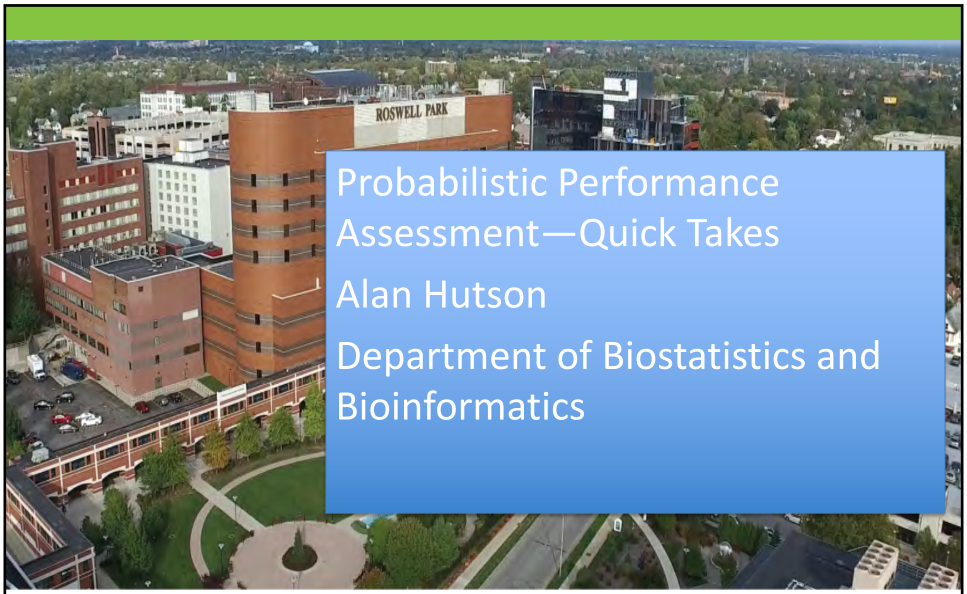

Probabilistic Performance Assessment—Quick Takes

Alan Hutson

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ROSWELL PARK
COMPREHENSIVE CANCER CENTER

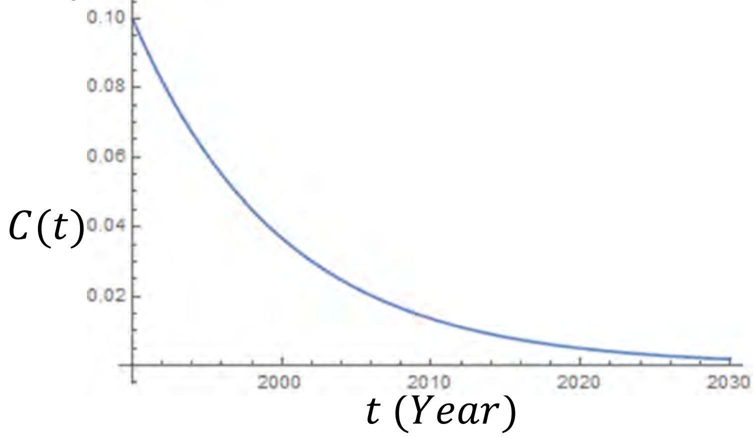
PPA model documents

- Fitting models to data
- Prediction
- Simulation
- Sensitivity Analysis
- Bayesian vs. Frequentist methods
- Spatial Smoothing
- My interpretation after reading several PPA documents

Toy Example-Fitting a Model

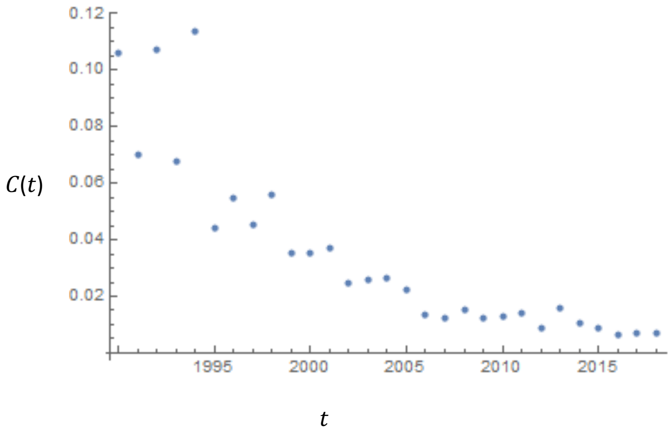
- $C(t) = \beta\, e^{-\lambda t}$
  - t = time
  - β=initial value at time t=0
  - λ= rate parameter
- The function $C(t)$ may be a “known” physical relationship or an approximation to a physical process
- The parameters β and λ may be known physical constants or estimated from the data

Toy Example-Known Parameters



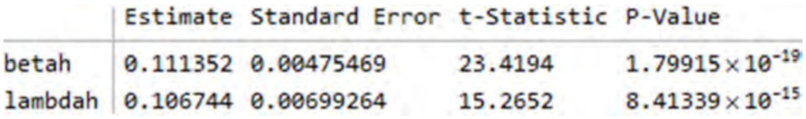
β=0.1 and λ= 0.1, time was offset by 1990

Real Life Data-Measurement Error



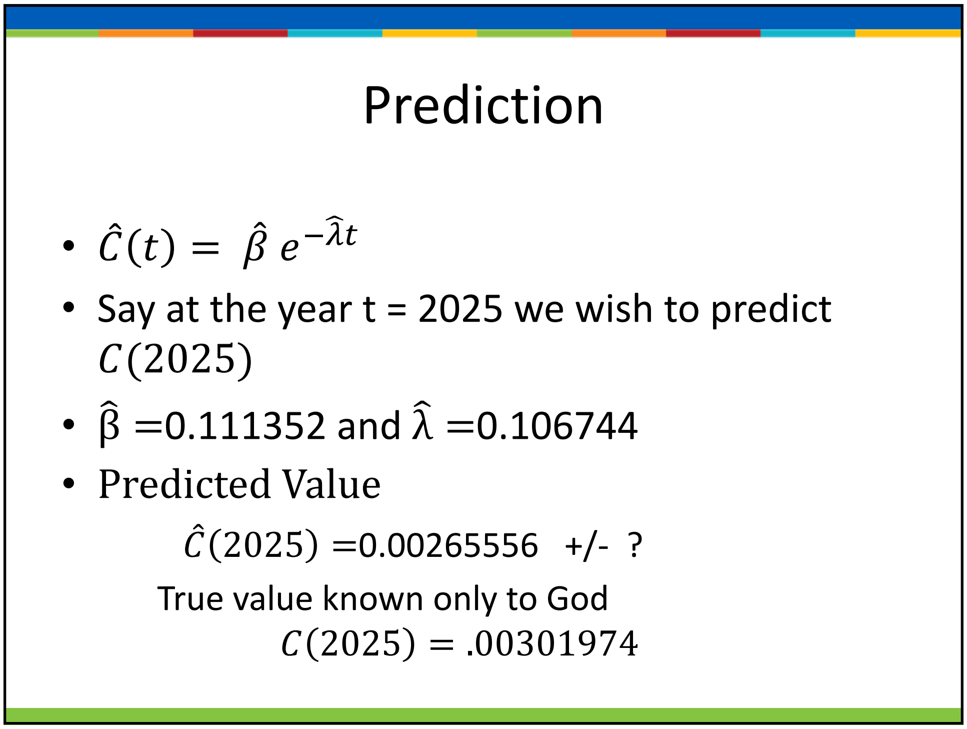
Parameter Estimates

- More data ⟶ less uncertainty
  - Uncertainty can be quantified multiple ways
- Several estimation methods



	Estimate	Standard Error	t-Statistic	P-Value
betah	0.111352	0.00475469	23.4194	1.79915×10^{-19}
lambdah	0.106744	0.00699264	15.2652	8.41339×10^{-15}

- Assumption of the model's functional form is critical



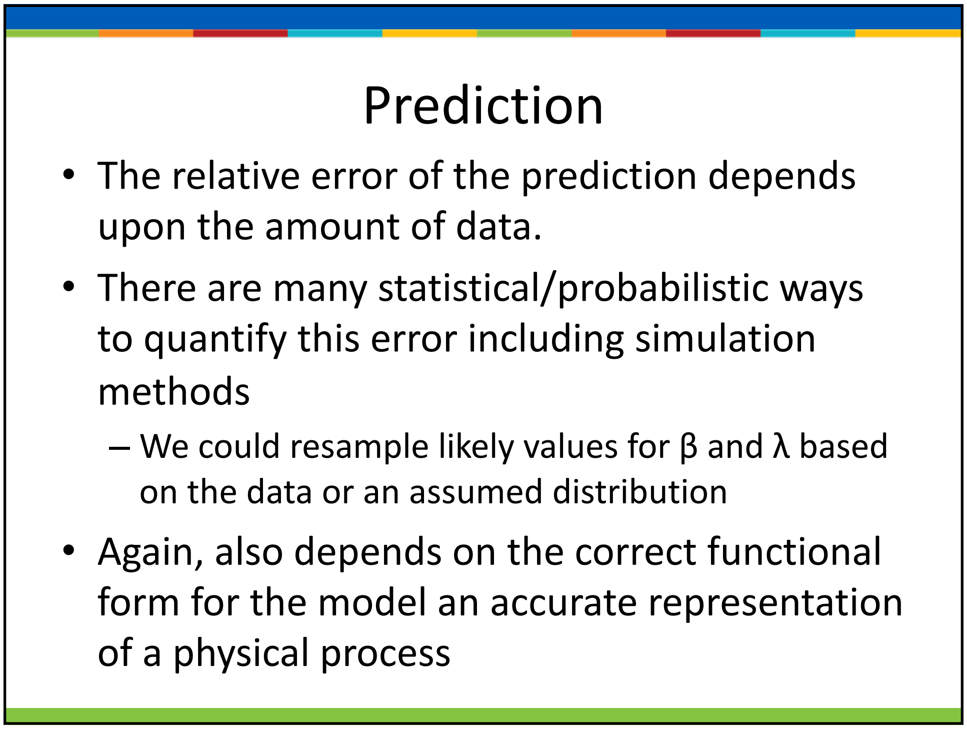
Prediction

- $\hat{C}(t) = \ \hat{\beta}\ e^{-\hat{\lambda}t}$
- Say at the year t = 2025 we wish to predict $C(2025)$
- $\hat{\beta}$ =0.111352 and $\hat{\lambda}$ =0.106744
- Predicted Value

  $\hat{C}(2025)$ =0.00265556 +/- ?

