Introduction to Bayesian Inference and Uncertainty Propagation

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Essentially, all models are wrong, but some are useful, George E.P. Box, Industrial Statistician.

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"We":
Zhengzheng Hu, Nate Burch, Allison Lewis, Kathleen Schmidt, Nikolas Bravo, Mami Wentworth (NCSU)
Michael Hays, Billy Oates (Florida State University)
Brian Williams (LANL), Russell Hooper, Brian Adams, Vince Mousseau (Sandia)
Emre Tatli and Yixing Sung (Westinghouse)
Modeling Strategy

**General Strategy:** Conservation of stuff

\[
\begin{array}{c|c}
\text{Stuff} & x \quad x + \Delta x \\
\end{array}
\]

\[
\frac{d\text{Stuff}}{dt} = \text{Stuff in} - \text{Stuff out} + \text{Stuff created} - \text{Stuff destroyed}
\]

**Continuity Equation:**

\[
\frac{\partial (\rho \Delta x)}{\partial t} = \phi(t, x) - \phi(t, x + \Delta x)
\]

\[
\Rightarrow \lim_{\Delta x \to 0} \frac{\partial \rho}{\partial t} = \lim_{\Delta x \to 0} \frac{\phi(t, x) - \phi(t, x + \Delta x)}{\Delta x}
\]

\[
\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = 0
\]

**Density:** \(\rho(t, x)\) - Stuff per unit length or volume

**Rate of Flow:** \(\phi(t, x)\) - Stuff per second

**More Generally:**

\[
\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources} - \text{Sinks}
\]
Example 1: Weather Models

Challenges:

• Coupling between temperature, pressure gradients, precipitation, aerosol, etc.;
• Models and inputs contain uncertainties;
• Numerical grids necessarily larger than many phenomena; e.g., clouds
• Sensors positions may be uncertain; e.g., weather balloons, ocean buoys.

Goal:

• Assimilate data to quantify uncertain initial conditions and parameters;
• Make predictions with quantified uncertainties.
Equations of Atmospheric Physics

Conservation Relations:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \]

Momentum

\[ \frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho} \nabla p - g \hat{k} - 2 \Omega \times \mathbf{v} \]

Energy

\[ \rho c_v \frac{\partial T}{\partial t} + p \nabla \cdot \mathbf{v} = -\nabla \cdot \mathbf{F} + \nabla \cdot (k \nabla T) + \rho \dot{q}(T, p, \rho) \]

\[ p = \rho RT \]

Water

\[ \frac{\partial m_j}{\partial t} = -\mathbf{v} \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho), \ j = 1, 2, 3, \]

Aerosol

\[ \frac{\partial \chi_j}{\partial t} = -\mathbf{v} \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho), \ j = 1, \cdots, J, \]

Constitutive Closure Relations: e.g.,

\[ S_{m_2} = S_1 + S_2 + S_3 - S_4 \]

where

\[ S_1 = \bar{\rho} (m_2 - m_2^*)^2 \left[ 1.2 \times 10^{-4} + \left( 1.569 \times 10^{-12} \frac{n_r}{d_0 (m_2 - m_2^*)} \right) \right]^{-1} \]
Ensemble Predictions:

Cone of Uncertainty:

00 UTC on August 26, 2005
12 UTC on August 26, 2005
Ensemble Predictions

Ensemble Predictions:

Cone of Uncertainty:

00 UTC on August 26, 2005
12 UTC on August 26, 2005

General Questions:

• What is expected rainfall in Research Triangle on February 25?
• What are average high and low temperatures?
• What is predicted average snow fall?
• Note: Quantities are statistical in nature.
Example 2: Pressurized Water Reactors (PWR)

Models:
- Involve neutron transport, thermal-hydraulics, chemistry.
- Inherently multi-scale, multi-physics.

CRUD Measurements: Consist of low resolution images at limited number of locations.
Challenges:
• Models linear in the state but function of 7 independent variables:
  \[ r = x, y, z; E; \Omega = \theta, \phi; t \]
• Very large number of inputs or parameters; e.g., 100,000. **Parameter selection critical.**
• Codes can take hours to days to run.

