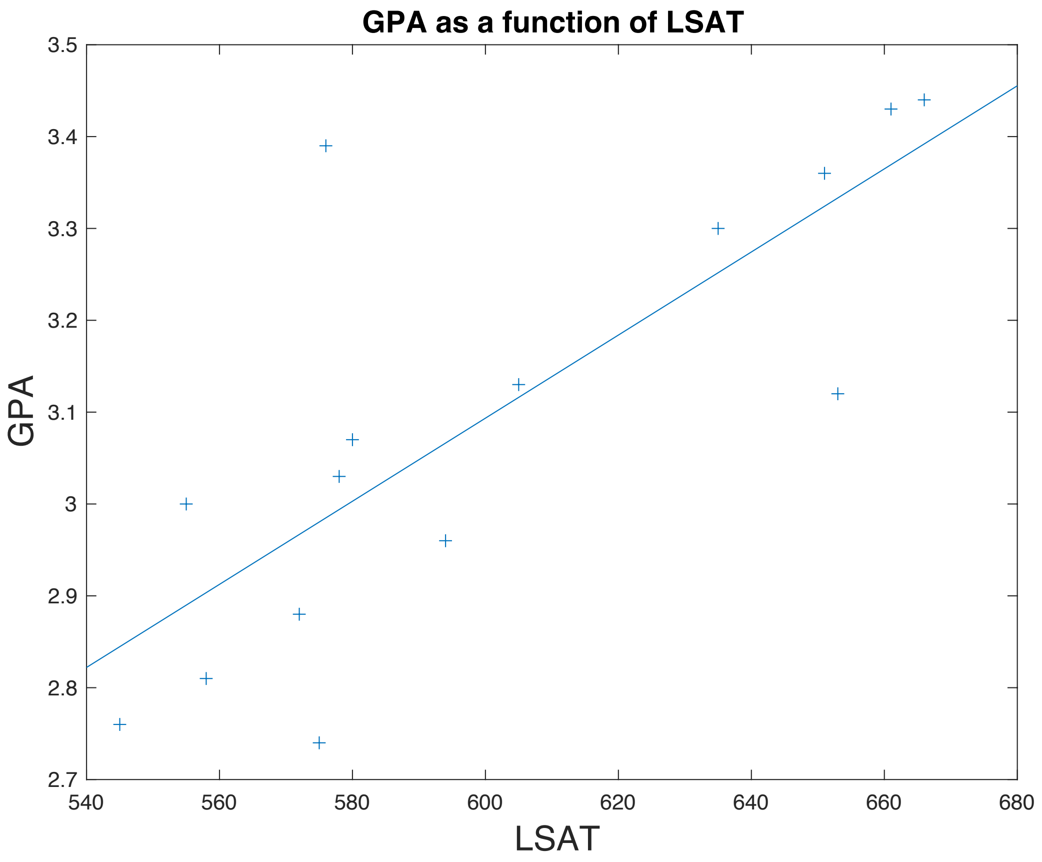
The mean of resamplings does not improve the original estimate! (Same data!)

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

bootstrap sampling example 2

```
%%
% The bootstrap procedure involves choosing random
% samples with replacement from a data set and analyzing each sample
% the same way. Sampling with replacement means that each observation
% is selected separately at random from the original dataset. So a particular
% data point from the original data set could appear multiple times
% in a given bootstrap sample. The number of elements in each bootstrap
% sample equals the number of elements in the original data set. The
% range of sample estimates you obtain enables you to establish the
% uncertainty of the quantity you are estimating.

%%
% This example from Efron and Tibshirani compares Law School Admission Test
% (LSAT) scores and subsequent law school grade point average (GPA) for a
% sample of 15 law schools.
load lawdata
plot(lsat,gpa,'+')
lsline
```

```
            LSAT                   GPA

   1.0e+02 *              1.0e+02 *
     5.760000000000000   0.033900000000000
     6.350000000000000   0.033000000000000
     5.580000000000000   0.028100000000000
     5.780000000000000   0.030300000000000
     6.660000000000000   0.034400000000000
     5.800000000000000   0.030700000000000
     5.550000000000000   0.030000000000000
     6.610000000000000   0.034300000000000
     6.510000000000000   0.033600000000000
     6.050000000000000   0.031300000000000
     6.530000000000000   0.031200000000000
     5.750000000000000   0.027400000000000
     5.450000000000000   0.027600000000000
     5.720000000000000   0.028800000000000
     5.940000000000000   0.029600000000000
```



```
%%
% The least-squares fit line indicates that higher LSAT scores go with
% higher law school GPAs. But how certain is this conclusion? The plot
% provides some intuition, but nothing quantitative.
```

