

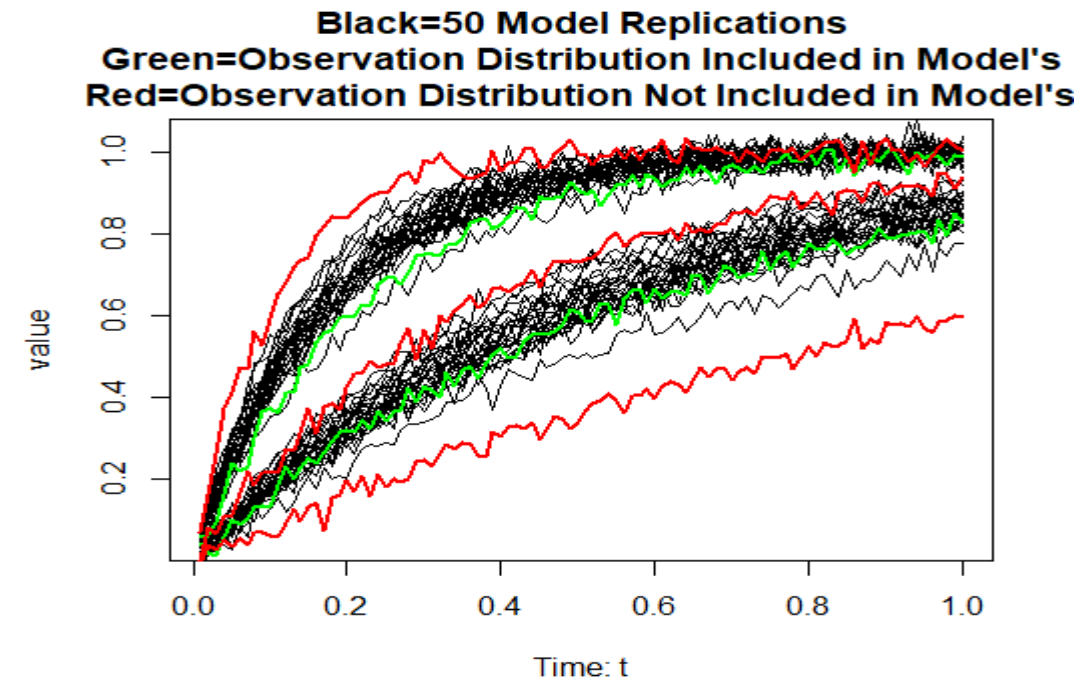
# A Kernel Density Procedure for Validation of a Computer Model with Multimodal Output

P. A. Jacobs

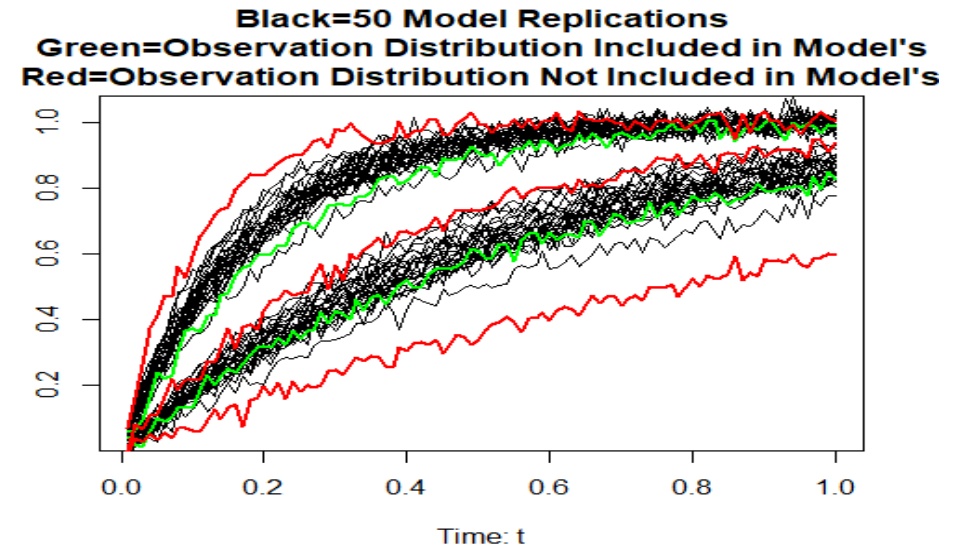
Naval Postgraduate School

# Question: How well does a computer model with multimodal output represent ONE observed time series?

- Test event results in one observed time series  $\{X(t); t=0.01, 0.02, \dots, 1\}$
- 300 independent and identically distributed replications of computer model of the time series;
  - $j$ th replication:  $\{Y_j(t); t=0, 0.01, 0.02, \dots, 1\}$



