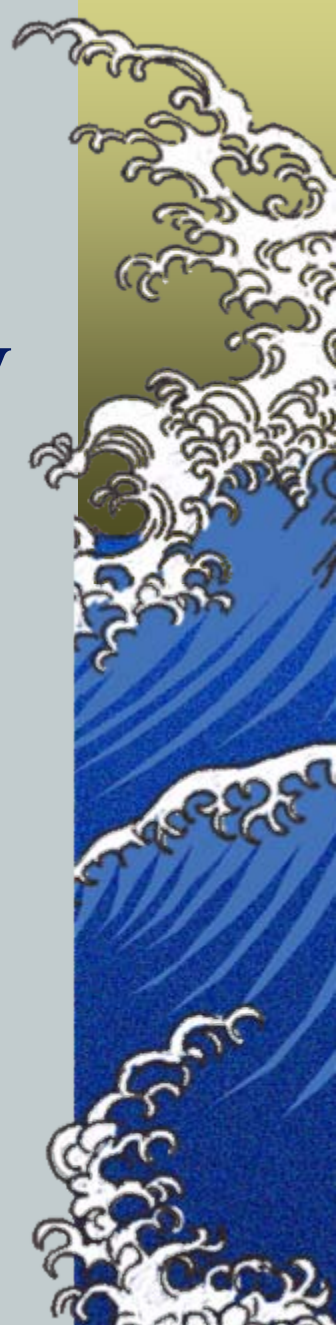
Estimating Non-Point Source Load and Measuring Uncertainty

Metropolitan Council Environmental Services

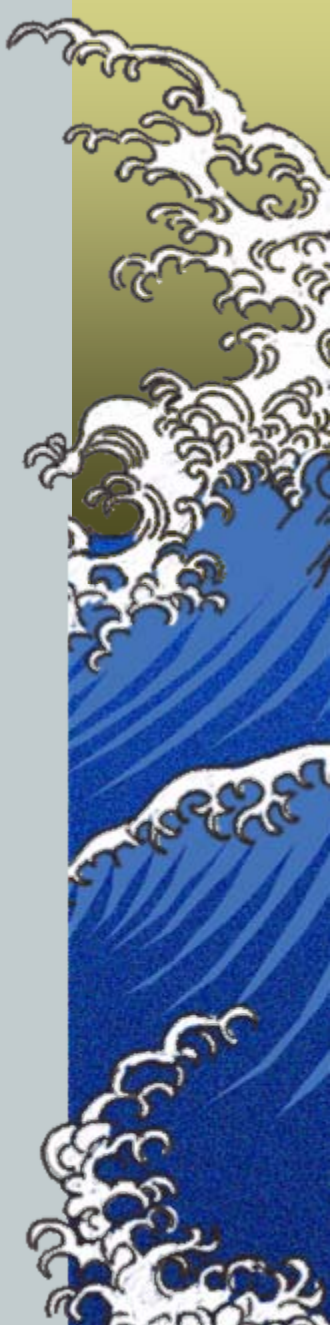
St. Olaf College Mathematics Practicum

January 2006



St. Olaf College Participants

- Haley Hedlin, Jostein Reiners, Phillip Schulte, Allan Trapp II, Molly Tuerk, and Stacey Wood
- Senior math majors
- Statistics concentrators



Mathematics Practicum?

- 3 different projects, 5-6 students each
- One month
- Real problem
- Gain experience

Motivating Questions

- Finding the best model for load estimation
  - Adjustments to current method
- Assessing the level of uncertainty
  - Major factors affecting variability

Stream Monitoring Program

Determining the amount of non-point source pollutant loading

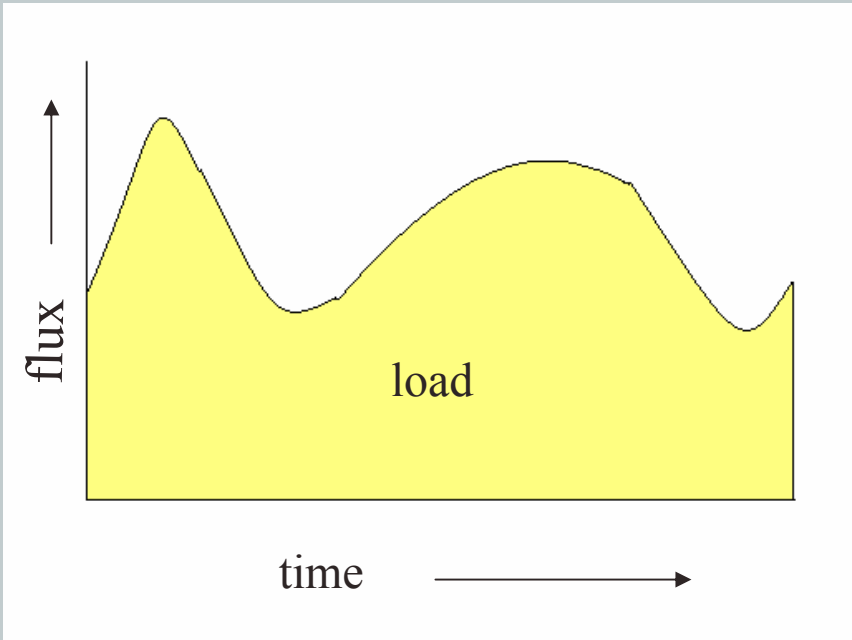
l to r: Haley Hedlin, Stacey Wood, Jostein Reiners, Phillip Schulte, Alan Trapp II, and Molly Tuerk

Loading Concept

- What is load?
- Flux=concentration*flow
  - Loading rate
  - Units in mass/time
- Load calculations

Load Estimation

- Integration approach



$$\text{Load} = \int \text{flux}(t)dt$$

$$\text{Load} = k \sum_{i=1}^{n} c_i \cdot q_i \cdot \Delta t_i$$

k=constant to convert units

c_i=concentration

q_i=flow

Δt_i=interval between observations

Issues with Current Methods

- Uncertainty with flow estimates
- Pollutant concentration samples limited
- Pollutant loading errors of 10%-40% are not unusual
- Flow rate can change rapidly

Our Focus

- Focused on three rivers:
  - Nine Mile Creek (urban)
  - Credit River (semi-urban)
  - Bevens Creek (rural)
- Focused on three pollutants:
  - Nitrates
  - Total Phosphorus
  - Total Suspended Solids

Presentation Outline

- Models for Load Estimation
  - FLUX (MCES)
  - Estimator (USGS)
  - Our Model
- Measures of Uncertainty
  - Methods
    - Jackknifing
    - Bootstrapping
  - Comparisons
- River Simulation

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FLUX Method 2

- Ratio estimate

$$W_2 = \text{Mean}(w) \cdot \frac{\text{Mean}(Q)}{\text{Mean}(q)}$$

W= total annual load (kg/yr)

w = daily sample loads (kg/yr)

q = daily sample flow (cf/s)

Q = average continuous daily flow (cf/s)

FLUX Method 4

- Regression estimate

$$W_4 = \text{Mean}(w) \cdot \left[\frac{\text{Mean}(Q)}{\text{Mean}(q)} \right]^{b+1}$$

W= total annual load (kg/yr)

w = daily sample loads (kg/yr)

q = daily sample flow (cf/s)

Q = average continuous daily flow (cf/s)

b = slope of ln(concentration) vs. ln(flow)

Estimator

- 7 parameter regression estimate predicting ln(concentration)

$$\ln(C) = \beta_0 + \beta_1 \ln [Q/Q_0] + \beta_2 (\ln [Q/Q_0])^2 + \beta_3 [T-T_0] +$$

$$\beta_4 [T-T_0]^2 + \beta_5 \sin[2\pi T] + \beta_6 \cos[2\pi T]$$

C = concentration (mg/L)

Q = flow (cf/s)

Q_0 = flow centering constant

T = time (years)

T_0 = time centering constant

Calculating Annual Load

sample loads

↓

regression model

↓

daily concentration

↓

daily flux

↓

daily load

↓

annual load

FLUX vs. Estimator

- FLUX
  - 6 methods from which to choose
  - Accounts only for flow
- Estimator
  - Choose from a list of predictors
  - Accounts only for season and flow

Our Model

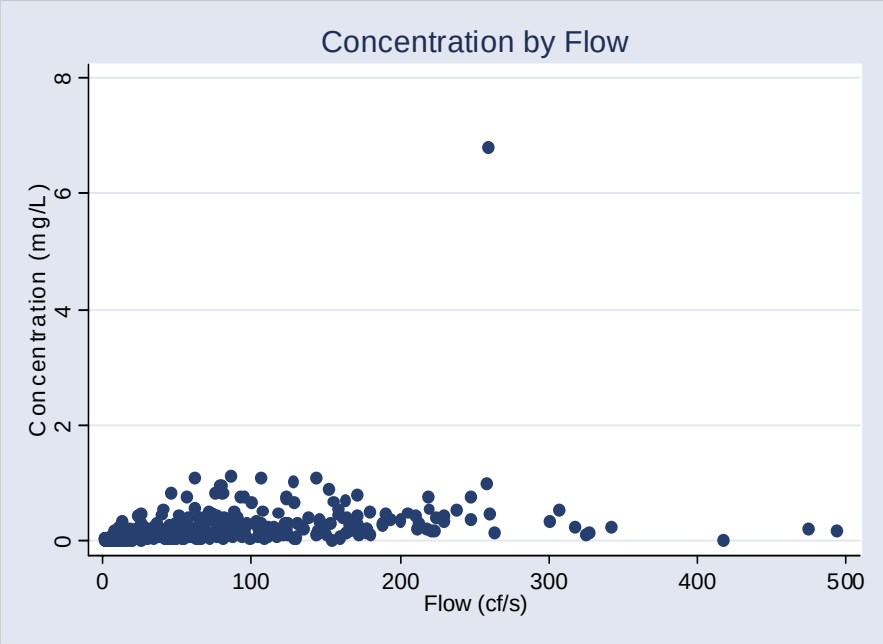
- Builds on Estimator and FLUX
- Predicts concentration in order to estimate annual load
- Uses linear regression model

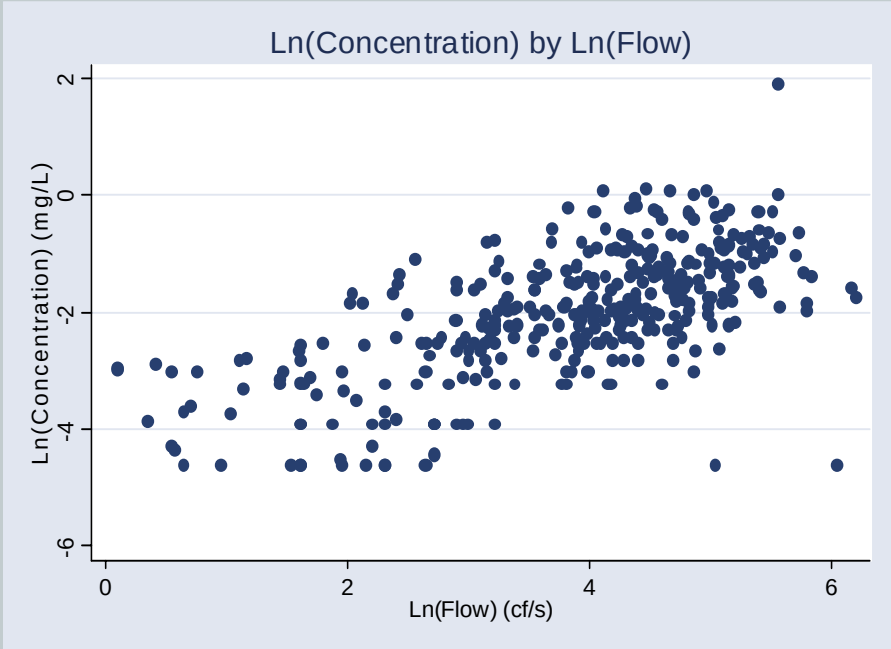
Choosing Our Predictors

- Brainstorm possibilities:
  - Flow, time of year, precipitation, air temperature
  - Logarithmic relationship, quadratic relationship, flow stratification
- Graphical exploration