Correlation Coefficient

The correlation coefficient of two random variables is a measure of their linear dependence. If each variable has *N* scalar observations, then the Pearson correlation coefficient is defined as

$$\rho(A,B) = \frac{1}{N-1}\sum_{i=1}^{N}\left(\frac{\overline{A_i - \mu_A}}{\sigma_A}\right)\left(\frac{B_i - \mu_B}{\sigma_B}\right),$$

where μ_A and σ_A are the mean and standard deviation of *A*, respectively, and μ_B and σ_B are the mean and standard deviation of *B*. Alternatively, you can define the correlation coefficient in terms of the covariance of *A* and *B*:

$$\rho(A,B) = \frac{\operatorname{cov}(A,B)}{\sigma_A \sigma_B}.$$

The correlation coefficient *matrix* of two random variables is the matrix of correlation coefficients for each pairwise variable combination,

$$R = \begin{pmatrix} \rho(A,A) & \rho(A,B) \\ \rho(B,A) & \rho(B,B) \end{pmatrix}.$$

Since *A* and *B* are always directly correlated to themselves, the diagonal entries are just 1, that is,

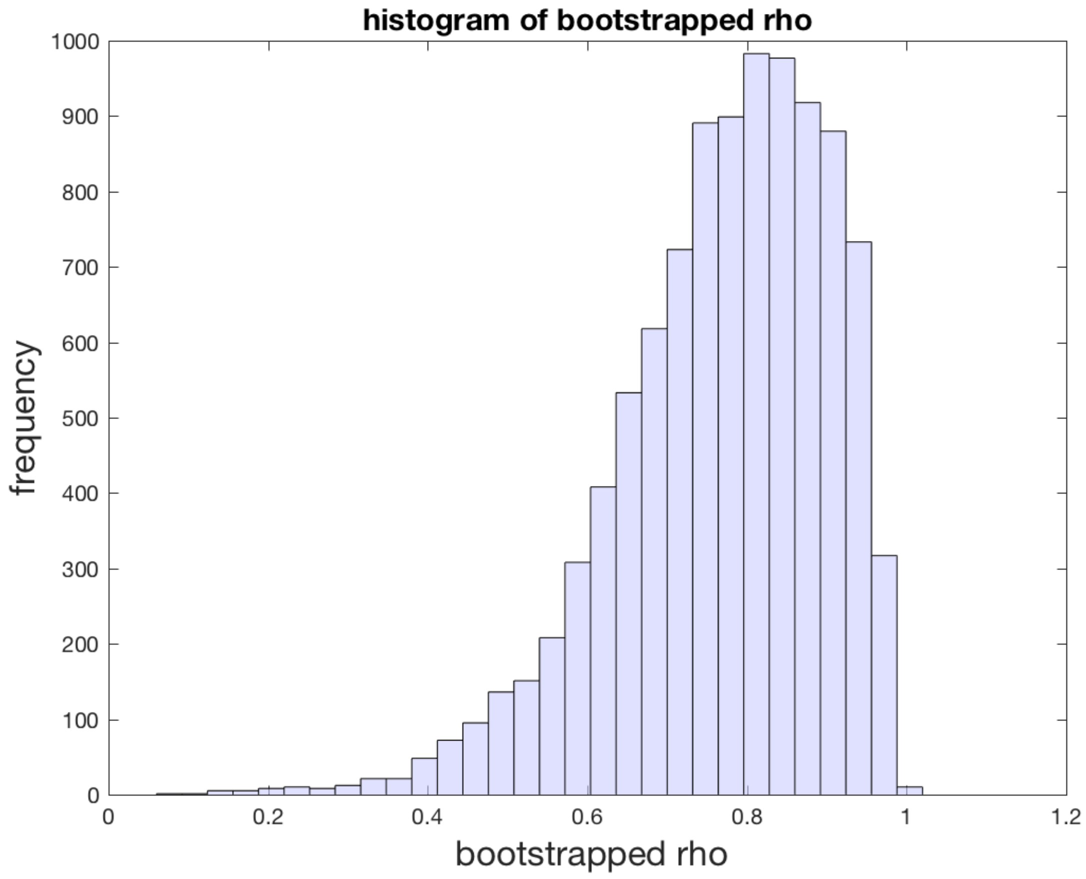
$$R = \begin{pmatrix} 1 & \rho(A,B) \\ \rho(B,A) & 1 \end{pmatrix}.$$