**Example:** Shearon Harris outside Raleigh

**UQ Questions:**
• What is peak operating temperature?
• What is expected level of CRUD buildup?
• What is associated risk?
• What is expected profit for new design?
Example 3: HIV Model for Characterization and Control Regimes

**HIV Model:**

\[ \dot{T}_1 = \lambda_1 - d_1 T_1 - (1 - \varepsilon_1) k_1 V T_1 \]
\[ \dot{T}_2 = \lambda_2 - d_2 T_2 - (1 - f \varepsilon_2) k_2 V T_2 \]
\[ \dot{T}^*_1 = (1 - \varepsilon_1) k_1 V T_1 - \delta T^*_1 - m_1 E T^*_1 \]
\[ \dot{T}^*_2 = (1 - f \varepsilon_2) k_2 V T_2 - \delta T^*_2 - m_2 E T^*_2 \]
\[ \dot{V} = N_T \delta (T^*_1 + T^*_2) - c V - [(1 - \varepsilon) \rho_1 k_1 T_1 + (1 - f \varepsilon) \rho_2 k_2 T_2] V \]
\[ \dot{E} = \lambda_E + \frac{b_E (T^*_1 + T^*_2)}{T^*_1 + T^*_2 + K_b} E - \frac{d_E (T^*_1 + T^*_2)}{T^*_1 + T^*_2 + K_d} E - \delta_E E \]

**Notes:** 21 parameters

[Adams, Banks et al., 2005, 2007]

**Notation:** \( \dot{E} \equiv \frac{dE}{dt} \)

**Compartmental Diagram:**

- **Uninfected Target Cells**
- **Infectious Virus**
- **Infected Target Cells**
- **Non-infectious Virus**
- **Immune Effectors (CTLs)**
Example: HIV Model for Characterization and Treatment Regimes

HIV Model: Several sources of uncertainty including viral measurement techniques

Example: Upper and lower limits to assay sensitivity

UQ Questions:

• What are the uncertainties in parameters that cannot be directly measured?
• What is optimal treatment regime that is “safe” for patient?
• What is expected viral load? Issue: very often requires high-dimensional integration!
• e.g., \( \mathbb{E}[V(t)] = \int_{\mathbb{R}^2} V(t, q) \rho(q) dq \)

Experimental results are believed by everyone, except for the person who ran the experiment, source anonymous, quoted by Max Gunzburger, Florida State University.
Example 4: SIR Cholera Model

Model:

\[
\begin{align*}
\frac{dS}{dt} &= bN - \beta_L S \frac{B_L}{\kappa_L + B_L} - \beta_H S \frac{B_H}{\kappa_H + B_H} - bS \\
\frac{dI}{dt} &= \beta_L S \frac{B_L}{\kappa_L + B_L} + \beta_H S \frac{B_H}{\kappa_H + B_H} - (\gamma + b)I \\
\frac{dR}{dt} &= \gamma I - bR \\
\frac{dB_H}{dt} &= \xi I - \chi B_H \\
\frac{dB_L}{dt} &= \chi B_H - \delta B_L
\end{align*}
\]

- **Model Parameter**
  - **Symbol**
  - **Units**
  - **Values**

| Rate of drinking $B_L$ cholera | $\beta_L$ | $\frac{1}{\text{week}}$ | 1.5 |
| Rate of drinking $B_H$ cholera | $\beta_H$ | $\frac{1}{\text{week}}$ | 7.5 ($\ast$) |
| $B_L$ cholera carrying capacity | $\kappa_L$ | $\frac{\text{# bacteria}}{m^6}$ | $10^6$ |
| $B_H$ cholera carrying capacity | $\kappa_H$ | $\frac{\text{# bacteria}}{m^6}$ | $\frac{\kappa_L}{700}$ |
| Human birth and death rate | $b$ | $\frac{1}{\text{week}}$ | $1560$ |
| Rate of decay from $B_H$ to $B_L$ | $\chi$ | $\frac{1}{\text{week}}$ | $168/5$ |
| Rate at which infectious individuals spread $B_H$ bacteria to water | $\xi$ | $\frac{\text{# bacteria}}{\text{# individuals} \cdot m^6 \cdot \text{week}}$ | $70$ |
| Death rate of $B_L$ cholera | $\delta$ | $\frac{1}{\text{week}}$ | $30$ |
| Rate of recovery from cholera | $\gamma$ | $\frac{1}{\text{week}}$ | $5$ |

[Diagram of the SIR model with nodes S, I, R, B_H, B_L, and arrows for transitions.]
Example: SIR Cholera Model

