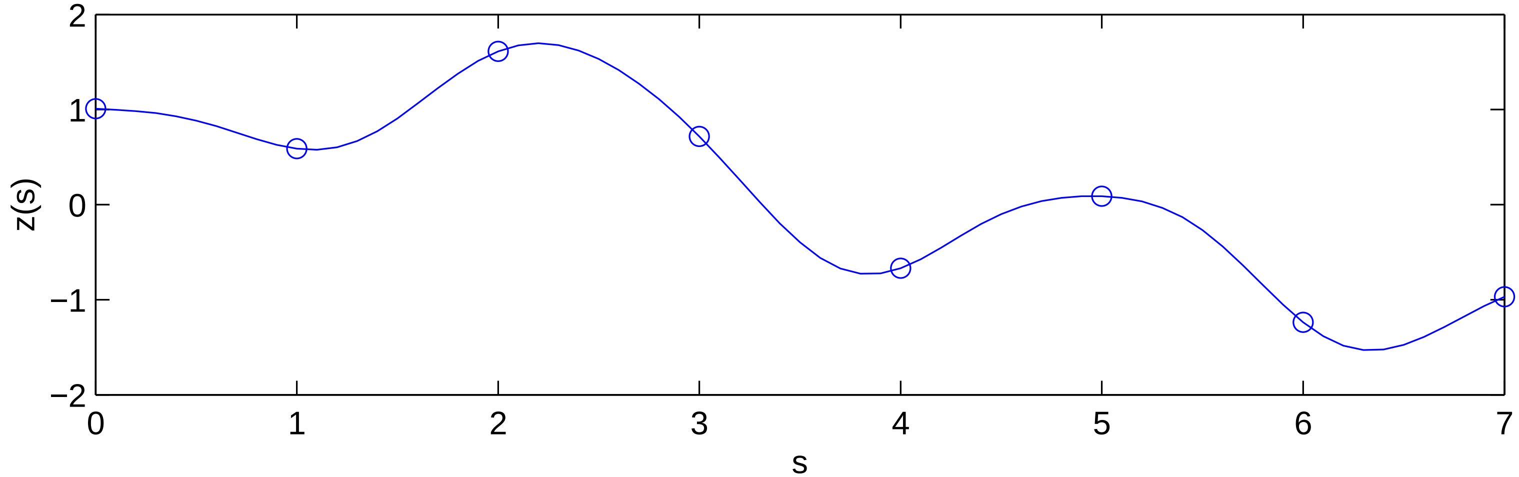
Gaussian process models for spatial phenomena



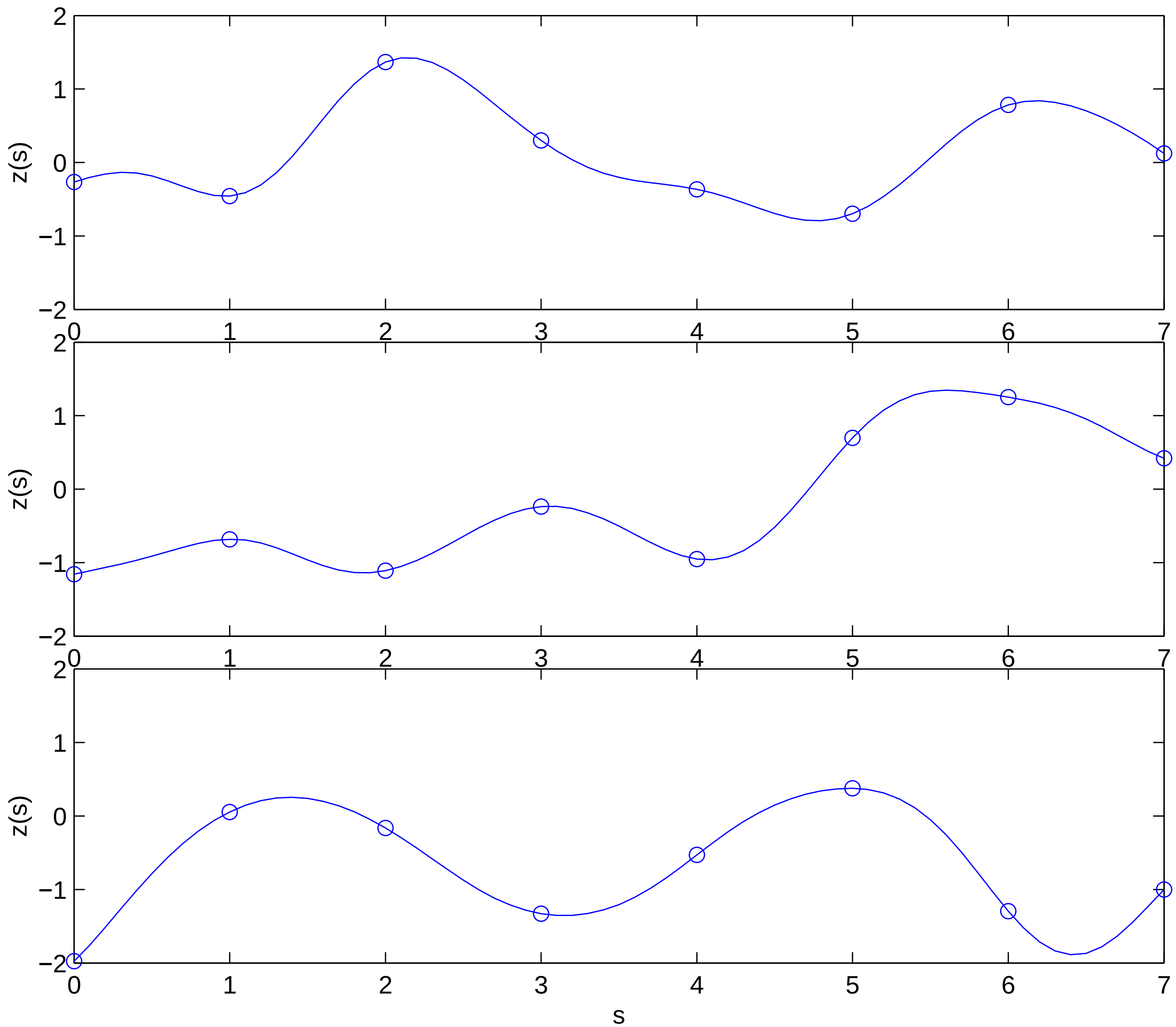
An example of $z(s)$ of a Gaussian process model on $s_1, \ldots, s_n$

$$z = \begin{pmatrix} z(s_1) \\ \vdots \\ z(s_n) \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} & & \\ & \Sigma & \\ & & \end{pmatrix} \right), \quad \text{with } \Sigma_{ij} = \exp\{-||s_i - s_j||^2\},$$

where $||s_i - s_j||$ denotes the distance between locations s_i and s_j.