bootstrap sampling   example 2

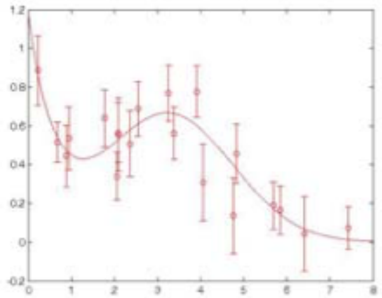
```
%%
% The bootstrap procedure involves choosing random
% samples with replacement from a data set and analyzing each sample
% the same way. Sampling with replacement means that each observation
% is selected separately at random from the original dataset. So a particular
% data point from the original data set could appear multiple times
% in a given bootstrap sample. The number of elements in each bootstrap
% sample equals the number of elements in the original data set. The
% range of sample estimates you obtain enables you to establish the
% uncertainty of the quantity you are estimating.

%%
% This example from Efron and Tibshirani compares Law School Admission Test
% (LSAT) scores and subsequent law school grade point average (GPA) for a
% sample of 15 law schools.
load lawdata
display([lsat gpa])
figure(1000)
hold on
box on
plot(lsat,gpa,'+')
lsline


%%
% Using the |bootstrp| function you can resample the |lsat| and |gpa|
% vectors as many times as you like and consider the variation in the
% resulting correlation coefficients.
rng default  % For reproducibility
rhos10000 = bootstrp(10000,'corr',lsat,gpa);

%%
% This resamples the |lsat| and |gpa| vectors 10000 times and computes the
% |corr| function on each sample. You can then plot the result in a
% histogram.
```