**Strategy:** Time-dependent global sensitivity indices; later talk by Pierre Gremaud

![Graph showing sensitivity indices over time]

**Conclusion:** Sensitive indices

- $\gamma$: Recovery rate
- $\beta_H$: Rate of drinking $B_H$ cholera
- $\kappa_L$: $B_L$ carrying capacity; Note $\kappa_H = \kappa_L/700$
- $\xi$: Rate at which $B_H$ bacteria spread
Example: SIR Cholera Model

Model:

\[
\frac{dS}{dt} = bN - \beta_L S \frac{B_L}{\kappa_L + B_L} - \beta_H S \frac{B_H}{\kappa_H + B_H} - bS
\]

\[
\frac{dI}{dt} = \beta_L S \frac{B_L}{\kappa_L + B_L} + \beta_H S \frac{B_H}{\kappa_H + B_H} - (\gamma + b)I
\]

\[
\frac{dR}{dt} = \gamma I - bR
\]

\[
\frac{dB_H}{dt} = \xi I - \chi B_H
\]

\[
\frac{dB_L}{dt} = \chi B_H - \delta B_L
\]

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<td>$\frac{5}{7}$</td>
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Steps in Uncertainty Quantification

Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.
Model Calibration and Uncertainty Propagation

Sources of Uncertainty:
- Model
- Parameters
- Sensor measurements
- Initial conditions

Strategy:
- Quantify uncertainty in parameters
- Propagate uncertainty through model

Example: HIV model
\[
\begin{align*}
\dot{T}_1 &= \lambda_1 - d_1 T_1 - (1 - \varepsilon) k_1 V T_1 \\
\dot{T}_2 &= \lambda_2 - d_2 T_2 - (1 - f\varepsilon) k_2 V T_2 \\
\dot{T}_1^* &= (1 - \varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^* \\
\dot{T}_2^* &= (1 - f\varepsilon) k_2 V T_2 - \delta T_2^* - m_2 E T_2^* \\
V &= N_T \delta(T_1^* + T_2^*) - cV - [(1 - \varepsilon)\rho_1 k_1 T_1 + (1 - f\varepsilon)\rho_2 k_2 T_2]V \\
\dot{E} &= \lambda_E + \frac{b_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E
\end{align*}
\]

Parameters: Reduced set
\[q = [b_E, \delta, d_1, k_2, \lambda_1, K_b]\]

Point Estimates: Ordinary least squares
\[q^0 = \arg\min_q \frac{1}{2} \sum_{j=1}^{N} [v_j - f(t_j, q)]^2\]

Note: Scaling critical since parameter values vary by 8 orders of magnitude.
Model Calibration and Predictions

Optimization Results:

<table>
<thead>
<tr>
<th>$b_E$</th>
<th>$\delta$</th>
<th>$d_1$</th>
<th>$k_2$</th>
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</tr>
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<tr>
<td>0.30</td>
<td>0.68</td>
<td>$9.1 \times 10^{-3}$</td>
<td>$1.22 \times 10^{-4}$</td>
<td>$9.95 \times 10^{3}$</td>
<td>88.5</td>
</tr>
</tbody>
</table>

Data and Prediction of Immune Effector Response $E$:

**Note:** Point estimates but no quantification of uncertainty in:
- Model
- Parameters
- Data

**Goals:**
- Replace point estimates with distributions.
- Construct credible and prediction intervals.
- Natural in a Bayesian framework
Statistical Inference

**Goal:** The goal in statistical inference is to make conclusions about a phenomenon based on observed data.

**Frequentist:** Observations made in the past are analyzed with a specified model. Result is regarded as confidence about state of real world.

- Probabilities defined as frequencies with which an event occurs if experiment is repeated several times.
- Parameter Estimation:
  - Relies on estimators derived from different data sets and a specific sampling distribution.
  - Parameters may be unknown but are fixed and deterministic.