# Interval Procedures



## Current: 2.5-sigma

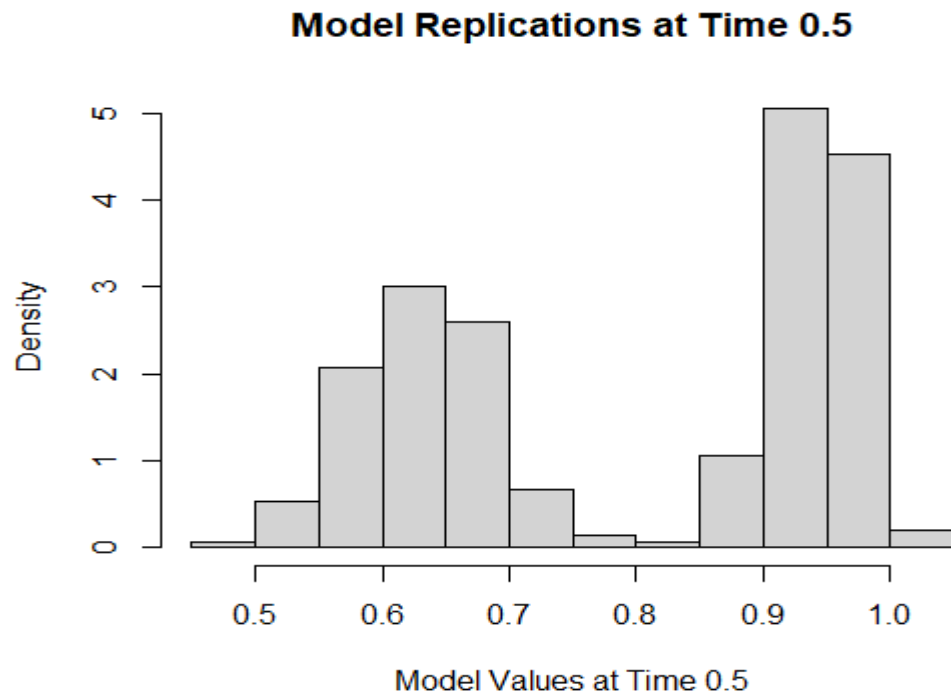
- Interval at each time= sample mean of model replications +/- 2.5 times the sample standard deviation of model replications
- Statistical evidence model does not well represent observation:
  - Observations outside of intervals more than 10% of the time

## Percentile

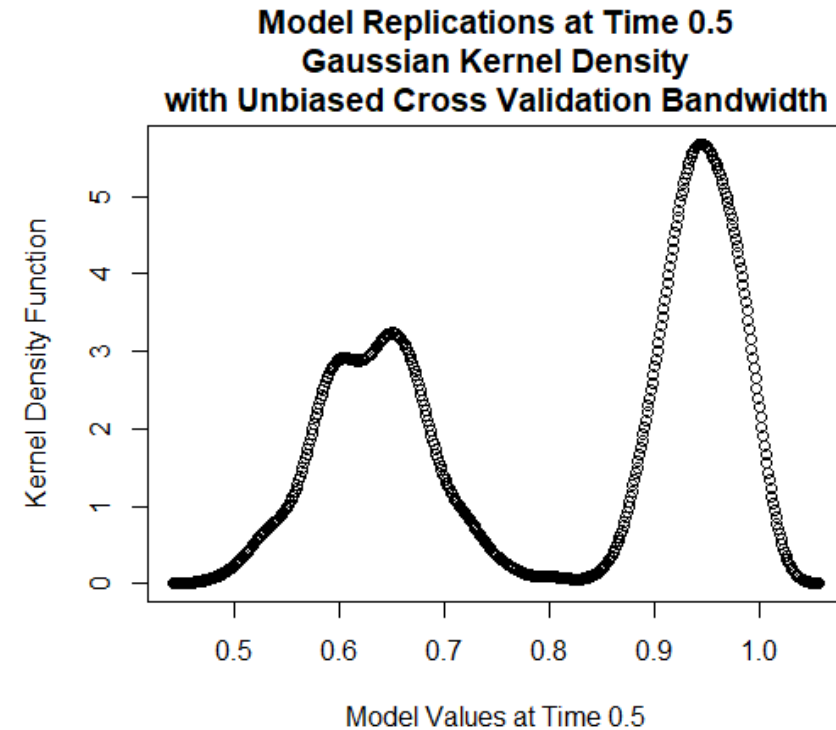
- Interval at each time: lower bound=0.005-quantile of model replications; upper bound=0.995-quantile of model replications
- Statistical evidence model does not well represent observation:
  - Observations outside of intervals more than 10% of the time