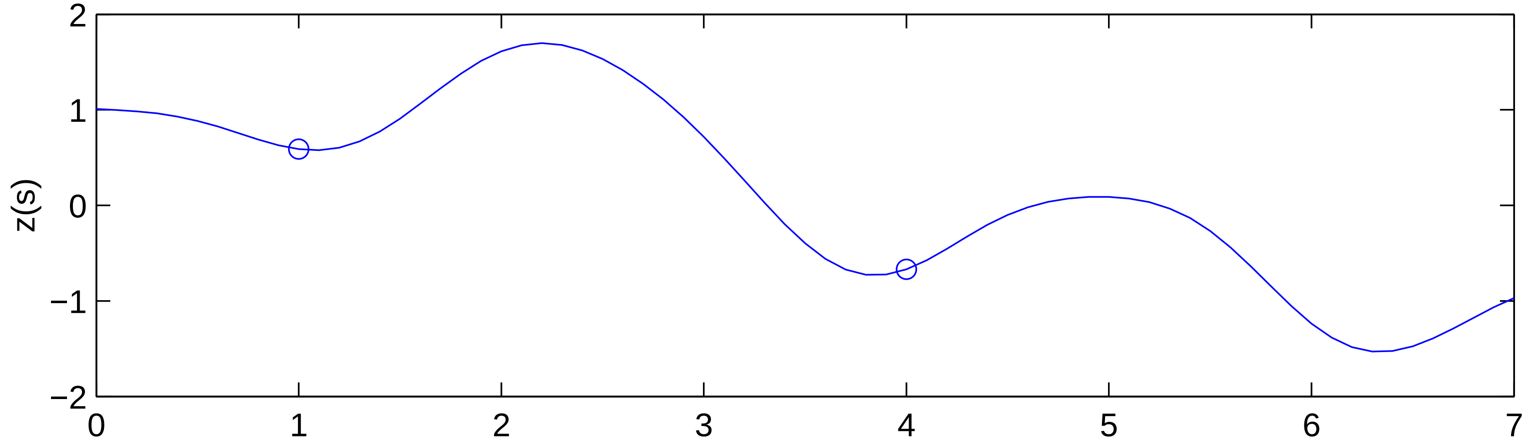
z has density $\pi(z) = (2\pi)^{-\frac{n}{2}} |\Sigma|^{-\frac{1}{2}} \exp\{-\frac{1}{2} z^T \Sigma^{-1} z\}$.

Realizations from $\pi(z) = (2\pi)^{-\frac{n}{2}}|\Sigma|^{-\frac{1}{2}}\exp\{-\frac{1}{2}z^T\Sigma^{-1}z\}$



model for $z(s)$ can be extended to continuous s

Conditioning on some observations of $z(s)$

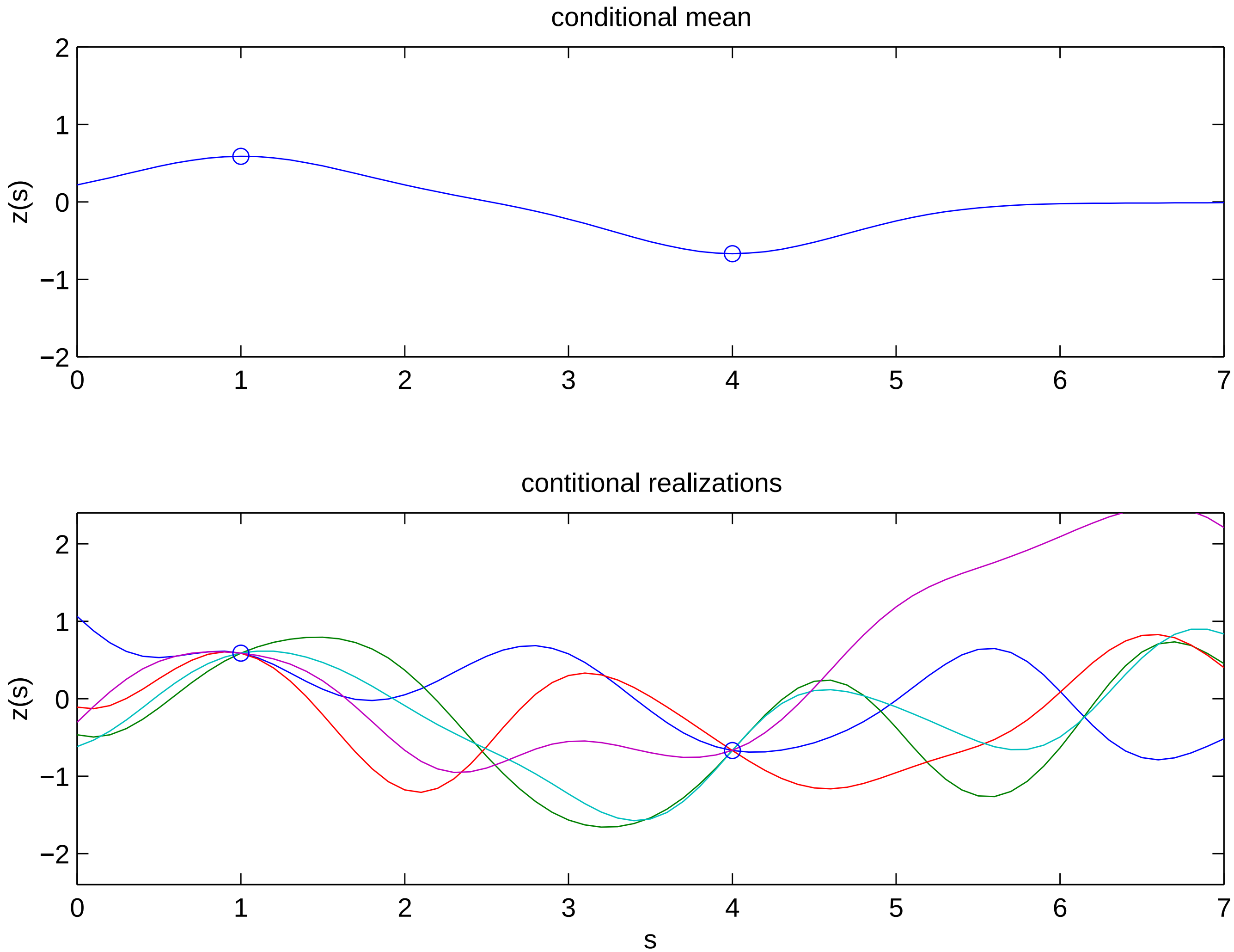


We observe $z(s_2)$ and $z(s_5)$ – what do we now know about $\{z(s_1), z(s_3), z(s_4), z(s_6), z(s_7), z(s_8)\}$?

