ASK THE EXPERT How Do I Use the Bootstrap Method in SAS[®]?



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THE ESSENTIAL GUIDE TO BOOTSTRAPPING IN SAS®



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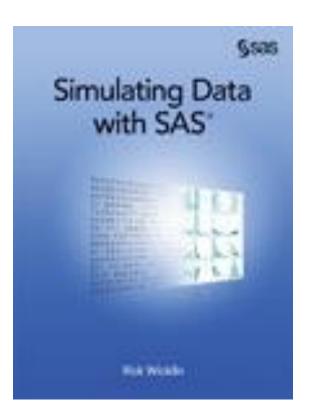
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The bootstrap method (Efron, 1979) is one of the most important innovations in statistics in the 20th century. This talk introduces the bootstrap method and discusses when it should be used. This example-driven presentation includes best practices for implementing bootstrap programs efficiently in SAS. An inefficient bootstrap program can take hours to run, whereas a well-written program can give you an answer in an instant. If you want to learn more about the bootstrap method and prefer "instants" to "hours," this talk is for you!



- The bootstrap method (Efron, 1979) is one of the most important innovations in statistics in the 20th century
- This talk includes tips for implementing bootstrap methods efficiently in SAS
- Some tips are from Simulating Data with SAS (Wicklin 2013, Chap 15)
- Others from The DO Loop blog: Search the internet for Essential Guide Bootstrapping SAS





- What is the bootstrap method?
- How to bootstrap a univariate statistic in SAS?
- Efficiency and details of the implementation
- How to bootstrap regression estimates in SAS?
- SAS procedures that support built-in bootstrapping



What is the bootstrap method?



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- Main assumption: Data are a random sample of size N from a population distribution
- A statistic is a sample estimate of a population parameter
- A different random sample gives a different estimate
- The distribution of a statistic over **all** possible samples of size *N* is the *sampling distribution*
- The bootstrap method is an *inferential* technique that estimates the sampling distribution by using **some** samples of size N
 - Standard error is the standard deviation of the sampling distribution
 - Confidence intervals (CIs) correspond to quantiles such as 5th to 95th



Use the bootstrap method when

- You want to estimate the precision of a point estimate
 - Standard error or confidence interval
- The sampling distribution is not known or is known only asymptotically (large N)
 - The sample size is small
 - The sample distribution is far from normal



ESSENTIAL BOOTSTRAPPING THE EMPIRICAL DISTRIBUTION REPLACES THE POPULATION

Why is it called the "bootstrap"?

- If you fit a *model* the data, you can use simulation to create random samples from the parametric model. Sometimes called *parametric bootstrap*, but that is a misnomer.
- The bootstrap replaces the unknown cumulative distribution function (CDF) with the known empirical CDF
- The bootstrap method is a *nonparametric* method, which "simulates" from the empirical CDF
 - You sample with replacement to obtain one of the N^N re-samples
 - The method approximates the population distribution by using only ONE sample!

