Bayesian Computer Modeling with Emulators
What are the odds?

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Main idea

1. Observe (maybe vector) \( X \in \mathcal{X} \) whose probability density function

\[
X \sim p(x \mid \theta)
\]

depends on an uncertain (maybe vector) \( \theta \in \Theta \)

2. Want to predict other quantities \( Y \in \mathcal{Y} \) whose distribution

\[
Y \sim p(y \mid \theta)
\]

depends on the same \( \theta \in \Theta \)

3. While being honest about the uncertainty:

\[
Y \mid X \sim p(y \mid X = x) = \int_{\Theta} p(y \mid \theta) p(\theta \mid x) \, d\theta
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Let $X$ be the number of successes in $n = 100$ independent trials, all with the same (unknown) probability $\theta$ of success. Suppose we observe $X = 68$.

- Could $\theta$ be as low as 0.10?
  - Probably not... $P[X \geq 68 | \theta = 0.10] = 2.7 \cdot 10^{-45}$.
- The MLE is $\hat{\theta} = 0.68$. Does $\theta$ equal 0.68?
  - Probably not... $P[X = 68 | \theta = 0.68] < 0.10$.
  - And $P[\theta = 0.68 | X = 68] = 0$. 
One-Dimensional (Toy) Example

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The Truth is Revealed...

Observe: \( X = 68 \)
Believe: \( X \sim \text{Bi}(n, p) \)
Know: \( n = 100 \)
Unaware: \( \theta = 0.60 \)

Likelihood (also \( \chi^2 \)):

\[
L(\theta) = \binom{100}{68} \theta^{68} (1 - \theta)^{32}
\]

\[
Q(\theta) = \frac{(100\theta - 68)^2}{100\theta}
\]

both optimized at \( \hat{\theta} = 0.68 \). Is that \( \theta \)?

No. Remember? Data were generated with (unknown!) \( \theta = 0.60 \).
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Observe: \( X = 68 \)
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Stochastic Optimization

Fix $\theta_0 = 1/2$ (or any other arbitrary point) and, at replicate $t \in \mathbb{N}$,

- Propose $\theta^* \sim q(\theta^* | \theta_{t-1})$ (SRW);
- Accept proposal if $L(\theta^*) \geq L(\theta_{t-1})$; Otherwise stay put.

Results of $10^2$ replicates with $q = \text{Un}(-0.10, 0.10)$ RW steps:

Unchanged after first 33 steps, with $\hat{\theta} \approx 0.6784$. Is that $\theta$? No.
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It’s an approximation to the posterior mode,

\[ \tilde{\theta} = \underset{\theta}{\text{argmax}} \ L(\theta) = 0.68 \]

That’s a data-based quantity, which might be far from \( \theta \).
Stochastic Optimization

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$$\tilde{\theta} = \text{argmax} \; L(\theta) = 0.68$$

That’s a data-based quantity, which might be far from $\theta$. 
Bayesian Posterior

Fix $\theta_0 = 1/2$ (or any other arbitrary point) and, at replicate $t \in \mathbb{N}$,

- Propose $\theta^* \sim q(\theta^* | \theta_{t-1})$ (SRW);
- Accept proposal with probability $1 \wedge H$ for Hastings Ratio

$$H = \frac{\pi(\theta^*) L(\theta^*) q(\theta | \theta^*)}{\pi(\theta) L(\theta) q(\theta^* | \theta)}$$

Note the difference to Stochastic Optimization—

$L(\theta^*) \geq L(\theta)$: SO Accepts  $H \geq 1$, $\Rightarrow$ MCMC Accepts

$L(\theta^*) < L(\theta)$: SO Rejects  $H < 1$, $\Rightarrow$ MCMC MIGHT accept

After $m = 100$ MCMC steps, $\bar{\theta}_m = 0.6621$ with sd 0.0443.