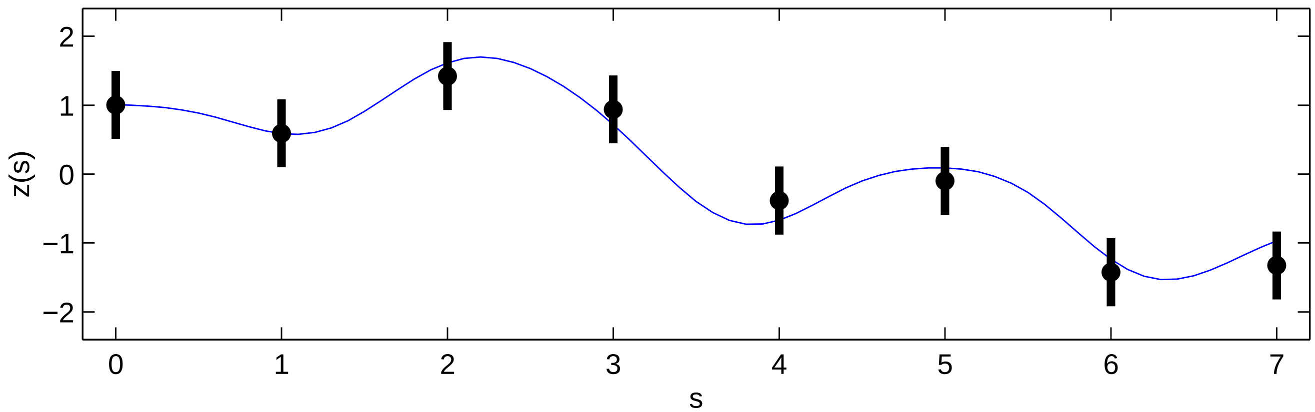
$$\begin{pmatrix} z(s_2) \\ z(s_5) \\ \hline z(s_1) \\ z(s_3) \\ z(s_4) \\ z(s_6) \\ z(s_7) \\ z(s_8) \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \\ \hline 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \left(\begin{array}{cc|ccc} 1 & .0001 & .3679 & \cdots & 0 \\ .0001 & 1 & 0 & \cdots & .0001 \\ \hline .3679 & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \vdots & \ddots & \vdots \\ 0 & .0001 & 0 & \cdots & 1 \end{array} \right) \right)$$

Conditioning on some observations of $z(s)$

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}\right), \quad z_2|z_1 \sim N(\Sigma_{21}\Sigma_{11}^{-1}z_1, \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$$



Soft Conditioning (Bayes Rule)



Observed data y are a noisy version of z

$$y(s_i) = z(s_i) + \epsilon(s_i) \text{ with } \epsilon(s_k) \overset{iid}{\sim} N(0, \sigma_y^2),\ \ k = 1, \ldots, n$$

Data

$$y \qquad \Sigma_y = \sigma_y^2 I_n$$

$$\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \quad \begin{pmatrix} \sigma_y^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_y^2 \end{pmatrix}$$

spatial process prior for $z(s)$

$$\mu_z \qquad \Sigma_z$$

$$\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \quad \begin{pmatrix} & & \\ & \Sigma_z & \\ & & \end{pmatrix}$$

$$L(y|z) \propto |\Sigma_y|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}(y-z)^T \Sigma_y^{-1}(y-z)\} \quad \pi(z) \propto |\Sigma_z|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2} z^T \Sigma_z^{-1} z\}$$

Soft Conditioning (Bayes Rule) ... continued

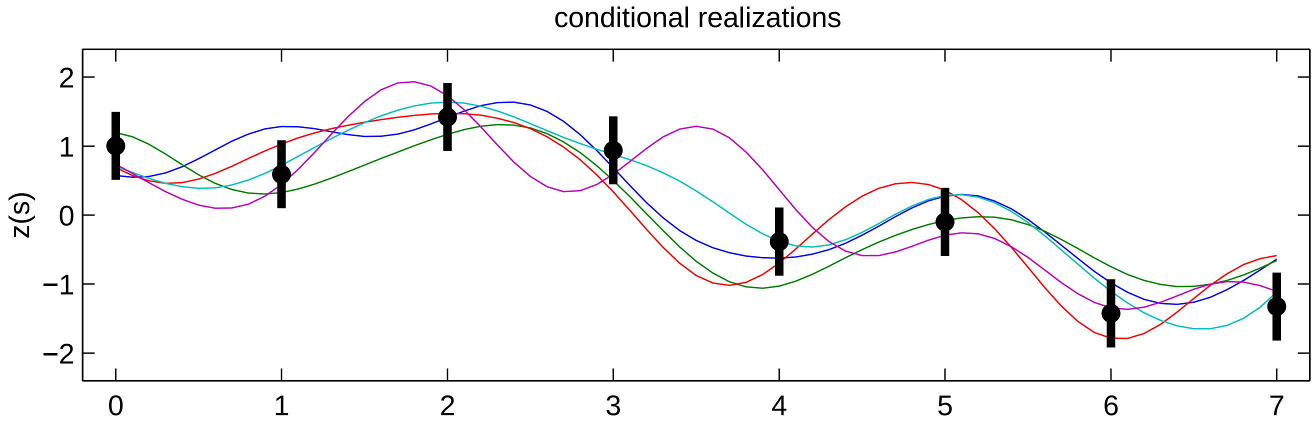
sampling model | spatial prior

$$L(y|z) \propto |\Sigma_y|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}(y-z)^T \Sigma_y^{-1}(y-z)\} \quad \pi(z) \propto |\Sigma_z|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2} z^T \Sigma_z^{-1} z\}$$