Log-Linear Relationship

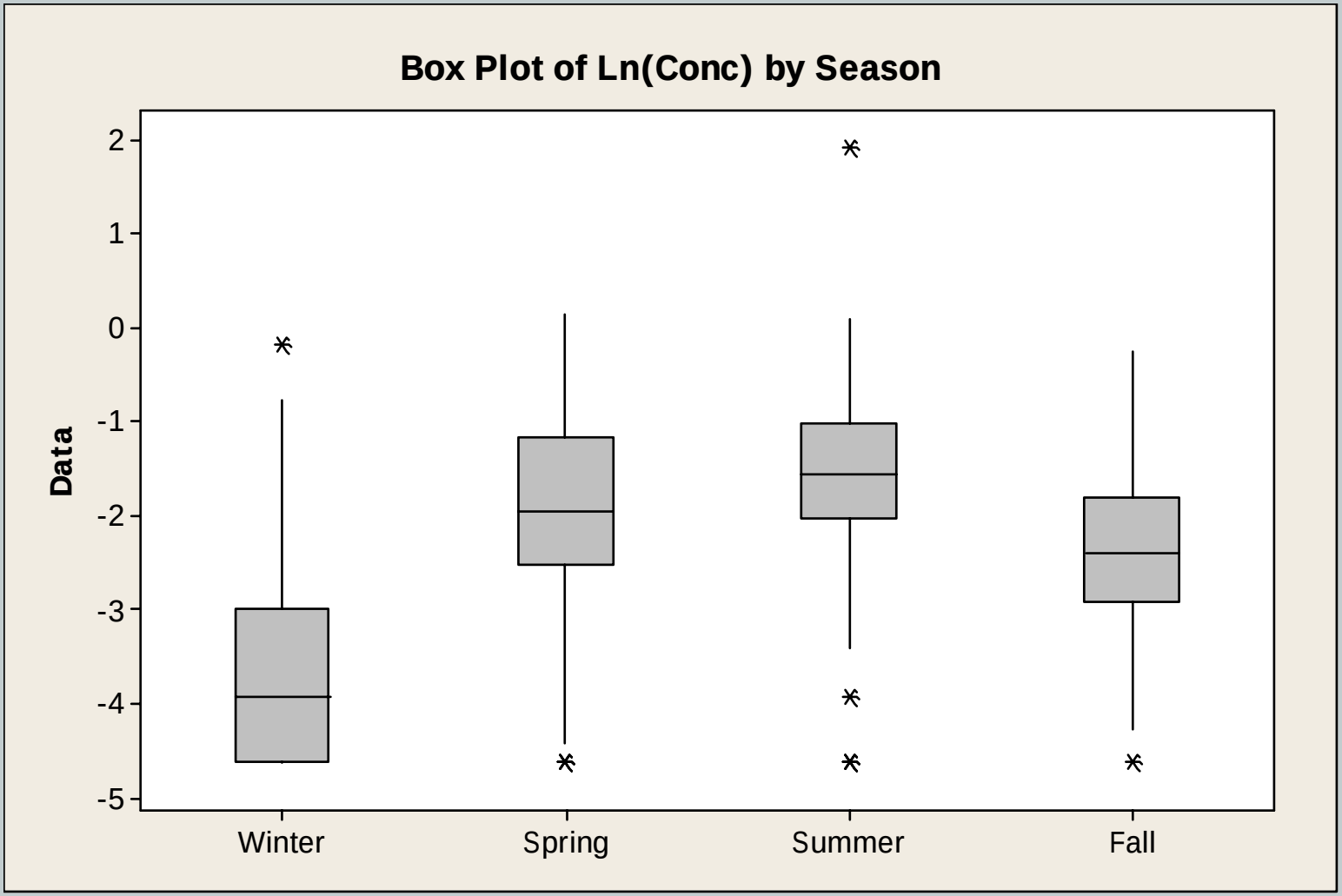
Nine Mile Creek Total Phosphorus





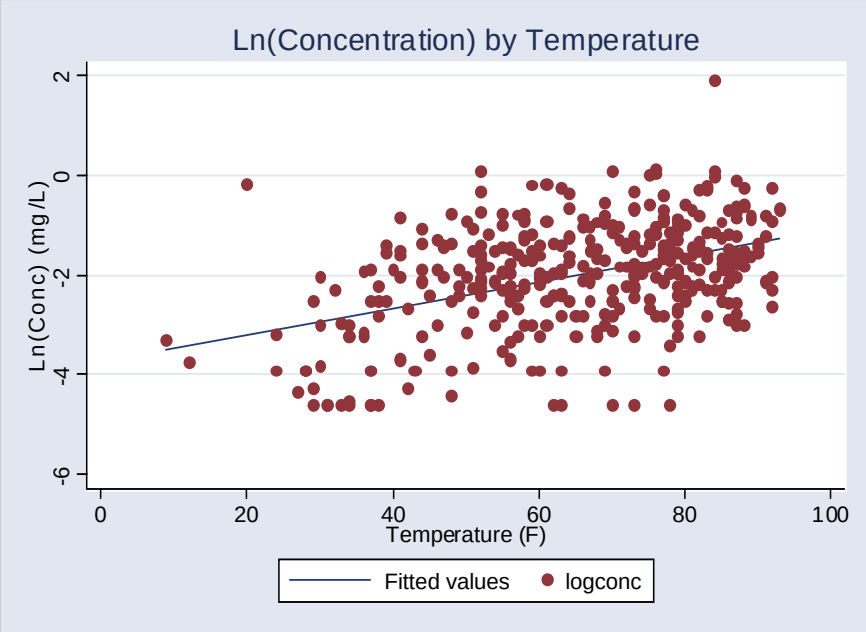
Boxplots of Seasonality

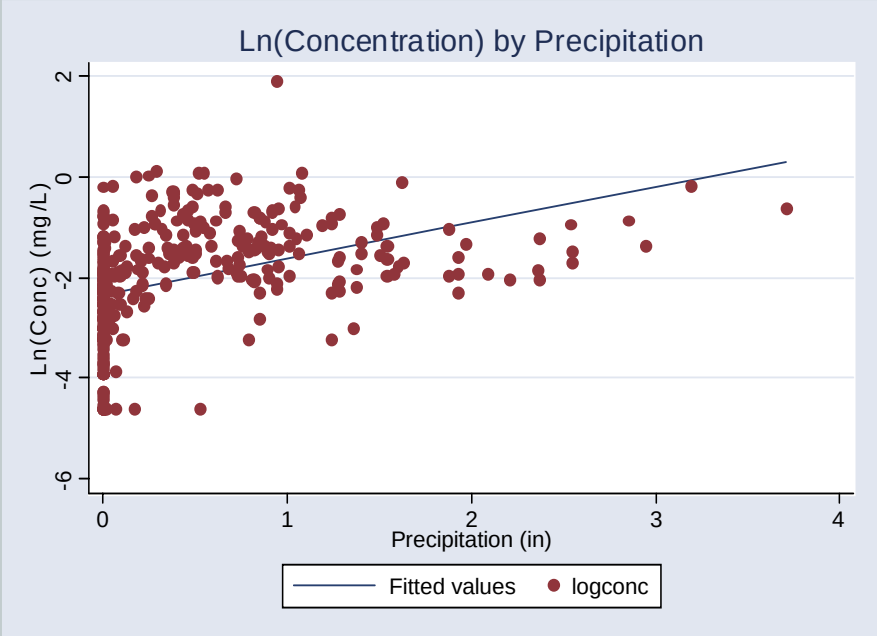
Nine Mile Creek Total Phosphorus



Temperature and Precipitation

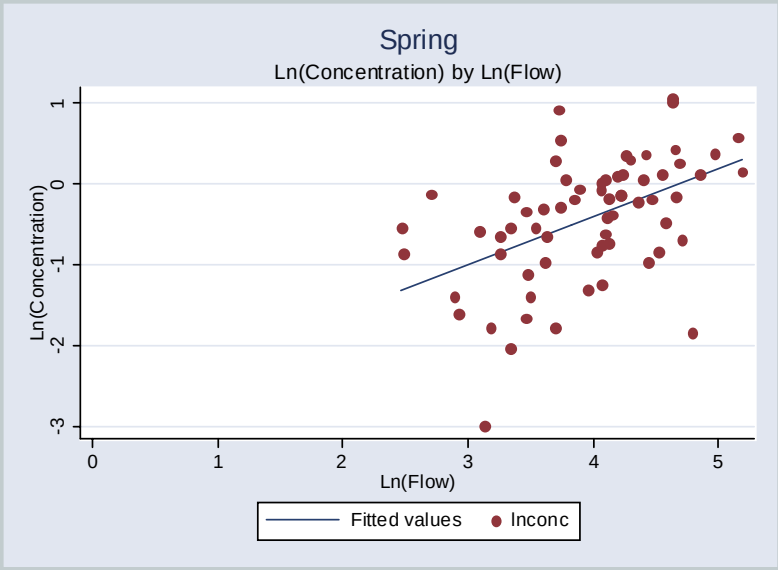
Nine Mile Creek Total Phosphorus

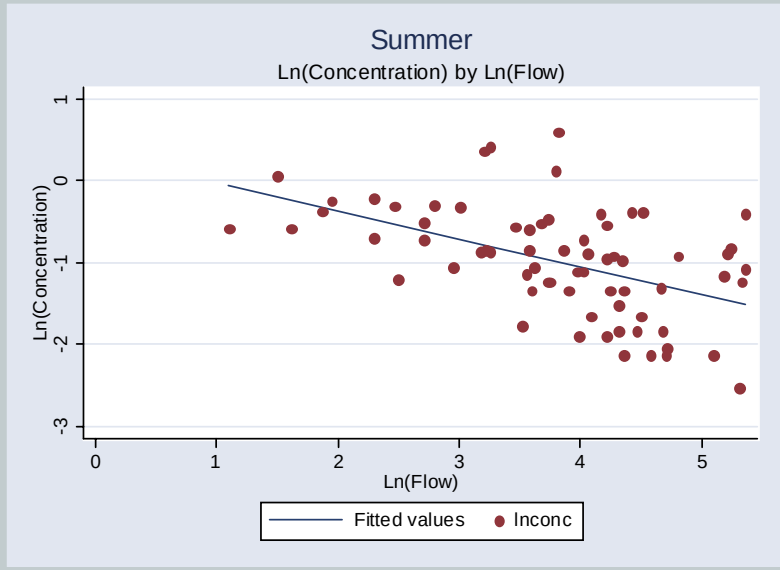


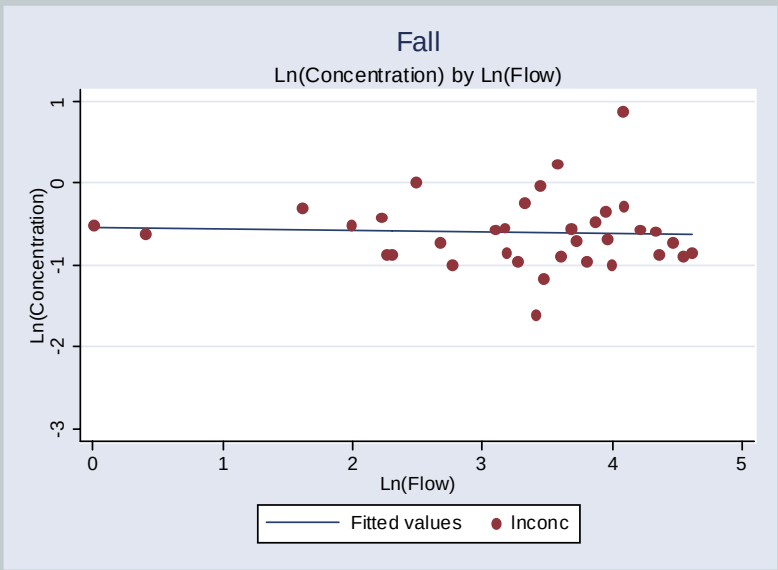


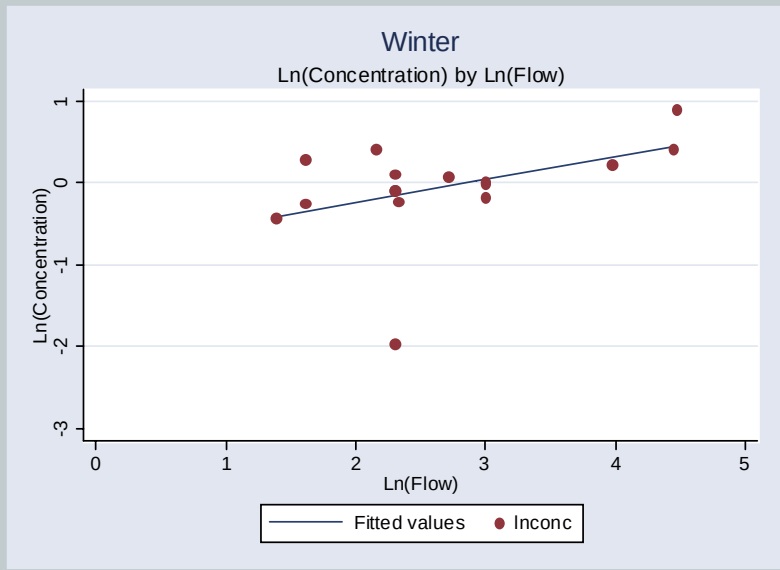
Effect of Seasonality

Credit River Nitrates



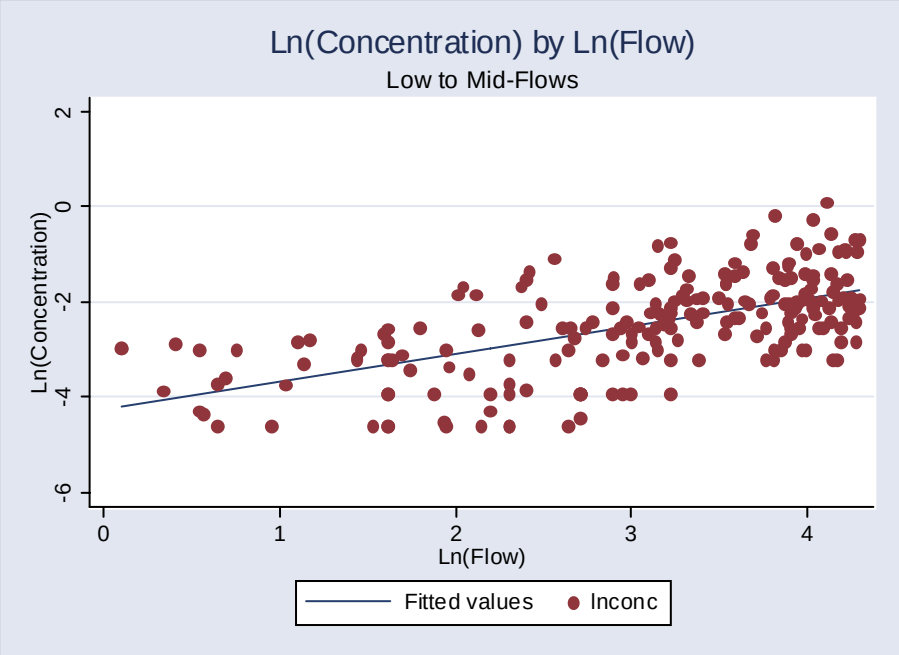


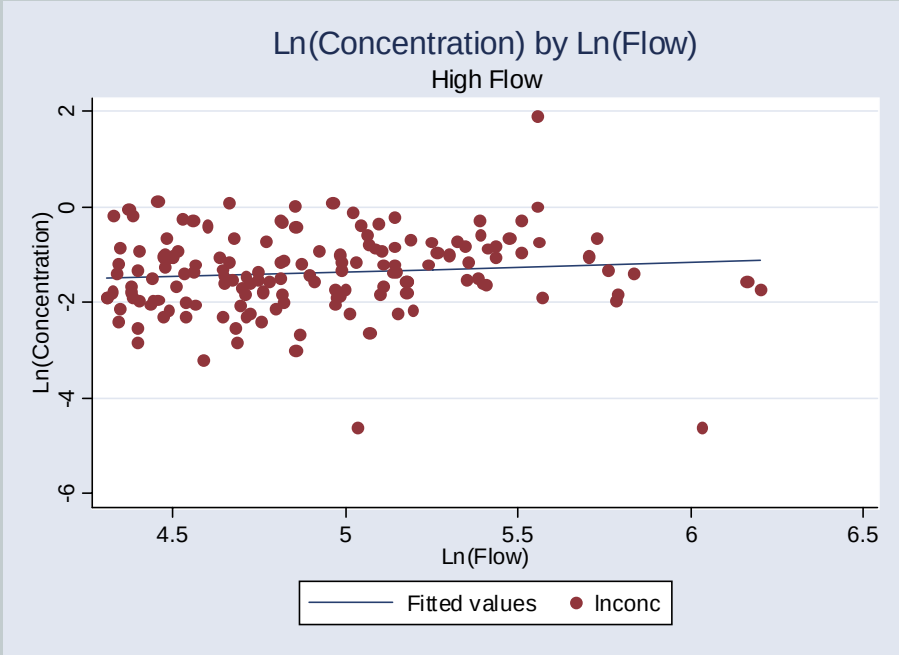




Flow Stratification

Nine Mile Creek Total Phosphorus





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Building our Model

- Began by predicting ln(conc) by ln(flow)
- Added predictors that seemed to best improve the model
- Consider factors we knew were most important
  - time or season
  - stratification of flow
- Followed good model building practices

Our Proposed Model

$$\ln[\text{conc}] = \beta_0 + \beta_1 \ln[\text{flow}] + \beta_2 (\ln[\text{flow}])^2 + \beta_3 \text{spring} + \beta_4 \text{summer} + \beta_5 \text{fall} + \beta_6 \text{temp} + \beta_7 \text{precip} + \beta_8 \text{highflow} + \beta_9 \ln[\text{flow}]*\text{highflow}$$

Model Selection

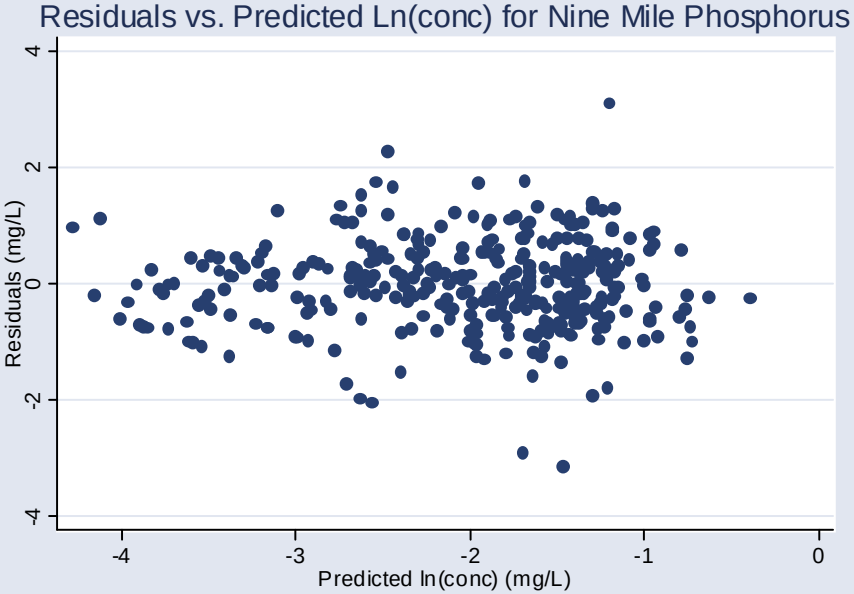
Model output for Nine Mile Creek Total Phosphorus

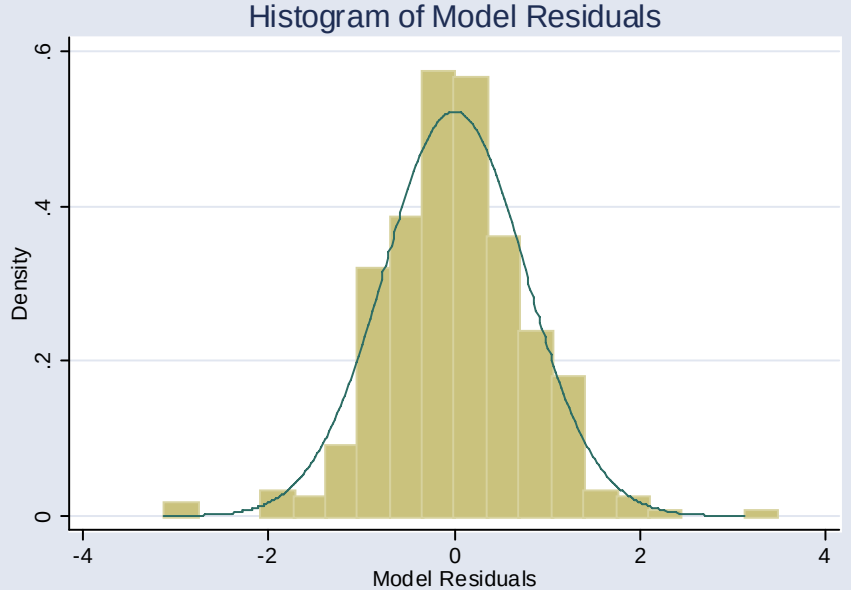
Source	SS	df	MS		
Model	221.339874	9	24.5933194	Number of obs	349