rho =
0.776374491289407

ci =
0.452682100239149
0.961268268870509



bootstrap sampling   example 3

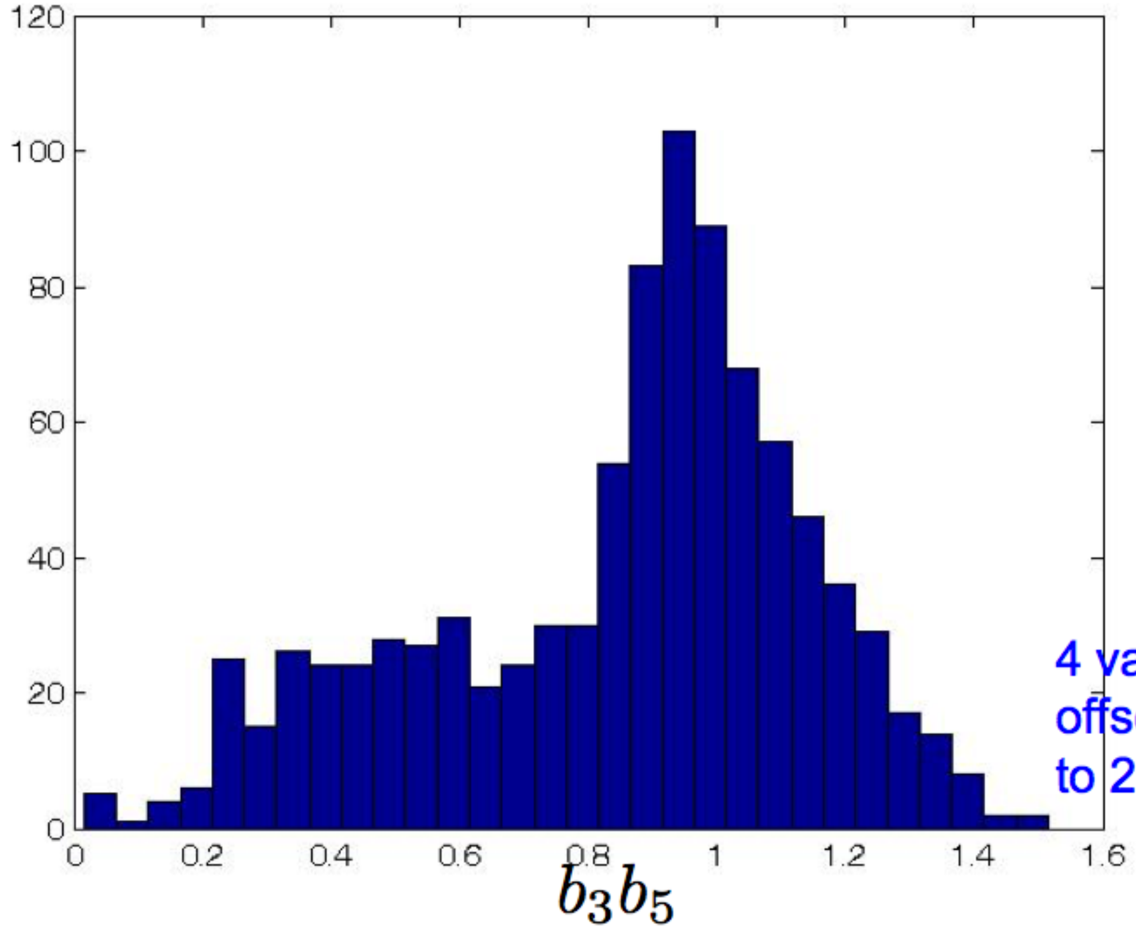


```
ndata = 20;
nboot = 1000;
vals = zeros(nboot,1);
ymodel = @(x,b) b(1)*exp(-b(2)*x)+b(3)*exp(-(1/2)*((x-b(4))/b(5)).^2);
for j=1:nboot,
   samp = randsample(ndata,ndata,true);
   xx = x(samp);
   yy = y(samp);
   ssig = sig(samp);
   chisqfun = @(b) sum(((ymodel(xx,b)-yy)./ssig).^2);
   bguess = [1 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
```