$$\Rightarrow \pi(z|y) \;\propto\; L(y|z) \times \pi(z)$$

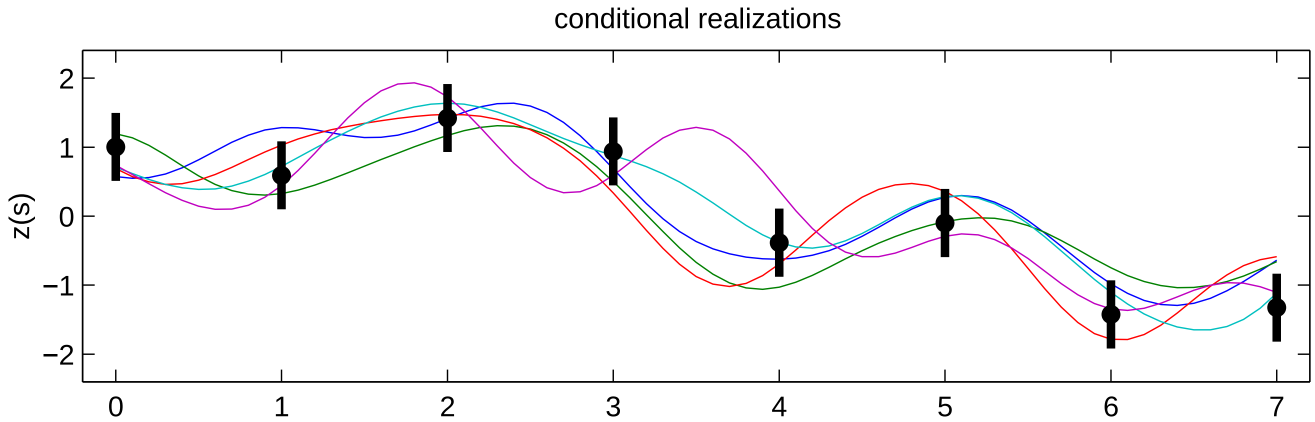
$$\Rightarrow \pi(z|y) \;\propto\; \exp\{-\tfrac{1}{2}[z^T(\Sigma_y^{-1} + \Sigma_z^{-1})z + z^T \Sigma_y^{-1} y + f(y)]\}$$

$$\Rightarrow \quad z|y \;\sim\; N(V\Sigma_y^{-1}y, V), \;\; \text{where } V = (\Sigma_y^{-1} + \Sigma_z^{-1})^{-1}$$



$\pi(z|y)$ describes the updated uncertainty about z given the observations.

Updated predictions for unobserved $z(s)$'s



$$\text{data locations} \quad y^d = (y(s_1), \ldots, y(s_n))^T \qquad z^d = (z(s_1), \ldots, z(s_n))^T$$

$$\text{prediction locations} \quad y^* = (y(s_1^*), \ldots, y(s_m^*))^T \qquad z^* = (z(s_1^*), \ldots, z(s_m^*))^T$$

$$\text{define} \quad y = (y^d; y^*) \qquad z = (z^d; z^*)$$

Data

$$y = \begin{pmatrix} y^d \\ y^* \end{pmatrix} = \begin{pmatrix} y^d \\ 0_m \end{pmatrix} \quad \Sigma_y = \begin{pmatrix} \sigma_y^2 I_n & 0 \\ 0 & \infty I_m \end{pmatrix}$$

spatial process prior for $z(s)$

$$\mu_z = \begin{pmatrix} 0_n \\ 0_m \end{pmatrix} \quad \Sigma_z = \begin{pmatrix} \text{cov rule applied} \\ \text{to } (s, s^*) \end{pmatrix}$$

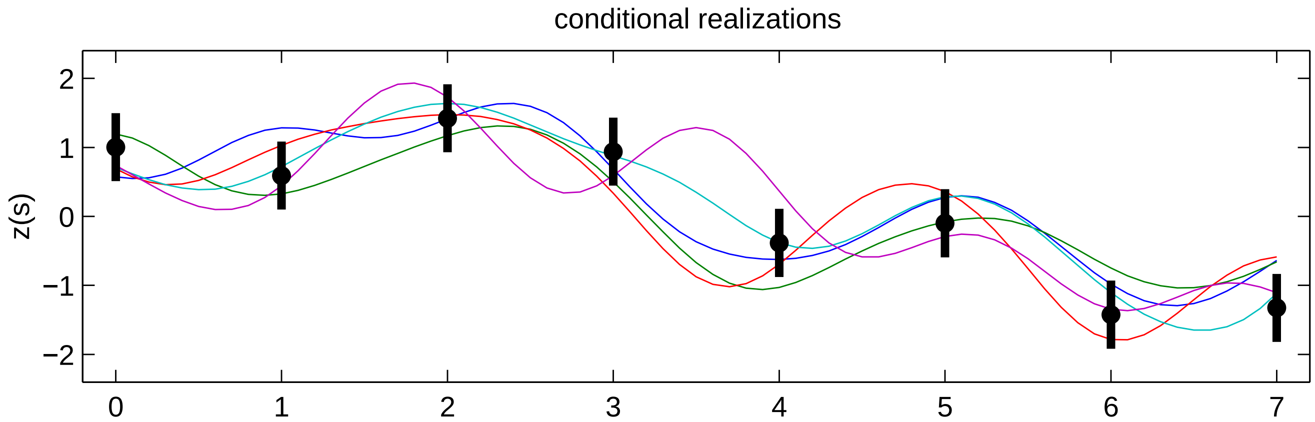
define $\Sigma_y^- = \begin{pmatrix} \frac{1}{\sigma_y^2} I_n & 0 \\ 0 & 0 \end{pmatrix}$

Now the posterior distribution for $z = (z^d, z^*)$ is

$$z|y \sim N(V\Sigma_y^- y, V), \quad \text{where } V = (\Sigma_y^- + \Sigma_z^{-1})^{-1}$$

Updated predictions for unobserved $z(s)$'s,

Alternative: use the conditional normal rules:



$$\text{data locations} \quad y = (y(s_1), \ldots, y(s_n))^T = (z(s_1) + \epsilon(s_1), \ldots, z(s_n) + \epsilon(s_n))^T$$
$$\text{prediction locations} \quad z^* = (z(s_1^*), \ldots, z(s_m^*))^T$$

$$\text{Jointly} \quad \begin{pmatrix} y \\ z^* \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_y^2 I_n & 0 \\ 0 & 0 \end{pmatrix} + \Sigma_z \right)$$

where

$$\Sigma_z = \begin{pmatrix} \Sigma_z(s,s) & \Sigma_z(s,s^*) \\ \Sigma_z(s^*,s) & \Sigma_z(s^*,s^*) \end{pmatrix} = \begin{pmatrix} \text{cov rule applied} \\ \text{to } (s, s^*) \end{pmatrix}_{(n+m)\times(n+m)}$$

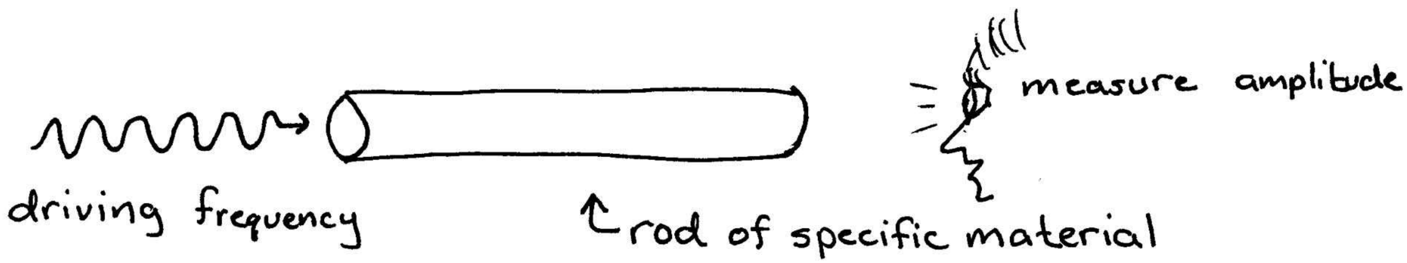
Therefore $z^*|y \sim N(\mu^*, \Sigma^*)$ where