  True value known only to God

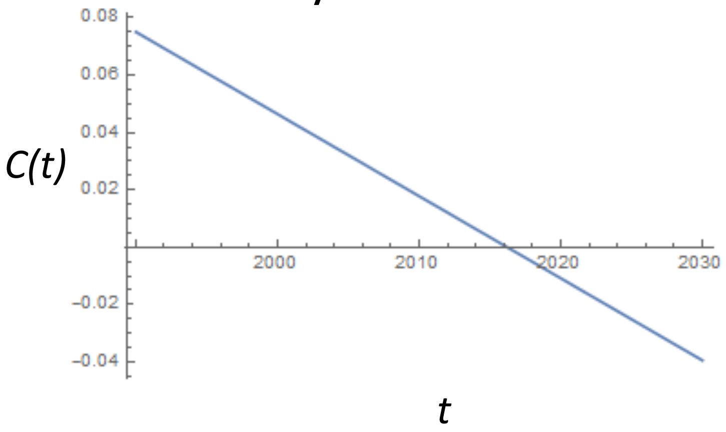
  $C(2025) = .00301974$



Prediction

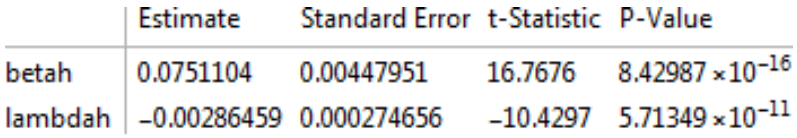
- The relative error of the prediction depends upon the amount of data.
- There are many statistical/probabilistic ways to quantify this error including simulation methods
  - We could resample likely values for β and λ based on the data or an assumed distribution
- Again, also depends on the correct functional form for the model an accurate representation of a physical process

Toy Example—Poor Model/Prediction

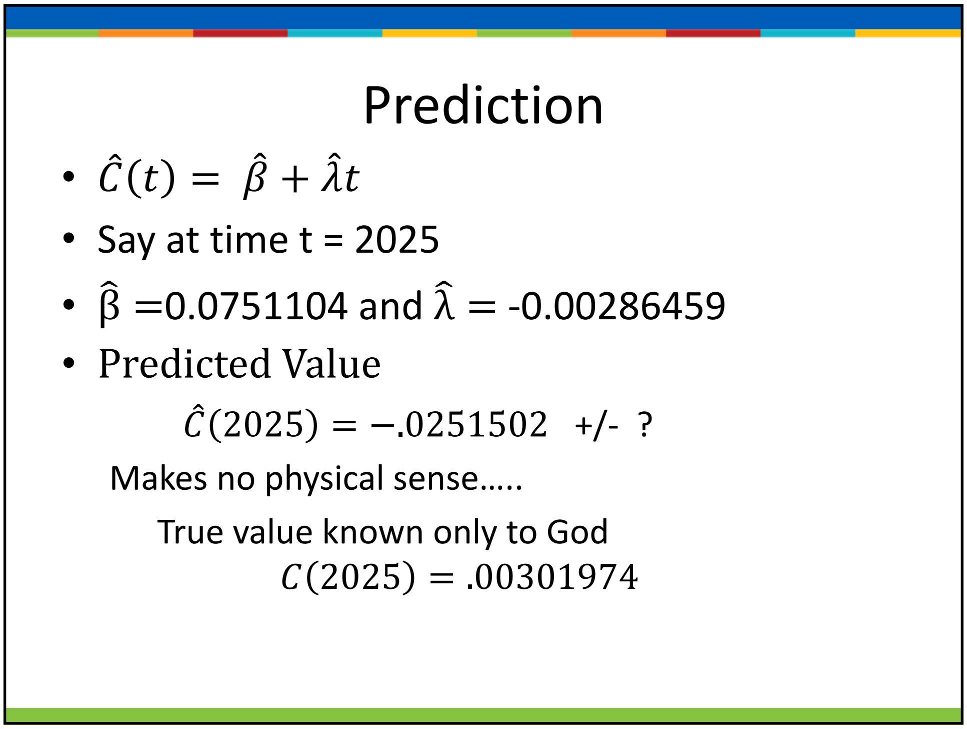


Toy Example—Wrong Model

- Assume incorrectly $C(t) = \beta + \lambda t$
- t = time
- β=initial value at time t=0
- λ= rate parameter
- Nothing stops one from fitting the wrong model



	Estimate	Standard Error	t-Statistic	P-Value
betah	0.0751104	0.00447951	16.7676	8.42987×10^{-16}
lambdah	−0.00286459	0.000274656	−10.4297	5.71349×10^{-11}



Prediction

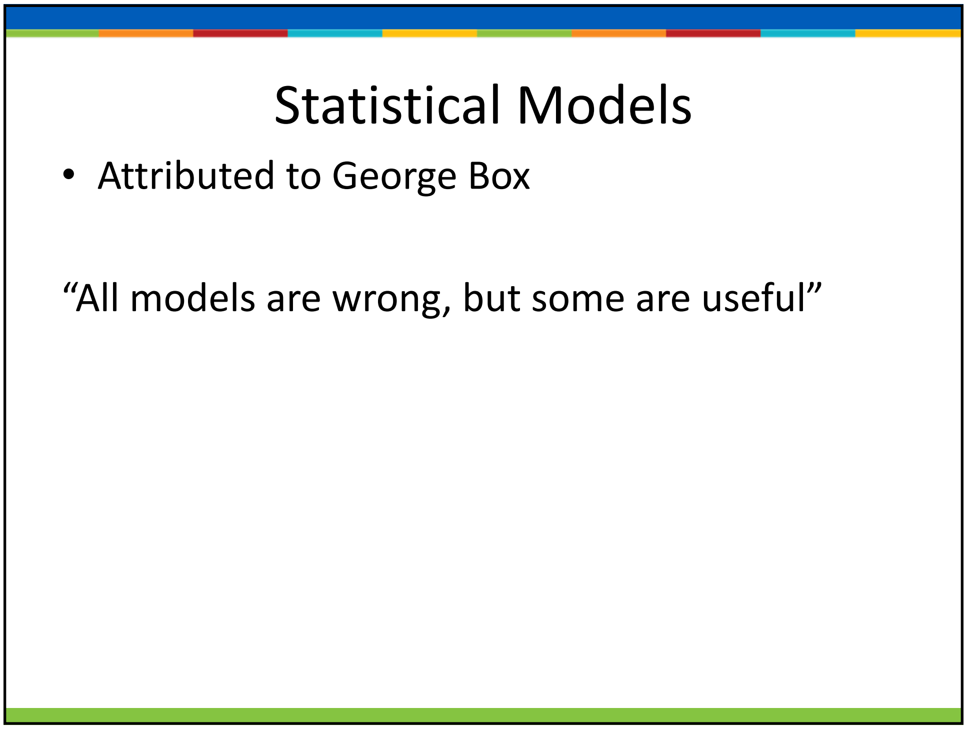
- $\hat{C}(t) = \hat{\beta} + \hat{\lambda}t$
- Say at time t = 2025
- $\hat{\beta}$ =0.0751104 and $\hat{\lambda}$ = -0.00286459
- Predicted Value

$\hat{C}(2025) = -.0251502$ +/- ?

Makes no physical sense…..

True value known only to God

$C(2025) = .00301974$



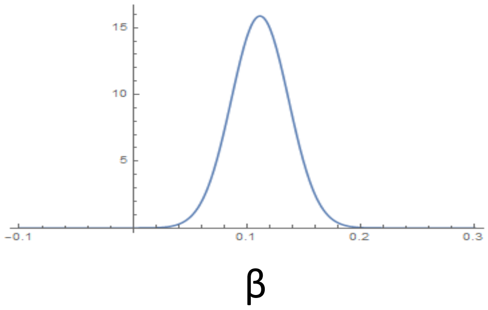
Statistical Models

- Attributed to George Box

“All models are wrong, but some are useful”

Simulation

- Simulation is useful for complex models in terms of prediction error, behavior, etc



- Resample values for β and λ to quantify the prediction error (or resample data)

Simulation

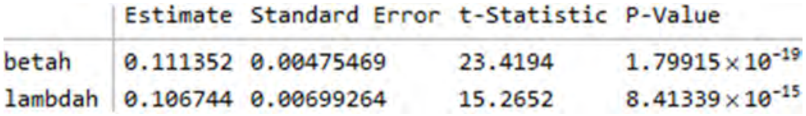
- Just like assuming the correct model there are several structural assumptions relative to the simulation of data
  - Correlation/dependence between the parameter distributions (temporal correlations)
  - Probability distribution for each parameter and/or joint distribution
    - Data based or assumed
    - Theoretical/large sample or physical properties
  - There are many simulation/resampling methodologies

Simulation

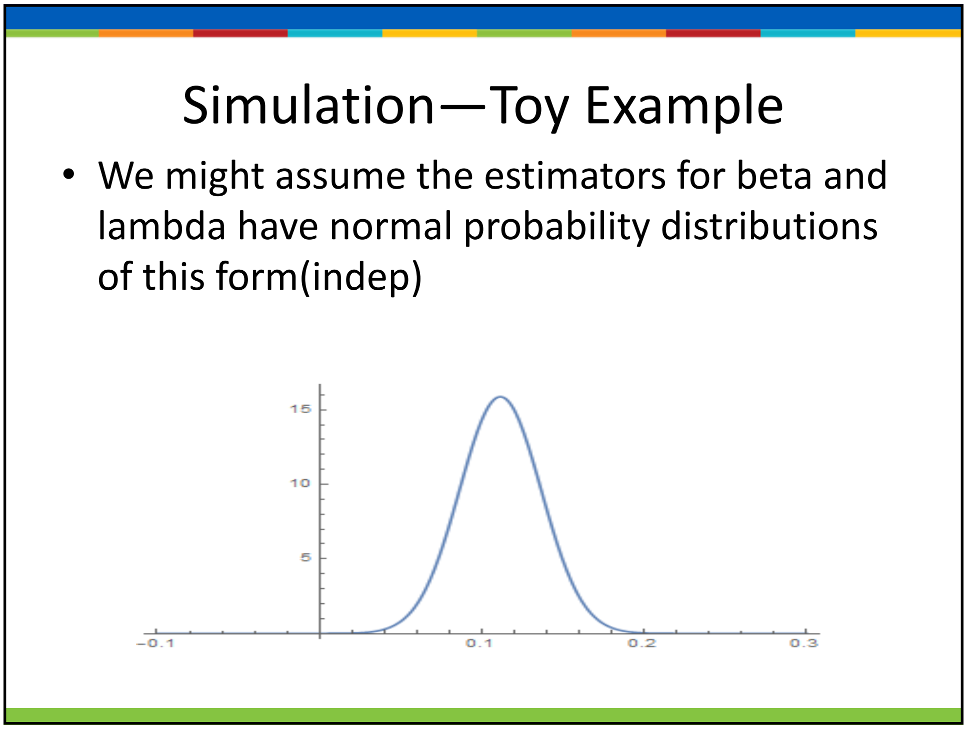
- There are theoretical approaches to “best” simulate data
- The goal is to approximate natural processes based on all of the available information to examine prediction error and the robustness of the assumed models