Residual	202.349277	339	.596900522	F(9, 339)	41.20
Total	423.689151	348	1.21749756	Prob > F	0.0000
				R-squared	**0.5224**
				Adj R-squared	0.5097
				Root MSE	.77259

logconc	Coef.	Std. Err.	t	P>|t|	[95% Conf.	Interval]
logflow	.0429734	.2380258	0.18	0.857	-.42522	.5111668
logflow2	.0791393	.0450354	1.76	**0.080**	-.0094448	.1677234
spring	.5285192	.1820339	2.90	**0.004**	.1704609	.8865774
summer	.2997691	.2191953	1.37	0.172	-.1313851	.7309233
fall	.0740877	.1942195	0.38	0.703	-.3079395	.4561148
temp	.0127285	.0033565	3.79	**0.000**	.0061263	.0193307
precip	.2729996	.0744209	3.67	**0.000**	.1266148	.4193844
highflow	4.04846	1.203126	3.36	**0.001**	1.681927	6.414993
logflowXhi~w	-.9031118	.2800664	-3.22	**0.001**	-1.453999	-.3522251
_cons	-4.547751	.3310143	-13.74	**0.000**	-5.198852	-3.89665

Model Validation

Residual Analysis for Nine Mile Creek Total Phosphorus





Possible Improvements

- Interaction terms
  - e.g. ln(flow) by season
- Custom building of models for best predictions
  - The model consistently fit well but not always best

Model Estimates of Annual Load

Credit River 1996 Total Phosphorus (in kg)

	Estimate
FLUX Method 2	5300
FLUX Method 4	2800
Estimator	4500
Our Model	3700

Model Estimates of Annual Load

Bevens Creek 2004 Total Phosphorus (in kg)

	Estimate
FLUX Method 2	590,000
FLUX Method 4	490,000
Estimator	660,000
Our Model	620,000

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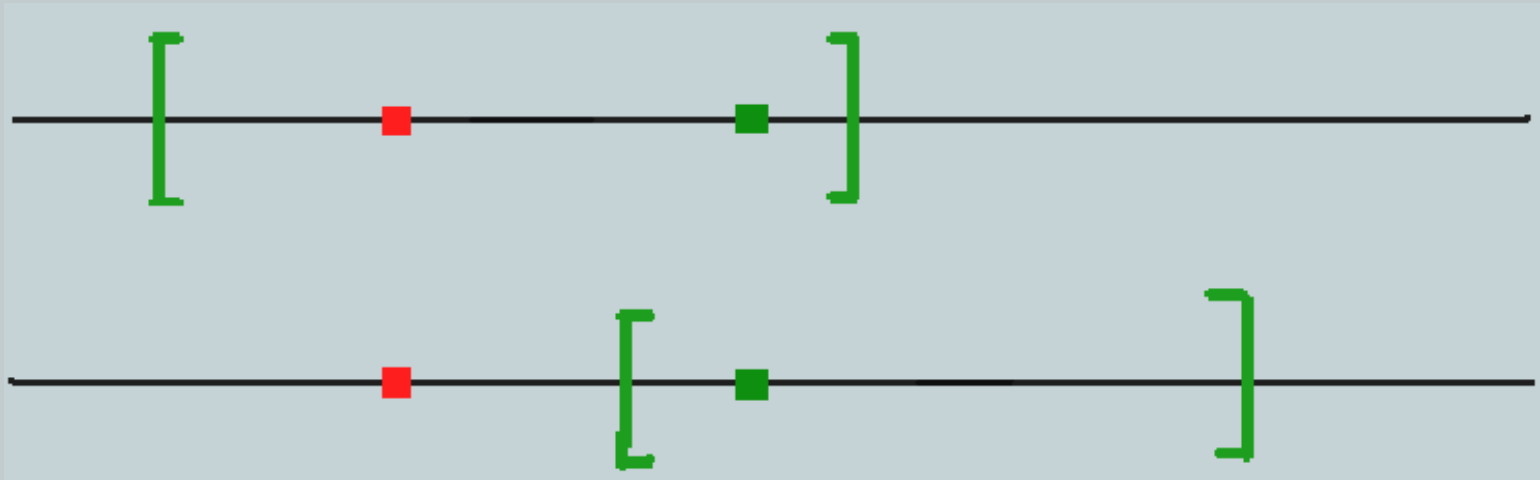
Assessing Levels of Uncertainty