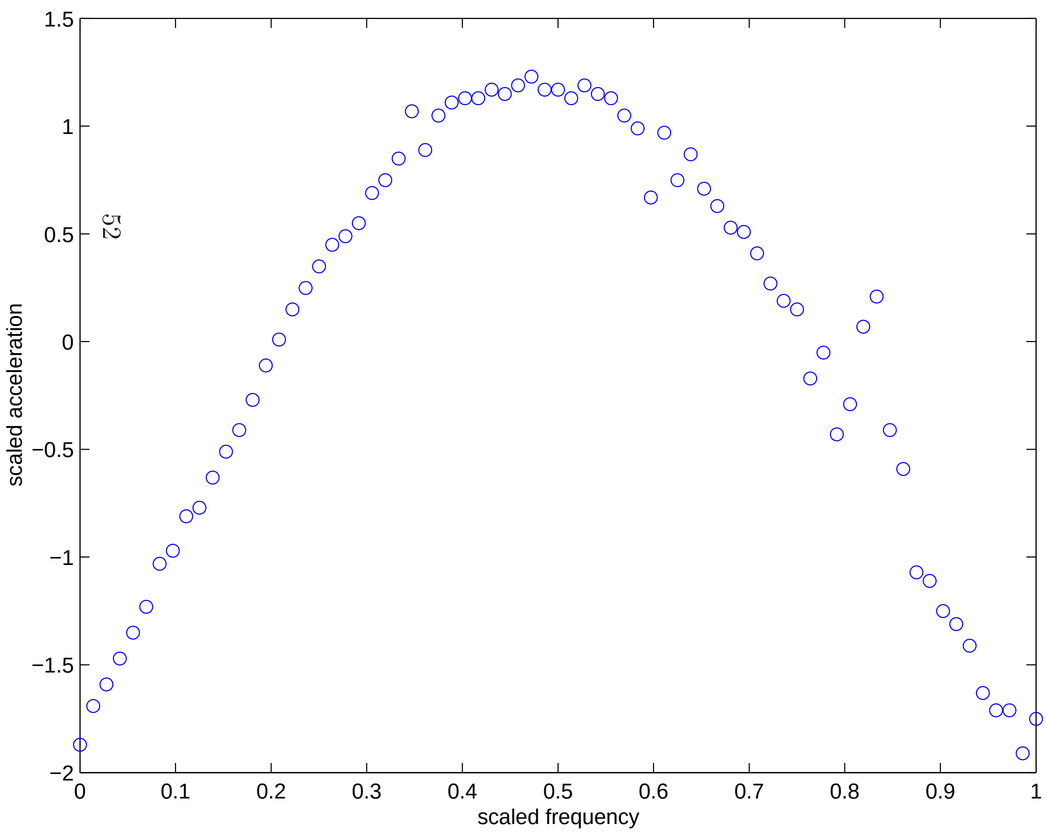
$$\mu^* = \Sigma_z(s^*,s)[\sigma_y^2 I_n + \Sigma_z(s,s)]^{-1} y$$
$$\Sigma^* = \Sigma_z(s^*,s^*) - \Sigma_z(s^*,s)[\sigma_z^2 I_n + \Sigma_z(s,s)]^{-1} \Sigma_z(s,s^*)$$

GAUSSIAN PROCESSES 2

Gaussian process models revisited

Application: finding in a rod of material

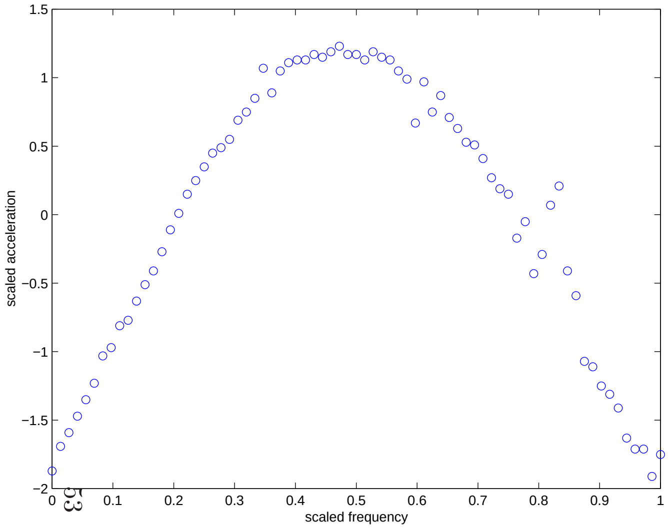




- for various driving frequencies, acceleration of rod recorded
- the true frequency-acceleration curve is smooth.
- we have noisy measurements of acceleration.
- estimate resonance frequency.
- use GP model for frequency-accel curve.
- smoothness of GP model important here.

Gaussian process models formulation

Take response y to be acceleration and spatial value s to be frequency.



data: $y = (y_1, \ldots, y_n)^T$ at spatial locations $s_1, \ldots, s_n$.

$z(s)$ is a mean 0 Gaussian process with covariance function

$$\text{Cov}(z(s), z(s')) = \frac{1}{\lambda_z} \exp\{-\beta(s - s')^2\}$$

β controls strength of dependence.

Take $z = (z(s_1), \ldots, z(s_n))^T$ to be $z(s)$ restricted to the data observations.

Model the data as:

$$y = z + \epsilon, \quad \text{where } \epsilon \sim N(0, \frac{1}{\lambda_y} I_n)$$

We want to find the posterior distribution for the frequency $s^\star$ where $z(s)$ is maximal.

Reparameterizing the spatial dependence parameter β

It is convenient to reparameterize β as:

$$\rho = \exp\{-\beta(1/2)^2\} \;\Leftrightarrow\; \beta = -4\log(\rho)$$

So ρ is the correlation between two points on $z(s)$ separated by $\frac{1}{2}$.

Hence z has spatial prior

$$z|\rho, \lambda_z \sim N(0, \frac{1}{\lambda_z} R(\rho; s))$$

54 where $R(\rho; s)$ is the correlation matrix with ij elements

$$R_{ij} = \rho^{4(s_i - s_j)^2}$$

Prior specification for $z(s)$ is completed by specfying priors for λ_z and ρ.