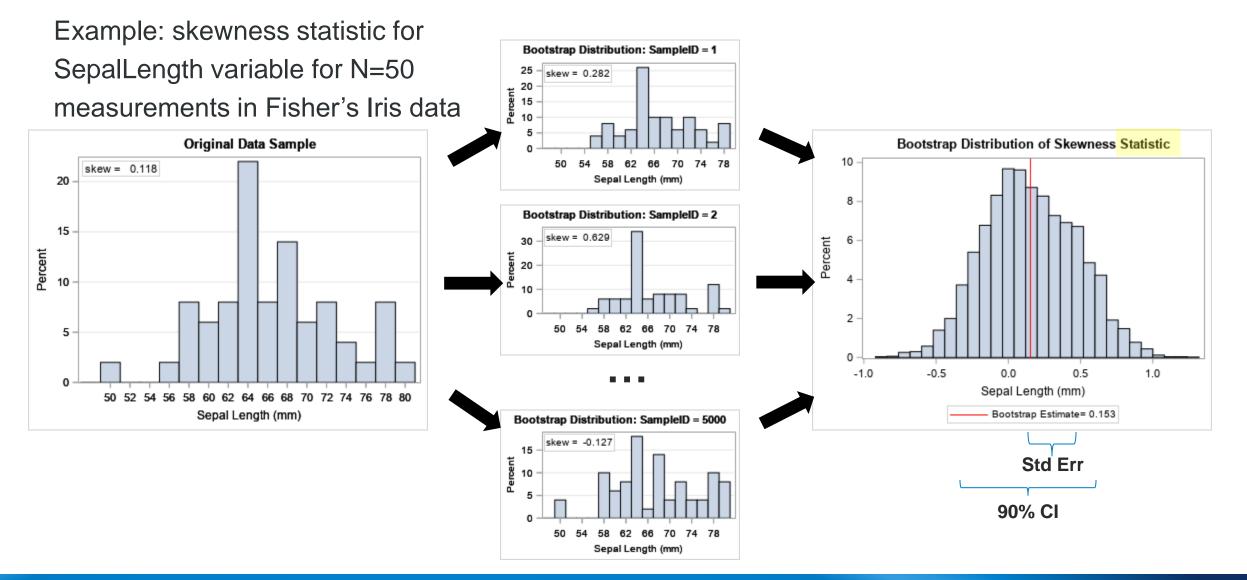


ESSENTIAL BOOTSTRAPPING THE BOOTSTRAP METHOD

- Repeat *B* times (*B* large):
 - Draw N observations with replacement from the data. This is a *bootstrap* sample, also called the *resample*.
- Compute the statistic on each bootstrap sample.
- Union of statistics is the *bootstrap distribution* (BD), which approximates the sampling distribution
 - Mean of BD is the bootstrap estimate
 - Standard deviation of BD is the bootstrap standard error
 - Percentiles of BD estimate a CI



THE BOOTSTRAP METHOD IN PICTURES





- Assumes the original sample is representative of the population
- Never uses values that are not in original sample (175 cm male)
- Rare events either ignored (if not in sample) or have undue influence (if in sample)
- Not useful for some statistics
 - Extreme quantiles, maximum, and minimum
- Bootstrap distribution might be non-smooth
 - Median of small sample
 - Can use variation called *smooth bootstrap*



How to bootstrap a univariate statistic in SAS?



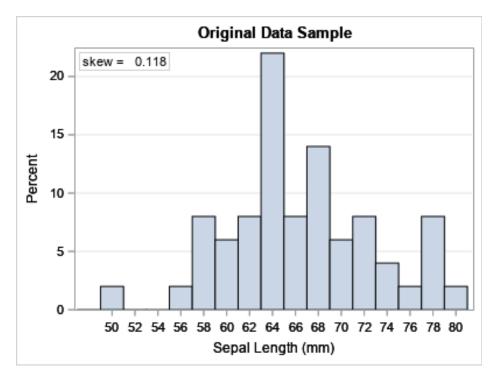
ESSENTIAL BOOTSTRAPPING HOW TO BOOTSTRAP IN SAS

- 1. Compute the statistic for the original data (the Sample data set)
- 2. Resample (with replacement) *B* times to form *B* bootstrap samples
 - Put all samples into ONE data set: the **BootSamp** data set
 - · How you resample might depend on the analysis
- 3. Compute the statistic on each bootstrap sample
 - BY-group processing
 - Put results in the BootStats data set
 - Avoid macro loops
- 4. Use bootstrap distribution to estimate standard error, confidence intervals, and evidence to reject null hypothesis



COMPUTE THE STATISTIC FOR THE ORIGINAL DATA

- Data: SepalLength variable in Fisher's Iris data, N=50 observations
- Statistic: Skewness
- **Goals:** Standard error, 90% CI for skewness, H_0 : Skewness = 0



Petal width /* Sample size N = 50 */ data Sample(keep=x); set Sashelp.Iris(rename=(SepalLength=x)); where Species="Virginica"; run; compute statistic on data */ /* proc means data=Sample nolabels Skew; var x; Skewness run; 0.1180151

Peta

ength



Sepal length

Sepal width



WHAT IS THE DISTRIBUTION OF THE SKEWNESS STATISTIC?

The sample skewness is 0.118. Can we infer that the skewness of the population is different from 0?

The sampling distribution of the skewness statistic is not known:→ Use the bootstrap!



