BASED ON WSC 2015 TUTORIAL

BOOTSTRAP CONFIDENCE BANDS
AND
GOODNESS-OF-FIT TESTS
IN
SIMULATION INPUT/OUTPUT MODELLING

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Introduction to Bootstrapping

First let me emphasise that Random Variables are a very important part of the Statistical Uncertainty that occurs in Simulation Modelling. Bootstrapping is a very simple method of studying this uncertainty, which it does by answering a question that we can ask of all Random Variables. Indeed it is the ONLY single question you can ask about a Random Variable.

Bootstrapping is all about answering this single question in a simple way!

Before we look at this question, let me summarise the Course so far: You will have been introduced to the idea of using Statistical Simulation Models to represent Real Life systems of interest. Use of the word Statistical highlights the fact that these systems are subject to statistical variation which can occur in the Input quantities, or which can occur within the System themselves. In a simulation model these quantities are treated as random variables which are generated by random variate generators.

A simple example is an M/M/1 queue where the first M denotes customers who arrive randomly with interarrival times that are exponentially distributed with PDF

$$\lambda e^{-\lambda t},\ t \geq 0$$

where λ is the mean arrival rate. These interarrival times are the Inputs.

Within the queue the customers are served by a single server indicated by the '1'. The times to serve each customer are system generated random quantities with the second M which indicating that the service times are also exponentially distributed

$$\mu e^{-\mu}\ ,\ t \geq 0$$

with μ the mean service rate of the server when busy.

In general, the quantity of interest is regarded as Output. This is will depend depend on the random input quantities and the system generated random quantities, so will also be a quantity that varies statistically.

In our example we might take the quantity of interest to be the mean waiting time in the queue, which happens to be known, with

$$W(\lambda, \mu) = \frac{\lambda}{\mu(\mu - \lambda)}$$

For more complicated queues the formula is not always so simple, which is why the simulation model is needed to estimate the Output value numerically.

Even when the formula for the output is known, numerical estimation is still required to estimate the parameters, as in our M/M/1. We could consider this numerical estimation to be part of Input Modelling, as parameter values are needed as inputs in order to run the Simulation

Model. But our real interest is in estimating the Output and its statistical variability. So estimating the parameters could equally be thought of as part of the Output Modelling.

Personally I think that trying to make a distinction between Input and Output Modelling is unhelpful and confusing. So though I will be paying lip service to these terms I will actually simply be focusing on Random Variables as these are a big source of uncertainty in Simulation.

You will have been shown, in the previous lectures, how to estimate the parameter using Maximum Likelihood (ML) estimation. This does this by fitting parameters to data. The data can have been obtained in different ways, but will depend on the parameters so are random variables which depend on the parameters. ML works by fitting the probability distributions to the data. Moreover, you will have been shown the attractive property of ML estimators in allowing the accuracy of the ML estimates to be assessed using Asymptotic Normal Theory, which shows that, as more data are obtained the parameter estimates become increasingly close to normally distributed which moreover can be estimated, so that confidence intervals can be obtained that allow one to gauge how accurate are the results.

Bootstrapping steps in here as it offers a simple alternative to Asymptotic Normal Theory.

One thing to realise at the outset is that there often is a common misconception that bootstrapping gives you something for nothing and that it somehow allows one to estimate parameters more accurately without having to obtain more data. This has led to an initial mistrust, when bootstrapping was first proposed. Bootstrapping is summarised in Chapter 4 of my book Cheng (2017).

What bootstrapping does is to give one an easy numerical way of assessing the accuracy of results wihout having to invoke the more complicated mathematics of asymptotic theory, moreover without requiring one to obtain more results by running more simulations.

A Point to Note: Though I have introduced bootstrapping as an attractive alternative to asymptotic normal theory when using ML, it has more **general uses**, as it solves the following

Basic Statistical Question

$$\boxed{F_Y(y)} \longrightarrow \boxed{\mathbf{Y}} \longrightarrow \boxed{T(\mathbf{Y})} \longrightarrow \boxed{F_T(t)}$$

Distribution of Y	Sample	Test Statistic	Distribution of T

What is the Distribution of $T(\mathbf{Y})$?

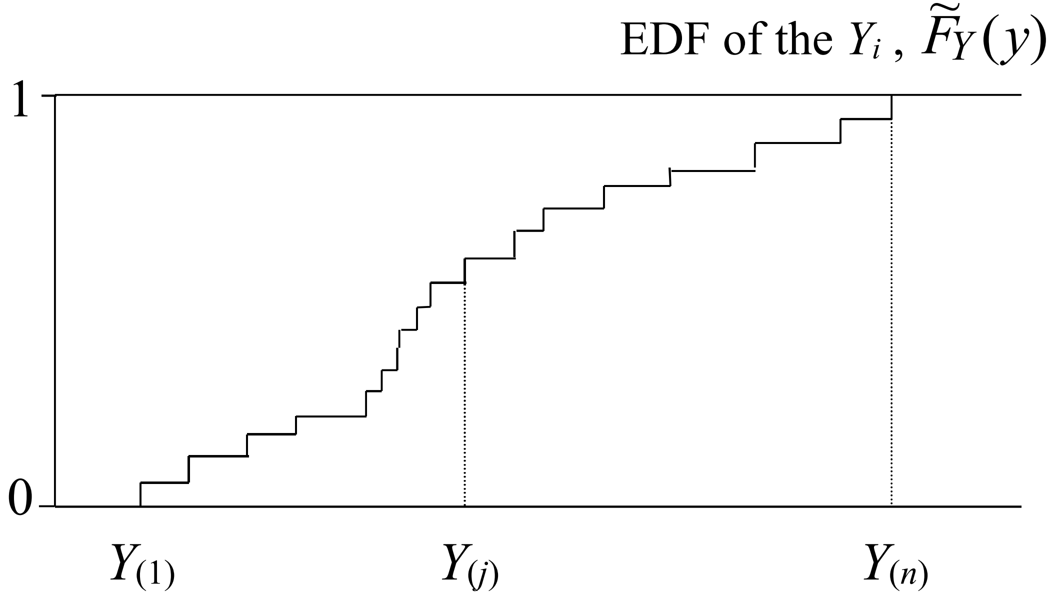
Example. Voting in an Election. We have a constituency of voters.
Distribution of interest is how they will vote.
Sample is an Opinion Poll.
Test Statistic of interest to a candidate is the proportion voting for her/him.

Bootstrapping depends on the properties of:

The ***empirical distribution function* (EDF)** defined as

$$\widetilde{F}_Y(y) = \frac{\#\ of\ \ Y's \le y}{n}$$

where Y_i, $i = 1, 2, \ldots, n$ is a *random sample*



The EDF estimates the *cumulative distribution function* (CDF) of *Y*.

Fundamental Theorem of Sampling

EDF → CDF with probability one, as n → ∞

? How does this and bootstrapping help with:

The Basic Sampling Question

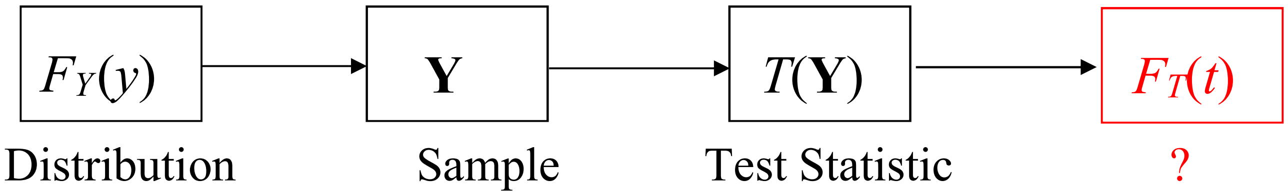
$$\boxed{F_Y(y)} \longrightarrow \boxed{\mathbf{Y}} \longrightarrow \boxed{T(\mathbf{Y})} \longrightarrow \boxed{F_T(t)}$$

Distribution	Sample	Test Statistic	?

What is the Distribution of T(Y)?