$\pi(\lambda_z) \propto \lambda_z^{a_z - 1}\exp\{-b_z\lambda_z\}$ if y is standardized, encourage λ_z to be close to 1 – eg.$a_z = b_z = 5$.

$\pi(\rho) \propto (1-\rho)^{-.5}$ encourages ρ to be large if possible

Bayesian model formulation

Likelihood

$$L(y|z, \lambda_y) \propto \lambda_y^{\frac{n}{2}} \exp\{-\tfrac{1}{2}\lambda_y (y-z)^T (y-z)\}$$

Priors

$$\pi(z|\lambda_z, \rho) \propto \lambda_z^{\frac{n}{2}} |R(\rho; s)|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}\lambda_z z^T R(\rho; s)^{-1} z\}$$

$$\pi(\lambda_y) \propto \lambda_y^{a_y - 1} e^{-b_y \lambda_y}, \text{ uninformative here – } a_y = 1,\ b_y = .005$$

$$\pi(\lambda_z) \propto \lambda_z^{a_z - 1} e^{-b_z \lambda_z}, \text{ fairly informative – } a_z = 5,\ b_z = 5$$

$$\pi(\rho) \propto (1-\rho)^{-.5}$$

Marginal likelihood (integrating out z)

$$L(y|\lambda_\epsilon, \lambda_z, \rho) \propto |\Lambda|^{\frac{1}{2}} \exp\{-\tfrac{1}{2} y^T \Lambda y\}$$

where $\Lambda^{-1} = \frac{1}{\lambda_y} I_n + \frac{1}{\lambda_z} R(\rho; s)$

Posterior

$$\pi(\lambda_y, \lambda_z, \rho | y) \propto |\Lambda|^{\frac{1}{2}} \exp\{-\tfrac{1}{2} y^T \Lambda y\} \times \lambda_y^{a_y - 1} e^{-b_y \lambda_y} \times \lambda_z^{a_z - 1} e^{-b_z \lambda_z} \times (1-\rho)^{-.5}$$

Posterior Simulation

Use Metropolis to simulate from the posterior

$$\pi(\lambda_y, \lambda_z, \rho|y) \propto |\Lambda|^{\frac{1}{2}} \exp\{-\tfrac{1}{2} y^T \Lambda y\} \times \lambda_y^{a_y-1} e^{-b_y\lambda_y} \times \lambda_z^{a_z-1} e^{-b_z\lambda_z} \times (1-\rho)^{-.5}$$

giving (after burn-in) $(\lambda_y, \lambda_z, \rho)^1, \ldots, (\lambda_y, \lambda_z, \rho)^T$

For any given realization $(\lambda_y, \lambda_z, \rho)^t$, one can generate $z^* = (z(s_1^*), \ldots, z(s_m^*))^T$ for any set of prediction locations $s_1^*, \ldots, s_m^*$.

From previous GP stuff, we know

$$\begin{pmatrix} z \\ z^* \end{pmatrix} | \cdots \sim N\left(V\Sigma_y^- \begin{pmatrix} y \\ 0_m \end{pmatrix}, V\right)$$

where

$$\Sigma_y^- = \begin{pmatrix} \lambda_\epsilon I_n & 0 \\ 0 & 0 \end{pmatrix} \text{ and } V^{-1} = \Sigma_y^- + \lambda_z R(\rho, (s, s^*))^{-1}$$

Hence, one can generate corresponding z^*'s for each posterior realization at a fine grid around the apparent resonance frequency $z^\star$.

Or use conditional normal formula with

$$\begin{pmatrix} y \\ z^* \end{pmatrix} | \cdots \sim N\left(\begin{pmatrix} 0_n \\ 0_m \end{pmatrix}, \begin{pmatrix} \lambda_\epsilon^{-1} I_n & 0 \\ 0 & 0 \end{pmatrix} + \lambda_z^{-1} R(\rho, (s, s^*)) \right)$$