GENERATE RESAMPLES: SAMPLE WITH REPLACEMENT

Three main techniques for sampling with replacement

- 1. DATA step: use the POINT= option
- 2. PROC SURVEYSELECT: use the METHOD=URS option to sample with replacement
 - 3. PROC IML: use the SAMPLE function



PROC SURVEYSELECT: SAMPLE WITH REPLACEMENT

Advantages of PROC SURVEYSELECT

- Requires no programming.
- About as fast as the DATA step
- Supports many sampling schemes
- Optional: create a frequency variable, which decreases the number of rows in the bootstrap samples



GENERATE MANY BOOTSTRAP SAMPLES

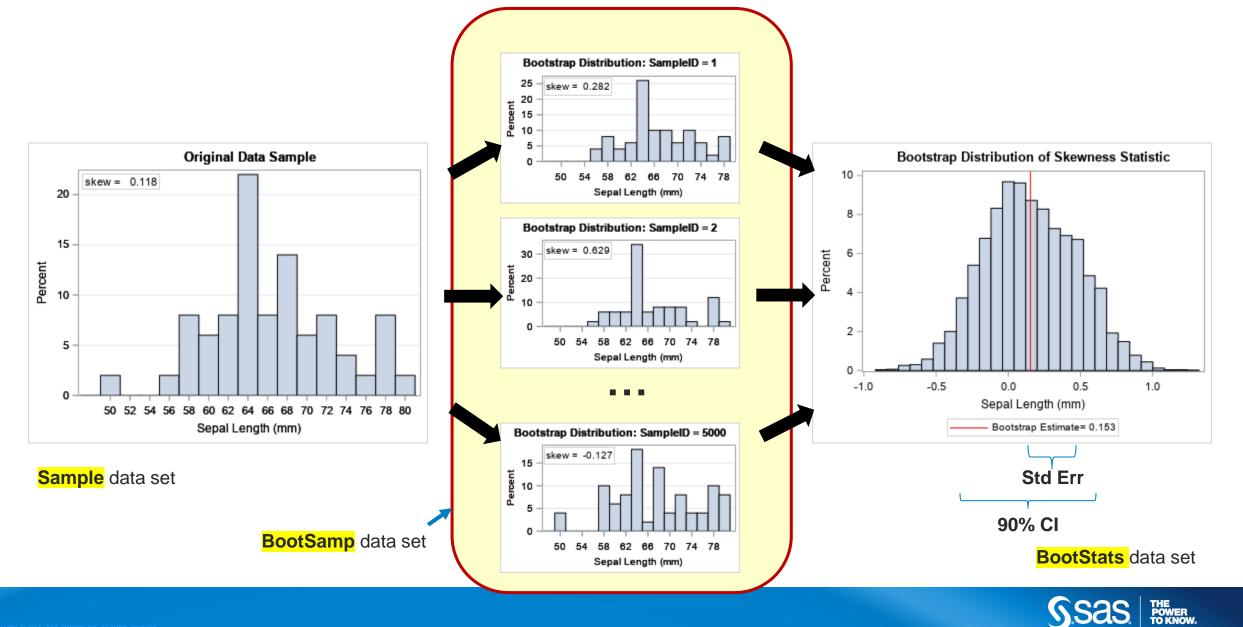
run;

When you use the OUTHITS option, the BootSamp data set contains N x NumSamples rows:

- N observations for SampleID = 1
- N observations for SampleID = 2
- And so on



THE BOOTSTRAP METHOD IN PICTURES



COMPUTE THE STATISTIC FOR EACH BOOTSTRAP SAMPLE

/*	3.	Compu	ite 1	the	stati	stic	for	each
		boots	strap	o sa	ample	*/		
pro	bc :	means	data	a= <mark>Bc</mark>	otSam	p NOI	PRIN	c ;

by SampleID;

ESSENTIAL

BOOTSTRAPPING

var x;

output out=BootStats skew=Skewness; /* bootstrap distribution */

run;

1	1	0.28206		
2	2	0.62902		
3	3	-0.08908		
4	4	0.59312		
5	5	0.55024		

Obs SampleID Skewness

~495~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∕~-0:20187
4995	4995	-0.21925
4996	4996	-0.39973
4997	4997	0.36382
4998	4998	-0.20712
4999	4999	0.23525
5000	5000	-0.12704



proc m

ESTIMATE STANDARD ERROR AND CONFIDENCE INTERVAL

proc means data=BootStats nolabels N Mean StdDev P5 P95;

var Skewness;

run;

Analysis Variable : Skewness					
Ν	Mean	Std Dev	5th Pctl	95th Pctl	
5000	0.1534985	0.3206183	-0.3482734	0.6766532	

Bootstrap estimates:

- Skewness = 0.153 (compare with 0.118 for sample)
- Standard error = 0.321
- 90% CI = [-0.348, 0.677] \rightarrow Do not reject H_0 . Assuming skewness = 0 is consistent with the data.