- 95% confidence intervals (CIs)
  - Based on chosen methods, we expect the interval to contain the true value (of load) 95% of the time



Confidence Interval Generation

- Traditional procedure

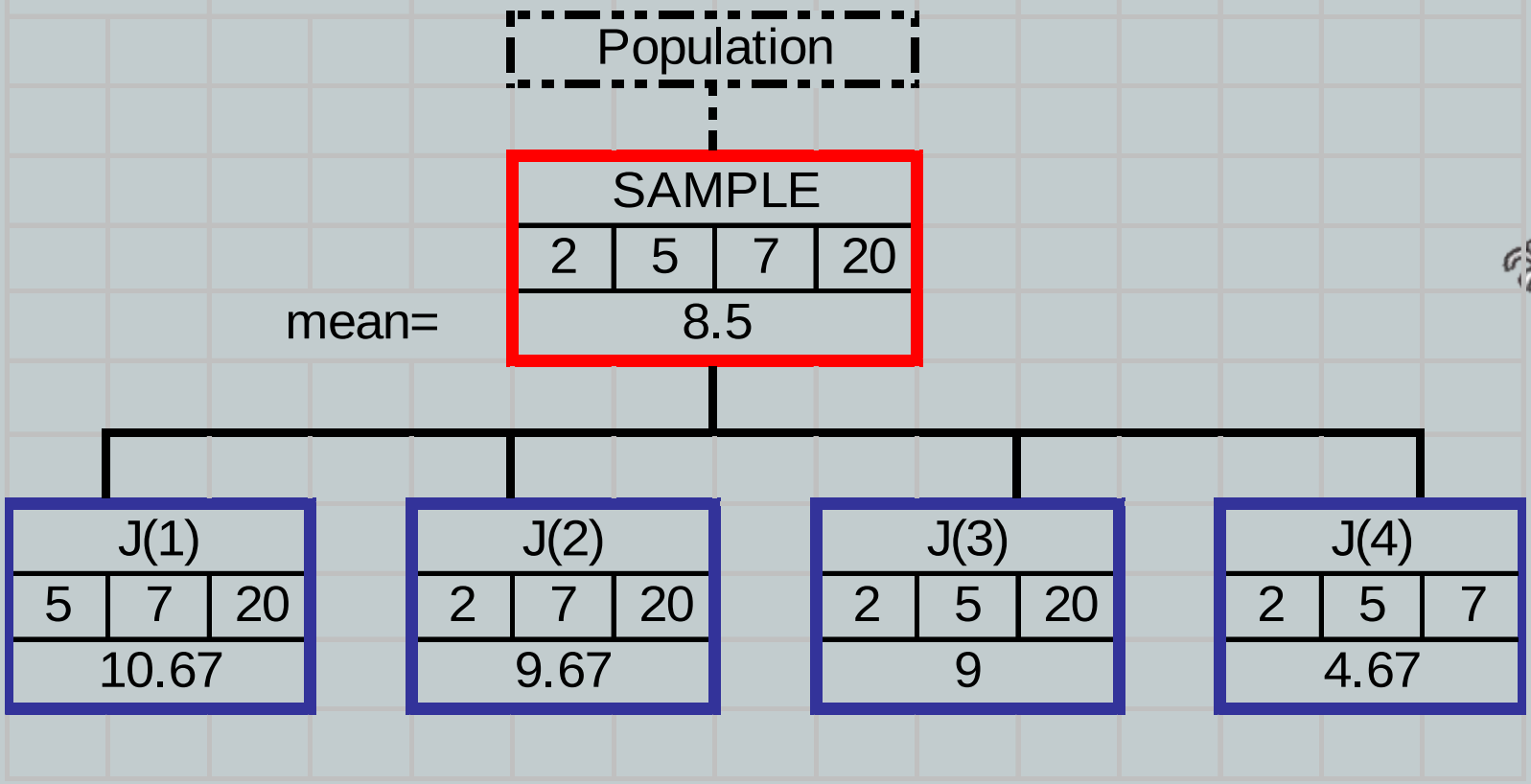
  CI = Mean ± 1.96 * Standard Error

- Resampling procedure
  - Draw multiple new samples from a given sample
  - Calculate the parameter of interest for each new sample
  - Obtain a distribution of the parameter

The Jackknife

- Used by FLUX
- Test model sensitivity to a particular observation
- Recalculate estimate after removing a particular observation

Jackknife Replication

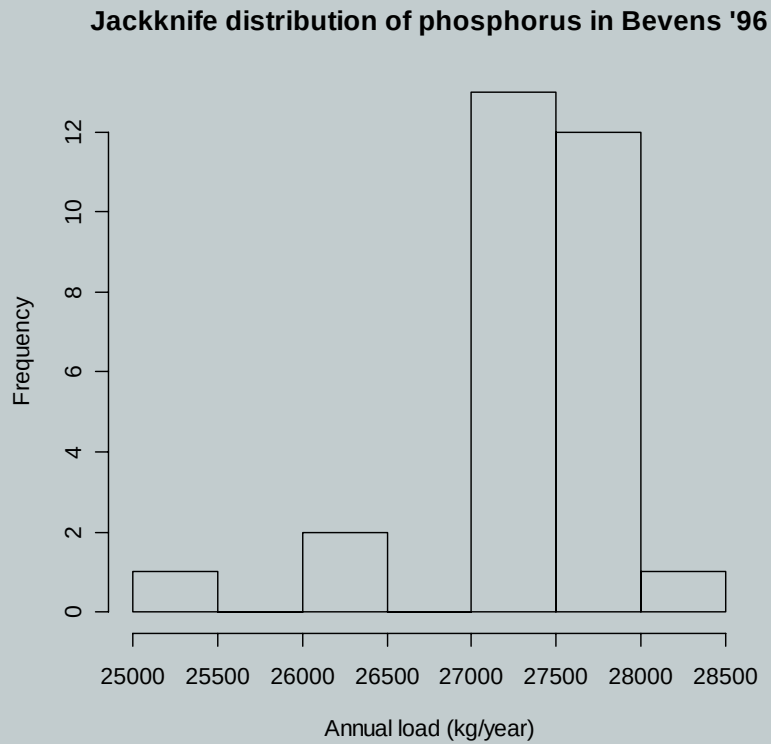


Standard Error (SE) of jackknifed values = 3.97

Mean = 8.5

95% CI = mean ± 1.96 * SE(jack) ⟶ (.72, 16.28)

Jackknife Application to Load Data

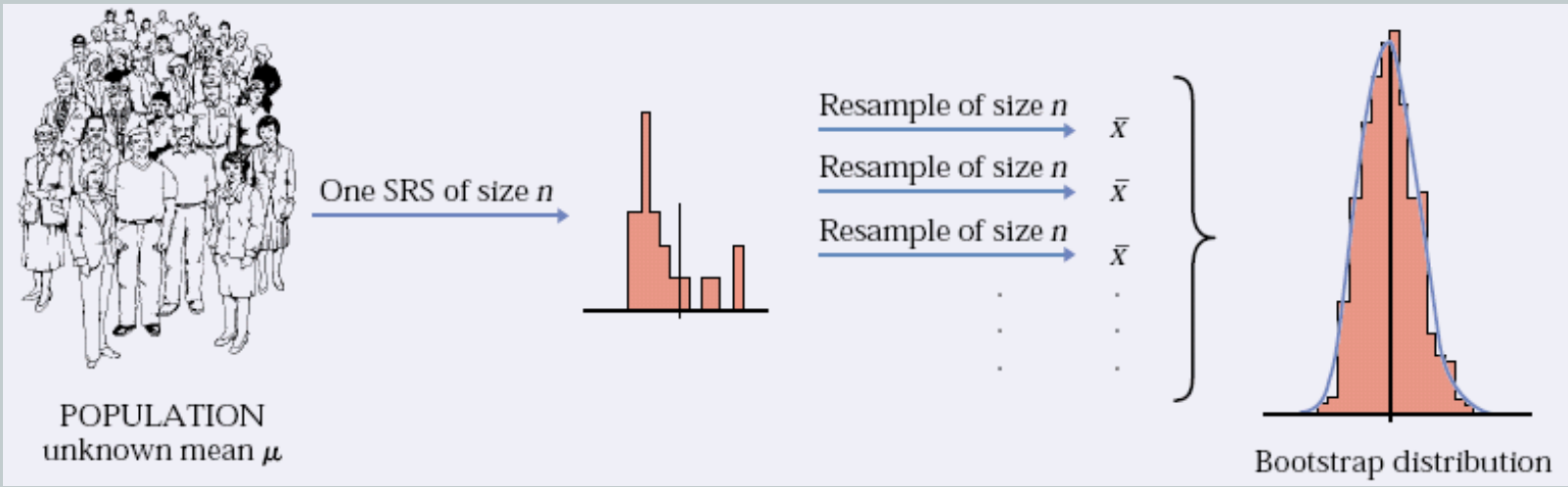


- Original sample size of 29
- Influential points within dataset
- 95% confidence interval →

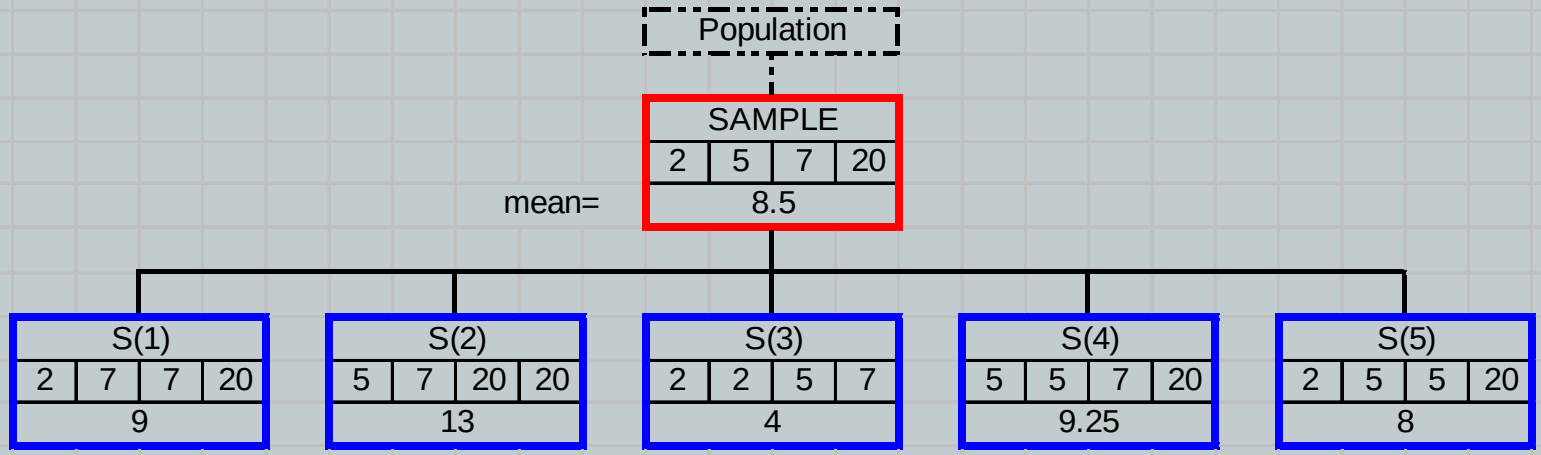
  (22000, 34100)

The Bootstrap

- Resample with replacement from the data set to simulate repeated samples
- Calculate uncertainty from the bootstrap distribution