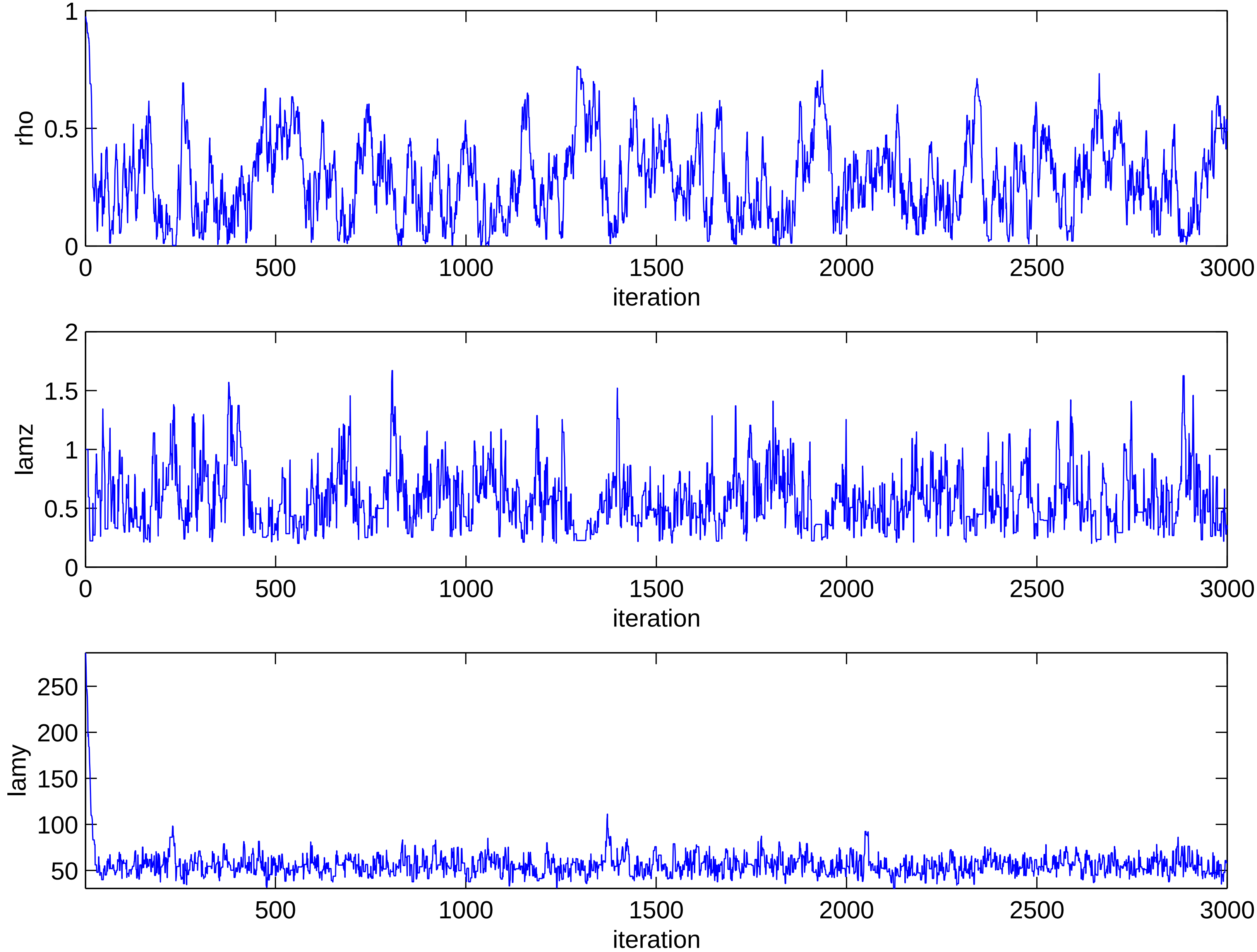
where

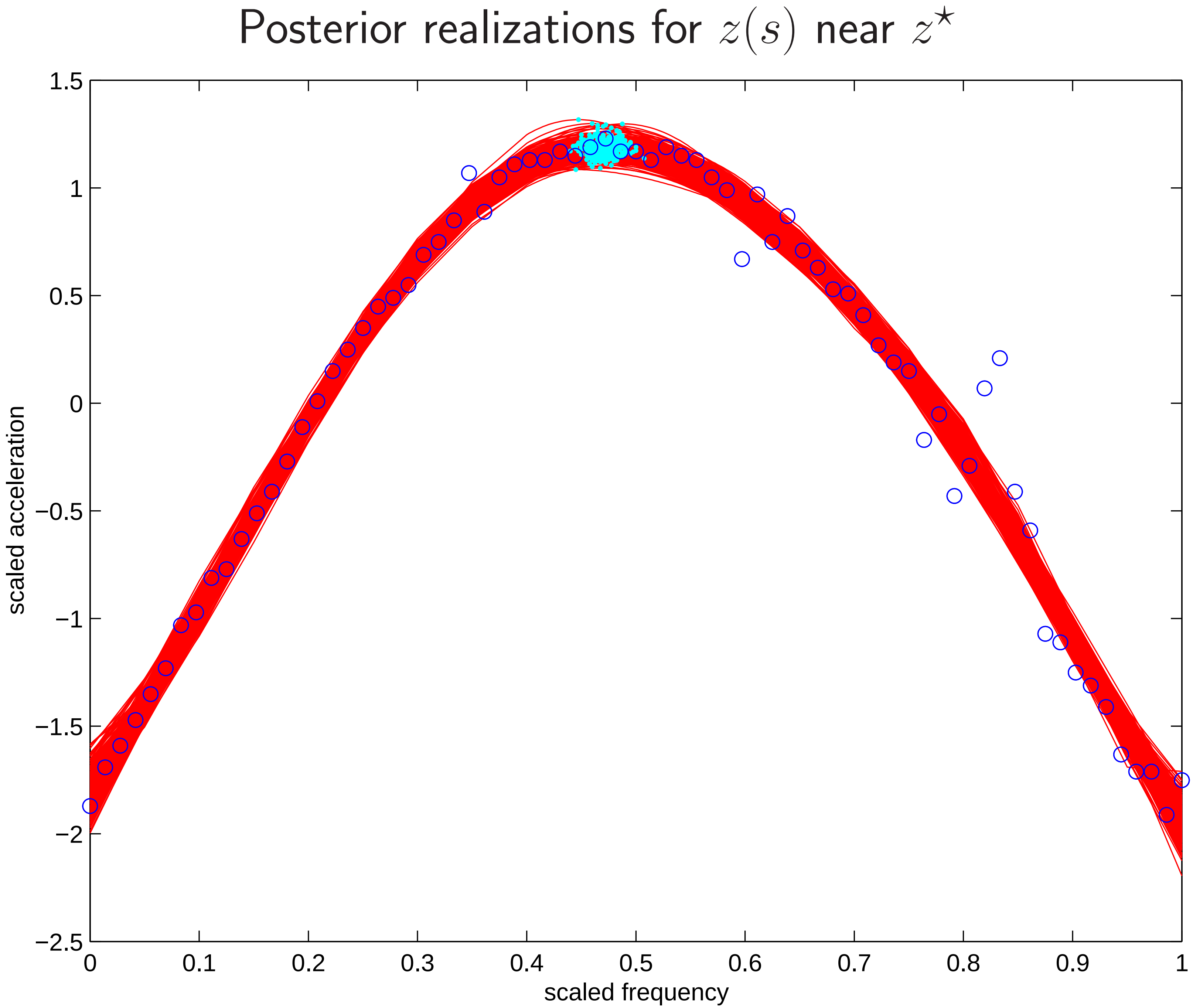
$$R(\rho, (s, s^*)) = \begin{pmatrix} R(\rho, (s, s)) & R(\rho, (s, s^*)) \\ R(\rho, (s^*, s)) & R(\rho, (s^*, s^*)) \end{pmatrix} = \begin{pmatrix} \text{cor rule applied} \\ \text{to } (s, s^*) \end{pmatrix}_{(n+m)\times(n+m)}$$