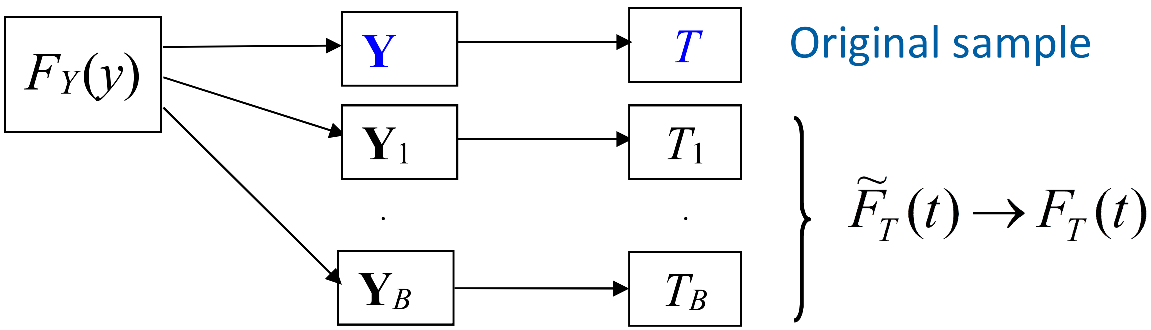
? How does this and bootstrapping help with:

The Basic Sampling Question



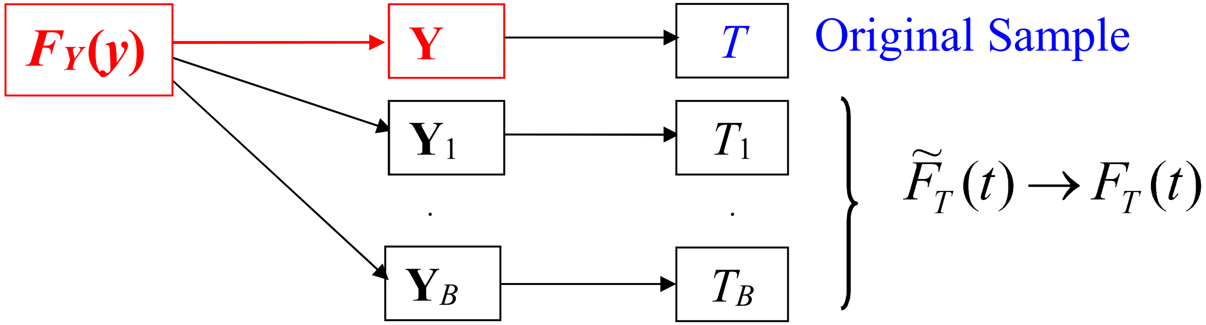
What is the Distribution of $T(\mathbf{Y})$?

The Basic Statistical Question is answered if we could replicate the process a large number of times



Problem: Sampling from the Distribution often difficult (Expensive, time consuming)

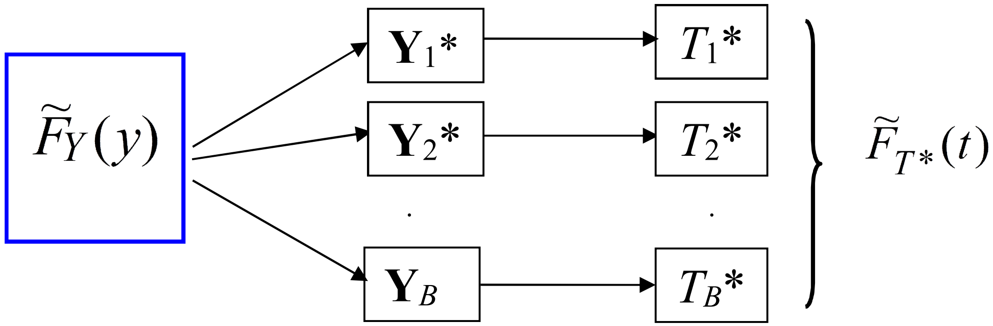
Let us focus on the difficult part:



Note that the Fundamental Theorem applies to this original sample Y:

EDF $\tilde{F}_Y(y) \to F_Y(y)$ **as** $n \to \infty$

Replace $F_Y(y)$ **by EDF** $\tilde{F}_Y(y)$ **of original sample to get the Bootstrap Version**



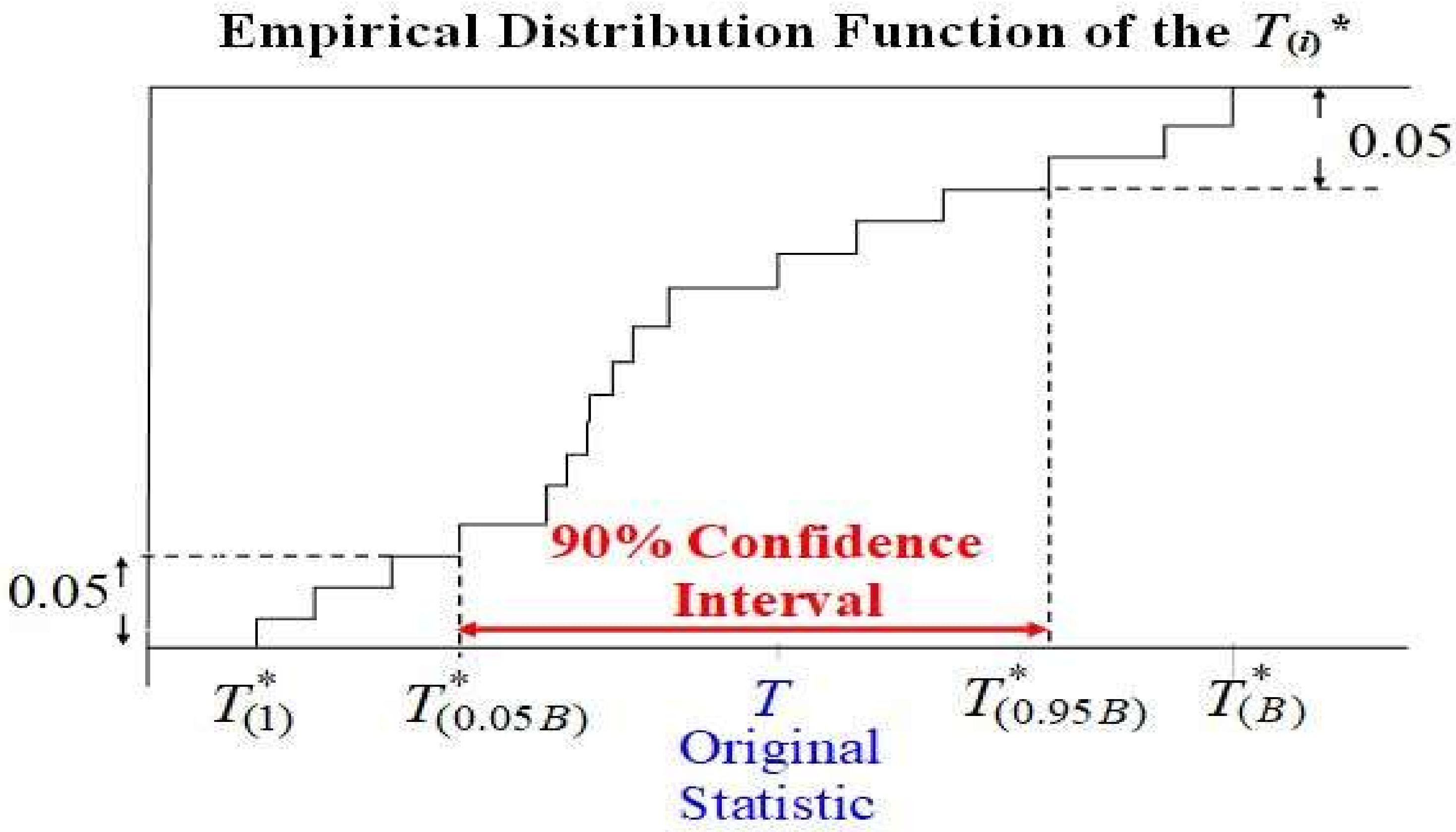
The pseudocode for the entire bootstrap process is as follows:

// $\boldsymbol{y} = (y(1), y(2), ..., y(n))$ is the original sample.
// $T=T(\boldsymbol{y})$ is the calculation that produced T from $\boldsymbol{y}$.

```
For k = 1 to B
{
  For i = 1 to n
  {
    j = Int [1 + n × Unif()]  // Unif ~ U(0,1)
    y*(i) = y(j)
  }
  T*(k) = T(y*)
}
```

Confidence Intervals

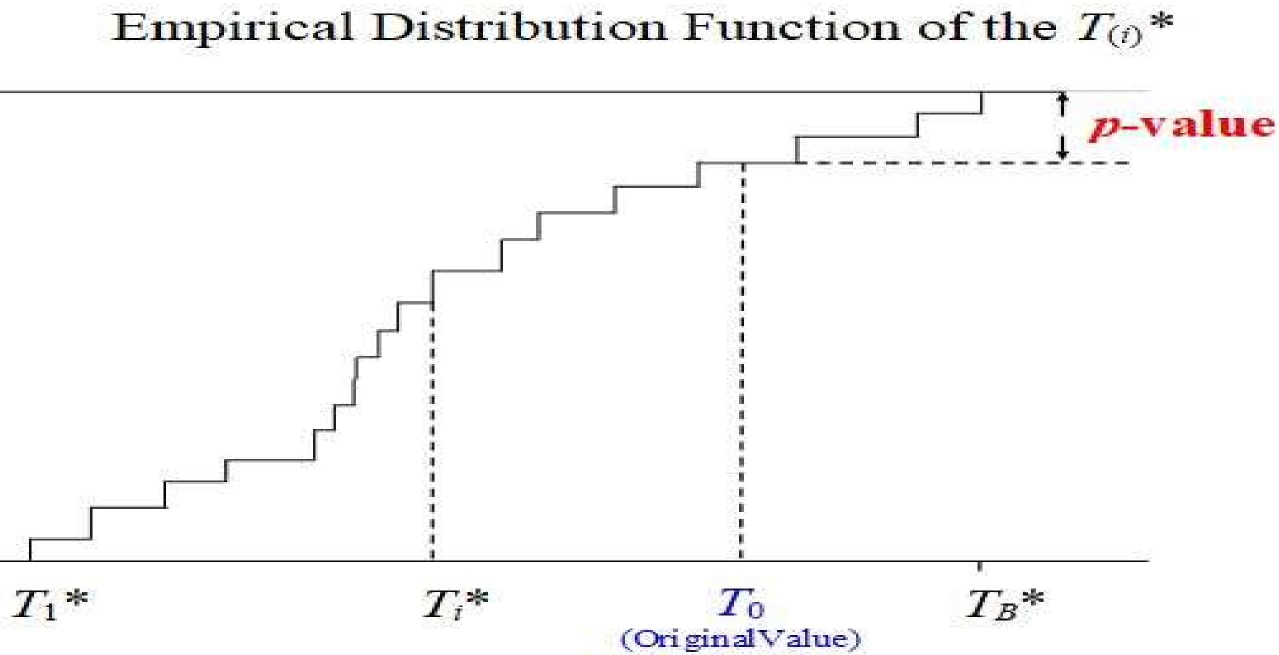
The EDF of the bootstrap sample estimates the distribution of *T*.



The *p*-value the original statistic value, T_0, is

$$p = 1 - \widetilde{F}^*(T_0).$$

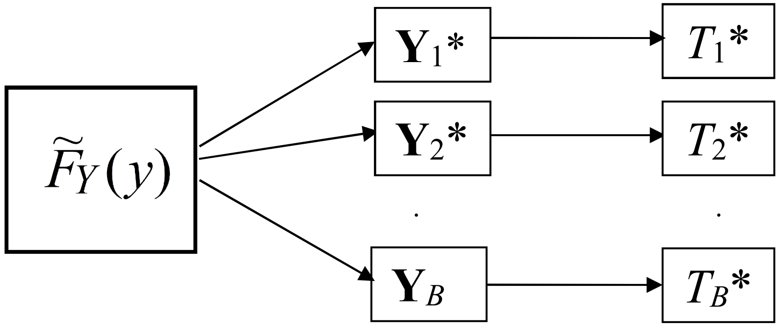
If the *p*-value is small then T_0 is in some sense unusual.



Excel Example 1 Here

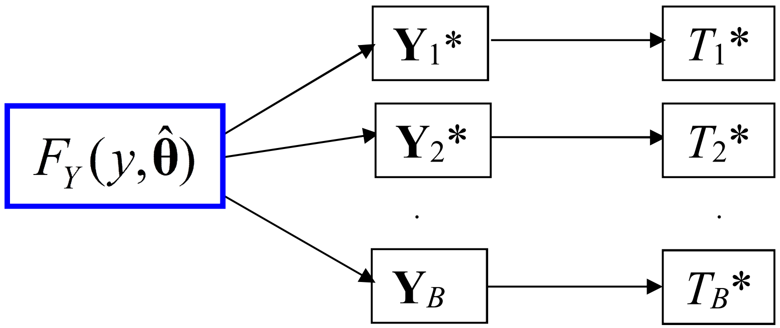
BasicBootstrapMeanMedian

Basic Bootstrap



If we have a parametric representation of $F_Y(y)$, possibly with estimated parameters
We can use the:

Parametric Bootstrap



Excel Example 2 Here ParametricBootstrap Mean/Median

We usually need to fit a parametric statistical model to data, as we did in our Example 2, need to use parametric bootstrapping. This has already been covered in the Course. We use a real data sample to remind you of what is needed.

The sample occurs in an Excel Toll Booth Example which we will also be using to discuss other issues in what follows.

The sample comprises47 observed times in seconds taken to process vehicles at a toll booth waiting to cross a bridge.

4.3	10.9	4.7	4.7	3.1	5.2	6.7	4.5	3.6	7.2
6.6	5.8	6.3	4.7	8.2	6.2	4.2	4.1	3.3	4.6
6.3	4.0	3.1	3.5	7.8	5.0	5.7	5.8	6.4	5.2
8.0	10.5	4.9	6.1	8.0	7.7	4.3	12.5	7.9	3.9
4.0	4.4	6.7	3.8	6.4	7.2	4.8			

We suppose that these are gamma variates with PDF:

$$f_G(y,\alpha,\beta)=\Gamma^{-1}(\alpha)\beta^{-\alpha}y^{\alpha-1}\exp(-y/\beta)$$

We shall use *Maximum Likelihood Estimation.* to obtain

ML Estimates $\hat{\alpha},\hat{\beta}$

Maximize the Log likelihood:

$L_G(\alpha,\beta,\mathbf{x})=-n[\log(\Gamma(\alpha))-\alpha\log\beta]-(\alpha-1)\sum_{j=1}^{n}\log(x_j)-\beta^{-1}\sum_{j=1}^{n}x_j$.A very convenient general numerical optimization method for doing this is the well-known simplex search procedure proposed by Nelder and Mead (1965).

$\boldsymbol{\theta}=(\alpha,\beta)$ ML estimator is $\hat{\boldsymbol{\theta}}=(\hat{\alpha},\hat{\beta})$

Asymptotic probability distribution of $\hat{\boldsymbol{\theta}}$ is known to be normal.

As the sample size $n \to \infty$,

$$\hat{\boldsymbol{\theta}} \sim N\{\boldsymbol{\theta}_0, \mathbf{V}(\boldsymbol{\theta}_0)\}$$

we can use

$$\hat{\boldsymbol{\theta}} \sim N\{\boldsymbol{\theta}_0, \mathbf{V}(\hat{\boldsymbol{\theta}})\}$$

where

$$\mathbf{V}(\hat{\boldsymbol{\theta}}) = [\, -\partial^2 \mathbf{L}(\boldsymbol{\theta}, \mathbf{y}) / \partial \boldsymbol{\theta}^2 \big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} \,]^{-1}$$

The second derivative of the loglikelihood, $\partial^2 \mathbf{L}(\boldsymbol{\theta}, \mathbf{y}) / \partial \boldsymbol{\theta}^2$, that appears in the expression for $\mathbf{V}(\hat{\boldsymbol{\theta}})$ is called the *Hessian* (of **L**). A numerical procedure is needed for this inversion.