Bootstrap Replication



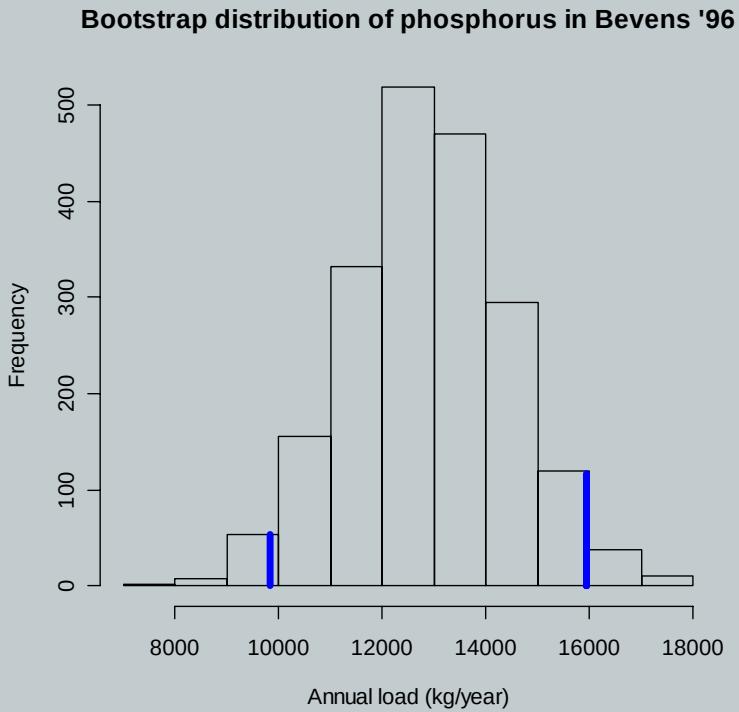
Mean of bootstrapped sample means = 8.65

Standard error = 3.22

95% confidence interval = 8.65 ± 1.96 * 3.22 →

(2.34, 14.96)

Bootstrap Application to Load Data



- Sampling of n = 29
- Randomly sampled 2000 times
- Quantiles CI →

  (9800, 16000)

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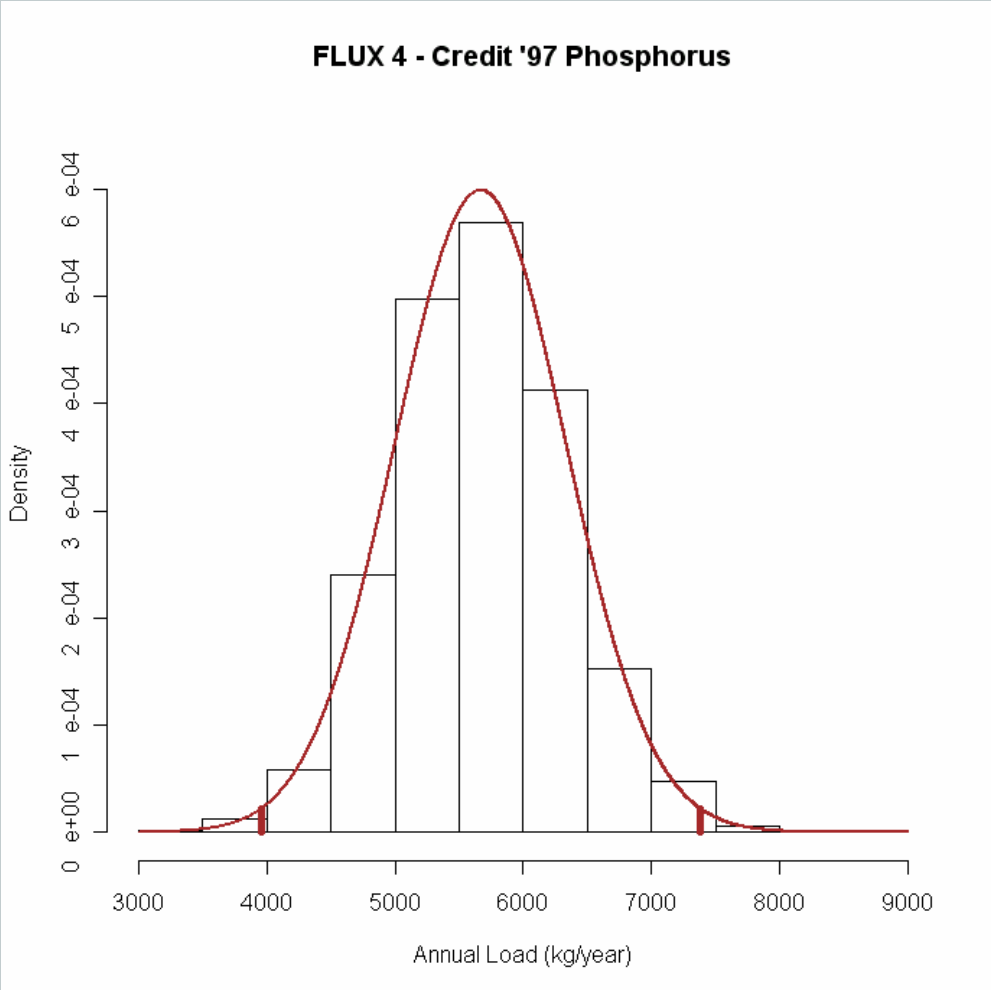
Types of Bootstrap Calculations

- Normality confidence interval
- t-confidence interval
- Quantiles
- Bias corrected and accelerated (BCa) quantiles

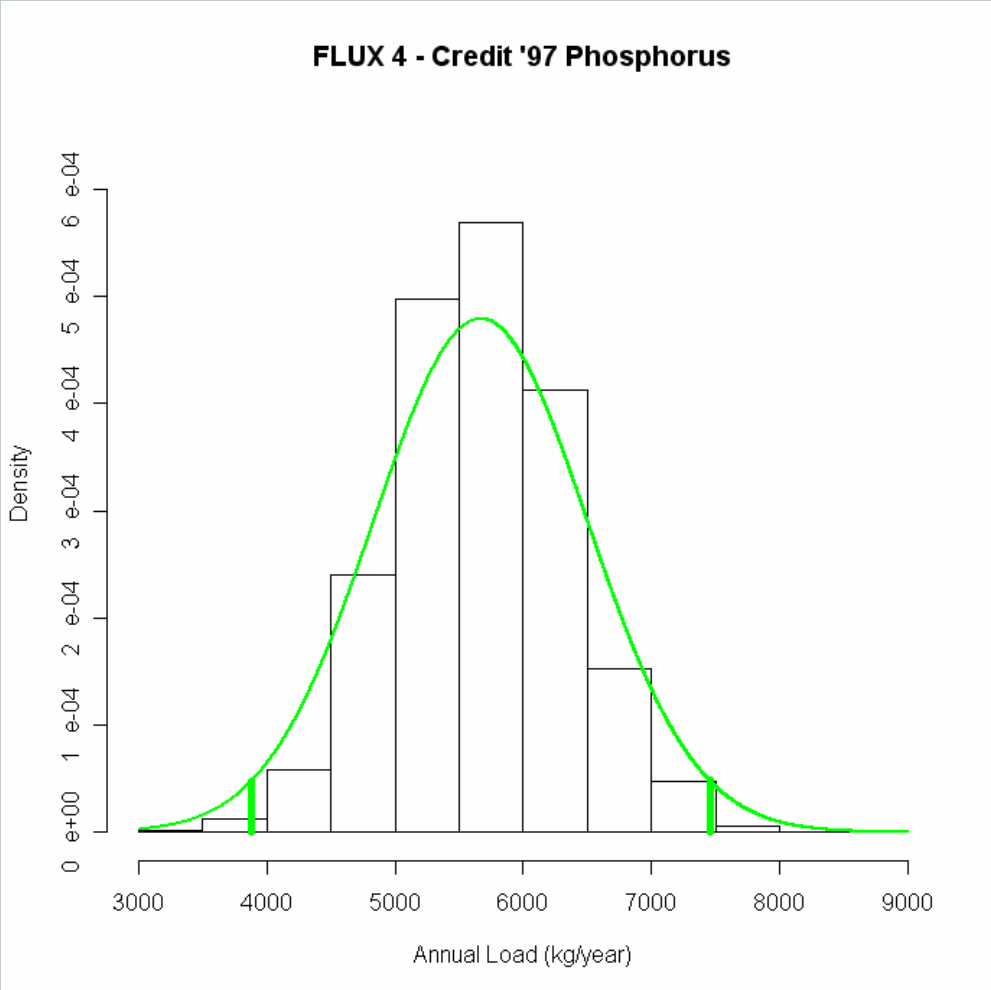
Assumptions of the Bootstrap Distribution

Normality



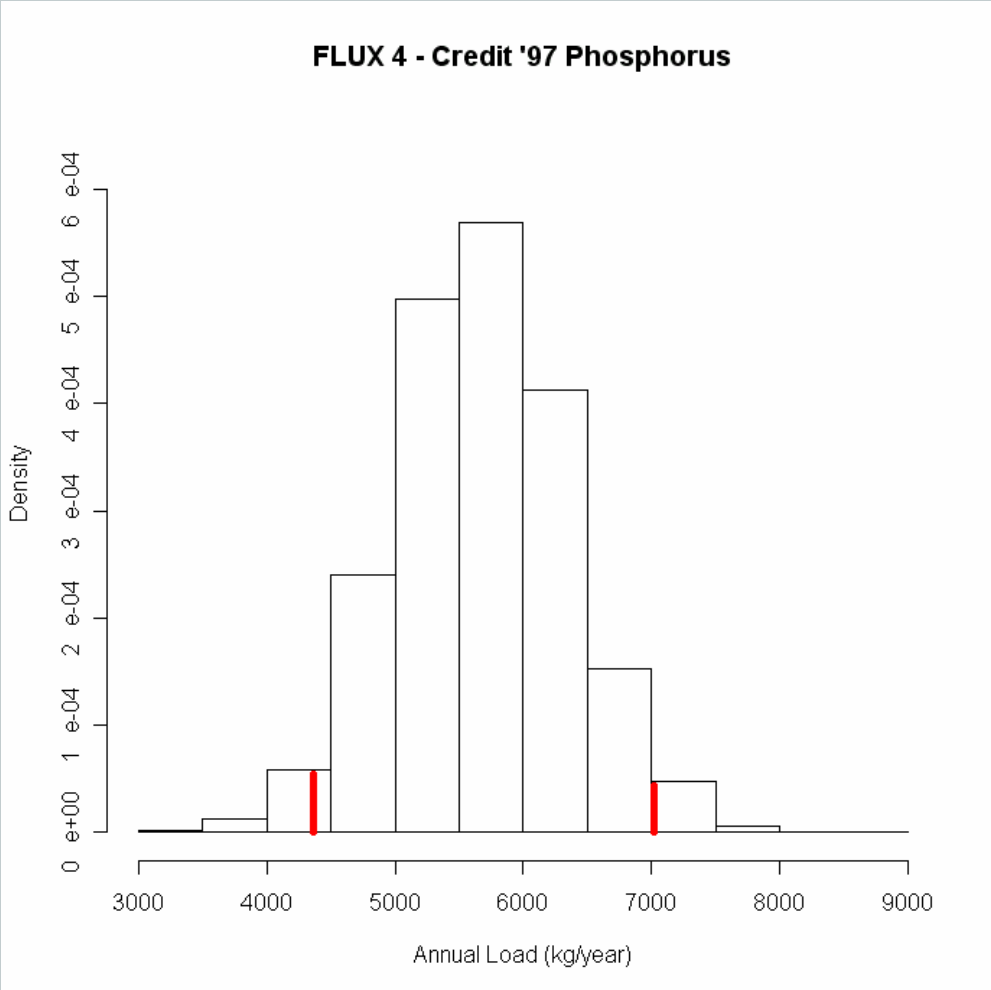
Assumptions of the Bootstrap Distribution