**Bayesian:** Interpretation of probability is subjective and can be updated with new data.

- Parameter Estimation: Parameters are considered to be random variables having associated densities.
Bayesian Inference: More General Model

**Example:** Displacement-force relation (Hooke’s Law)

\[ s_i = E e_i + \epsilon_i , \ i = 1, \ldots, N \]

\[ \epsilon_i \sim N(0, \sigma^2) \]

**Parameter:** Stiffness \( E \)

**Strategy:** Use model fit to data to update prior information

\[
\pi_0(E) e^{-\sum_{i=1}^{N} [s_i - E e_i]^2 / 2\sigma^2} \quad \Rightarrow \quad \pi(E|s)
\]

**Non-normalized Bayes’ Relation:**

\[
\pi(E|s) = e^{-\sum_{i=1}^{N} [s_i - E e_i]^2 / 2\sigma^2} \pi_0(E)
\]
Bayesian Inference

**Bayes’ Relation:** Specifies posterior in terms of likelihood and prior

\[
\pi(q|\nu) = \frac{\pi(\nu|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\nu|q)\pi_0(q)\,dq}
\]

\[\text{Likelihood: } e^{-\sum_{i=1}^{N}[s_i-Ee_i]^2/2\sigma^2}, \quad q = E\nu = [s_1, \ldots, s_N]\]

- **Prior Distribution:** Quantifies prior knowledge of parameter values
- **Likelihood:** Probability of observing a data given set of parameter values.
- **Posterior Distribution:** Conditional distribution of parameters given observed data.

**Problem:** Can require high-dimensional integration

- e.g., HIV Model: \(p = 6 - 23!\)

**Solution:** Sampling-based Markov Chain Monte Carlo (MCMC) algorithms.

- Metropolis algorithms first used by nuclear physicists during Manhattan Project in 1940’s to understand particle movement underlying first atomic bomb.
Markov Chain Monte Carlo Methods

Strategy:

- Sample values from proposal distribution $J(q^*|q^{k-1})$ that reflects geometry of posterior distribution
- Compute $r(q^*|q^{k-1}) = \frac{\pi(v|q^*)\pi_0(q^*)}{\pi(v|q^{k-1})\pi_0(q^{k-1})}$
  * If $r \geq 1$, accept with probability $\alpha = 1$
  * If $r < 1$, accept with probability $\alpha = r$

Intuition: Consider flat prior $\pi_0(q) = 1$ and Gaussian observation model

$$\pi(v|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}$$

$$SS_q = \sum_{i=1}^{N} [v_i - f(t_i, q)]^2$$
Delayed Rejection Adaptive Metropolis (DRAM)

**Algorithm:** [Haario et al., 2006] – MATLAB, Python

1. Determine \( q^0 = \text{arg min}_q \sum_{i=1}^{N} [u_i - f(t_i, q)]^2 \)

2. For \( k = 1, \cdots, M \)
   (a) Construct candidate \( q^* \sim N(q^{k-1}, V) \)
   (b) Compute likelihood
      \[
      SS_{q^*} = \sum_{i=1}^{N} [u_i - f(t_i, q^*)]^2
      \]
      \[
      \pi(u|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}
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   (c) Accept $q^*$ with probability dictated by likelihood
Bayesian Model Calibration – HIV Example

Model: \[
\begin{align*}
\dot{\lambda}_1 &= \omega_1 - d_1 \lambda_1 - (1 - \varepsilon)k_1 VT_1 \\
\dot{\lambda}_2 &= \omega_2 - d_2 \lambda_2 - (1 - f\varepsilon)k_2 VT_2 \\
\dot{T}_1^* &= (1 - \varepsilon)k_1 VT_1 - \delta T_1^* - m_1 ET_1^* \\
\dot{T}_2^* &= (1 - f\varepsilon)k_2 VT_2 - \delta T_2^* - m_2 ET_2^* \\
\dot{V} &= N_T \delta(T_1^* + T_2^*) - cV - [(1 - \varepsilon)\rho_1 \lambda_1 T_1 + (1 - f\varepsilon)\rho_2 \lambda_2 T_2]V \\
\dot{E} &= \lambda_E + \frac{b_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta E E
\end{align*}
\]

Verification: Why do we trust results??

- Compare results from different algorithms; e.g., DRAM and Gibbs

Parameter Chains and Densities: \[q = [b_E, \delta, d_1, k_2, \lambda_1, K_b]\]
Chain Convergence (Burn-In)

Techniques:

• Visually check chains
• Statistical tests
• Often abused in the literature
Propagation of Uncertainty in Models – HIV Example

**Parameter Densities:**

- $b_L$
- $\delta$
- $d_1$
- $k_2$
- $\lambda_1$
- $K_b$

**Techniques:**

- Sample from parameter densities to construct prediction intervals for QoI.
- Slow convergence rate $O(1/\sqrt{M})$
- 100-fold more evaluations required to gain additional place of accuracy.
- Significant numerical analysis used to efficiently propagate densities.