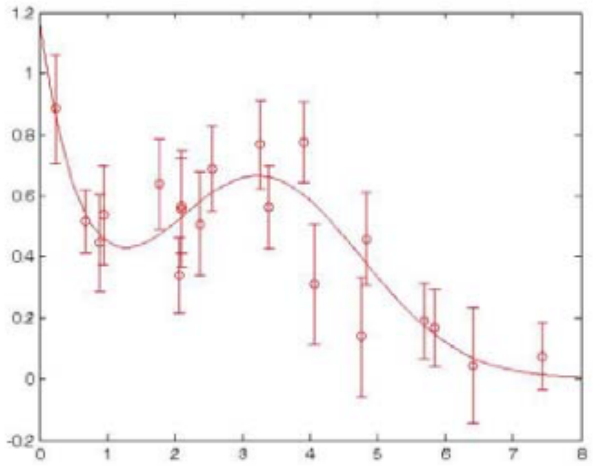


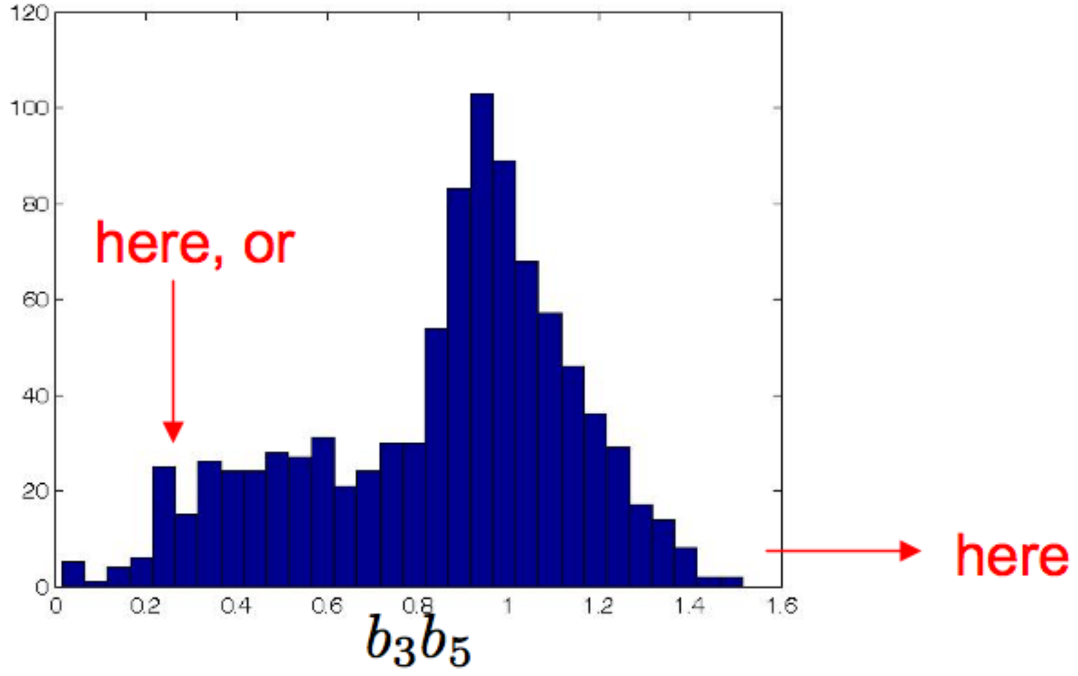
4 values offscale (up to 27!)

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

bootstrap sampling   example 3

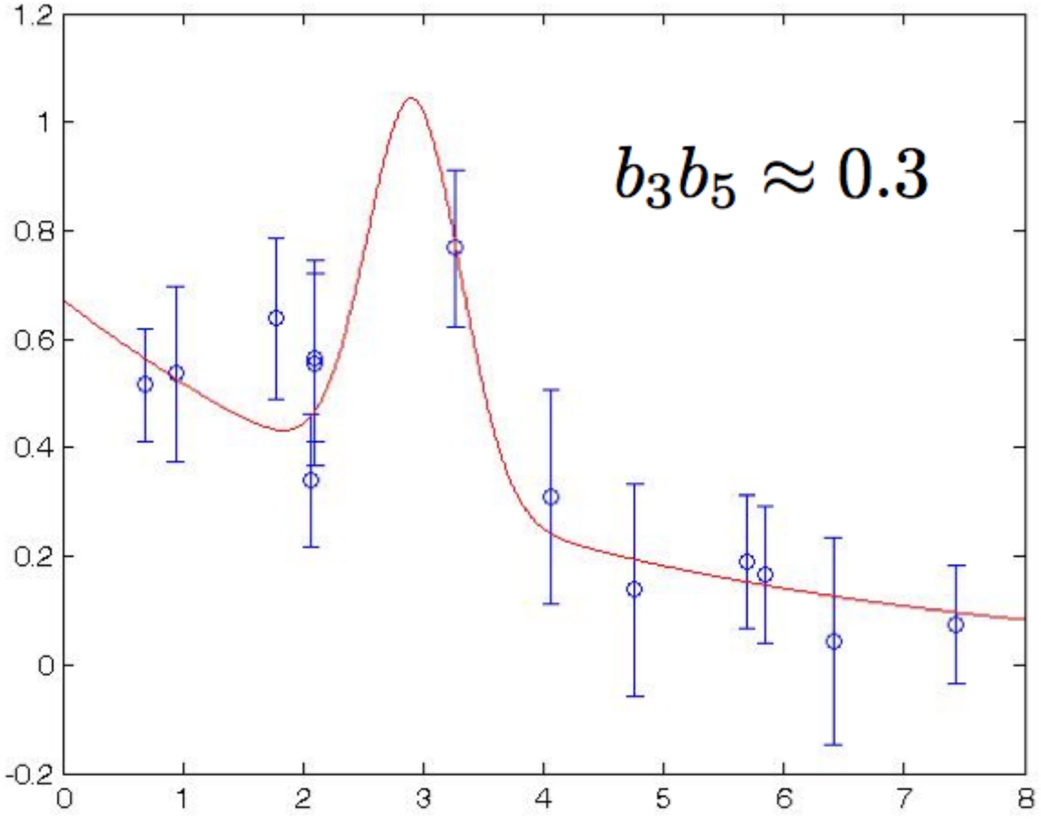
Can you guess what the extreme bootstrap cases look like, compared to the full data?