A (1-α)100% confidence interval for the coefficient θ_1 is

$$\hat{\theta}_1 \pm z_{\alpha/2} \sqrt{V_{11}(\hat{\boldsymbol{\theta}})}$$

where $z_{\alpha/2}$ is the upper 100α/2 percentage point of the standard normal distribution.

Show Excel Examples 3 and 4 here

Example 3 gives the Gamma fit to Toll Booth Data. (show Optimize & Fit Sheets)

For comparison:

Example 4 gives the Normal fit to Toll Booth Data. (shoe Optimize & Fit Sheets)

Question: are either fits satisfactory?

Classical Goodness of Fit

Does the model that we have fitted actually fit the data very well?

Use a *goodness of fit test* (GOF test).
A popular test is the *chi-squared goodness of fit test*.
(i) The test statistic is easy to calculate
(ii) It has a *known* chi-squared distribution, under the null.

But (i) It is not all that powerful
(ii) The user has to decide how to group the data

The best GOF tests compare the fitted CDF $F_Y(y, \hat{\boldsymbol{\theta}})$ with the EDF $\tilde{F}_Y(y)$

Such tests are called *EDF goodness of fit tests*.

The ***Anderson - Darling*** test, is the best by far. (Stephens, 1974)

But The critical values are very dependent on the model being tested

This means that different tables of test values are required for different models (see d'Agostino and Stephens, 1986).

***Anderson-Darling test statistic*:**

$$A^2 = \int \frac{\left(\widetilde{F}_Y(y) - F_Y(y)\right)^2}{F_Y(y)(1 - F_Y(y))} dF_Y(y)$$

$$= -\sum_{i=1}^{n} (2i-1)[\ln Z_i + \ln(1 - Z_{n+1-i})]/n) - n$$

where $Z_i = F(Y_{(i)}, \hat{\boldsymbol{\theta}})$

The basic idea in using a goodness of fit test statistic is as follows:

If the sample has really been drawn from $F_0(y)$ then A^2 will not be large.

This follows from the Fundamental Theorem $\widetilde{F}(y) \to F_0(y)$

Thus A^2 will be a typical value. But what is a typical value?

Typical values given by its null distribution

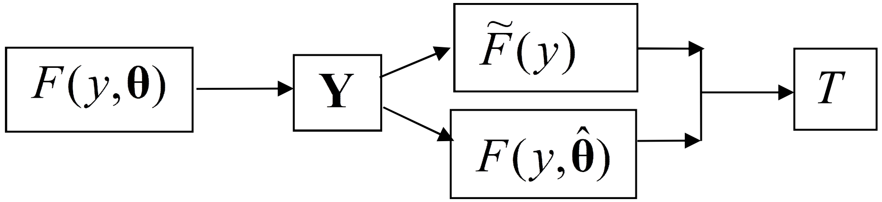
If the sample is drawn from a distribution different from $F_0(y)$ then A^2 will be large.

Its *p - value* will then be small.

This indicates that T has *not* been drawn from the supposed null distribution.

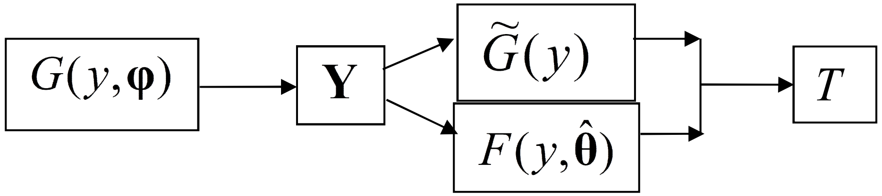
How a GOF Test Works

Null Case: Fitted model $F(y,\hat{\boldsymbol{\theta}})$ is the correct



Null Distribution where T is likely to be small

Alternative Case: Fitted model $F(y,\hat{\boldsymbol{\theta}})$ is an incorrect



Non-Null Distribution where T is likely to be large

GOF test hinges on being able to calculate the null distribution of *T*.

The null distribution of the Anderson-Darling statistic is difficult to obtain. So not used as often as it should in practice.

Bootstrapping provides a simple and accurate way of resolving this problem.

Bootstrap Calculation of the Null Distribution of a GOF Test Statistic, *T*

$$
\begin{tikzcd}
 & & \boxed{\tilde{F}(y \mid \mathbf{Y}_i^*)} \arrow[dr] & \\
\boxed{F(y,\hat{\boldsymbol{\theta}})} \arrow[r] & \boxed{\mathbf{Y}_i^*} \arrow[ur] \arrow[dr] & & \boxed{T_i^*} \\
 & & \boxed{F(y,\hat{\boldsymbol{\theta}}_i^*)} \arrow[ur] &
\end{tikzcd}
$$

$i = 1,2, \ldots, B$

Show Excel Example 3 here again

GammaFitToll Booth Example only now including Bootstrapping Sheet

Model Uncertainty:

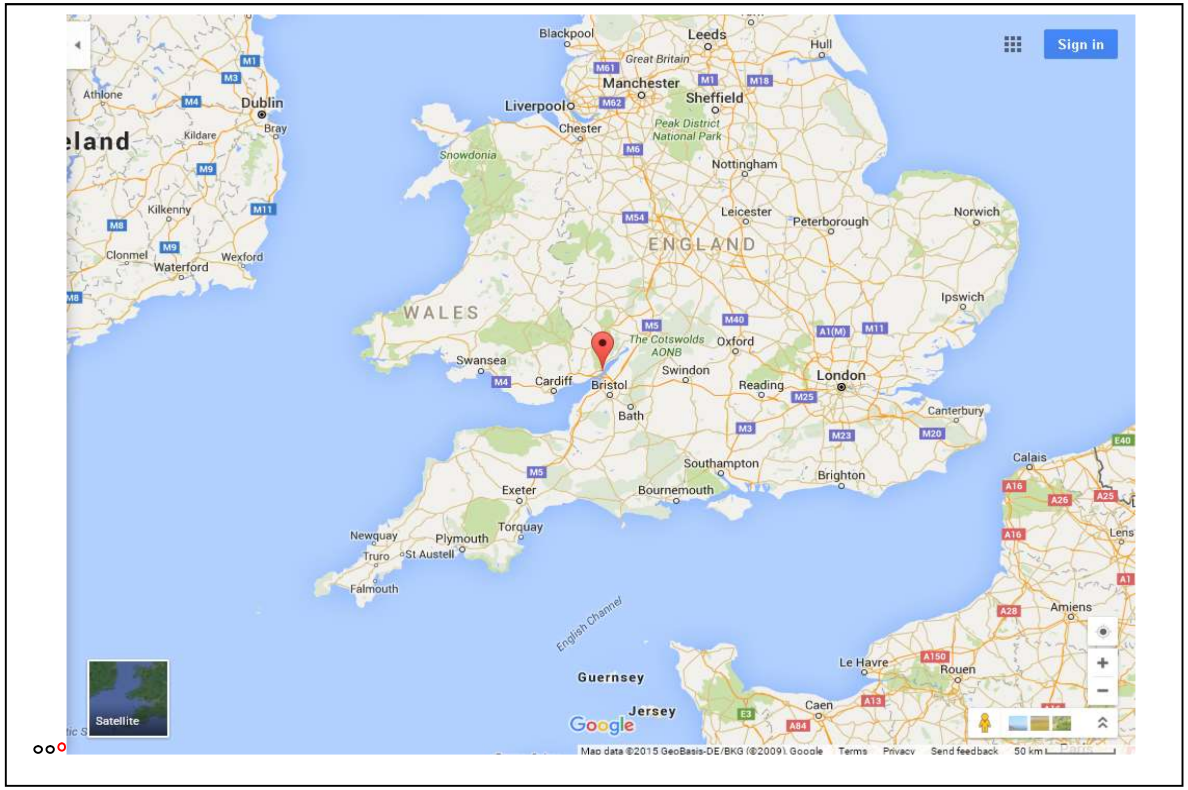
Our discussion so far has focused on how bootstrapping is useful for measuring the variability of a statistical quantity of interest.
In the basic bootstrap the actual probability distribution of the statistical quantity is not particular concern. However when using parametric bootstrapping which applies to particular distribution like the example of the M/M/1 queue involves only the exponential distribution.