**Samples from Chain**

**Data, Credible Intervals and Prediction Intervals**

**Non-Gaussian Credible and Prediction Intervals**
Use of Prediction Intervals: Nuclear Power Plant Design

Subchannel Code (COBRA-TF): numerous closure relations, ~70 parameters

e.g., Dittus—Boelter Relation

\[ Nu = 0.023 Re^{0.8} Pr^{0.4} \]

\( Nu \): Nusselt number
\( Re \): Reynolds number
\( Pr \): Prandtl number

Industry Standard: Employ conservative, uniform, bounds

i.e., [0, 0.046], [0, 1.6], [0, 0.8]

Bayesian Analysis: Employ conservative bounds as priors

Note: Substantial reduction in parameter uncertainty
Use of Prediction Intervals: Nuclear Power Plant Design

**Strategy:** Propagate parameter uncertainties through COBRA-TF to determine uncertainty in maximum fuel temperature

**Notes:**
- Temperature uncertainty reduced from 40 degrees to 5 degrees
- Can run plant 20 degrees hotter, which significantly improves efficiency

**Ramification:** Savings of **10 billion dollars per year** for US power plants

**Issues:**
- We considered only one of many physical relations
- Nuclear regulatory commission takes years to change requirements and codes

**Good News:** We are now working with Westinghouse to reduce uncertainties.
Parameter Selection: Required for models with unidentifiable or noninfluential inputs

- e.g., HIV and SIR model
Parameter Selection Techniques

**Issue:** Parameters often *not identifiable* in the sense that they are uniquely determined by the data.

**SIR Model:**

\[
\begin{align*}
\frac{dS}{dt} &= \delta N - \delta S - \gamma k IS, \quad S(0) = S_0 \quad \text{Susceptible} \\
\frac{dI}{dt} &= \gamma k IS - (r + \delta)I, \quad I(0) = I_0 \quad \text{Infectious} \\
\frac{dR}{dt} &= r I - \delta R, \quad R(0) = R_0 \quad \text{Recovered}
\end{align*}
\]

**Response:**

\[y = \int_{0}^{5} R(t, q) dt\]

**Note:** Parameter set \( q = [\gamma, k, r, \delta] \) is not identifiable

**Later Talk:** Pierre Gremaud -- *A Biased Introduction to Global Sensitivity Analysis*
SIR Disease Example

SIR Model:

\[
\frac{dS}{dt} = \delta N - \delta S - \gamma kS \quad , \quad S(0) = S_0 \quad \text{Susceptible}
\]

\[
\frac{dI}{dt} = \gamma kS - (r + \delta)I \quad , \quad I(0) = I_0 \quad \text{Infectious}
\]

\[
\frac{dR}{dt} = rI - \delta R \quad , \quad R(0) = R_0 \quad \text{Recovered}
\]

Typical Realization:
Local Sensitivity Analysis

Local Sensitivities: Consider

\[
\frac{\partial y}{\partial \gamma}, \frac{\partial y}{\partial r}, \frac{\partial y}{\partial \delta}, \frac{\partial y}{\partial k}
\]

Conclusion: Response most sensitive to \( r \) and \( \delta \)

Limitations:

- Does not accommodate potential uncertainty in parameters.
- Sensitive to units and magnitudes of parameters.
Global Sensitivity Analysis

**Global Sensitivities:** Sample parameters from uniform distributions; e.g.,

\[ \gamma \sim U(\gamma_l, \gamma_r) \]
\[ \gamma_l = \gamma_{nom} - 0.2\gamma_{nom} \]
\[ \gamma_r = \gamma_{nom} + 0.2\gamma_{nom} \]

**Recall:** MATLAB command to sample M samples from U(a,b)

\[ >> q = a + (b - a) \times \text{rand}(M, 1) \]

**Conclusion:** Response most sensitive to \( r \) and \( \delta \)

**Advantage:**

- Quantifies how uncertainties in response apportioned to uncertainties in parameters -- Basis for Analysis of Variance (ANOVA).
Variance-Based Methods