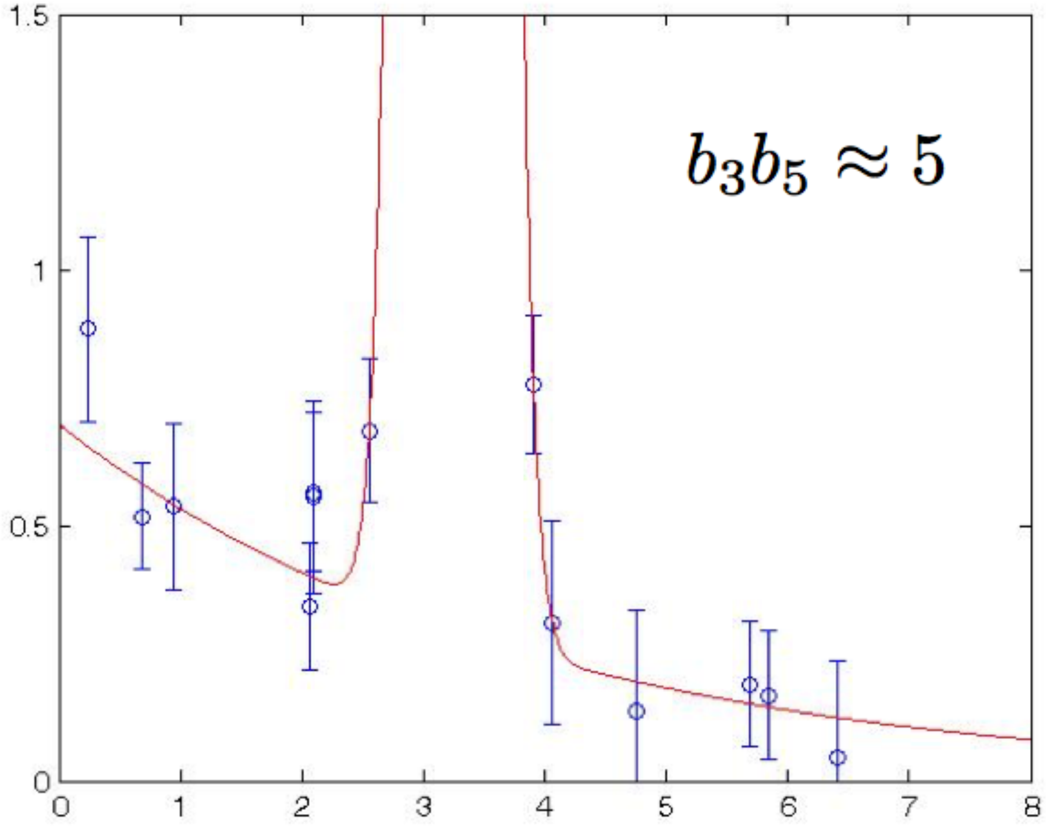


here, or

here



$b_3b_5 \approx 0.3$

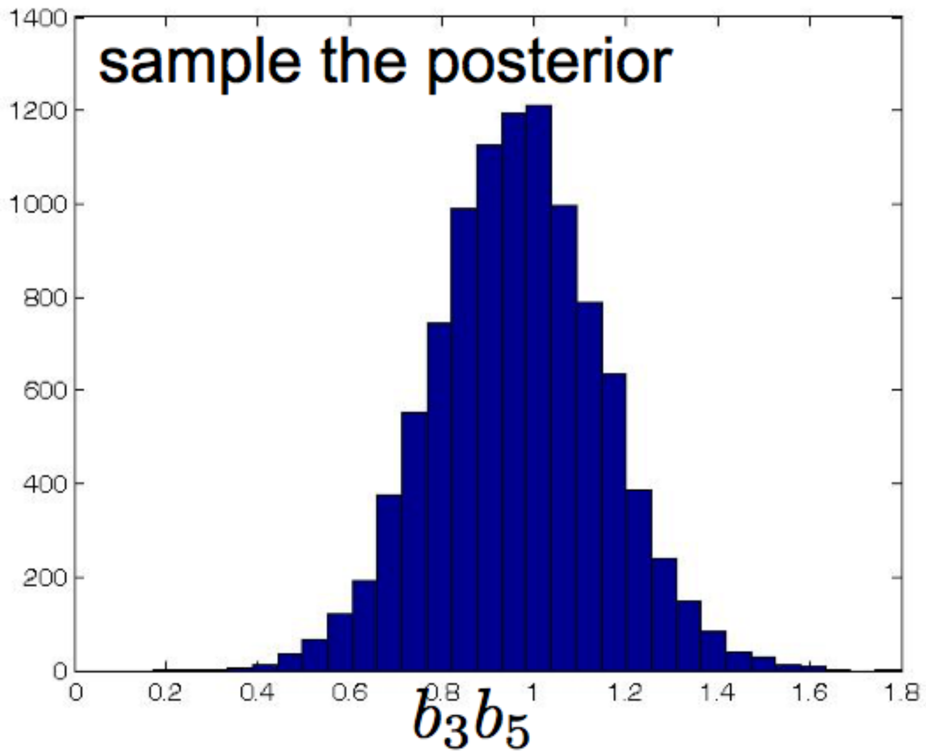


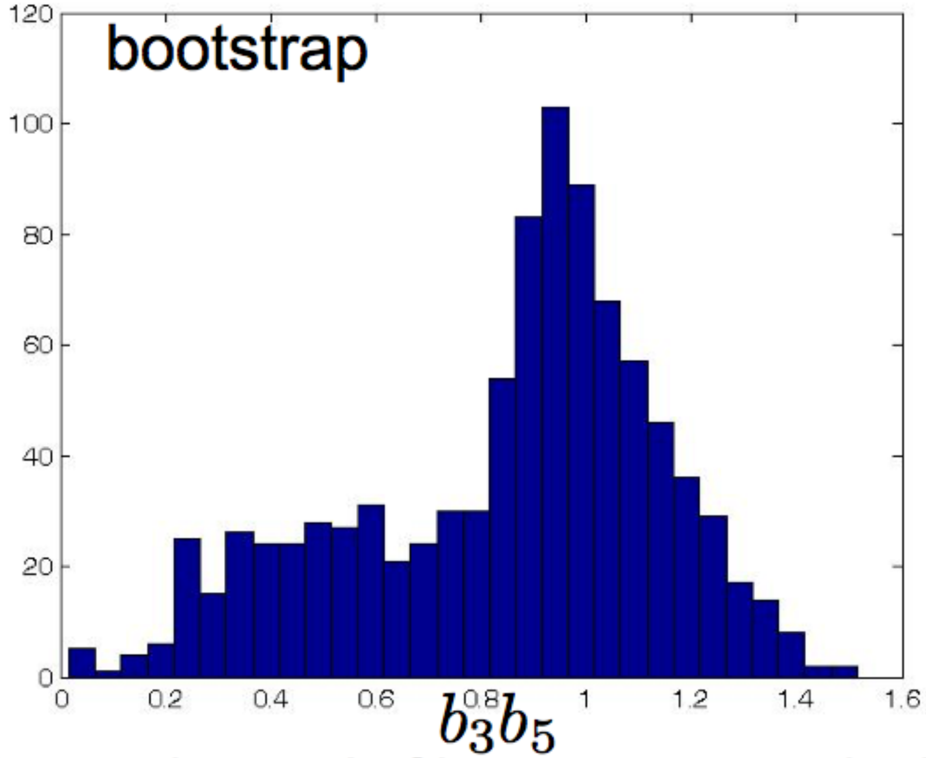
$b_3b_5 \approx 5$

frequentist is concerned about error estimate

bootstrap sampling example 3