Simulation—Toy Example

- Let us assume our model assumptions were “accurate” or even “known”

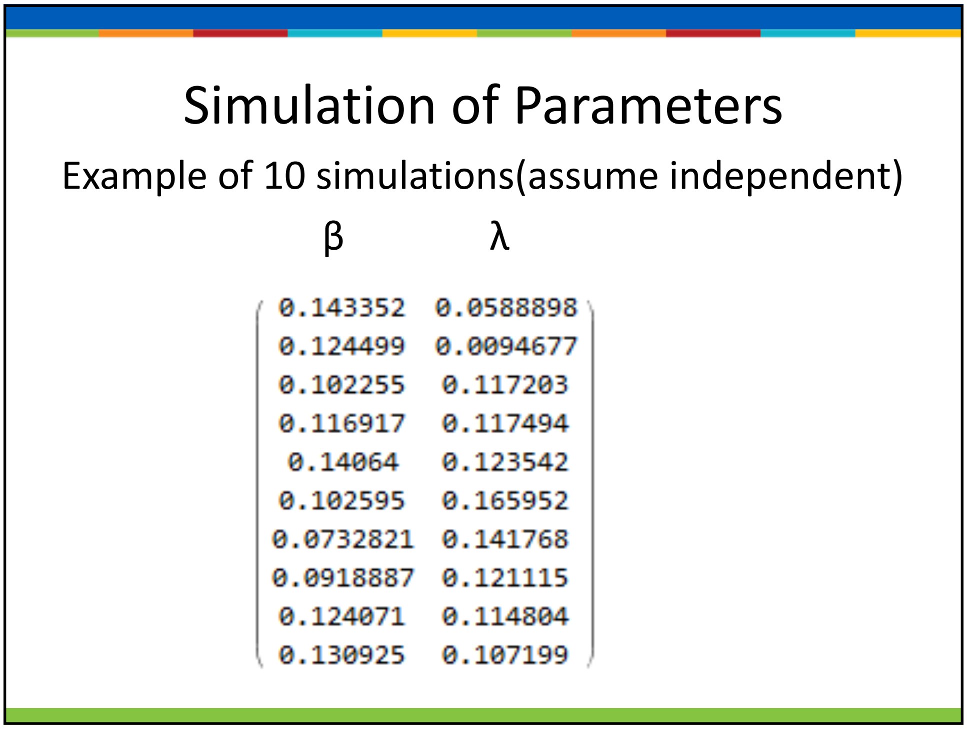


	Estimate	Standard Error	t-Statistic	P-Value
betah	0.111352	0.00475469	23.4194	1.79915×10^{-19}
lambdah	0.106744	0.00699264	15.2652	8.41339×10^{-15}



Simulation—Toy Example

- We might assume the estimators for beta and lambda have normal probability distributions of this form(indep)



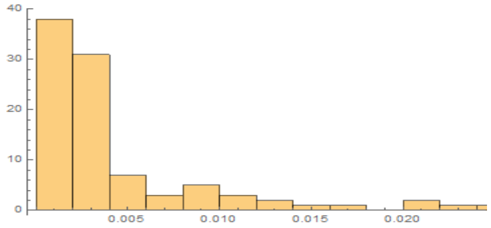
Simulation of Parameters

Example of 10 simulations(assume independent)

$$\begin{array}{c} \begin{array}{cc} \beta & \qquad \lambda \end{array} \\ \begin{pmatrix} 0.143352 & 0.0588898 \\ 0.124499 & 0.0094677 \\ 0.102255 & 0.117203 \\ 0.116917 & 0.117494 \\ 0.14064 & 0.123542 \\ 0.102595 & 0.165952 \\ 0.0732821 & 0.141768 \\ 0.0918887 & 0.121115 \\ 0.124071 & 0.114804 \\ 0.130925 & 0.107199 \end{pmatrix} \end{array}$$

Simulation of Parameters

- From 100 simulations at time t=2025 we get 100 predicted C(2025) values

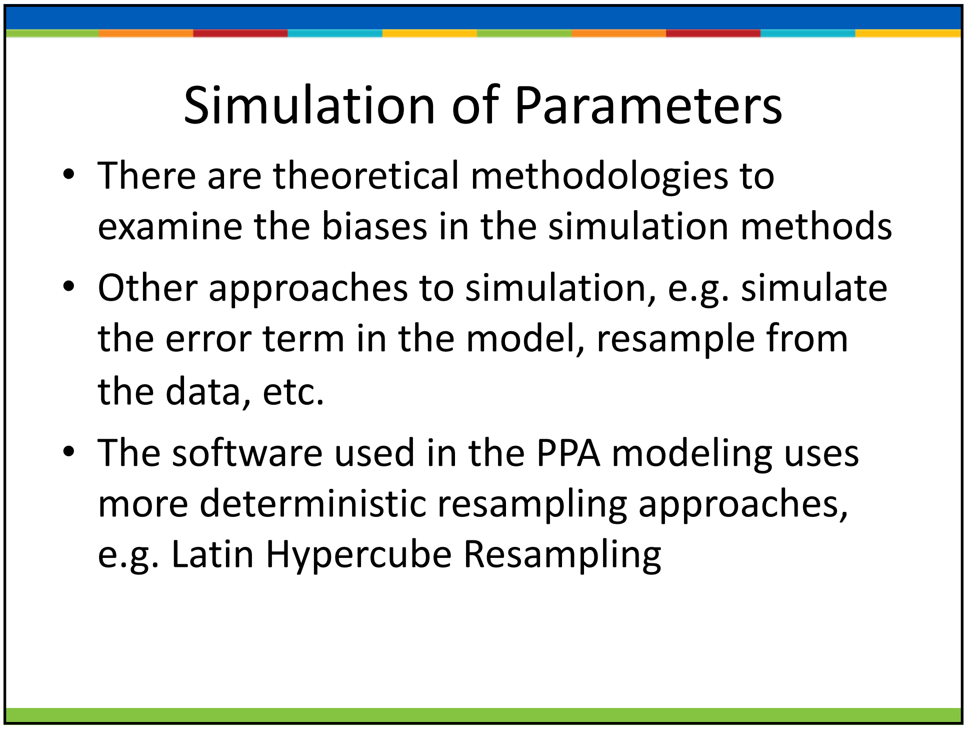


Estimated C(t)

- C(2025) Mean=0.006 Standard Deviation=0.012 (biased estimate)
- Recall: True value is $C(2025)$=.00301974

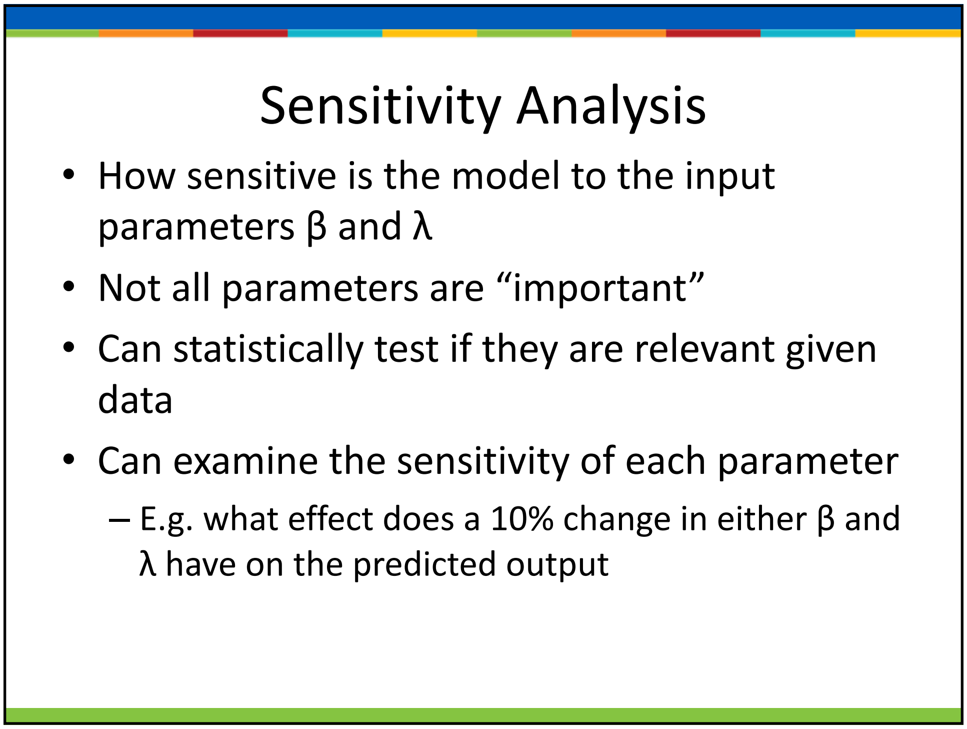
Simulation of Parameters

- Where might we be “off-base”
- Likely picked the wrong probability distributions for β and λ estimates. For small samples in this scenario the distributions are likely to be asymmetrical
- Ignored the potential correlation structure between β and λ estimates
- We used estimates for β and λ ..random chance