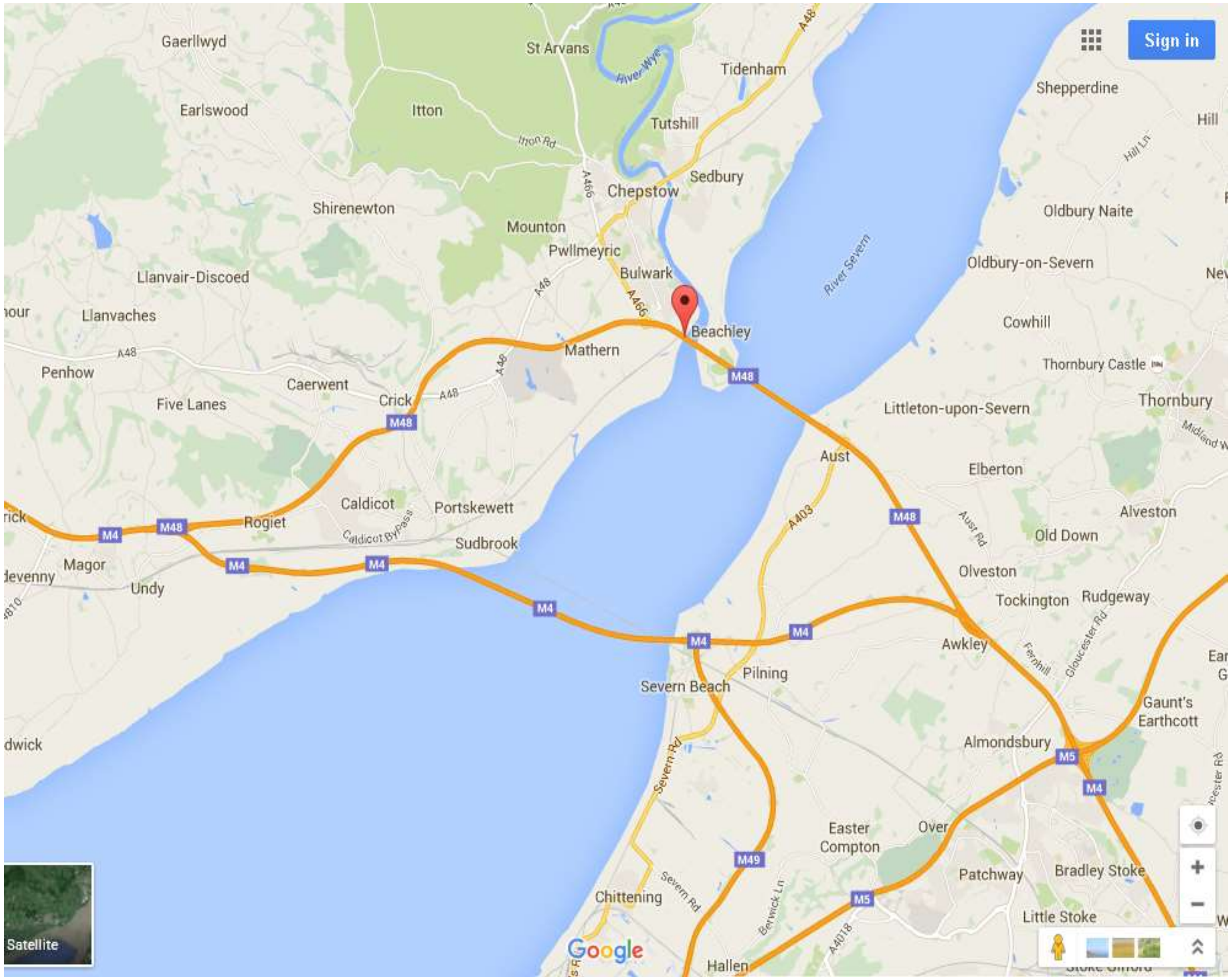
In a full simulation model, various different probability distributions may be involved. In the M/M/1 queue, the interarrival times and the service times are both assumed to have the Exponential Distribution. This is often okay for interarrival times but the service times can be different.

We have already mentioned one example, the Toll Booth Example where we have tried both the gamma and normal distributions. We now describe this example in more detail, as it is a good example of or next topic which focuses on use of Bootstrapping in Output Analysis.

Toll Booth Example

Operation of toll booths of the old Severn River bridge, UK, Griffiths and Williams (1984)




Sign in
Gaerllwyd
St Arvans
Tidenham
Shepperdine
Earlswood
Itton
Tutshill
Sedbury
Chepstow
Shirenewton
Mounton
Pwllmeyric
Bulwark
Oldbury Naite
Oldbury-on-Severn
Llanvair-Discoed
Llanvaches
River Severn
Beachley
Cowhill
Penhow
Mathern
Thornbury Castle
Five Lanes
Caerwent
Crick
Thornbury
Littleton-upon-Severn
Aust
Elberton
Caldicot
Portskewett
Alveston
Rogiet
Old Down
Sudbrook
Magor
Olveston
Undy
Tockington
Rudgeway
Awkley
Pilning
Severn Beach
Gaunt's Earthcott
Almondsbury
Easter Compton
Over
Patchway
Bradley Stoke
Chittening
Little Stoke
Hallen
Satellite
Google
M4
M48
M5
M49
A48
A466
A403

Unsatisfactory Original Bridge. Can you see why?

Each toll booth was modelled as a single server queue

Simulation model simulates the service of *l* vehicles.

Of interest: W - the average vehicle waiting time in the queue.

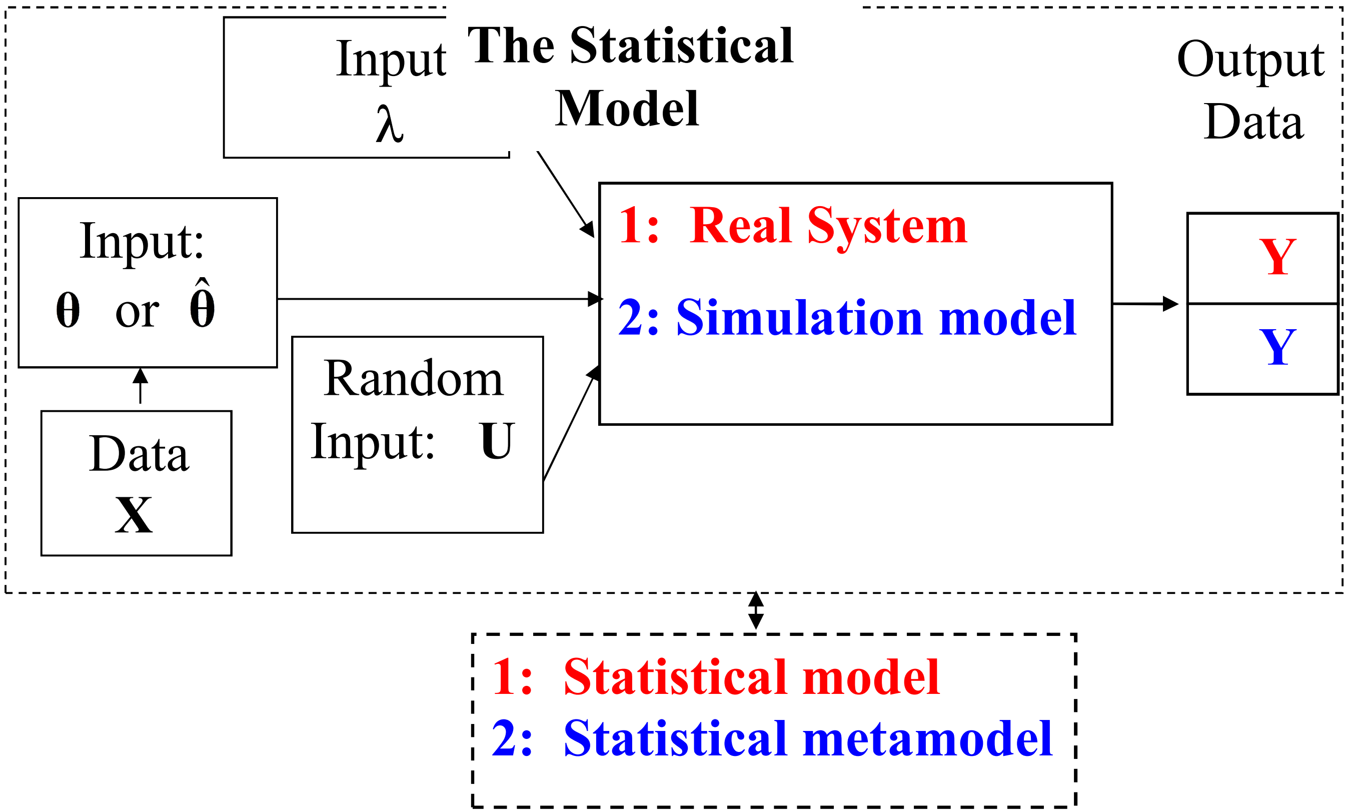
Service time data: Time taken for a vehicle to pay at the toll booth before crossing the bridge.