Is that $\theta$?  Yes!  Why?
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Bayesian Posterior, $m = 10^2$ MCMC Steps:

Mean $\pm 2 \text{ S.D.} = 0.6621 \pm 0.0886$
Bayesian Posterior, $m = 10^4$ MCMC Steps:

**MCMC Posterior Stream for Bayes Model**

**Posterior pdf**

Mean ±2 S.D. = 0.6734 ± 0.0963
Bayesian Posterior, \( m = 10^6 \) Steps:

MCMC Posterior Stream for Bayes Model

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\[ \text{Mean } \pm 2 \text{ S.D. } = 0.6673 \pm 0.1092 \]

Why aren’t the intervals getting narrower???
Bayesian Posterior, $m = 10^6$ Steps:

**MCMC Posterior Stream for Bayes Model**

![MCMC Replicates Graph]

**Posterior pdf**

![Density Graph]

Mean $\pm$ 2 S.D. = $0.6673 \pm 0.1092$

Why aren’t the intervals getting narrower???
Bayesian Posterior, \( m = \infty \) MCMC Steps:

Q: Why don’t the intervals home in on the truth as \( n \to \infty \)?
A: Because they shouldn’t!

We only observed \( x = 68 \) successes in \( n = 100 \) trials.

Recall— True \( \theta = 0.60 \) was used to generate data!
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Exact Mean $\pm 2$ S.D. $= 69/102 = 0.6764706 \pm 0.0922$

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Recall—True \( \theta = 0.60 \) was used to generate data!
What is Playful about this Toy Example?

- In **One-Dimension**, “Highest Posterior Density” (HPD) regions are **Intervals**;
  - HPD Intervals are more useful than optima—
    - $q=50\%$: $[0.6482, 0.7107]$ Doesn’t contain $\theta = 0.60$
    - $q=90\%$: $[0.6011, 0.7525]$ Doesn’t contain $\theta = 0.60$
    - $q=95\%$: $[0.5855, 0.7655]$ Does contain $\theta = 0.60$
    - $q=99\%$: $[0.5548, 0.7898]$ Does contain $\theta = 0.60$
  - In **2+ Dim**, HPDs are **High-dimensional bananas**.
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- In **2+ Dim**, HPDs are **High-dimensional bananas**.
Typical Log LLHs

At best the log likelihood will have banana-shaped contours:

with LOTS of (nearly) equally-likely $\theta$’s, and “TRUTH” unlikely to be near center!
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Optimize?

One idea... optimize and hope for the best:

Perhaps

\[ Y \mid X = x \sim p(y \mid \hat{\theta}(x)) \]

Understates uncertainty; gives wrong answer.
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Understates uncertainty; gives wrong answer.
Integrate?

Another idea... obey the **Laws of Probability**

\[
p(x, \theta) = p(x | \theta) p(\theta)
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p(x) = \int_\Theta p(x | \theta) p(\theta) \, d\theta
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p(\theta | x) = \frac{p(x, \theta)}{p(x)} = \frac{p(x | \theta) p(\theta)}{\int_\Theta p(x | \vartheta) p(\vartheta) \, d\vartheta}
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p(y | x) = \int_\Theta p(y | \theta) p(\theta | x) \, d\theta
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One problem: Where did the marginal density \( p(\theta) \) come from?
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Prior Distributions:

Where does $p(\theta)$ come from? 

**Historical experience, informed opinion, or ignorance:**

- **Historical Experience:** If we’ve seen 200 successes in 300 previous trials, we might use $p(\theta) = \text{Be}(200, 100)$ prior;

- **Informed Opinion:** If a subject-matter expert tells us s/he is certain $0.5 < \theta < 0.75$ but unsure within that interval, we might use $p(\theta) = \text{Un}(0.50 - \epsilon, 0.75 + \epsilon)$;

- **Ignorance:** In the absence of other information, we might use a conventional choice of $p(\theta) \sim \text{Un}(0, 1)$ or $p(\theta) \sim \text{Be}(\frac{1}{2}, \frac{1}{2})$. 
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What if the Integrals are hard in low dimensions?

1. Euler, Simpson, or Runge-Kutta Quadrature:

\[
p(y \mid x) = \frac{\int p(y \mid \theta)p(x \mid \theta)p(\theta) \, d\theta}{\int p(x \mid \vartheta)p(\vartheta) \, d\vartheta} \approx \sum p(y \mid \theta_j)w_j
\]

Error \( \epsilon \approx n^{-4/d} \) for \( \Theta \subseteq \mathbb{R}^d \) so need \( n = O(\epsilon^{-d/4}) \) evaluations; OK in dimension \( d \leq 4 \) for Simpson, \( d \leq 8 \) for RK4.
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- Bayes: Integrating over Parameter Space
- MC Importance Sampling:

What if the Integrals are harder?