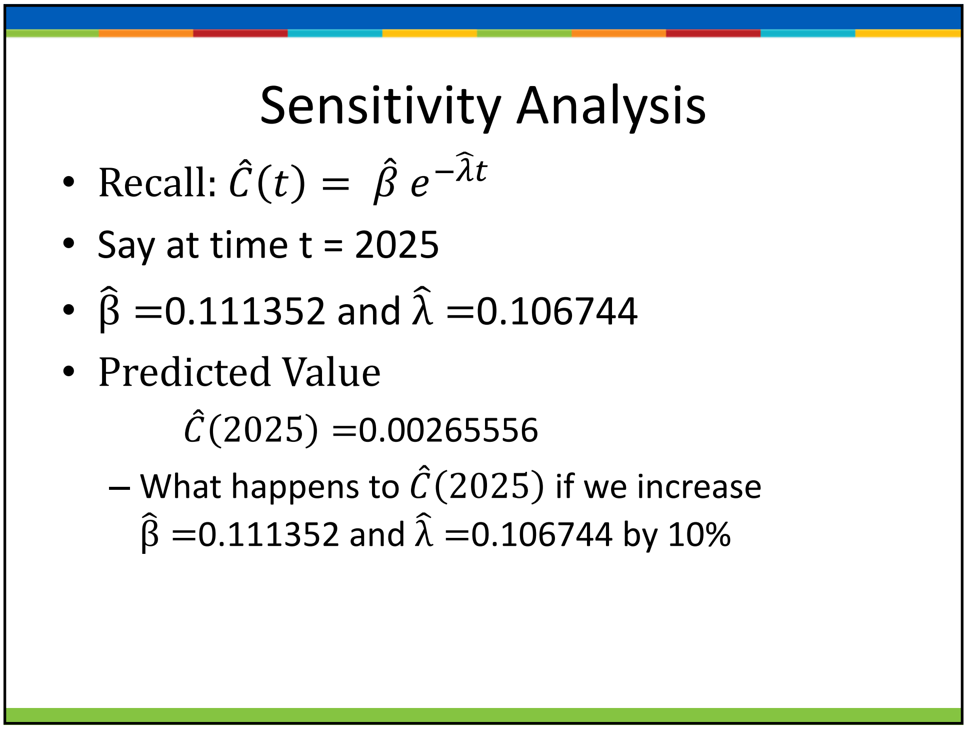
Simulation of Parameters

- There are theoretical methodologies to examine the biases in the simulation methods
- Other approaches to simulation, e.g. simulate the error term in the model, resample from the data, etc.
- The software used in the PPA modeling uses more deterministic resampling approaches, e.g. Latin Hypercube Resampling



Sensitivity Analysis

- How sensitive is the model to the input parameters β and λ
- Not all parameters are "important"
- Can statistically test if they are relevant given data
- Can examine the sensitivity of each parameter
  - E.g. what effect does a 10% change in either β and λ have on the predicted output

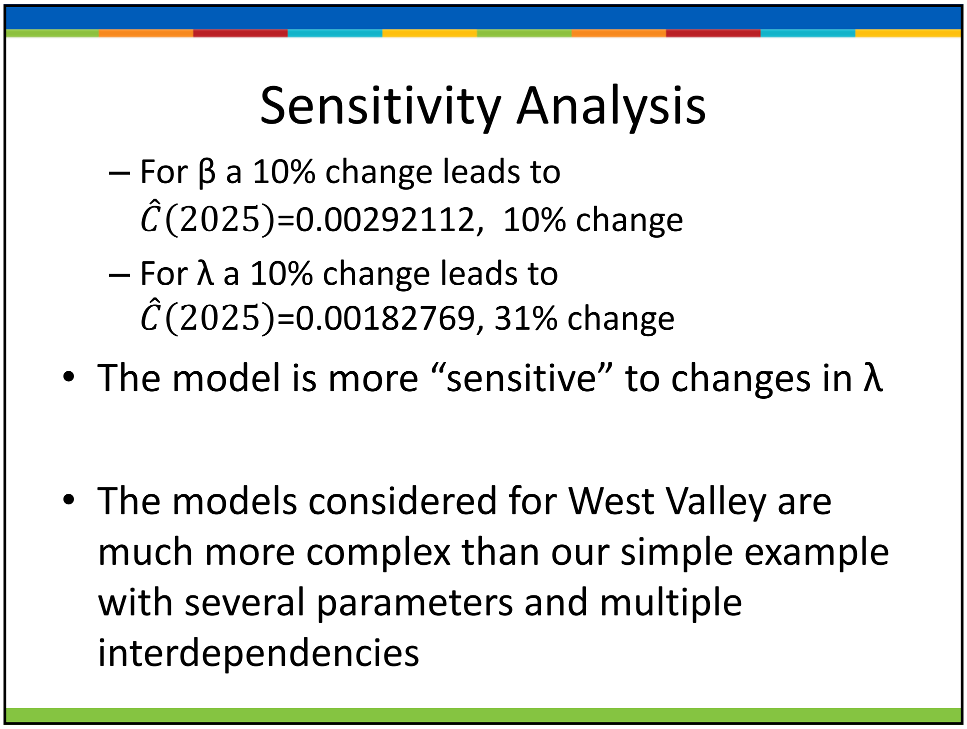


Sensitivity Analysis

- Recall: $\hat{C}(t) = \hat{\beta}\, e^{-\hat{\lambda} t}$
- Say at time t = 2025
- $\hat{\beta}$ =0.111352 and $\hat{\lambda}$ =0.106744
- Predicted Value

  $\hat{C}(2025)$ =0.00265556

  – What happens to $\hat{C}(2025)$ if we increase $\hat{\beta}$ =0.111352 and $\hat{\lambda}$ =0.106744 by 10%

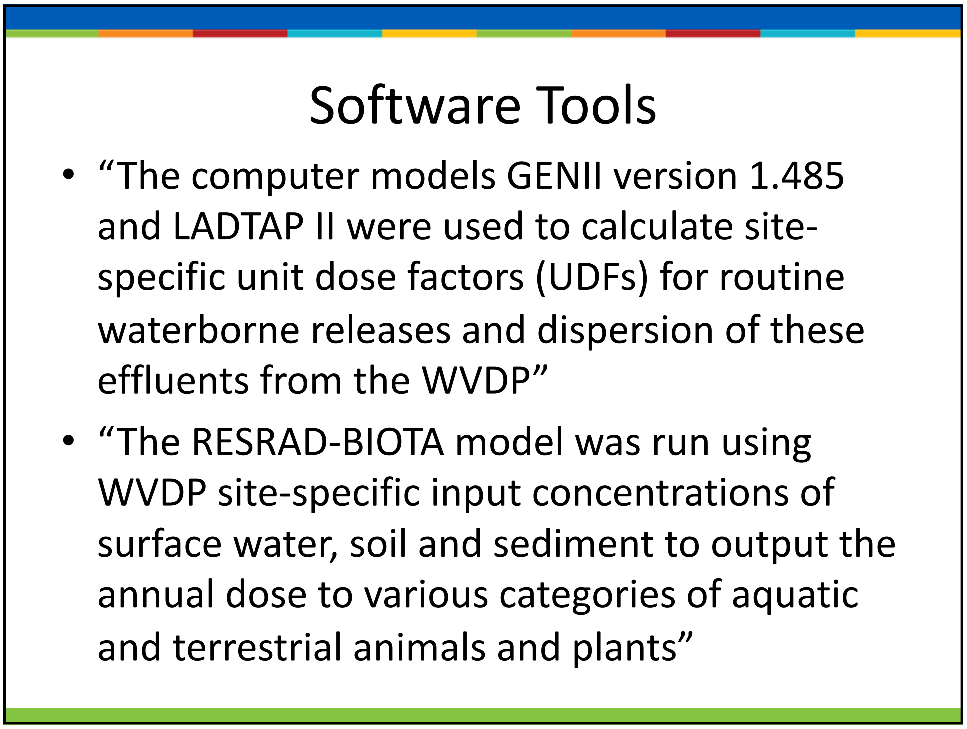


Sensitivity Analysis

  – For β a 10% change leads to $\hat{C}(2025)$=0.00292112, 10% change

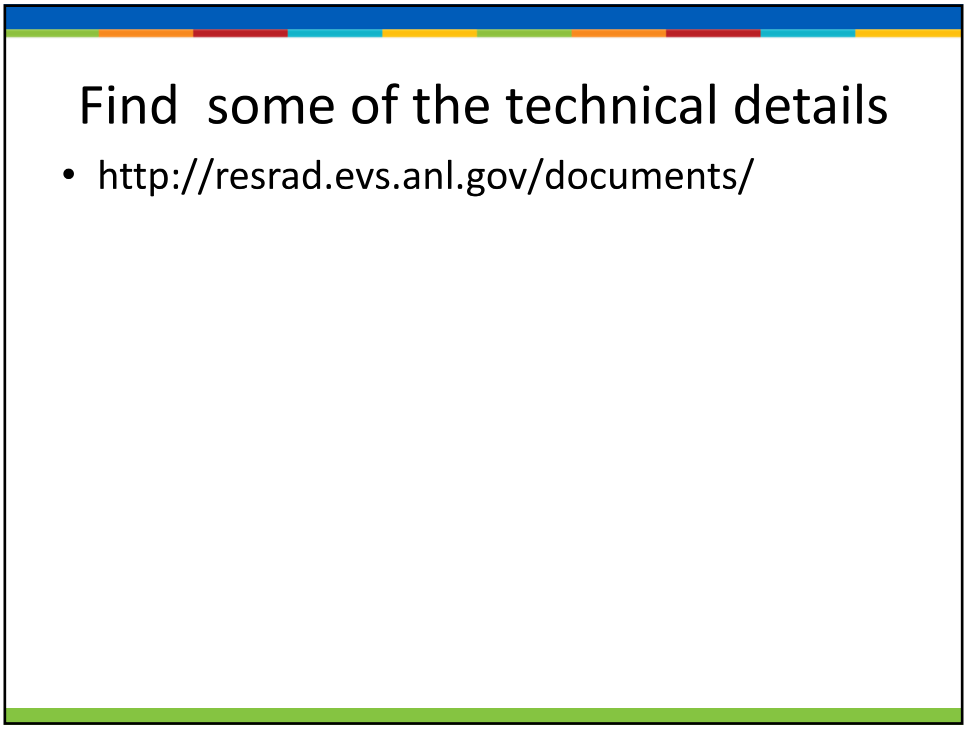
  – For λ a 10% change leads to $\hat{C}(2025)$=0.00182769, 31% change

- The model is more “sensitive” to changes in λ
- The models considered for West Valley are much more complex than our simple example with several parameters and multiple interdependencies