# Estimate of Model Distribution at a Single Time: Model Values Corresponding to Small Values Unlikely to Occur

**Histogram: 300 Model Replications**



**Gaussian Kernel Density**

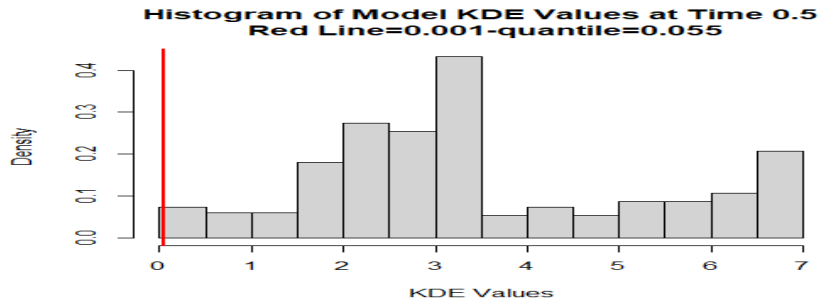


# Kernel Density Estimate (KDE) Procedure

## KDEs of observation too small too many times?

For each time & each model replication:  
find KDE of the model replication value using  
all other model replications.

For each time:  
find 0.001-quantile of all model's KDEs



For each model replication:

find number of times its KDEs are less than model KDE  
0.001-quantiles.

Choose bound from number of times model replication  
KDEs < 0.001 quantiles

Max number?

2<sup>nd</sup> largest number?

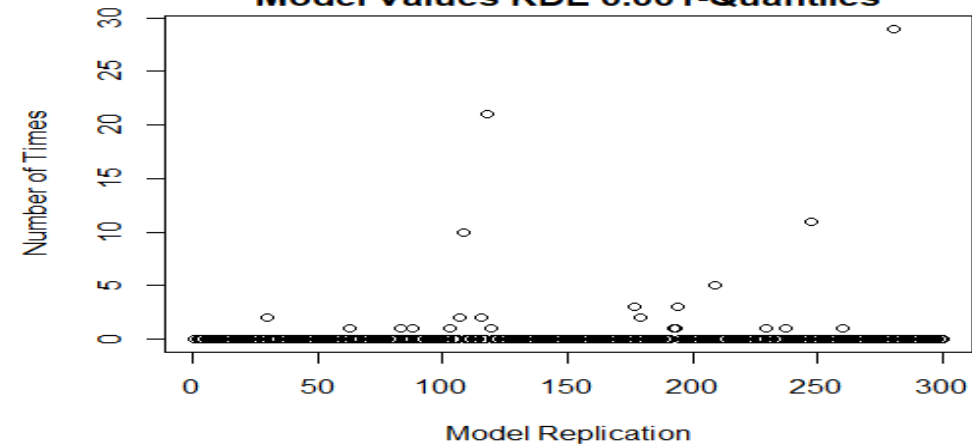
For each time:

find KDE of observation value using all model  
replications

Observation KDEs too small too many times  
=statistical evidence model distribution does  
not include that of observation