t-confidence



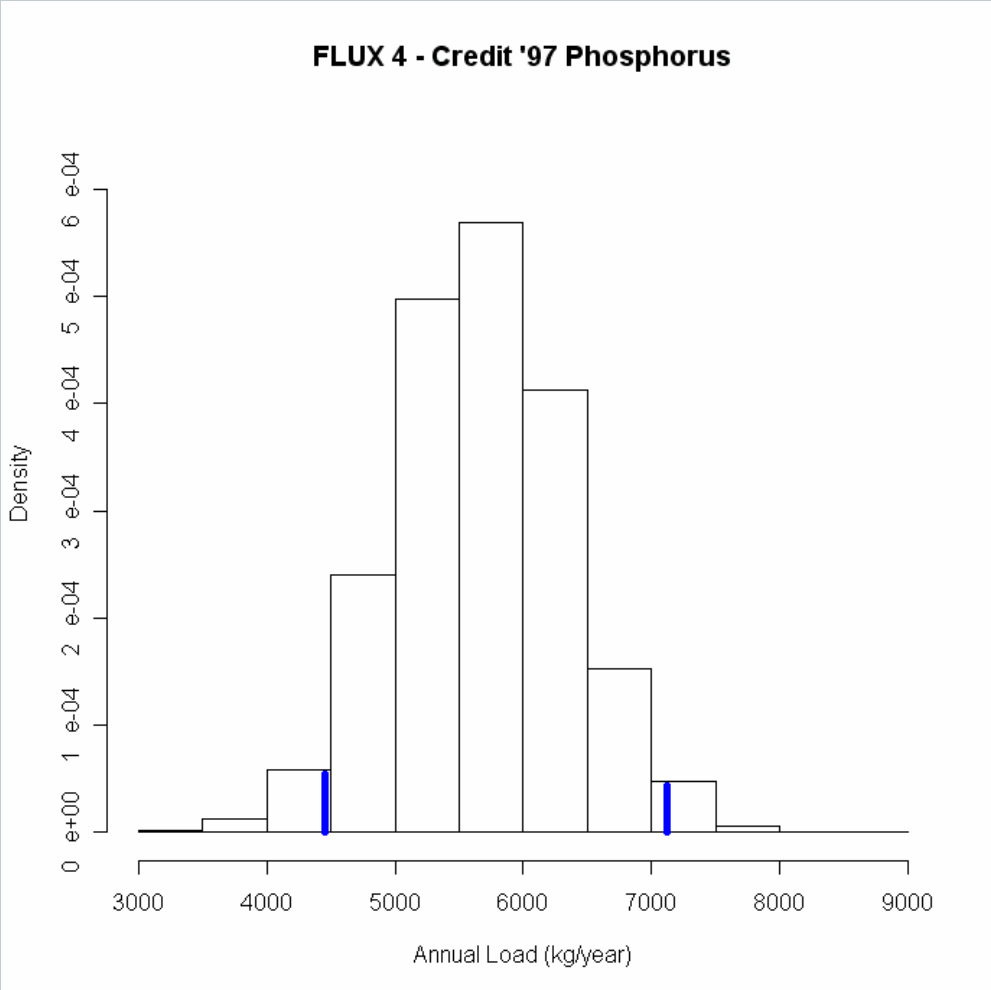
Assumptions of the Bootstrap Distribution

Quantiles

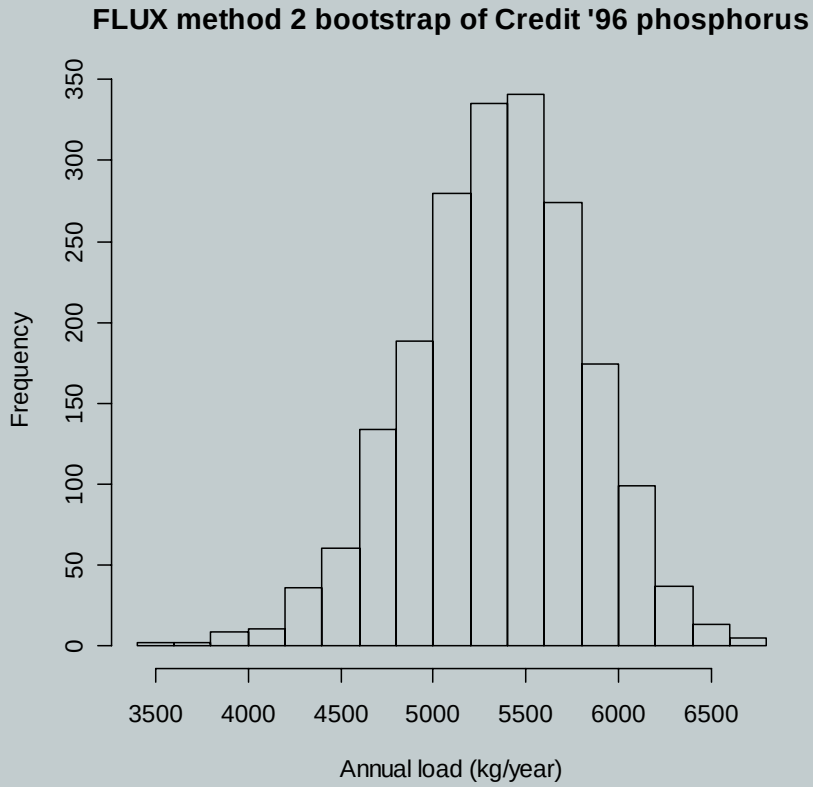


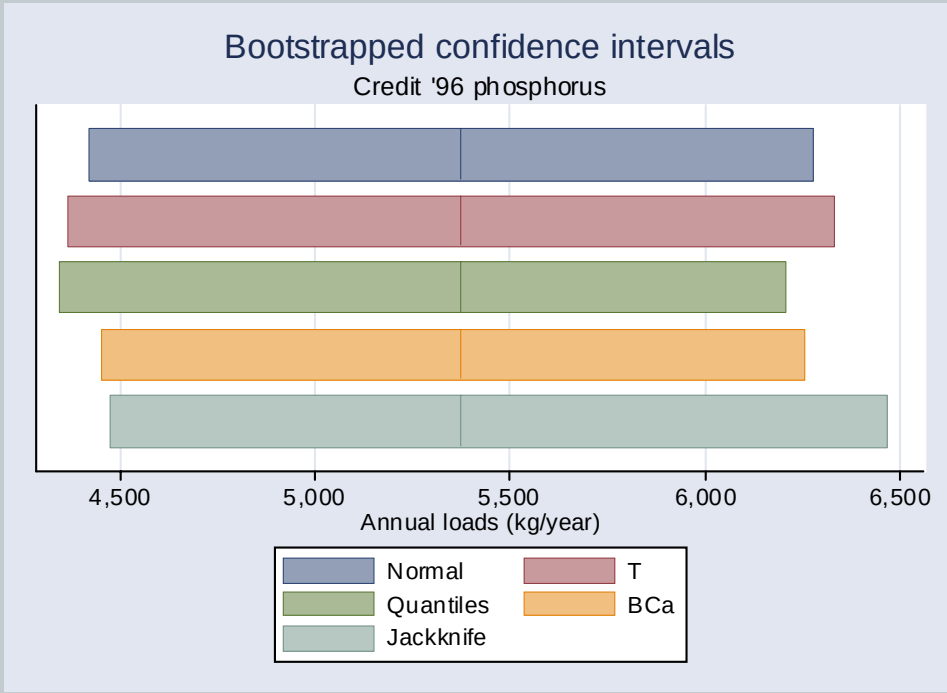
Assumptions of the Bootstrap Distribution