Software Tools

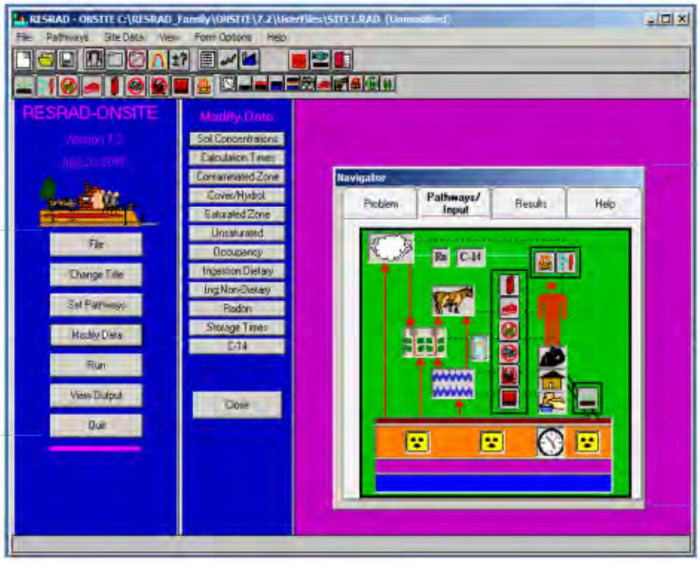
- “The computer models GENII version 1.485 and LADTAP II were used to calculate site-specific unit dose factors (UDFs) for routine waterborne releases and dispersion of these effluents from the WVDP”
- “The RESRAD-BIOTA model was run using WVDP site-specific input concentrations of surface water, soil and sediment to output the annual dose to various categories of aquatic and terrestrial animals and plants”



Find some of the technical details

- http://resrad.evs.anl.gov/documents/

RESRAD



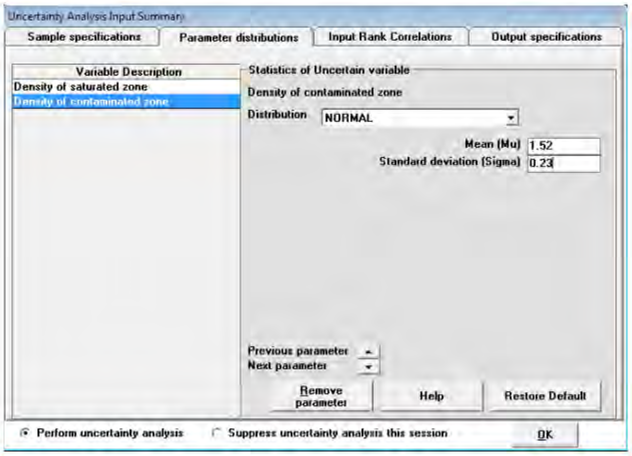
Menu

Toolbars

DOS Emulator

Navigator Window

RESRAD Simulations


Uncertainty Analysis Input Summary

Variable Description

Density of saturated zone

Density of contaminated zone

Statistics of Uncertain variable

Density of contaminated zone

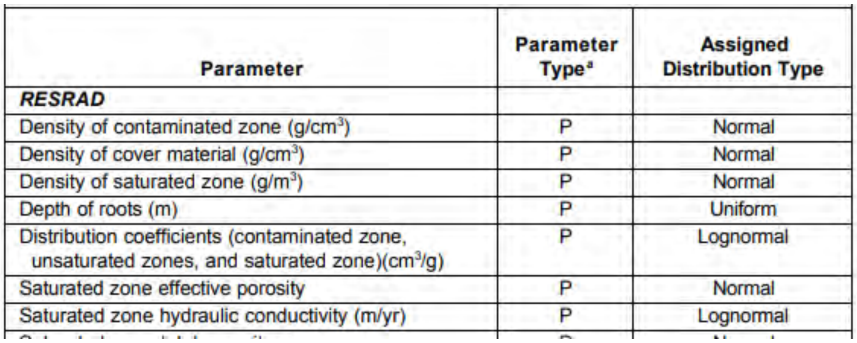
Distribution: NORMAL

Mean (Mu): 1.52

Standard deviation (Sigma): 0.23

● Perform uncertainty analysis ○ Suppress uncertainty analysis this session

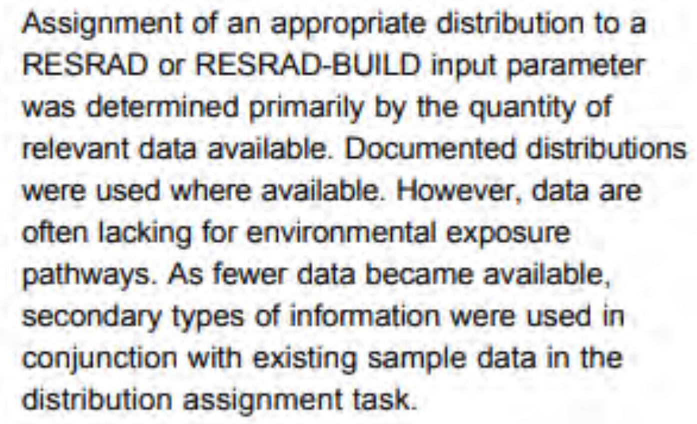
RESRAD Simulations



Parameter	Parameter Type[a]	Assigned Distribution Type
RESRAD		
Density of contaminated zone (g/cm^3)	P	Normal
Density of cover material (g/cm^3)	P	Normal
Density of saturated zone (g/m^3)	P	Normal
Depth of roots (m)	P	Uniform
Distribution coefficients (contaminated zone, unsaturated zones, and saturated zone)(cm^3/g)	P	Lognormal
Saturated zone effective porosity	P	Normal
Saturated zone hydraulic conductivity (m/yr)	P	Lognormal

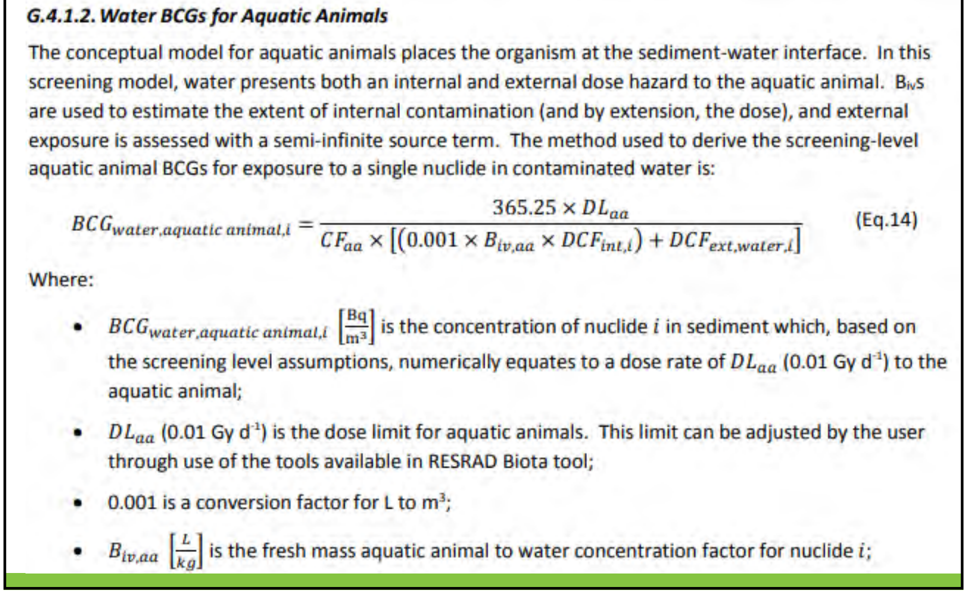
RESRAD Simulations

- Typical documented language, not necessarily specific to this project



Assignment of an appropriate distribution to a RESRAD or RESRAD-BUILD input parameter was determined primarily by the quantity of relevant data available. Documented distributions were used where available. However, data are often lacking for environmental exposure pathways. As fewer data became available, secondary types of information were used in conjunction with existing sample data in the distribution assignment task.

Technical Documentation



G.4.1.2. Water BCGs for Aquatic Animals

The conceptual model for aquatic animals places the organism at the sediment-water interface. In this screening model, water presents both an internal and external dose hazard to the aquatic animal. B_{iv}s are used to estimate the extent of internal contamination (and by extension, the dose), and external exposure is assessed with a semi-infinite source term. The method used to derive the screening-level aquatic animal BCGs for exposure to a single nuclide in contaminated water is:

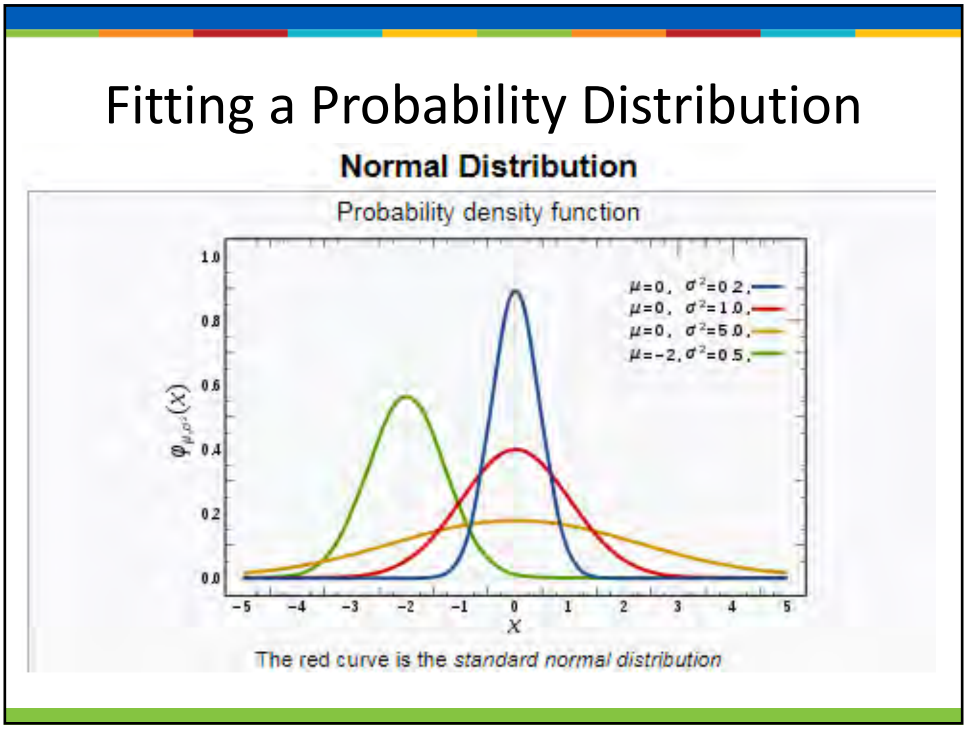
$$BCG_{water,aquatic\ animal,i} = \frac{365.25 \times DL_{aa}}{CF_{aa} \times [(0.001 \times B_{iv,aa} \times DCF_{int,i}) + DCF_{ext,water,i}]} \quad \text{(Eq.14)}$$