1 Parameter Uncertainty

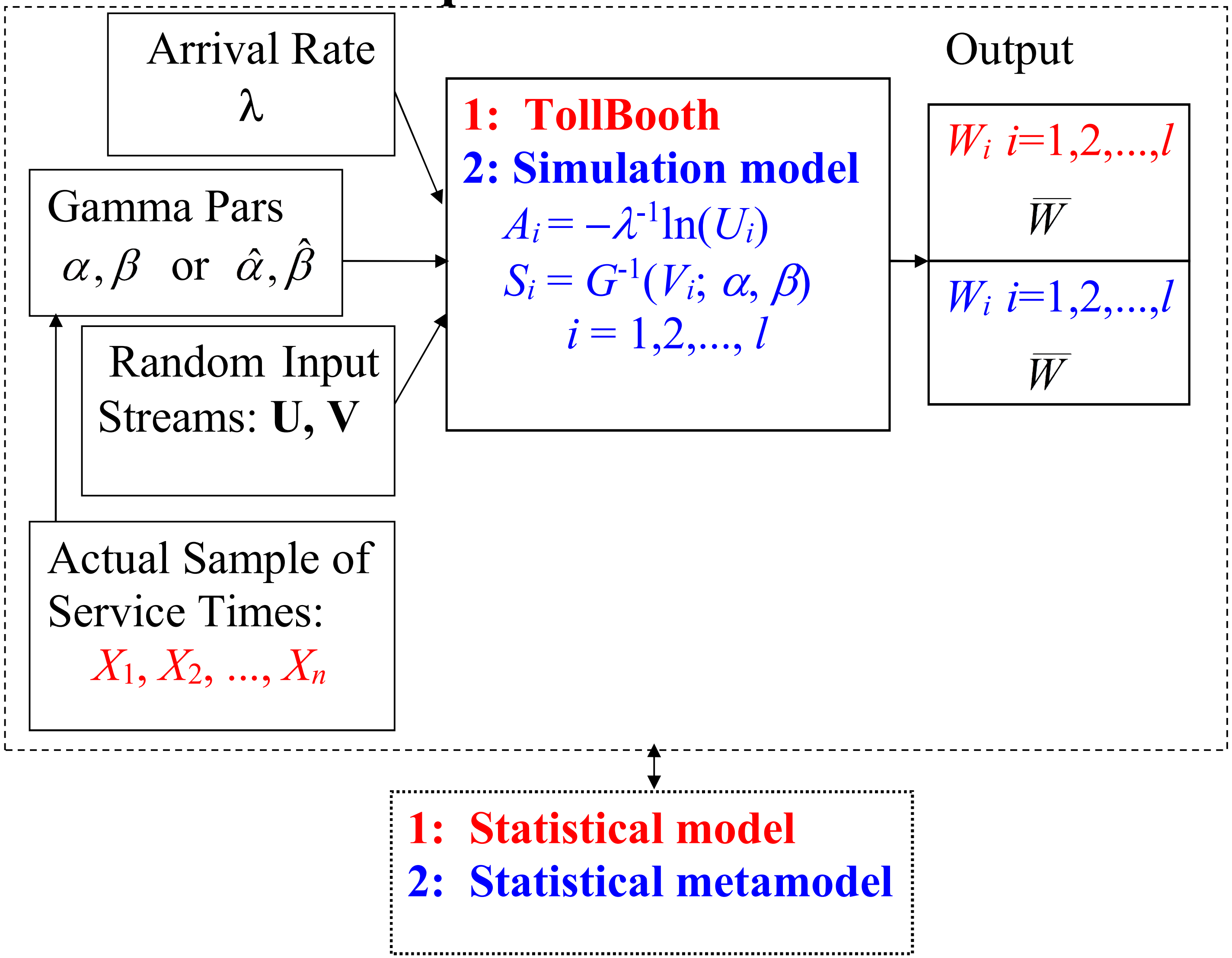
Poisson arrivals (Exponential Interarrivals)
Gamma service times (Both part of the Input Uncertainty in this Course)

2 Simulation Uncertainty

Vehicle Waiting Time (Simulation Uncertainty in this Course)


The Statistical Model
Input
λ
Input:
θ or θ̂
Data
X
Random Input: U
1: Real System
2: Simulation model
Output Data
Y
Y
1: Statistical model
2: Statistical metamodel

Toll BoothExample



Use of Parametric Functions in Output Analysis

Suppose are real interest is not in the parameters themselves but in a function of $\boldsymbol{\theta}$, $g(\lambda, \boldsymbol{\theta})$, say, where $g(\lambda, \boldsymbol{\theta})$ is a function of λ, $\lambda_0 < \lambda < \lambda_1$

What is the MLE of $g(\lambda, \theta)$, $\lambda_0 < \lambda < \lambda_1$?

Answer is simple: The MLE of g is $\hat{g} = g(\lambda, \hat{\boldsymbol{\theta}})$.

Toll booth example: The steady state mean waiting time in the queue is known to be

$$\boldsymbol{W}(\boldsymbol{\lambda}|\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{\boldsymbol{\lambda}(\mathbf{1}+\boldsymbol{\alpha})\boldsymbol{\alpha}\boldsymbol{\beta}^{\mathbf{2}}}{\mathbf{2}[\mathbf{1}-\boldsymbol{\alpha}\boldsymbol{\beta}\boldsymbol{\lambda}]} \quad \lambda_0 < \lambda < \lambda_1$$

Its ML estimated is simply $W(\lambda|\hat{\alpha},\hat{\beta})$ where we have replaced α, β by $\hat{\alpha},\hat{\beta}$:

An approximate (1-α)100% confidence interval for $g(\lambda, \boldsymbol{\theta})$ at a given λ is then

$$g(\lambda,\hat{\boldsymbol{\theta}}) \pm z_{\alpha/2}\sqrt{(\partial g/\partial\boldsymbol{\theta})\big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}^{T}\,\mathbf{V}(\hat{\boldsymbol{\theta}})(\partial g/\partial\boldsymbol{\theta})\big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}}$$

This is conventionally called **the delta-method**.