ESSENTIAL BOOTSTRAPPING VISUALIZE THE SAMPLING DISTRIBUTION

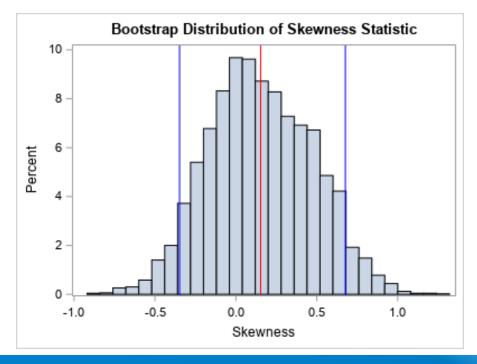
title "Bootstrap Distribution of Skewness Statistic";
proc sgplot data=BootStats;

histogram Skewness;

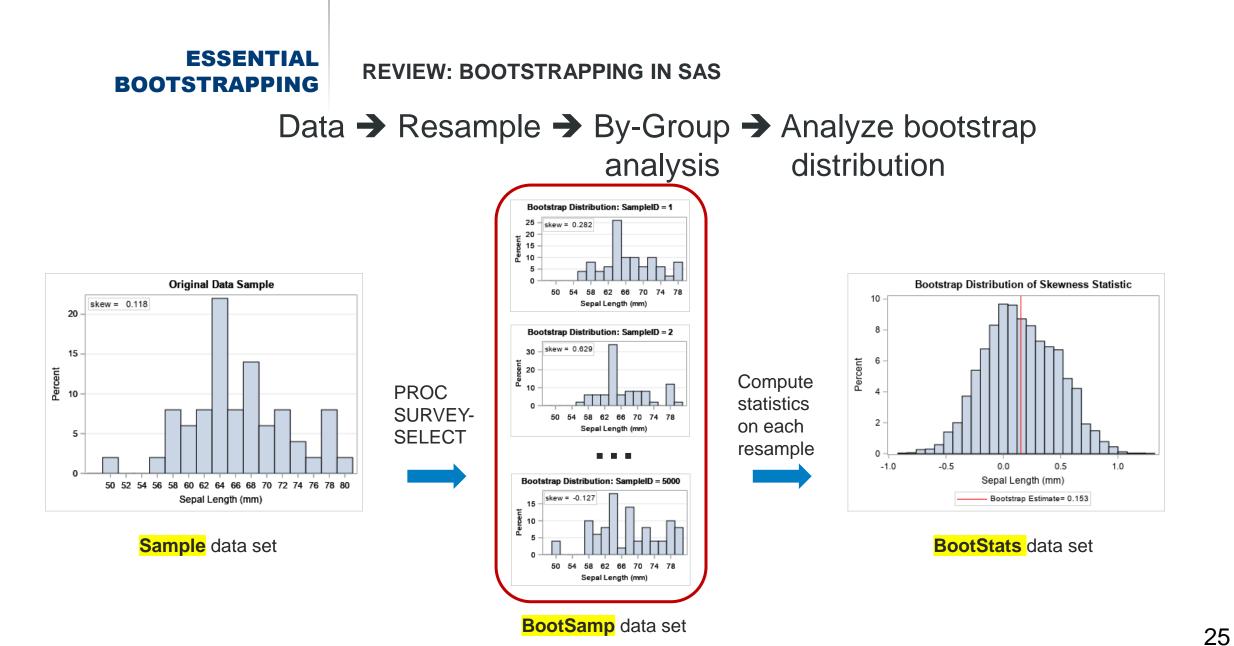
refline 0.153 / axis=x lineattrs=(color=red);

refline -0.348 0.677 / axis=x lineattrs=(color=blue);

run;









Efficiency and details of the implementation



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Every program in this presentation runs in less than 1 second!