Where:

- $BCG_{water,aquatic\ animal,i}$ $\left[\frac{\text{Bq}}{\text{m}^3}\right]$ is the concentration of nuclide i in sediment which, based on the screening level assumptions, numerically equates to a dose rate of DL_{aa} (0.01 Gy d^{-1}) to the aquatic animal;
- DL_{aa} (0.01 Gy d^{-1}) is the dose limit for aquatic animals. This limit can be adjusted by the user through use of the tools available in RESRAD Biota tool;
- 0.001 is a conversion factor for L to m^3;
- $B_{iv,aa}$ $\left[\frac{L}{kg}\right]$ is the fresh mass aquatic animal to water concentration factor for nuclide i;

Fitting a Probability Distribution

- Several functional("zillions") forms to capture the shape and support(range) of a random variable. What to use?
- Can statistically test the "fit" of a distribution to the observed data
- Parametric distributions are typically defined by one to three parameters

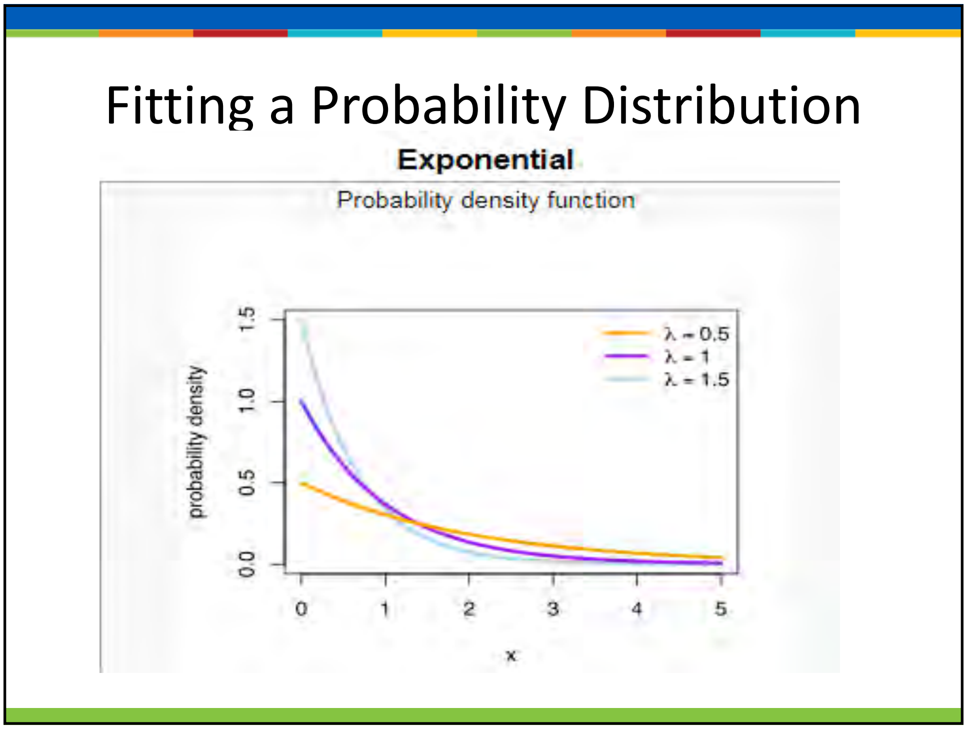


Fitting a Probability Distribution

Normal Distribution

Probability density function

The red curve is the *standard normal distribution*



Fitting a Probability Distribution

Exponential

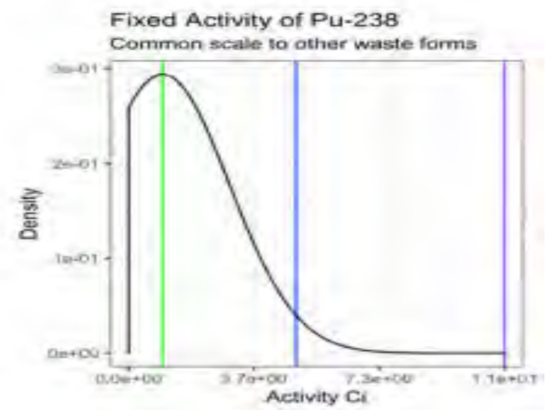
Probability density function

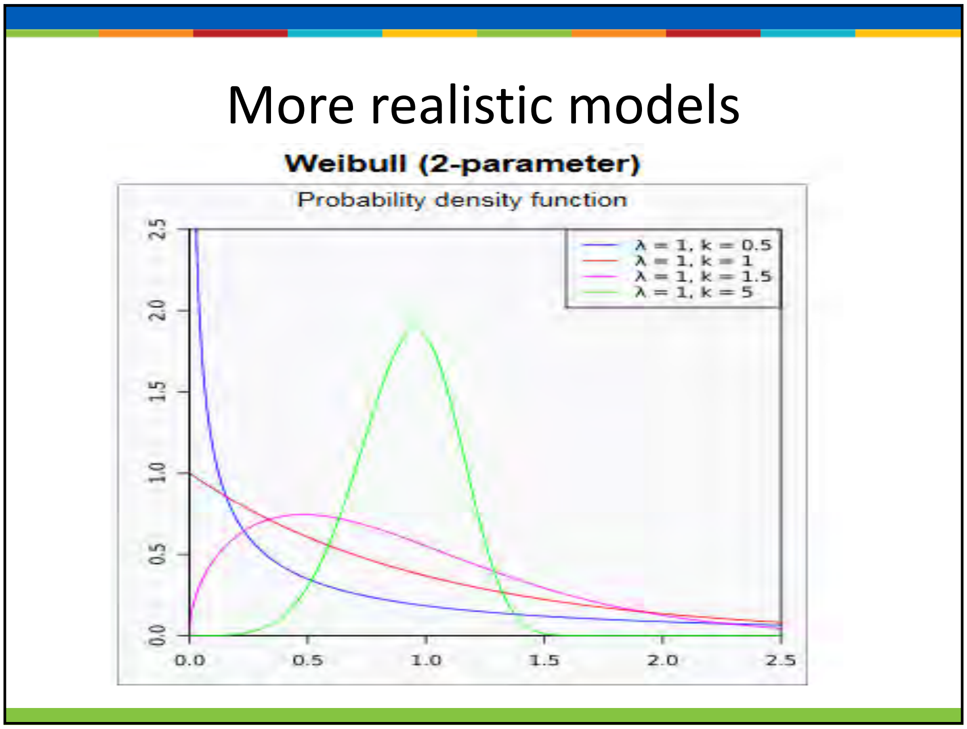
Fitting a Probability Distribution

- The more data ⟶ more accurate parameter estimates
- Can pick the wrong distribution(can be tested)
- Several estimation methods
  - Maximum likelihood most well-known
  - Bayesian methods are also a likelihood based approach
  - i.e. given the data, what is the most likely values of the parameters that lead to that data
- One may consider “nonparametric” methods

Flag-WVDP Feb 2019 Inv Update

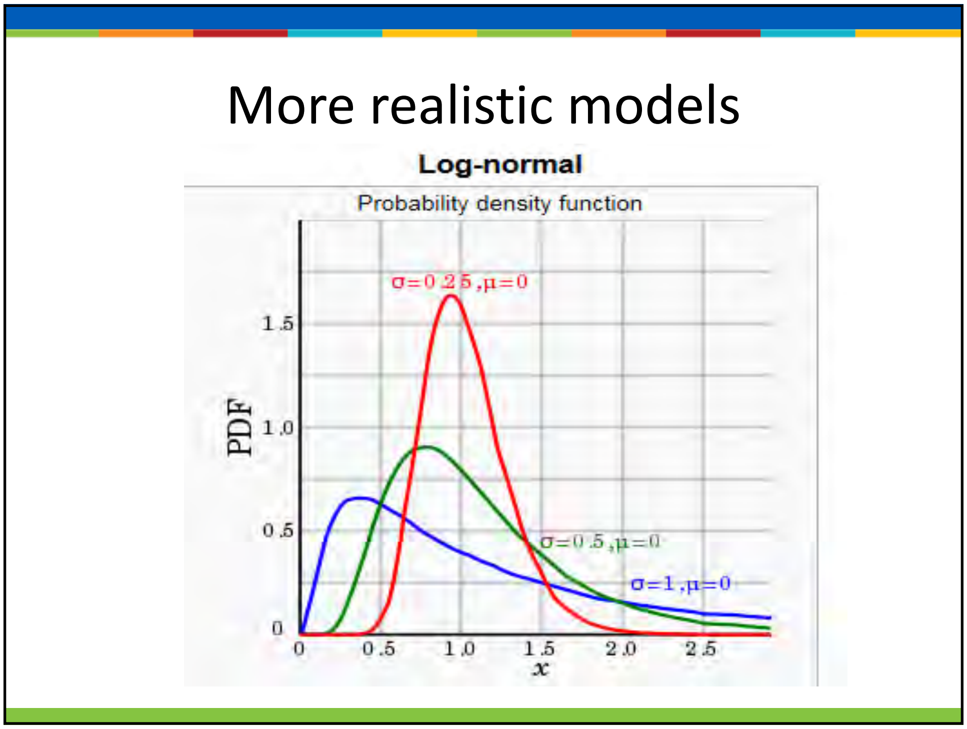
- Overutilization of truncated normal models
- Highly unlikely natural process