The above shows how to calculate Confidence Intervals for $g(\lambda, \theta)$**, but these apply only for individual λ and are not suitable if confidence intervals for several diferent λ are needed simultaneously.**

Excel Examples 3 here again to give the Bootstrap Answer
Gamma Fit to Toll Booth Data now including the PerformanceIndex page

Note
I have used Performance Index (PI) and Performance Measure (PM) synonymously. In the case of the Toll Booth example the PI/PM is simply the expected waiting time W

Confidence Bands for Functions with Estimated Parameters

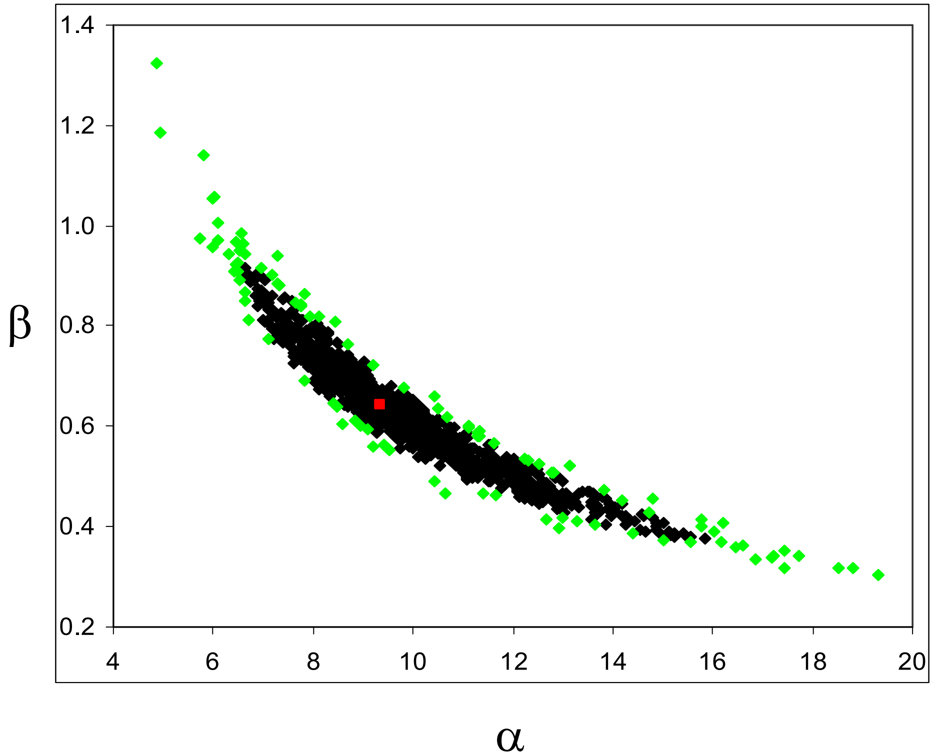
As we have aleady seen, a confidence interval for the case $W(\lambda|\hat{\alpha},\hat{\beta})$ at a given λ. is straightforward. But what about constructing a Band with upper and lower limits

$$\boldsymbol{WU(\lambda|\hat{\alpha},\hat{\beta})} \quad \lambda_0 < \lambda < \lambda_1$$
$$\boldsymbol{WL(\lambda|\hat{\alpha},\hat{\beta})} \quad \lambda_0 < \lambda < \lambda_1$$

Within which the **entire** MLestimate $\boldsymbol{W(\lambda|\hat{\alpha},\hat{\beta})} \quad \lambda_0 < \lambda < \lambda_1$ **lies?**

This question can be answered using Bootstrapping.

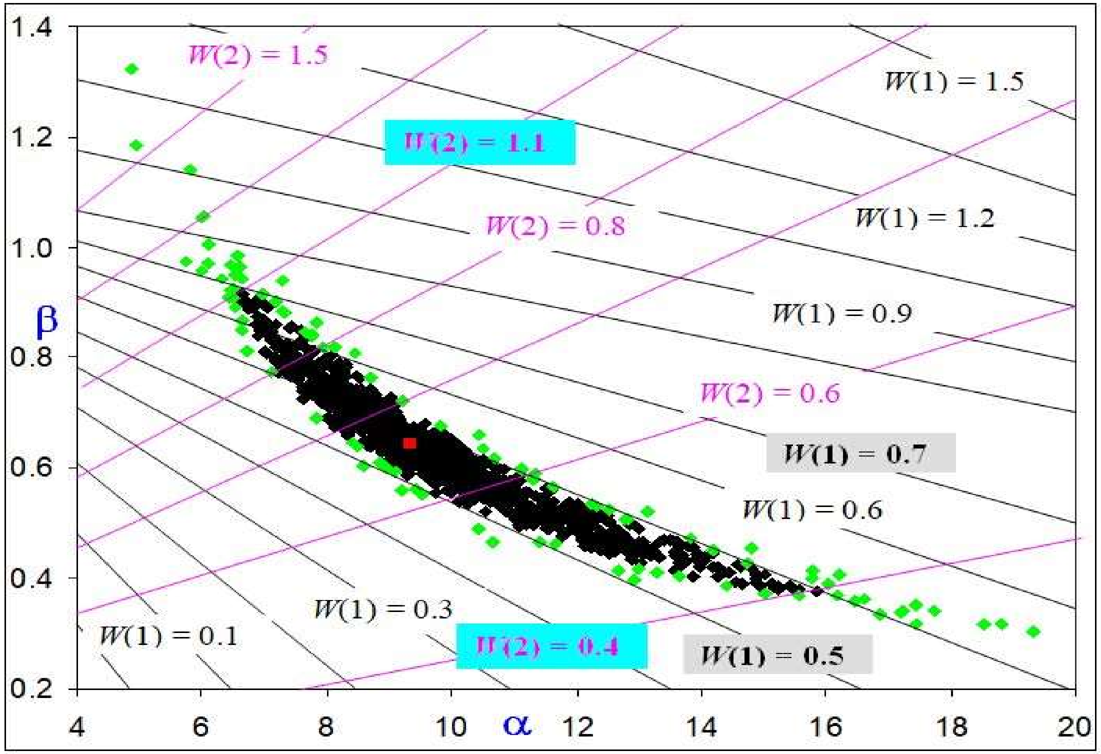
Use of ScatterPlot for calculating confidence bands



Red point: Location of the parameter MLEs $\hat{\alpha}, \hat{\beta}$

Black points:{ **R**} = 90% of the total number of points with highest likelihood values

Green points: {**Not in R**} = 10%, the Rest of the points with lowest likelihood values



Contours of $W = [\lambda(1+\alpha)\alpha\beta^2]/[2(1-\alpha\beta\lambda)]$ at a given λ

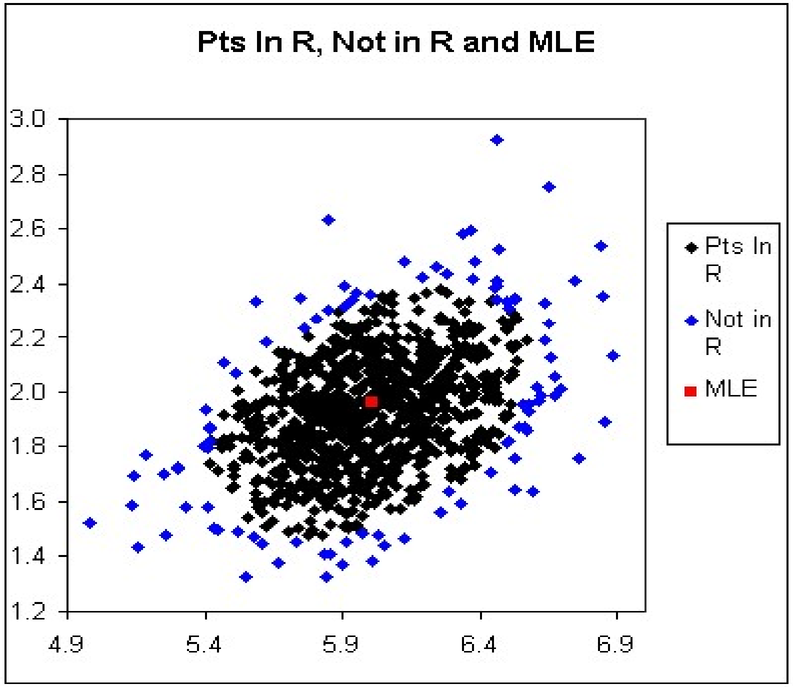
Confidence band is

$W_{min}(\lambda) = \min_R W(\boldsymbol{\lambda} | \alpha,\beta)$ $W_{max}(\lambda) = \max_R W(\boldsymbol{\lambda} | \alpha,\beta)$ $\lambda_0 < \lambda < \lambda_1$