Observe these SAS **efficiency** programming tips:

- ✓ 1. Put all resamples in one data set
 - 2. Use BY-group analysis to analyze all resamples
 - 3. Suppress output during BY-group analysis
 - 4. Avoid writing macro loops
 - 5. To get smaller data set, omit the OUTHITS option in PROC SURVEYSELECT



USE THE BY STATEMENT TO ANALYZE EACH SAMPLE

/* Use BY-group analysis to analyze resamples.
 Suppress output during BY-group analysis */
proc means data=BootSamp NOPRINT;

BY SampleID;

var x;

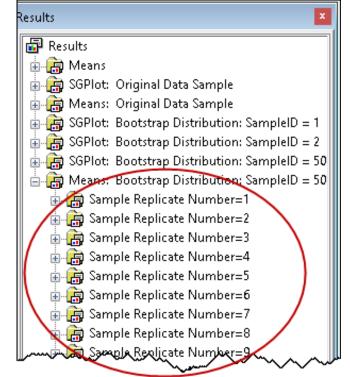
output out=BootStats skew=Skewness;

run;

Obs	SampleID	Skewness
1	1	0.28206
2	2	0.62902
3	3	-0.08908
4	4	0.59312
5	5	0.55024
ma manan		

SUPPRESS OUTPUT DURING BY-GROUP ANALYSIS

- SAS procedures can create a LOT of output!
- For simple computations, it takes longer to print 5,000 tables than it does to compute them
- Suppress display of intermediate graphs and tables
 - About 50 procedures support the NOPRINT option
 - Use ODS to suppress output in other procedures
- Any unnecessary output will slow the bootstrap analysis
 - NOTES can fill up the SAS Log
 - ODS Results window makes a node in a tree for every BY group





ESSENTIAL BOOTSTRAPPING SAS MACROS FOR CONTROLLING OUTPUT

```
%macro ODSOff(); /* call prior to BY-group processing */
   ods graphics off;
   ods exclude all; /* all open destinations */
   ods noresults; /* no updates to tree view */
   options nonotes; /* sometimes useful */
%mend;
```

```
%macro ODSOn();  /* call after BY-group processing */
    ods graphics on;
    ods exclude none;
    ods results;
    options notes;
%mend;
```

ESSENTIAL BOOTSTRAPPING TEMPLATE FOR BOOTSTRAP

```
proc surveyselect data=Sample NOPRINT seed=1
    method=urs samprate=1 reps=&NumSamples outhits /* Optional */
    out=BootSamp(rename=(Replicate=SampleID));
run;
```

```
%ODSOff /* or use NOPRINT option in procedure */
proc WhatEver data=BootSamp;
    by SampleID; /* Optional: FREQ NumberHits; */
    /* generate statistic for each resample */
    output out=BootStats ...;
run;
%ODSOn
/* use bootstrap distribution of statistic to answer
    questions about CIs, hypothesis tests, and more */
proc means data=BootStats; /* or PROC UNIVARIATE */
    var Stats;
```

```
run;
```



ESSENTIAL AVOID WR

AVOID WRITING MACRO LOOPS

Do NOT write a SAS macro that creates and analyzes one resample at a time!

```
%macro Bootstrap(...);
%do i = 1 %to 5000;
   data a; ...; run;
   proc means data=a;
     output out=out skew=Skew;
   run;
   proc append base=out;
   run;
%end;
%mend;
```

Novikov (2003) compares times for his application: **Macro** > 7 minutes **BY group** < 5 secs

→ 100x faster!



- Each PROC or DATA step call requires overhead
 - Start procedure, parse statements, load data,...
 - [Do computation]
 - Close data, exit procedure
- The macro code repeats these steps 5,000 times; the overhead costs large relative to the computation
- In contrast, BY group processing uses one call to generate the resamples and one call to analyze the statistics; overhead costs small relative to the computation



ESSENTIAL BOOTSTRAPPING THE OUTHITS OPTION IN PROC SURVEYSELECT

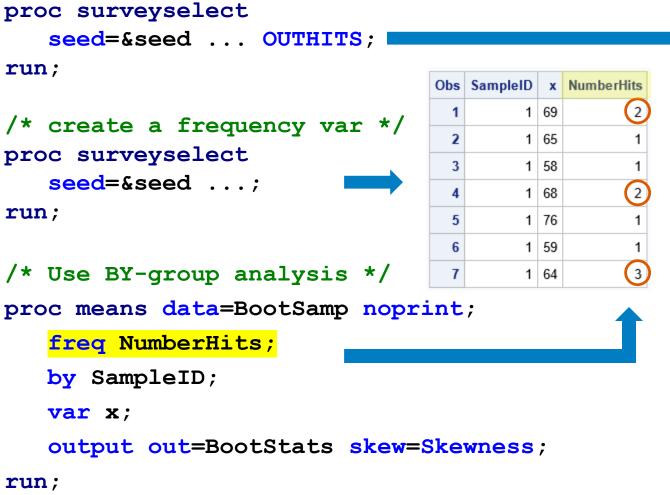
- The bootstrap method samples *N* observations *with replacement* from the data
- The average bootstrap sample contains 63.2% of the observations
 - Example: Data are {1,2,3,4,5,6,7,8,9,10}. A possible bootstrap sample is {1,2,2,2,5,5,6,7,8,8}, which contains 60% of values.
- If the analysis procedure supports a FREQ statement:
 - > Omit the **OUTHITS** option to get a BootSamp data set that has 37% fewer rows