BCa

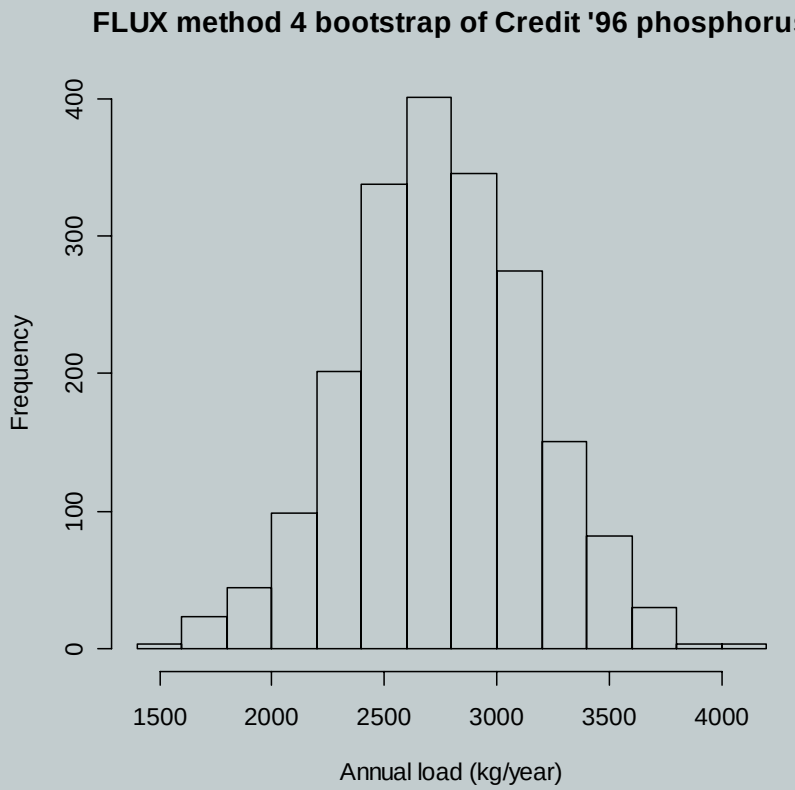


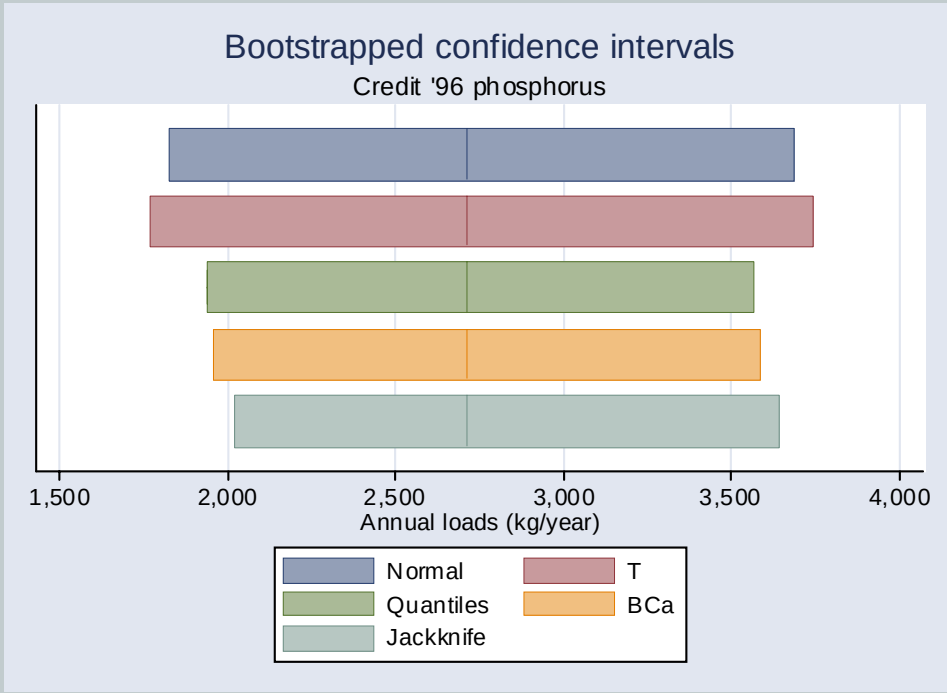
FLUX Method 2



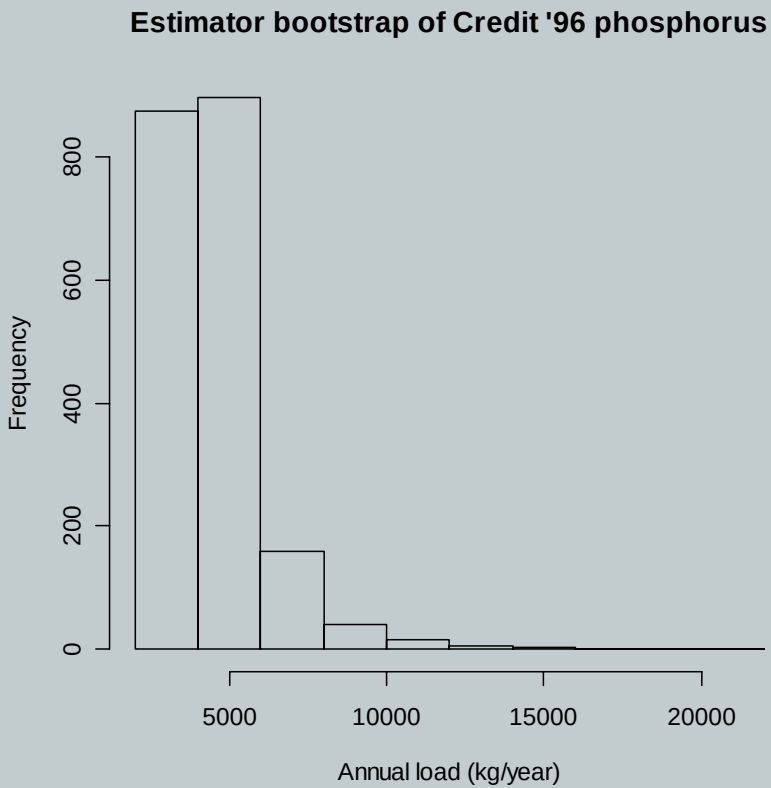


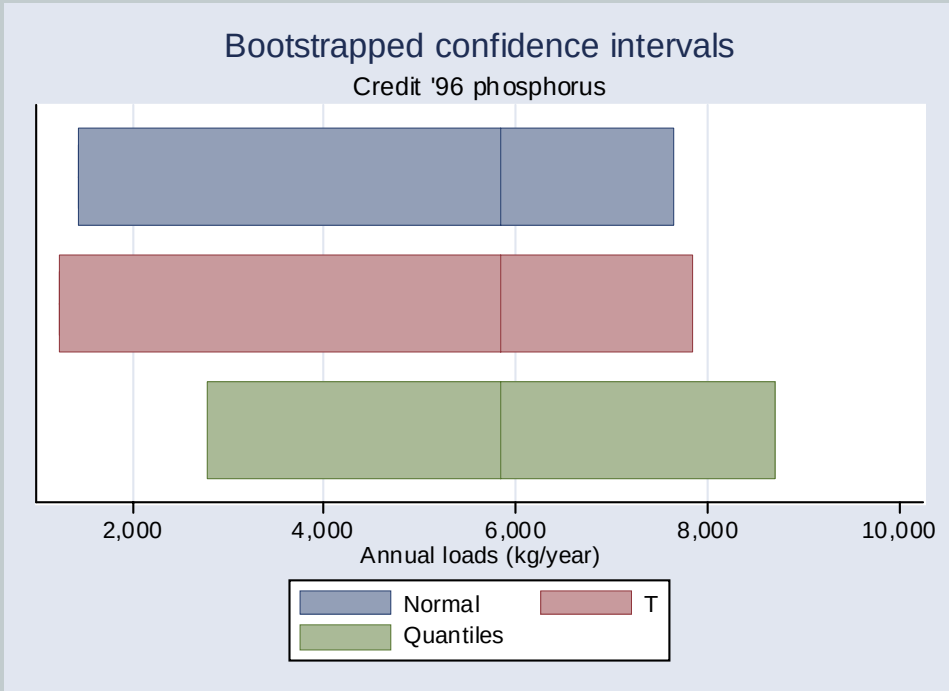
FLUX Method 4



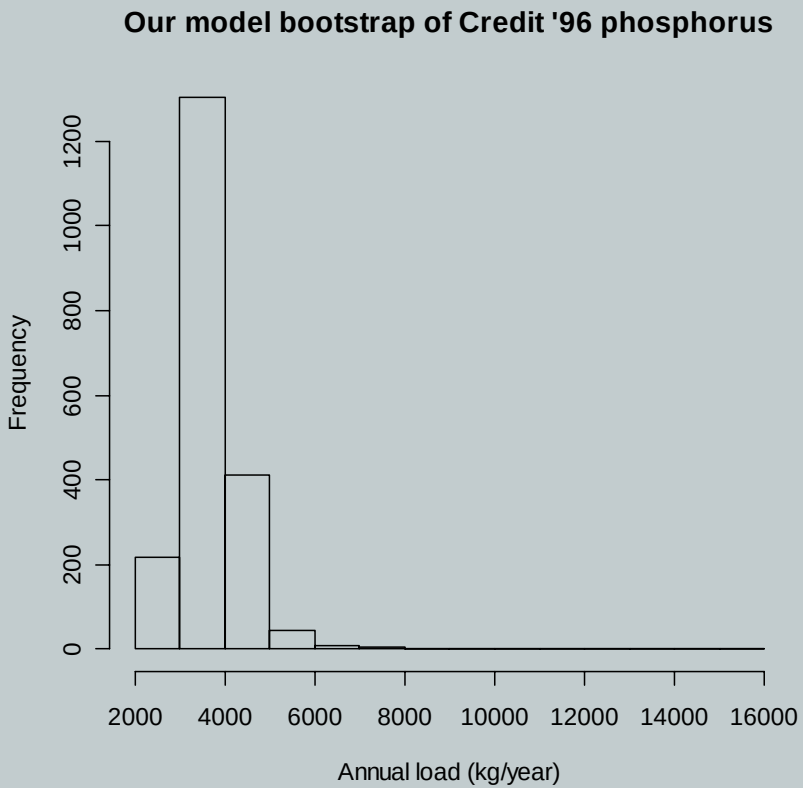


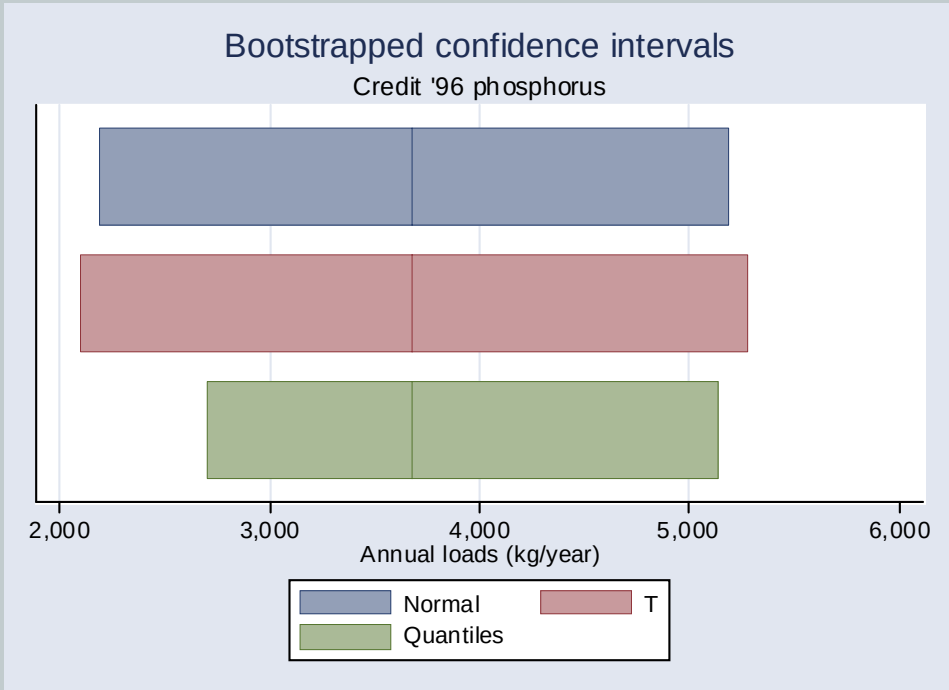
Estimator


Estimator bootstrap of Credit '96 phosphorus
Frequency
0
200
400
600
800
5000
10000
15000
20000
Annual load (kg/year)

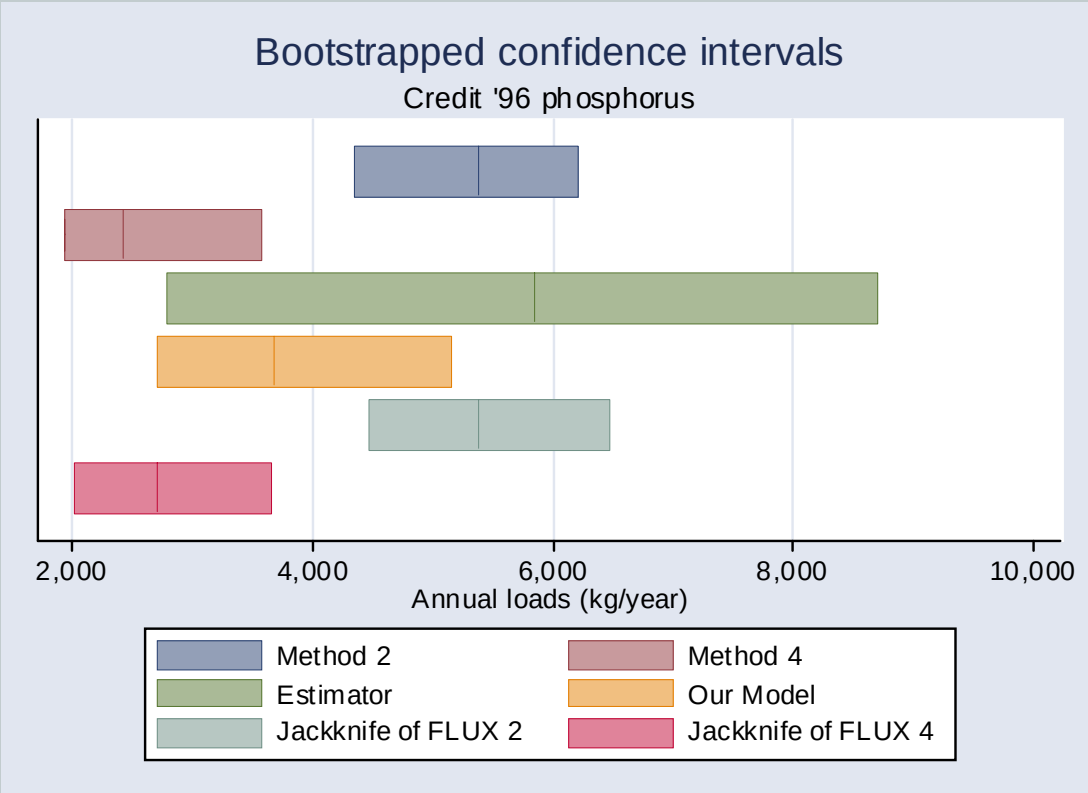

Bootstrapped confidence intervals
Credit '96 phosphorus
2,000
4,000
6,000
8,000
10,000
Annual loads (kg/year)
Normal
T
Quantiles

Our Model

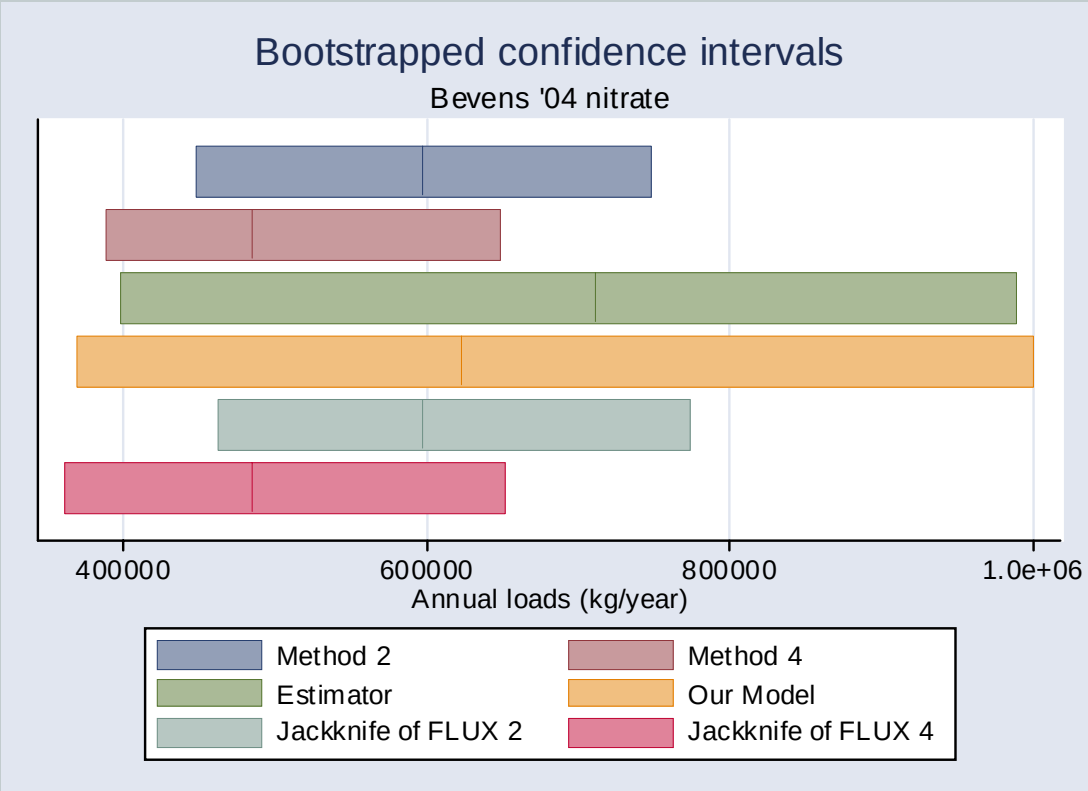

Our model bootstrap of Credit '96 phosphorus
Frequency
0
200
400
600
800
1000
1200
2000
4000
6000
8000
10000
12000
14000
16000
Annual load (kg/year)