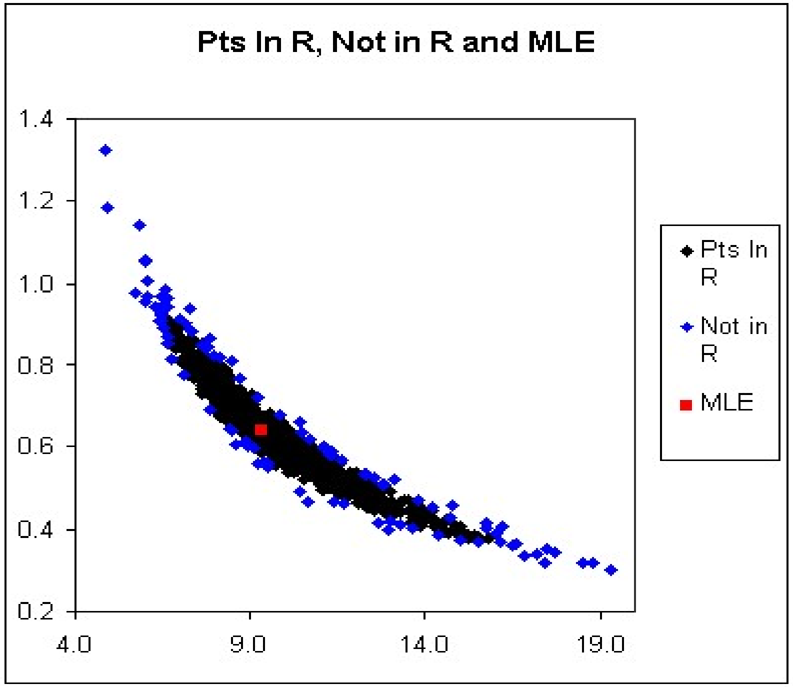
Example 5 Here to show difference between CIs and Bands

Reparametrized parameters makes the band more accurate and symmetrical

$\mu = \alpha\beta \quad \sigma = \alpha\beta^2$

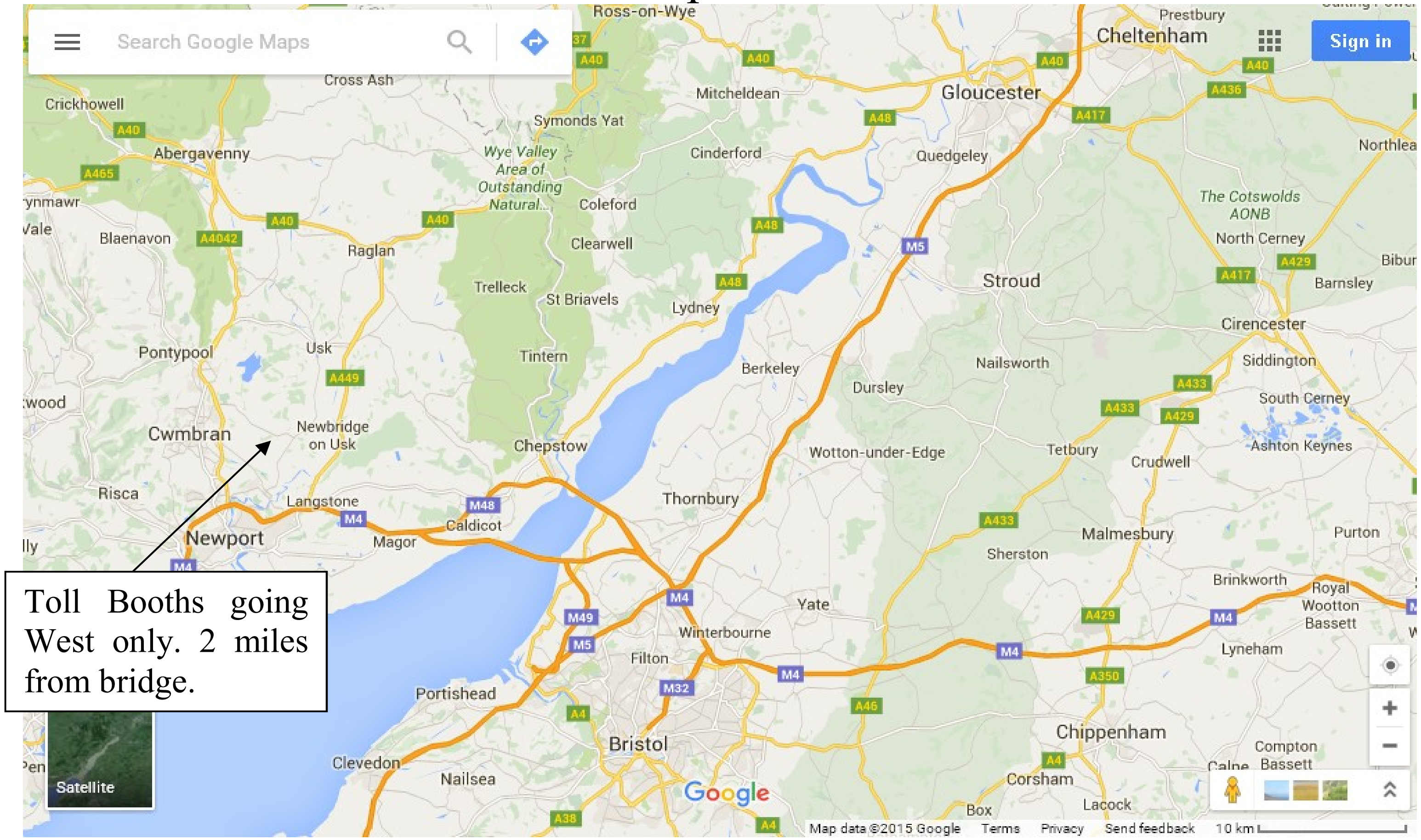


$\alpha = \mu^2/\sigma \quad \beta = \sigma/\mu$



Second Bridge. Built after OR Simulation Study

Additional Recommendation Adopted



Review of the Role of Parametric Bootstrapping (BS) as so far used in the Toll Booth Example.

(1) It enables the accuracy of estimate of the parameters to be assessed of the assumed Gamma service times. (By BS sampling of the estimates)

(2) It enables the suitability of the assumption of the gamma service times to be assessed. (Using BS GoF Testing)

(3) It enables the accuracy of the estimate of the Performance Measure (PM) to be assessed when its mathematical form is a known function of the parameters. (By BS sampling of estimates of the PM)

Note that (1) and (2) are issues that arise from Input Uncertainty, whereas (3) is an issue of Output Analysis, In the present context of Simulation Modelling. these two issues were respectively termed Parameter Uncertainty and Simulation Uncertainty by Cheng and Holland (1997)

Question: What happens when the Performance Measure is not a known mathematical function, but instead is a quantity that is obtained numerically from runs of the Simulation Model, so that it becomes an issue of Simulation Uncertainty?

The interesting answer is that, to first order of approximation, the overall variability of the PM is measured as a statistical variance, the the overall variance is simply the sum of the variance of the Parameter Uncertainty and the variance of the Simulation Uncertainty. This was first pointed by Cheng and Holland (1997).

We can therefore do the following

Simply make B independent runs of the Simulation Model, where, in the ith run, the ith BS estimate, $\hat{\theta}^{(i)}$, of the vector of parameters as obtained in (1) above, is used. This allows us to estimate simultaneously the overall variability of the PM's obtained from these runs.

Excel Example 5 Here

References

Cheng, R C H and Holland, W. (1997). Sensitivity of Computer Simulation Erros in Input Data. *J. Statist. Comput. Simul.*, **57**, 219-241.

Cheng, R C H (2017) *Non-Standard Parametric Statistical Inference*, Oxford University Press.