≻ Add

FREQ NumberHits;
to the analysis procedure



OMIT THE OUTHITS OPTION (CONTINUED)



/* OUTHITS ==> suppress frequency var */

Obs	SampleID	x	
1	1	69]
2	1	69	ſ
3	1	65	
4	1	58	
5	1	68	l
6	1	68	ſ
7	1	76	
8	1	59	
9	1	64	1
10	1	64	╞
11	1	64	



ESSENTIAL BOOTSTRAPPING DETAILS OF SAS IMPLEMENTATION

- 1. Results depend on the random number stream
- 2. How to get a bootstrap p-value for a hypothesis test
- 3. Bootstrap in the SAS/IML language
- 4. Alternatives to percentile confidence intervals



DEPENDENCE ON THE RANDOM NUMBER STREAM

- You perform a bootstrap analysis, not THE bootstrap analysis
- The resamples depend on the random number stream, which is set by the SEED= option in PROC SURVEYSELECT
 - DATA step uses CALL STREAMINIT to set the seed
 - PROC IML uses CALL RANDSEED to set the seed
- All numbers will change if you change the seed
- Decisions (reject/fail to reject) should rarely change

Bootstrap Analysis of Skewness SEED = 1

The MEANS Procedure

Analysis Variable : Skewness							
N	Mean	Std Dev	5th Pctl	95th Pctl			
5000	0.1534985	0.3206183	-0.3482734	0.6766532			

Bootstrap Analysis of Skewness SEED = 321

The MEANS Procedure

Analysis Variable : Skewness						
Ν	Mean	Std Dev	5th Pctl	95th Pctl		
5000	0.1580319	0.3233697	-0.3581482	0.6849739		

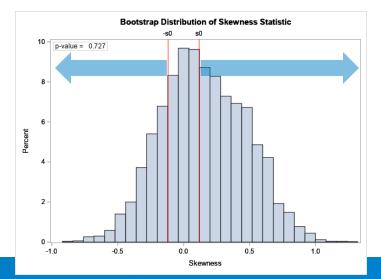


(TWO-SIDED) P-VALUES FOR THE NULL HYPOTHESIS

 H_0 : Skewness = 0.

A bootstrap p-value is the proportion of bootstrap statistics that are more extreme than the observed statistic:

 $p = \sum_{i=1}^{B} I(|s_i| > |s_0|)/B$ or Davidson-Hinkley correction $p = (1 + \sum_{i=1}^{B} I(|s_i| > |s_0|))/(B + 1)$



```
%let Skew0 = 0.1180151;
proc iml;
use BootStats; read all var "Skewness";
/* Two-sided p-value for H0: Skewness = 0 */
B = nrow(Skewness);
s0 = abs(&Skew0);
p = sum(abs(Skewness) >= s0) / B;
pDH = (1 + sum(abs(Skewness) >= s0)) / (B+1);
print p pDH;
```

р	pDH
0.727	0.7270546

For large *B*, the two estimates are very close



BOOTSTRAP IN SAS/IML LANGUAGE

proc iml;

```
/* Function to eval stat for each col of a matrix */
start EvalStat(M);
  return skewness(M); /* <== put computation here */
finish;
```

```
call randseed(1); alpha=0.1; B=5000; /* B = num bootstrap samples */
use Sample; read all var "x"; close; /* read data into x */
```

```
/* 1. observed stat */
s0 = EvalStat(x);
s = sample(x, B // nrow(x));
                                    /* 2. sample WR: s is N x B matrix
                                                                        */
bStat = T( EvalStat(s) );
                                    /* 3. compute stat for each column
                                                                        */
                                                                        */
                                    /* 4. summarize bootstrap distrib:
bootEst = mean(bStat);
                                    /*
SE = std(bStat);
                                          mean, standard deviation,
                                                                        */
call qntl(CI, bStat, alpha/2 || 1-alpha/2); /* general percentile CI */
```

Bootstrap Analysis in SAS/IML							
Obs	BootEst	StdErr	LowerCL	UpperCL			
0.1180	0.1511	0.3192	-0.3611	0.6843			

Bootstrap estimates are similar. Results differ only because random samples are different.