**Sobol Representation:** For now, take $Q_i \sim \mathcal{U}(0, 1)$ and $\Gamma = [0, 1]^p$

Take

$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{1 \leq i < j \leq p} f_{ij}(q_i, q_j)$$

With appropriate assumptions,

$$f_0 = \int_{\Gamma} f(q) dq$$

$$f_i(q_i) = \int_{\Gamma^{p-1}} f(q) dq_{\sim i} - f_0$$

**Variances:**

$$D_i = \int_{0}^{1} f_i^2(q_i) dq_i$$

$$D = \text{var}(Y)$$

**Sobol Indices:** $S_i = \frac{D_i}{D}$

**Statistical Interpretation:**

$$D_i = \text{var}[E(Y|q_i)] \Rightarrow S_i = \frac{\text{var}[E(Y|q_i)]}{\text{var}(Y)}$$
Morris Screening: Random Sampling of Approximated Derivatives

Example: Consider uniformly distributed parameters on \( \Gamma = [0, 1]^p \)

Elementary Effect:

\[
d_i^j = \frac{f(q^j + \Delta e_i) - F(q^j)}{\Delta}, \quad i^{th} \text{ parameter, } j^{th} \text{ sample}
\]

Global Sensitivity Measures: \( r \) samples

\[
\mu_i^* = \frac{1}{r} \sum_{j=1}^{r} |d_i^j(q)|
\]

\[
\sigma_i^2 = \frac{1}{r-1} \sum_{j=1}^{r} \left(d_i^j(q) - \mu_i\right)^2, \quad \mu_i = \frac{1}{r} \sum_{j=1}^{r} d_i^j(q)
\]
SIR Disease Example

SIR Model:

\[
\begin{align*}
\frac{dS}{dt} &= \delta N - \delta S - \gamma kIS, \quad S(0) = S_0 \quad \text{Susceptible} \\
\frac{dI}{dt} &= \gamma kIS - (r + \delta)I, \quad I(0) = I_0 \quad \text{Infectious} \\
\frac{dR}{dt} &= rl - \delta R, \quad R(0) = R_0 \quad \text{Recovered}
\end{align*}
\]

Note: Parameter set \( q = [\gamma, k, r, \delta] \) is not identifiable

Assumed Parameter Distribution:

\[
\begin{align*}
\gamma &\sim \mathcal{U}(0, 1), \quad k \sim \text{Beta}(\alpha, \beta), \quad r \sim \mathcal{U}(0, 1), \quad \delta \sim \mathcal{U}(0, 1)
\end{align*}
\]

Infection \quad Interaction \quad Recovery \quad Birth/death
Coefficient \quad Coefficient \quad Rate \quad Rate

Response:

\[
y = \int_{0}^{5} R(t, q) dt
\]
SIR Disease Example

Global Sensitivity Measures:

<table>
<thead>
<tr>
<th></th>
<th>$\gamma$</th>
<th>$k$</th>
<th>$r$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sobol $S_i$</td>
<td>0.0997</td>
<td>0.0312</td>
<td>0.7901</td>
<td>0.1750</td>
</tr>
<tr>
<td>Sobol $S_{T_i}$</td>
<td>-0.0637</td>
<td>-0.0541</td>
<td>0.5634</td>
<td>0.2029</td>
</tr>
<tr>
<td>Morris $\mu_i^* (\times 10^3)$</td>
<td>0.2532</td>
<td>0.2812</td>
<td>2.0184</td>
<td>1.2328</td>
</tr>
<tr>
<td>Morris $\sigma_i (\times 10^3)$</td>
<td>0.9539</td>
<td>1.6245</td>
<td>6.6748</td>
<td>3.9886</td>
</tr>
</tbody>
</table>

Result: Densities for $R(t_f)$ at $t_f = 5$

Note: Can fix non-influential parameters $\gamma$, $k$

Note: More during the project!
Concluding Remarks

Notes:

• UQ requires a synergy between engineering, statistics, and applied mathematics.

• Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.

• Goal is to predict model responses with quantified and reduced uncertainties.

• Parameter selection is critical to isolate identifiable and influential parameters.

• Surrogate models critical for computationally intensive simulation codes.

• Codes and packages: Sandia Dakota, R, MATLAB, Python, nanoHUB.

• Prediction is very difficult, especially if it’s about the future, Niels Bohr.