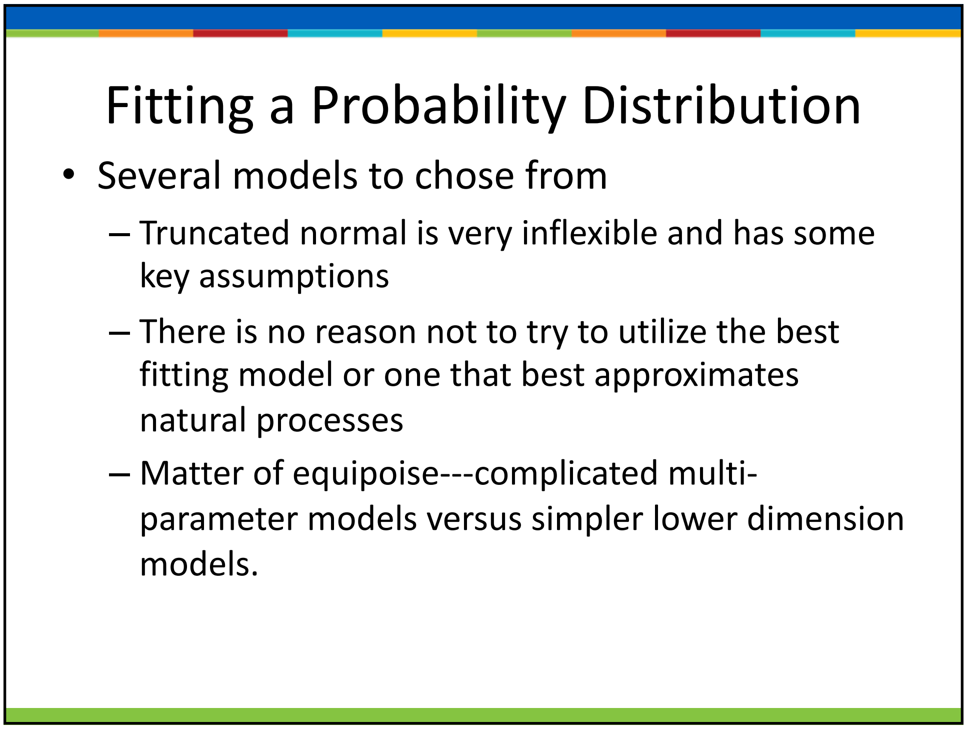
More realistic models

Weibull (2-parameter)



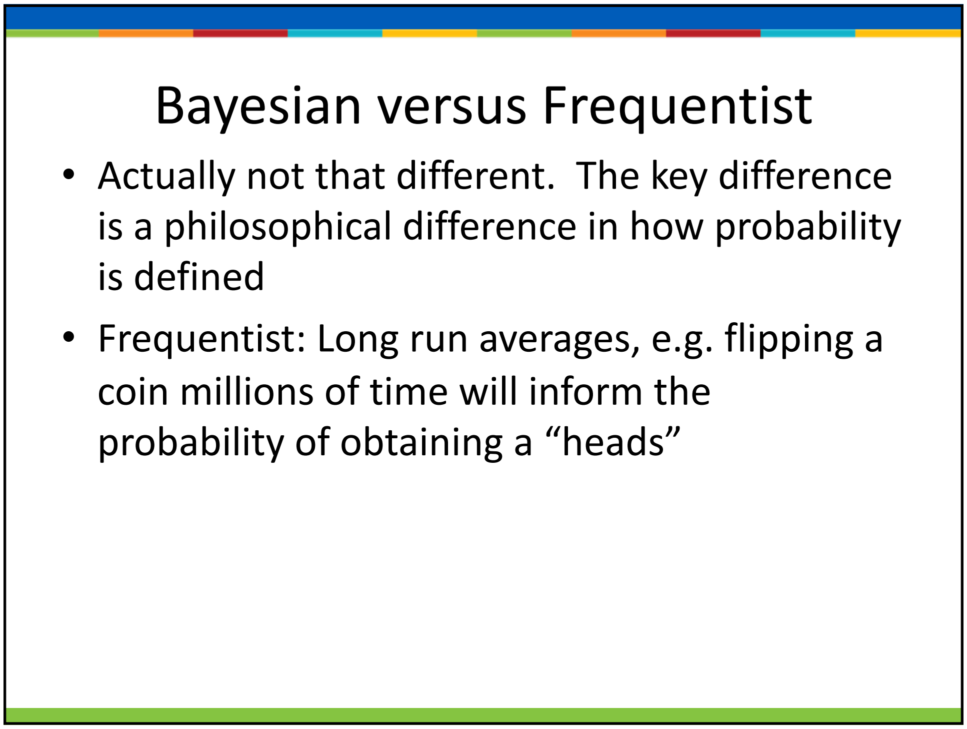
More realistic models

Log-normal



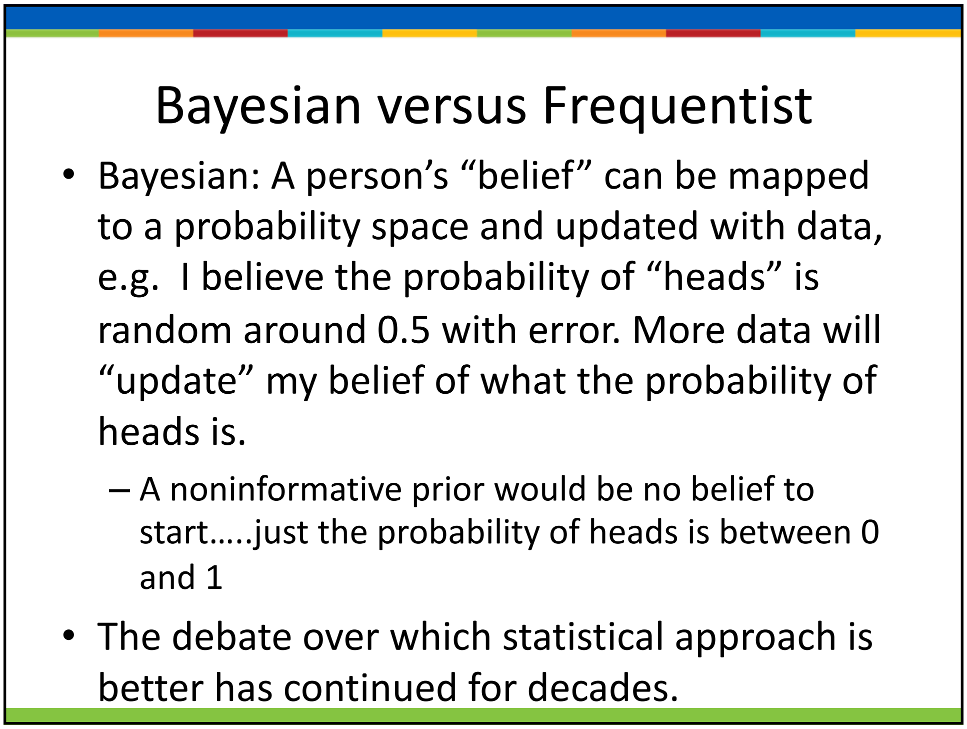
Fitting a Probability Distribution

- Several models to chose from
  - Truncated normal is very inflexible and has some key assumptions
  - There is no reason not to try to utilize the best fitting model or one that best approximates natural processes
  - Matter of equipoise---complicated multi-parameter models versus simpler lower dimension models.



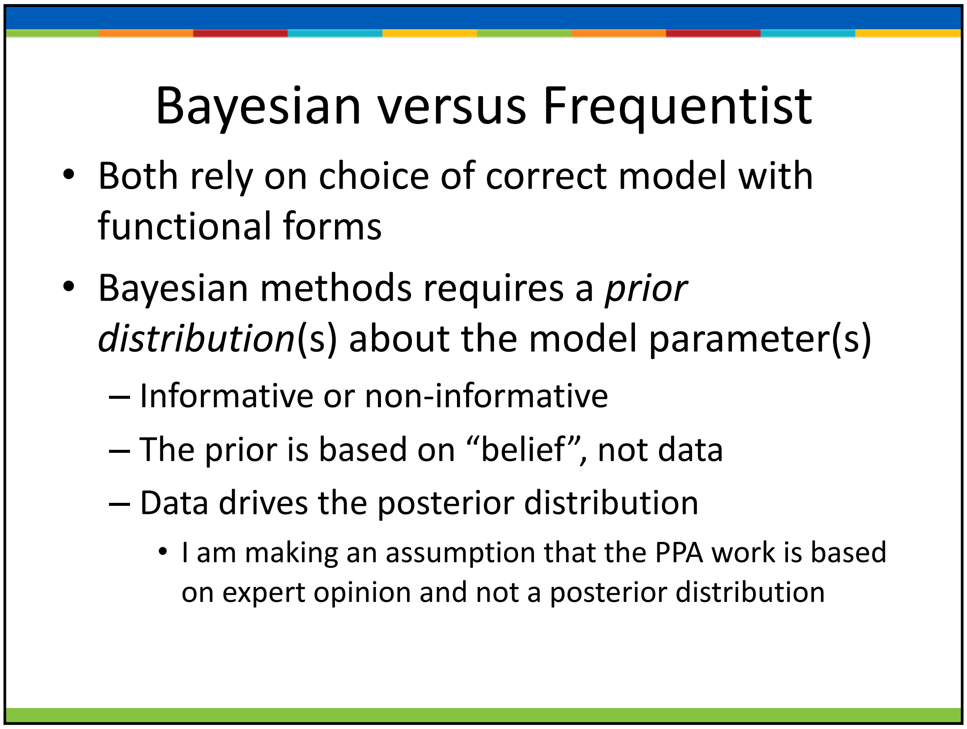
Bayesian versus Frequentist

- Actually not that different. The key difference is a philosophical difference in how probability is defined
- Frequentist: Long run averages, e.g. flipping a coin millions of time will inform the probability of obtaining a "heads"



Bayesian versus Frequentist

- Bayesian: A person's "belief" can be mapped to a probability space and updated with data, e.g. I believe the probability of "heads" is random around 0.5 with error. More data will "update" my belief of what the probability of heads is.
  - A noninformative prior would be no belief to start…..just the probability of heads is between 0 and 1
- The debate over which statistical approach is better has continued for decades.