ESSENTIAL BOOTSTRAPPING BETTER

- The percentile CI is first-order accurate
 - Does not use estimate from original data
 - Does not adjust for skewness of the bootstrap distribution
- The bias-corrected and accelerated interval (BCa interval) is second-order accurate
 - Estimate bias-correction parameter, z_0 , from difference between sample and bootstrap estimates
 - Estimate acceleration parameter, *a*, based on the skewness
 - Obtain adjusted percentiles to use for CI
 - Ex: Instead of using 5th and 95th quantiles for 90% CI, might use 13th and 99th for the CI
- Details

Wicklin, R (2017) "The bias-corrected and accelerated (BCa) bootstrap interval" <u>https://blogs.sas.com/content/iml/2017/07/12/bootstrap-bca-interval.html</u>



How to bootstrap regression estimates in SAS?



ESSENTIAL BOOTSTRAPPING BOOTSTRAP REGRESSION ESTIMATES

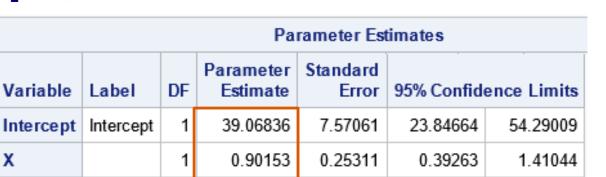
- The multivariate bootstrap is similar to the univariate bootstrap
- Regression models:
- Case resampling: Randomly select observations with replacement
- Residual resampling (semi-parametric): Predict $\hat{Y}_i = f(x_i)$. Form residuals $r_i = Y_i \hat{Y}_i$. Bootstrap *residuals* and form bootstrap samples $\hat{Y}_i + r_k$ where r_k is random residual.
- Block bootstrap: For time-series and repeated-measures models with correlated errors



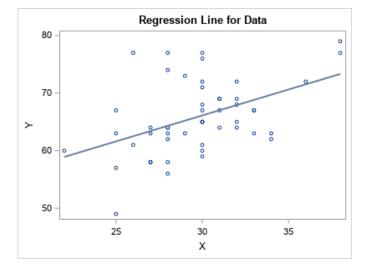
ESSENTIAL BOOTSTRAPPING BOOTSTRAP REGRESSION EXAMPLE

You want to bootstrap the regression coefficients. Asymptotically, $\hat{\beta} \sim MVN$

```
/* 1. compute statistics on the original data (N=50) */
proc reg data=Sample plots(only)=FitPlot(noclm nocli);
   model Y = X / CLB covb; /* original estimates */
quit;
```



Covariance of Estimates					
Variable	Intercept	Х			
Intercept	57.314064817	-1.905215711			
х	-1.905215711	0.0640623978			





ESSENTIAL BOOTSTRAPPING BOOTSTRAP REGRESSION EXAMPLE

```
/* 3. Compute the statistic for each bootstrap sample */
proc reg data=BootCases outest=PEBoot noprint;
    freq NumberHits;
    by SampleID;
    model Y = X;
```

```
quit;
```



BOOTSTRAP REGRESSION RESULTS

```
/* 4. Visualize bootstrap distribution */
```

proc means data=PEBoot N Mean Std P5 P95;

var Intercept X;

run;

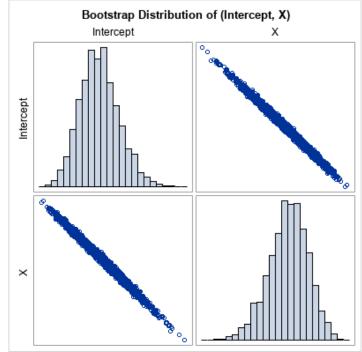
```
proc corr data=PEBoot cov vardef=N
```

plots(maxpoints=none)=matrix(histogram);

var Intercept X;

run;