Bootstrapped confidence intervals
Credit '96 phosphorus
2,000
3,000
4,000
5,000
6,000
Annual loads (kg/year)
Normal
T
Quantiles

Comparison of Quantile and Jackknife Confidence Intervals



Comparison of Quantile and Jackknife Confidence Intervals



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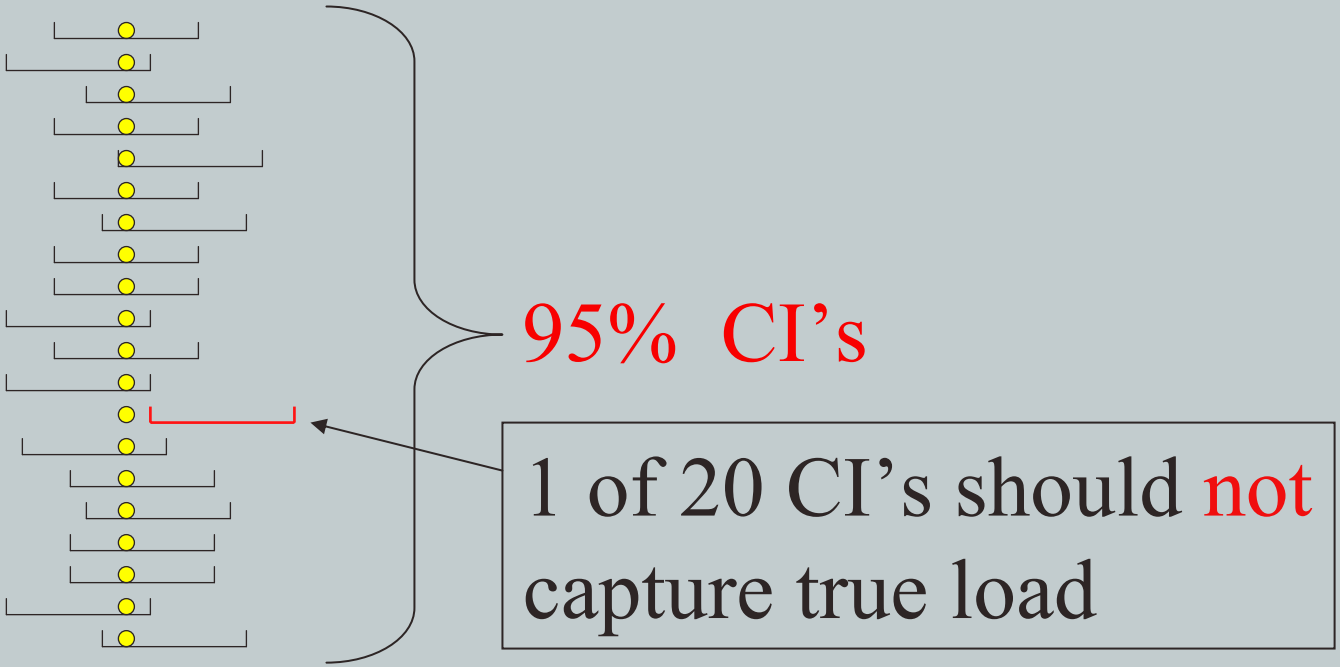
River Simulation

- Confidence Intervals (CI's)
- How frequently do our CI's capture true load?

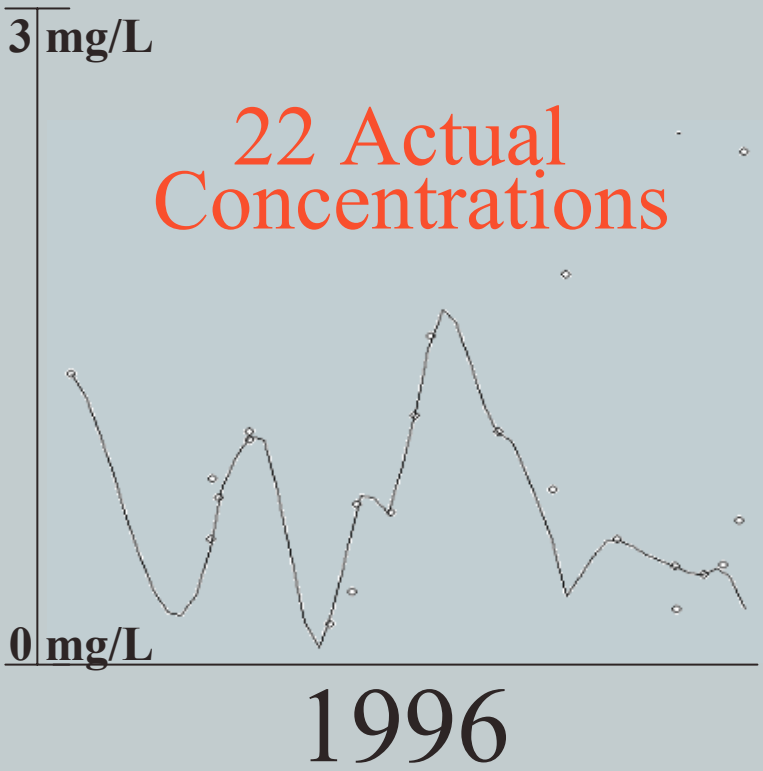


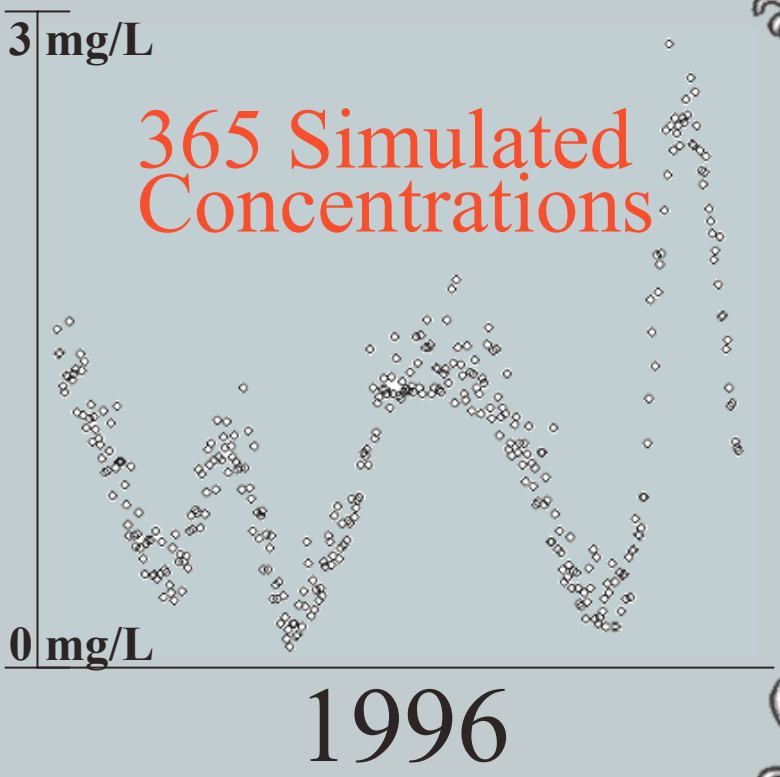
River Simulation

- Create a river with known yearly load
- Incorporate realistic characteristics
  - Based on Credit River in 1996
- Simulation fills in missing sample data

River Simulation

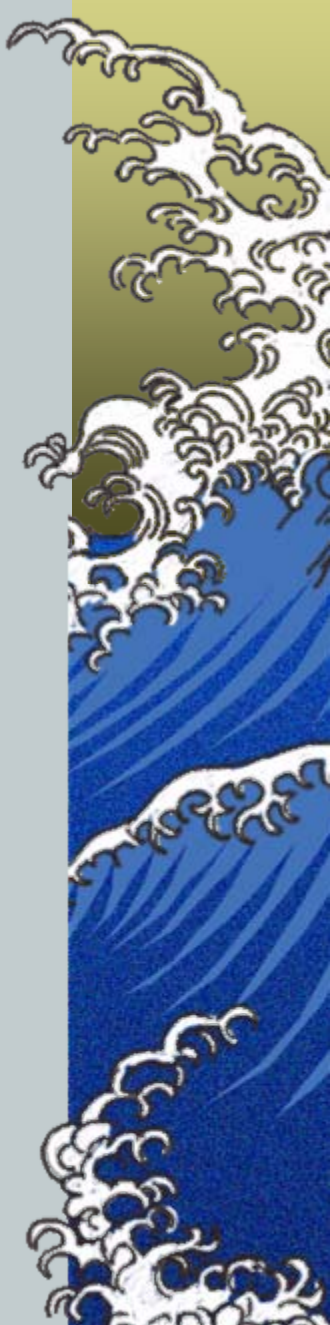
- Credit River 1996 Nitrate Concentration





Creating CI's by Bootstrapping

- Sample from simulated concentrations
- Bootstrap the sample
- Generate load estimates (FLUX 2 and 4)
- Repeat the process 1000 times to get 1000 CI's
- What percentage of CI's capture true load?



Evaluating Confidence Intervals

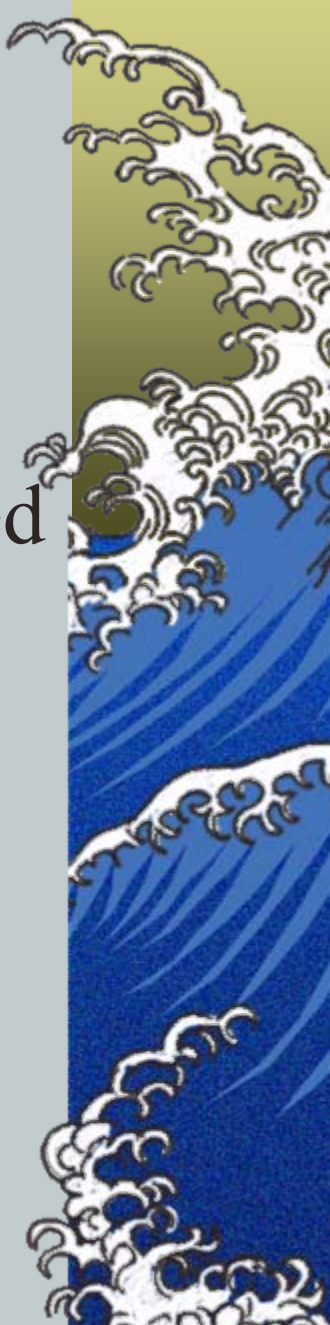
Percentage of 95% CI's capturing simulated true loads

	Bootstrapping				Jackknifing
	Normal	T-Dist	Quantile	BCa	Jackknife
FLUX 2	98.0	98.4	98.1	98.0	98.8
FLUX 4	92.1	93.2	93.0	88.8	93.2

- 95% of the CI's should capture true load
- Methods produce similar coverage rates
- Narrow interval is preferable

CI's: Bootstrapping vs. Jackknifing

- Bootstrapped quantile intervals are approximately 17% smaller than jackknifed intervals
- Smaller interval with same coverage rate means less estimate uncertainty



Simulation Improvements

- Broaden the scope of simulation
  - Begin with different sample data
  - Incorporate other concentration simulations
  - Implement other sampling strategies

Conclusion

- Bootstrapping provides tighter CI's than jackknifing
- FLUX estimates load sufficiently
  - Additional predictors may improve accuracy
- Further simulations would enhance results

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