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

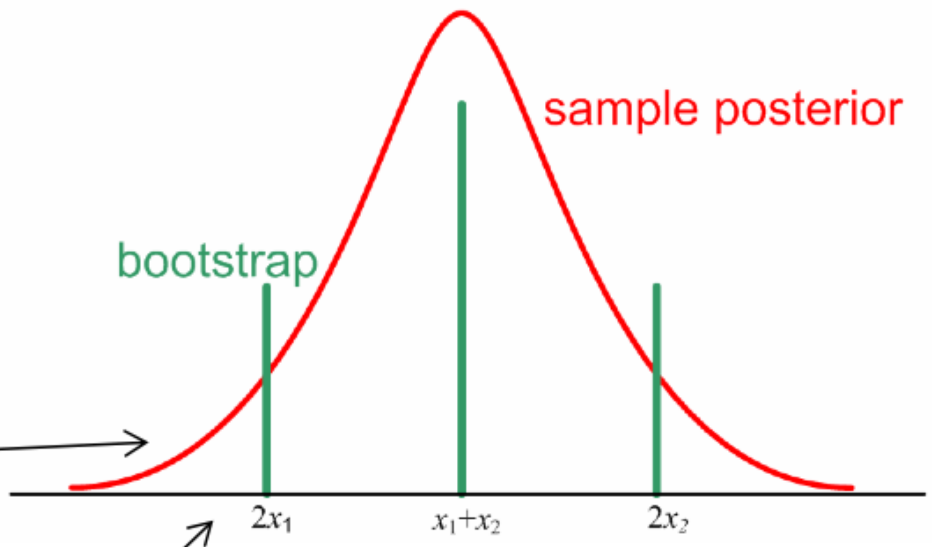
Note that sampling the posterior "honors" the stated measurement errors. Bootstrap doesn't. That can be good!

Suppose (very toy example) the "statistic" is

$$s = x_1 + x_2$$

then the posterior probability is

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

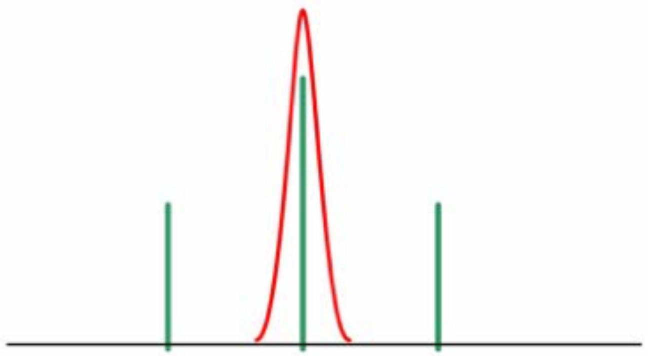


Note that this depends on the σ's!

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