Variable	N	Mean	Std Dev	5th Pctl	95th Pctl
Intercept X				27.2820239 0.4321832	



Covariance Matrix, DF = 5000							
Intercept							
Intercept	Intercept	62.78133221	-2.02605471				
x		-2.02605471	0.06598298				



SAS procedures that support built-in bootstrapping



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SAS/STAT PROCEDURES THAT SUPPORT BOOTSTRAP ESTIMATES

- Many confidence intervals are based on distributional assumptions
- Bootstrap estimates are distribution-free!
- The following procedures support bootstrap estimates:
 - PROC CAUSALMED and CAUSALTRT: standard errors and confidence intervals
 - PROC MULTTEST: p-values
 - PROC NLIN: confidence intervals for parameters and the covariance of the parameter estimates
 - PROC QUANTREG: regression quantiles
 - The SURVEY* procedures: variance
 - PROC TTEST: standard errors, bias, and confidence intervals

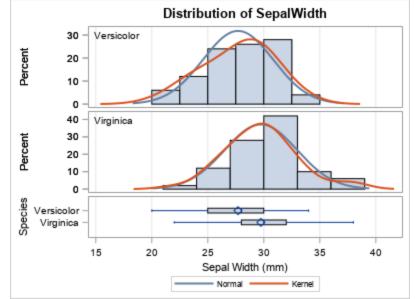


PROC TTEST EXAMPLE

- PROC TTEST supports the BOOTSTRAP statement
- Can run a bootstrap analysis of the difference of means:
 - Is the mean of the Species='Versicolor' group different from the mean of the Species='Virginica' group?

run;

Data might not be normal!





OUTPUT FROM PROC TTEST BOOTSTRAP STATEMENT

Species	Method	Mean	95% CL Mean		Std Dev	
Versicolor		27.7000	26.8082	28.5918	3.1380	
Virginica		29.7400	28.8235	30.6565	3.2250	
Diff (1-2)	Pooled	-2.0400	-3.3028	-0.7772	3.1818	

Bootstrap Statistics and Confidence Limits								
Species	Method	Parameter	Std Error	Bias	95% CL			
Diff (1-2)		Mean	0.6221	0.00752	-3.3000	-0.8200		

Bootstrap *t* test:

Conclusion: group means are different. **No parametric assumptions.**

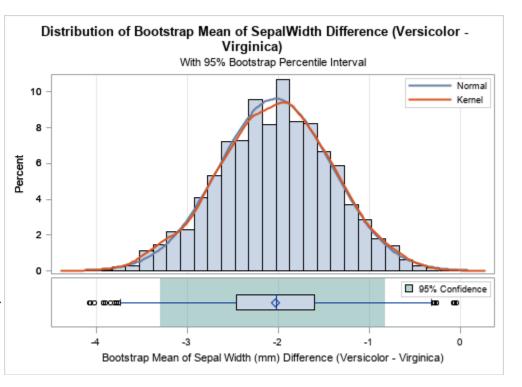
Reports Bias = Observed – Bootstrap estimate

Graph produced automatically! →

Classical parametric *t* test:

Conclusion: group means are different.

Assumes normality of data and equal variances.





ESSENTIAL BOOTSTRAPPING SUMMARY

The bootstrap method estimates a standard error for a statistic (or CI)

- Use when the sampling distribution of a statistic is unknown
- Efficiency matters! Use the tips:
 - Use PROC SURVEYSELECT and METHOD=URS to generate bootstrap samples
 - Use BY statement to analyze bootstrap samples and create a bootstrap distribution
- The results depend (slightly) on the random number stream
- The SAS/IML language enables compact implementation of univariate and multivariate bootstrapping
- Several SAS/STAT procedures support built-in bootstrap analyses



ESSENTIAL BOOTSTRAPPING FURTHER READING

- Theory and practice:
 - Chernick, M. (1999) Bootstrap methods: A practitioner's guide
 - Davison, A.C. and Hinkley, D.V. (1997) Bootstrap methods and their application
- Implementation in SAS: The DO Loop blog
 - <u>http://blogs.sas.com/content/iml</u>
 - Click on Bootstrap and Resampling in the word cloud to see articles
 - "The Essential Guide to Bootstrapping in SAS" links to more than 30 blog posts that demonstrate bootstrapping in SAS



TWITTER: @RICKWICKLIN LINKEDIN: WWW.LINKEDIN.COM/IN/RICKWICKLIN/ **BLOG:** blogs.sas.com/content/iml





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