2. Monte Carlo Importance Sampling:

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\theta_j \overset{\text{iid}}{\sim} f(\theta) d\theta, \quad w_j = \frac{p(x \mid \theta_j)p(\theta_j)}{f(\theta_j)}
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Error $\epsilon \lesssim n^{-1/2}$ for any dimension

Hard to find good “importance function” $f(\theta)$ if $d$ big.
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Hard to find good "importance function" \( f(\theta) \) if \( d \) big.
What if the Integrals are still too hard?

3. Metropolis/Hastings Markov Chain Monte Carlo:

\[ p(y \mid x) \approx \frac{\sum p(y \mid \theta_j)}{N}, \quad \{\theta_j\} \sim p(\theta \mid x) \]

\[ \theta_{j+1} = \begin{cases} 
\theta_j^* & \text{w/prob } [1 \wedge H_j] \\
\theta_j & \text{otherwise}
\end{cases} \]

\[ \theta_j \sim \theta_j^* \sim g(\theta_j^* \mid \theta_j), \quad H_j = \frac{p(\theta_j^*) g(\theta_j \mid \theta_j^*)}{p(\theta_j) g(\theta_j^* \mid \theta_j)} \]

Works well in high-dimensional problems (despite autocorrelation). Just a technique for approximating integrals— not optimization.
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Deterministic Computer Models

How can *Probability* help us with *Deterministic* computer models?
What’s **random** about a deterministic computer model?

Well... our *uncertainty* about it! Here’s an analogy:

- Find the book closest to you—
- How long is 2\textsuperscript{nd} text line on page 50? Call length “X”
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- Uh oh, paragraph could end... 15–70 chars, w/prob 0.75?
- Answer (for me): $X = 61$ (Doob), so now $P[X = 61] = 1$.

**Observation changes probabilities!**

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Computer Models and Reality

Denote by $Y^F(x_j)$ the value of a Field measurement taken at settable and observable input value $x_j$. Typically this will differ by some measurement error $\epsilon^F_j$ from the Real value:

$$Y^F(x_j) = Y^R(x_j) + \epsilon^F_j, \quad \epsilon^F_j \sim \text{No}(0, 1/\lambda^F).$$

Our computer Model will include additional tuning parameters and, alas, may also exhibit bias or discrepancy:

$$Y^R(x) = Y^M(x, u) + \delta_u(x).$$

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Uncertainty for Complex Models

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Complex model uncertainty is much more than measurement error and systematic errors.

In studying the “Galform” model for Galaxy Formation, Vernon, Goldstein & Bower (2004) identify five aspects:

1. **Observational error**
   \[ \epsilon^F_j = ??? \]

2. **Parameter uncertainty**
   \[ x, u = ??? \]

3. **Simulator uncertainty**
   \[ Y^M(x, u) = ??? \]

4. **Structural uncertainty**
   \[ \delta_u(x) = ??? \]

5. **Initial condition and forcing function uncertainty**
   All the other variables & missing physics...

Want to see a modest (3-dim) example? Or Wrap Up?
Uncertainty for Complex Models

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Pedagogic Example

The mass $y(t)$ of Silane gas $\text{SiH}_4$ decreases in the manufacture of silicon solar cells through the reaction $\text{SiH}_4 \rightarrow \text{Si} + 2\text{H}_2$; a plausible model is linear decay:

$$\frac{d}{dt} y(t) = -u y(t), \quad y(0) = y_0$$

for (unknown) reaction rate $u$ and (known) initial concentration $y_0$. The obvious solution to this ODE is our “computer model”

$$Y^M(t, u) = y_0 \exp(-u t)$$

Imagine however that a portion $c$ remains unreacted, however, so the model is (a little) wrong— the real mass is

$$Y^R(t) = (y_0 - c) \exp(-u_* t) + c = Y^M(t, u_*) + \delta_u(x).$$
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### Field Data