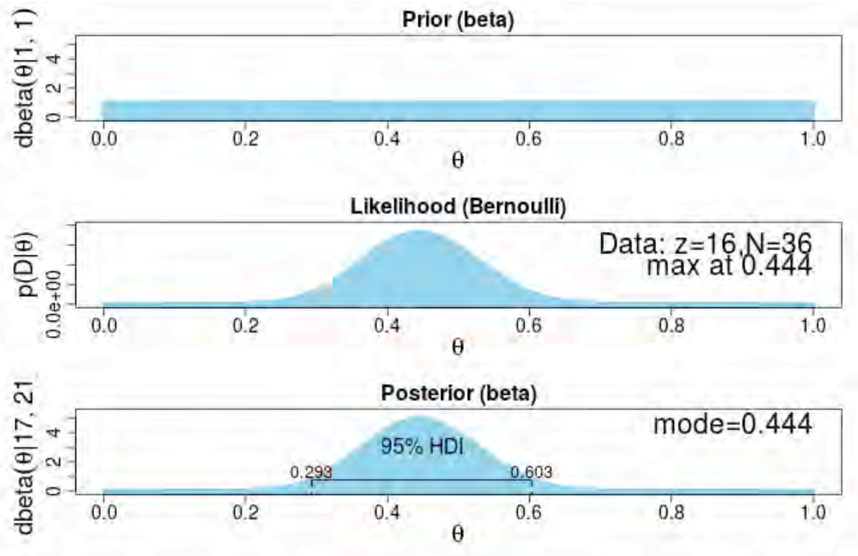
Bayesian versus Frequentist

- Both rely on choice of correct model with functional forms
- Bayesian methods requires a *prior distribution*(s) about the model parameter(s)
  - Informative or non-informative
  - The prior is based on "belief", not data
  - Data drives the posterior distribution
    - I am making an assumption that the PPA work is based on expert opinion and not a posterior distribution

Bayesian versus Frequentist

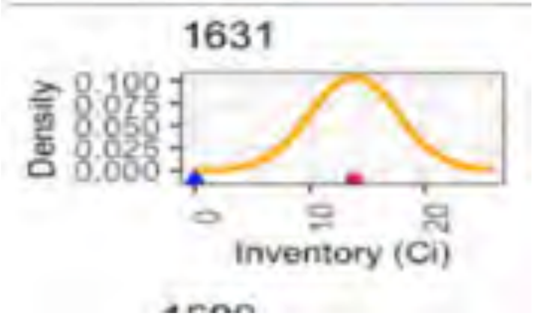
- Both approaches rely on data to provide accurate predictions
- In general, frequentist and Bayesian methods (should) yield similar results

Probability of heads (say we see 16 heads out of 36 flips)



Activity Distribution by Burial Record

- Page 16 PPA document.

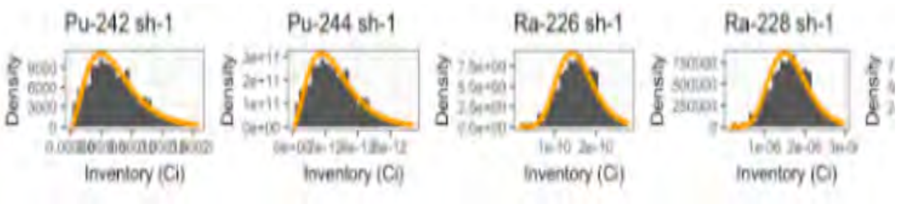


Activity Distribution by Burial Record

- My guess is that they used a normal prior distribution and normal posterior distribution and fit the density model with one observation. Or this is just an illustration
- Had to assume some scale value not based on data…seems to be some pooled value
- Not exactly sure what these figures represent

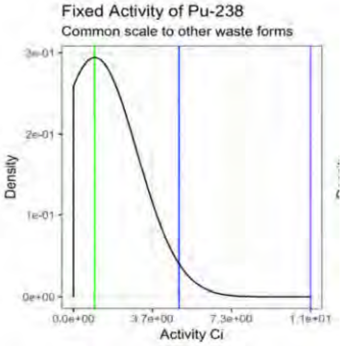
Total Inventory

- Not sure what is going on here…..certainly fitting non-normal distributions…Bayesian or frequentist…..probably nonparametric



Tank 8D-1 non-STS

- Unclear if this is a prior or posterior?? Is based on one data point or no data or much data
- Choice of scale seems to be pooled across waste forms

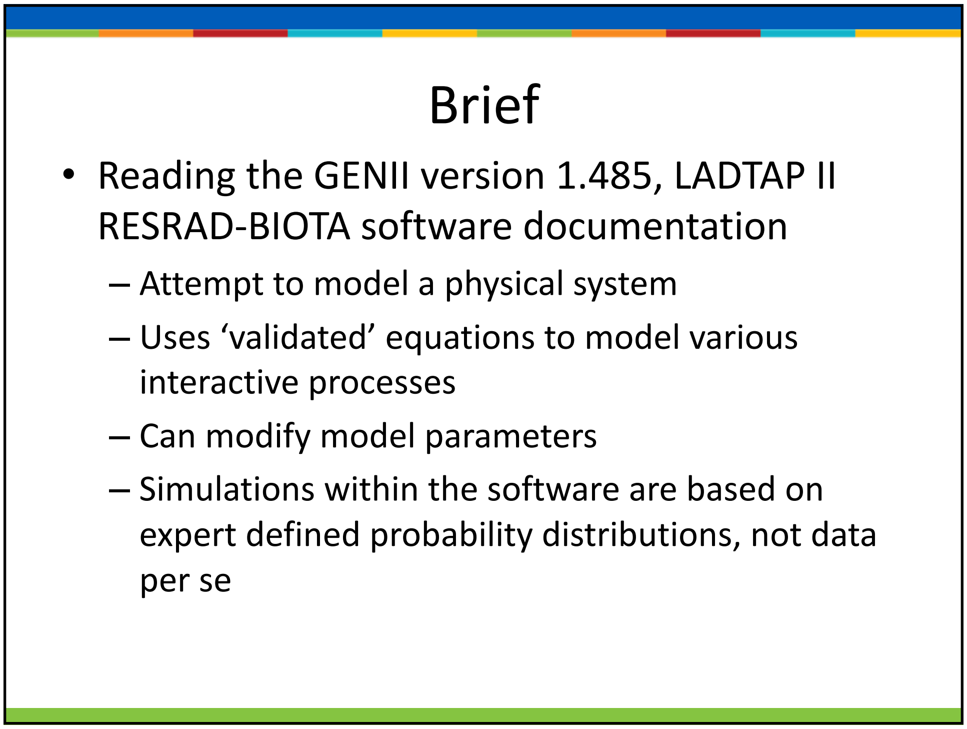


Brief

- Poor choice of models is generally not overcome by data (other approaches) for either frequentist or Bayesian parametric methods
- Bayesian methods tend to be anti-conservative, i.e. one can incorporate strong ‘beliefs’, higher likelihood of false positive results but can be more efficient if ‘correct’ prior distribution is chosen

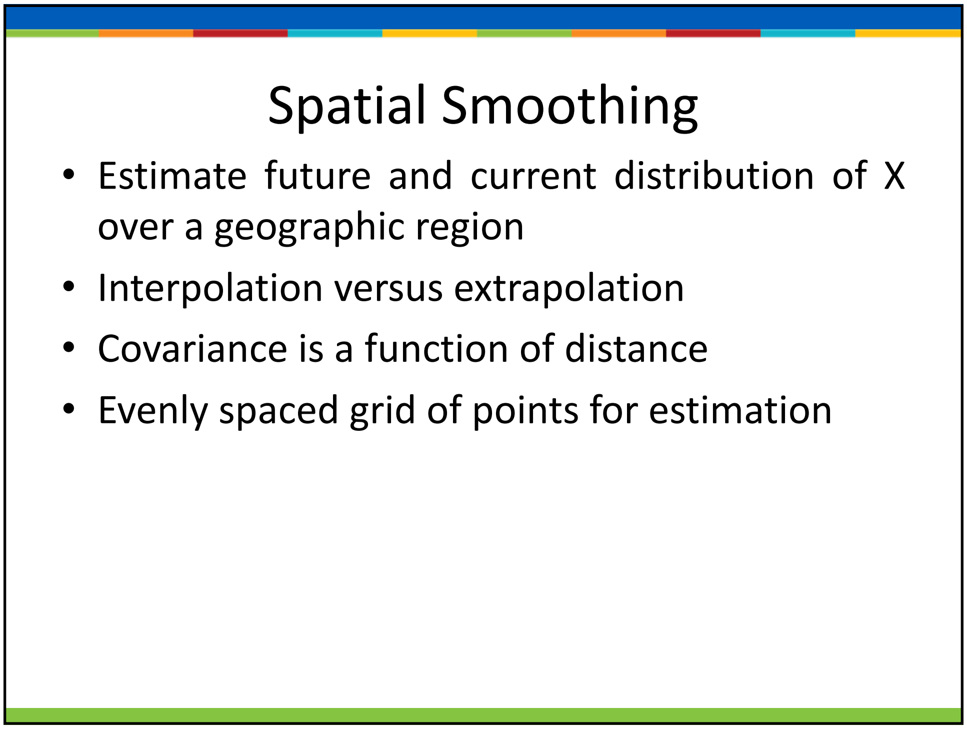
Brief

- Frequentist methods are data driven only, conservative
- With the same ‘base’ distribution both tend to converge to the same answer as more data is gathered
- very similar mathematical properties when a non-informative prior is utilized.



Brief

- Reading the GENII version 1.485, LADTAP II RESRAD-BIOTA software documentation
  - Attempt to model a physical system
  - Uses ‘validated’ equations to model various interactive processes
  - Can modify model parameters
  - Simulations within the software are based on expert defined probability distributions, not data per se

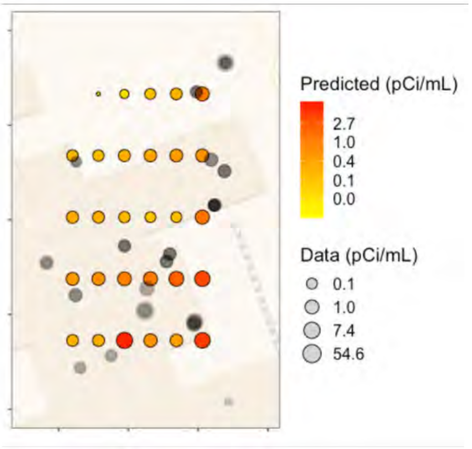


Spatial Smoothing

- Estimate future and current distribution of X over a geographic region
- Interpolation versus extrapolation
- Covariance is a function of distance
- Evenly spaced grid of points for estimation

Flag-WVDP Feb 2019 Inv Update

Convex Hull-interpolation vs extrapolation


Predicted (pCi/mL)
Data (pCi/mL)