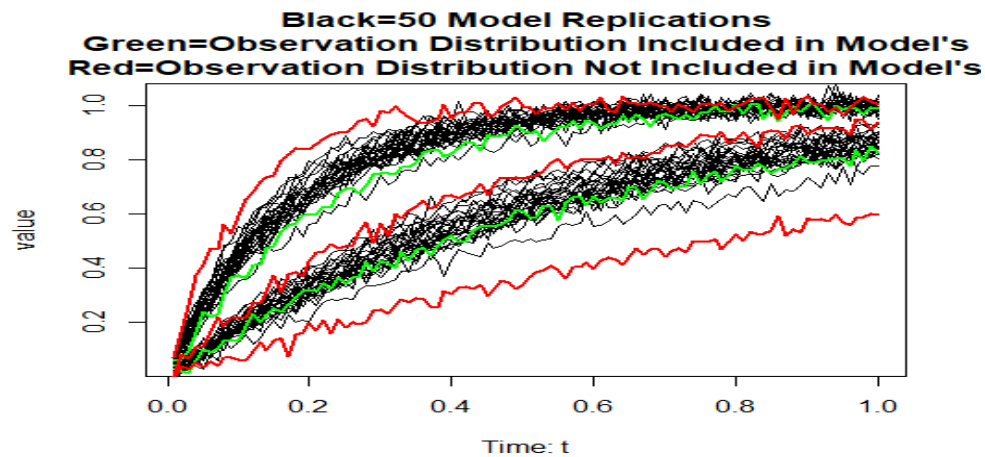
number of times observation KDEs less than  
model's KDE 0.001-quantiles is greater than  
chosen bound

**Number of Times  
Model Replication's Value KDEs <  
Model Values KDE 0.001-Quantiles**

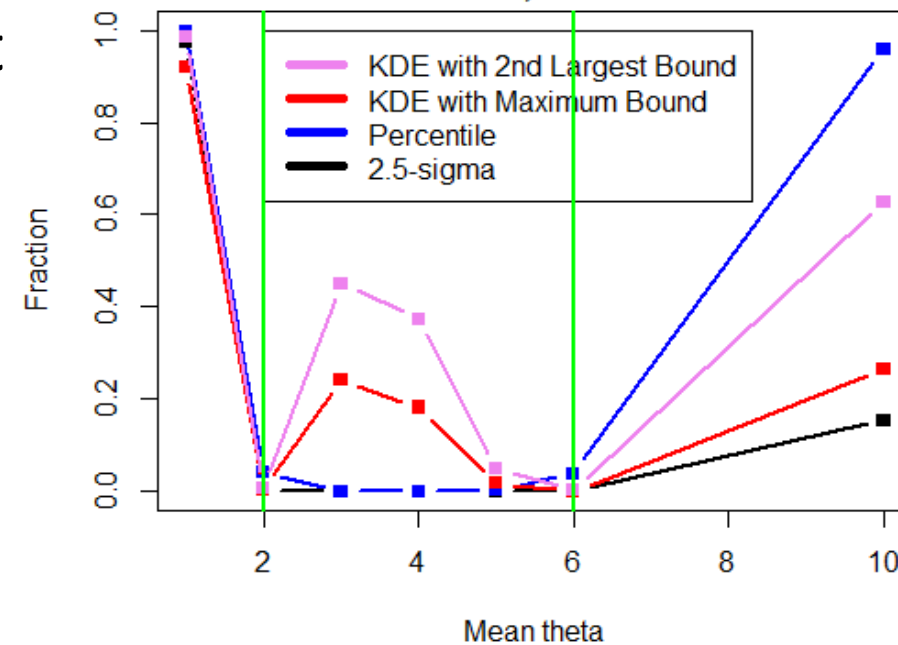


# Fraction 500 Simulation Replications (each with 300 model replications) with Statistical Evidence Model Distribution Does Not Include that of Observation

- 2 cases incorrect: Green Lines @ 2 & 6
- Ideal fraction=0
- 2.5-sigma=best; percentile =worst