<table>
<thead>
<tr>
<th>$t$</th>
<th>$Y^F(t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.110</td>
<td>4.730</td>
</tr>
<tr>
<td>0.432</td>
<td>3.177</td>
</tr>
<tr>
<td>0.754</td>
<td>1.970</td>
</tr>
<tr>
<td>1.077</td>
<td>2.079</td>
</tr>
<tr>
<td>1.399</td>
<td>1.908</td>
</tr>
<tr>
<td>1.721</td>
<td>1.773</td>
</tr>
<tr>
<td>2.043</td>
<td>1.370</td>
</tr>
<tr>
<td>2.366</td>
<td>1.868</td>
</tr>
<tr>
<td>2.688</td>
<td>1.390</td>
</tr>
<tr>
<td>3.010</td>
<td>1.461</td>
</tr>
</tbody>
</table>

Three noisy replicates at each of 10 field points
Minimum occurs at $\hat{u} \approx 0.6364$— how good is model at $\hat{u}$?
Model Fit and Field Data

\[ Y^F(t) \]

Time \( t \)

Not very!  Maybe there's discrepancy...
Example: Model Fit and Field Data

Not very! Maybe there’s discrepancy...
Discrepancy

\[ Y^F(x_j) = Y^M(x, u) + \epsilon_j^F + \delta_u(x) \]

We were uncertain about the:

- Tuning parameter \( u \) \( (\hat{u} \approx 0.6364) \);
- Field m.e. precision \( \lambda^F \) \( (\hat{\lambda}^F \approx 21.74) \);
- Discrepancy function \( \delta_u(x) \) (probably not zero!).

Let’s pick independent prior distributions:

- \( u \sim \text{Un}(0.2, 2.0) \)
- \( \lambda^F \sim \text{Ex}\left(\frac{1}{5\times21.74}\right) \)
- \( \delta_u(\cdot) \sim \text{GP}(0, c^B(\cdot, \cdot | \beta^y_b)) \)

and then find the posterior!
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Correcting for Discrepancy

Discrepancy-corrected predictions of $Y^F$ with 90% intervals

*Post’r dist’n of $\delta_u(\cdot)$ for $u = E[u|\text{Dat}]$*
What did we do?

We identified the model discrepancy $\delta_u(t)$ and learned $u$.

For this simulation the Truth was:

$$Y^F(t_i) = 1.5 + (3.5) e^{-1.7 t_i} \pm \epsilon_i$$

$$\delta_{u*}(t) = Y^R(t) - Y^M(t, 1.7)$$

$$= 1.5 (1 - e^{-1.7 t})$$

$$\lambda = 1/(0.3^2) \approx 11.11$$

With these, we were able to correct for the discrepancy and make reliable out-of-sample predictions of $Y^F(t')$ at unobserved times $t'$, with honest reflection of uncertainty.
How did we do it?

To simulate the posterior distribution of $u$, $\lambda^F$, and $\delta_u(\cdot)$, at each Monte Carlo step $m$ we had to:

- Draw a random $u^*$, and consider replacing $u^{m-1}$ with $u^*$; the “consideration” entails evaluating $Y^M(t_i, u^*)$ at each field location $t_i \in D$.

- Draw a new random $\lambda^{F \cdot m}$ from its complete conditional distribution given $u^{m-1}$ and $\delta_{u}^{m-1}(t)$ (easy).

- Draw a new random $\delta_{u}^{m}(t)$ from its complete conditional distribution (high-dimensional $\Rightarrow$ hard if $|D|$ is big).

All inside a loop, for $m = 1$ to $m = 1,000,000$!
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- Draw a new random $\delta^m_u(t)$ from its complete conditional distribution (high-dimensional $\Rightarrow$ hard if $|\mathcal{D}|$ is big).

All inside a loop, for $m = 1$ to $m = 1,000,000$!
A way out...

- For RHIC (for example) it may take 1 hr to evaluate $Y^M(t_i, u)$
- We don’t have 1,000,000 hours.
- If evaluating the model $Y^M(t_i, u)$ at all field locations $t_i \in D$ and tuning values $u$ is too slow, consider an Emulator
- Fit a new GaSP $Y^E(x, u) \sim \text{GP}($Mean, Cov$)$ as a fast surrogate for $Y^M(t_i, u)$, with honest reflection of uncertainty.
- The “fitting” is done at a carefully chosen set of data values:
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<th>$u_i$</th>
<th>$Y^M(t_i, u_i)$</th>
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</thead>
<tbody>
<tr>
<td>2.159</td>
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<td>0.935</td>
<td>1.174</td>
</tr>
<tr>
<td>2.594</td>
<td>0.815</td>
<td>0.604</td>
<td>2.797</td>
<td>1.790</td>
<td>0.033</td>
</tr>
<tr>
<td>1.347</td>
<td>1.460</td>
<td>0.700</td>
<td>0.100</td>
<td>1.355</td>
<td>4.366</td>
</tr>
<tr>
<td>3.000</td>
<td>1.250</td>
<td>0.0118</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fifteen points $(t_i, u_i) \in [0, 3] \times [0.5, 2]$, space-filling LHC design
Unlike a lattice, the 1-dim projections are spread widely.
Space-filling LHC design

Unlike a lattice, the 1-dim projections are spread widely.
Model our Uncertainty about $Y^M(x, u)$ with a GaSP

$Y^M(x_i, u_i)$ \hspace{1cm} Model output at input (vector) $x_i \in \mathcal{X}$, tuning parameter (vector) $u_i \in \mathcal{U}$
Only observed at a few points $\mathcal{D}^M = \{x_i, u_i\}_{i \in I}$

$Y^E(x, u)$ \hspace{1cm} Emulator: $Y^E(x, u) \sim \text{GP}(\text{Mean}, \text{Cov})$
Prior: \hspace{0.5cm} Mean $= \Psi'(x, u)\beta^m$, Cov $= c^M(\cdot, \cdot; \beta^v)$
Post’r: \hspace{0.5cm} Usual Gaussian updating formulas

Emulator is just an interpolator, with uncertainty measure
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A few details...

Mean, Covariance:
Set $\mathbf{z} = (\mathbf{x}, \mathbf{u})$, $\beta = (\beta^m, \beta^v)$:

$$
E[Y^E(\mathbf{z}) \mid \mathbf{y}^M, \beta] = \Psi'(\mathbf{z}) \beta^m + r'_z [\Gamma^M]^{-1} (\mathbf{y}^M - \Psi'(\mathbf{z}^M) \beta^m)
$$

$$
V[Y^E(\mathbf{z}), Y^E(\mathbf{z}^*) \mid \mathbf{y}^M, \beta] = c^M(\mathbf{z}, \mathbf{z}^*; \beta^v) - r'_z [\Gamma^M]^{-1} r_{z^*}
$$

where $\Gamma^M = c^M(\mathbf{z}^M, \mathbf{z}^M; \beta^v)$, $r_z = c^M(\mathbf{z}, \mathbf{z}^M; \beta^v)$.

Given $\beta^m, \beta^v$ these are usual Kalman filter formulae.
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Mean & Variance Hyperparameters $\beta^m, \beta^v$:

- **MLE**: Weighted linear regression using Model Data:
  Find $\hat{\beta}^m, \hat{\beta}^v$ by maximizing Gaussian LLH for:
  \[
  Y^M(z_i) \sim \text{No}\left(\Psi'(z_i)\beta^m, c^M(z_i, z_j; \beta^v)\right)
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General consensus is that MLE is good enough approximation at this level of hierarchy.
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Most common covariance function is isotropic **Power Exponential**:

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where \( \beta^v = (\lambda, \{\alpha_i, \rho_i\}) \)

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- Learning physics from complex models is hard, but
- **Bayesian Statistics** and meso-scale **Model Emulators** can help.
- We can use them to help identify **Regions of Parameter Space** that lead to model predictions consistent with observations—
- Or, if **no part** of parameter space works, that can shine light on model discrepancies and perhaps lead to **new insights**.

The approach has been applied successfully in up to 50 or so dimensions (but try to stay below 20 or so if you can).

**Thanks for your attention and interest!**

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(or just Google me: Robert Wolpert)
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