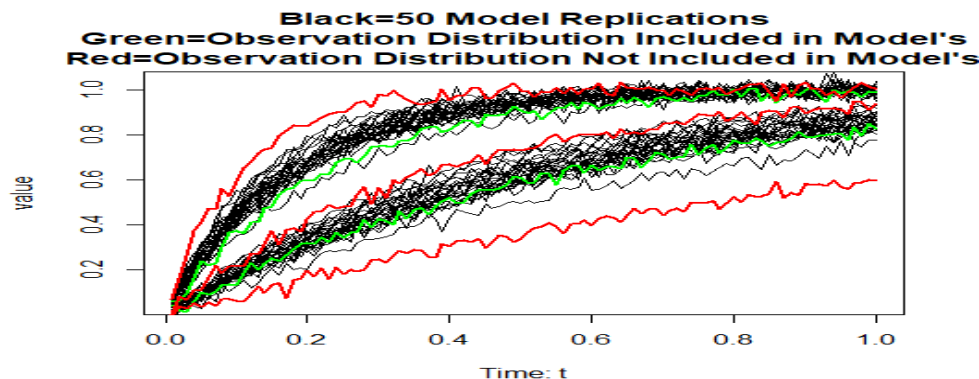


Fraction 500 Replications with Statistical Evidence  
Mixture Model Distribution Does not Include  
that of Observation; KDE Quantile=0.001

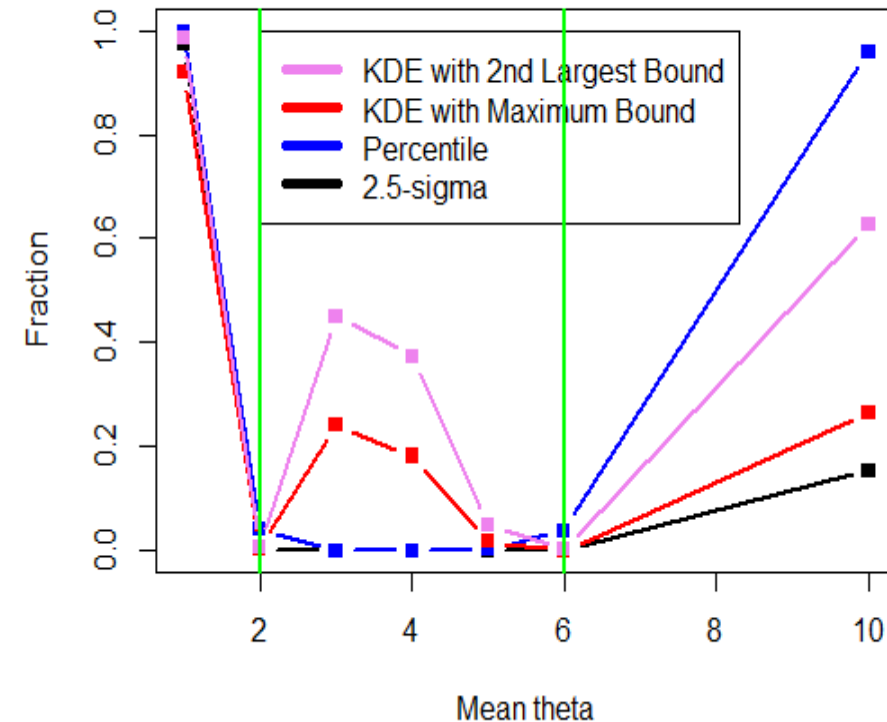


# Fraction of 500 Simulation Replications that Result in Statistical Evidence Model Distribution Does Not Include that of Observation

- 5 cases correct evidence: ideal fraction=1
- x-axis @ 1 & 10
  - Best=percentile;
  - 2<sup>nd</sup> best=KDE with 2<sup>nd</sup> largest bound
- x-axis @ 3, 4, 5
  - Worst=2.5-Sigma
  - Best=KDE with 2<sup>nd</sup> largest lower bound



Fraction 500 Replications with Statistical Evidence Mixture Model Distribution Does not Include that of Observation; KDE Quantile=0.001



# Summary

- The currently used 2.5-sigma procedure is less likely to produce correct statistical evidence a multimodal mixture model distribution does not include that of the observed times series than kernel density estimation procedure