Therefore $z^*|y \sim N(\mu^*, \Sigma^*)$ where

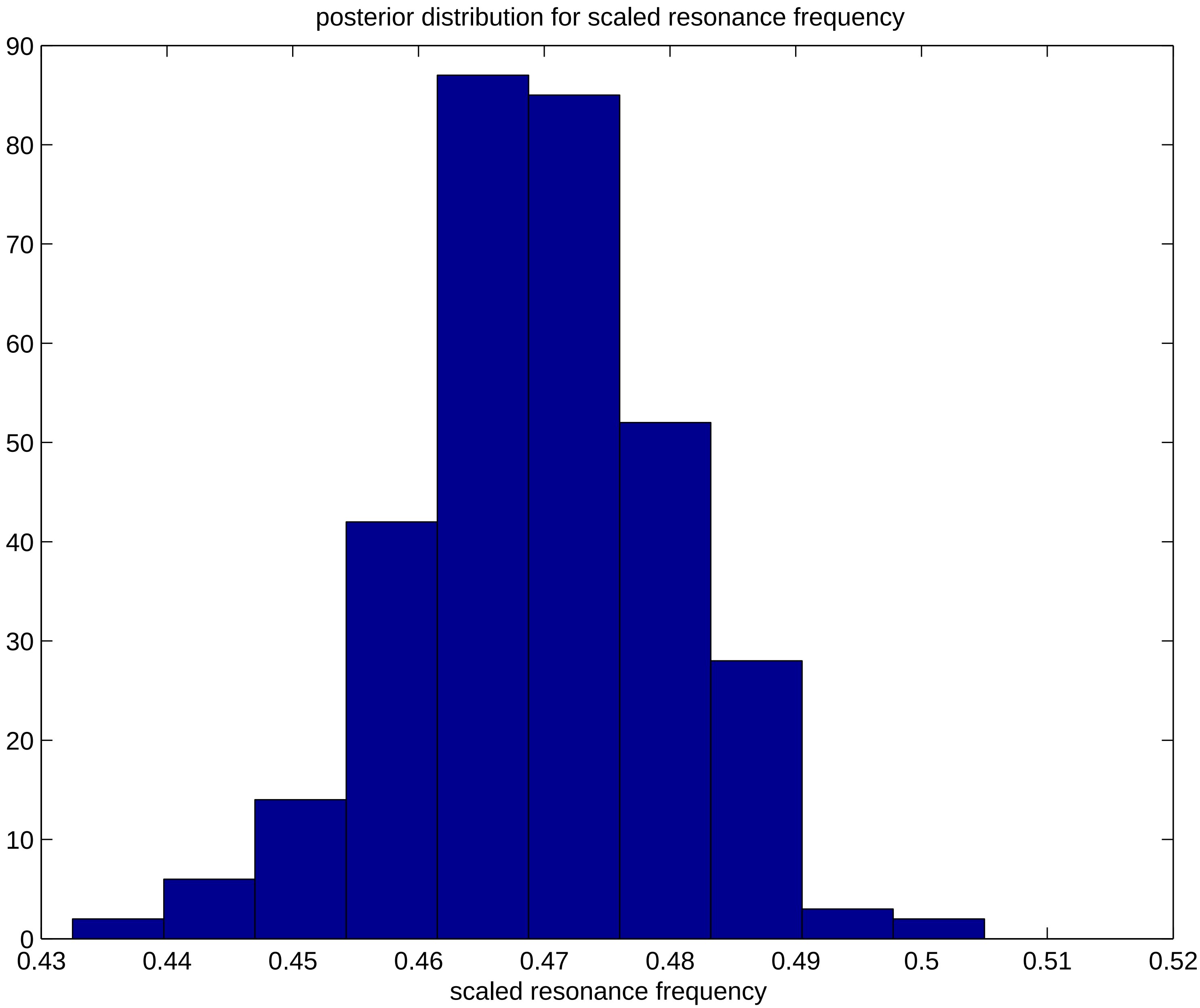
$$\begin{aligned} \mu^* &= \lambda_z^{-1} R(\rho, (s^*, s))[\lambda_\epsilon^{-1} I_n + \lambda_z^{-1} R(\rho, (s, s))]^{-1} y \\ \Sigma^* &= \lambda_z^{-1} R(\rho, (s^*, s^*)) - \\ &\quad \lambda_z^{-1} R(\rho, (s^*, s))[\lambda_\epsilon^{-1} I_n + \lambda_z^{-1} R(\rho, (s, s))]^{-1} \lambda_z^{-1} R(\rho, (s, s^*)) \end{aligned}$$

MCMC output for $(\lambda_y, \lambda_z, \rho)$




Posterior realizations for $z(s)$ near $z^\star$
scaled acceleration
scaled frequency
1.5
1
0.5
0
−0.5
−1
−1.5
−2
−2.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Posterior for resonance frequency $z^\star$



Gaussian Processes for modeling complex computer simulators

data input settings (spatial locations)

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \qquad S = \begin{pmatrix} s_1 \\ \vdots \\ s_n \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ \vdots & \vdots & \vdots & \vdots \\ s_{n1} & s_{n2} & \cdots & s_{np} \end{pmatrix}$$

Model responses y as a (stochastic) function of s

$$y(s) = z(s) + \epsilon(s)$$

Vector form – restricting to the n data points

$$y = z + \epsilon$$

Model response as a Gaussian processes

$$y(s) = z(s) + \epsilon$$

Likelihood

$$L(y|z, \lambda_\epsilon) \;\propto\; \lambda_\epsilon^{\frac{n}{2}} \exp\{-\tfrac{1}{2}\lambda_\epsilon (y - z)^T (y - z)\}$$

Priors

$$\pi(z|\lambda_z, \beta) \;\propto\; \lambda_z^{\frac{n}{2}} |R(\beta)|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}\lambda_z z^T R(\beta)^{-1} z\}$$

$$\pi(\lambda_\epsilon) \;\propto\; \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon}, \text{ perhaps quite informative}$$

$$\pi(\lambda_z) \;\propto\; \lambda_z^{a_z - 1} e^{-b_z \lambda_z}, \text{ fairly informative if data have been standardized}$$

$$\pi(\rho) \;\propto\; \prod_{k=1}^{p} (1 - \rho_k)^{-.5}$$

Marginal likelihood (integrating out z)

$$L(y|\lambda_\epsilon, \lambda_z, \beta) \;\propto\; |\Lambda|^{\frac{1}{2}} \exp\{-\tfrac{1}{2} y^T \Lambda y\}$$

where $\Lambda^{-1} = \frac{1}{\lambda_\epsilon} I_n + \frac{1}{\lambda_z} R(\beta)$

GASP Covariance model for $z(s)$

$$\text{Cov}(z(s_i), z(s_j)) = \frac{1}{\lambda_z} R(\beta) = \frac{1}{\lambda_z} \prod_{k=1}^{p} \exp\{-\beta_k (s_{ik} - s_{jk})^\alpha\}$$

- Typically $\alpha = 2 \Rightarrow z(s)$ is smooth.
- Separable covariance – a product of componentwise covariances.
- Can handle large number of covariates/inputs p.
- Can allow for multiway interactions.
- $\beta_k = 0 \Rightarrow$ input k is "inactive" $\Rightarrow$ variable selection
- reparameterize: $\rho_k = \exp\{-\beta_k d_0^\alpha\}$ – typically d_0 is a halfwidth.

Posterior Distribution and MCMC

$$\pi(\lambda_\epsilon, \lambda_z, \rho | y) \;\propto\; |\Lambda_{\lambda,\rho}|^{\frac{1}{2}} \exp\{-\tfrac{1}{2} y^T \Lambda_{\lambda,\rho} y\} \times \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon} \times$$
$$\lambda_z^{a_z - 1} e^{-b_z \lambda_z} \times \prod_{k=1}^{p} (1 - \rho_k)^{-.5}$$

- MCMC implementation requires Metropolis updates.
- Realizations of $z(s)|\lambda, \rho, y$ can be obtained post-hoc:

– define $z^* = (z(s_1^*), \ldots, z(s_m^*))^T$ to be predictions at locations $s_1^*, \ldots, s_m^*$, then

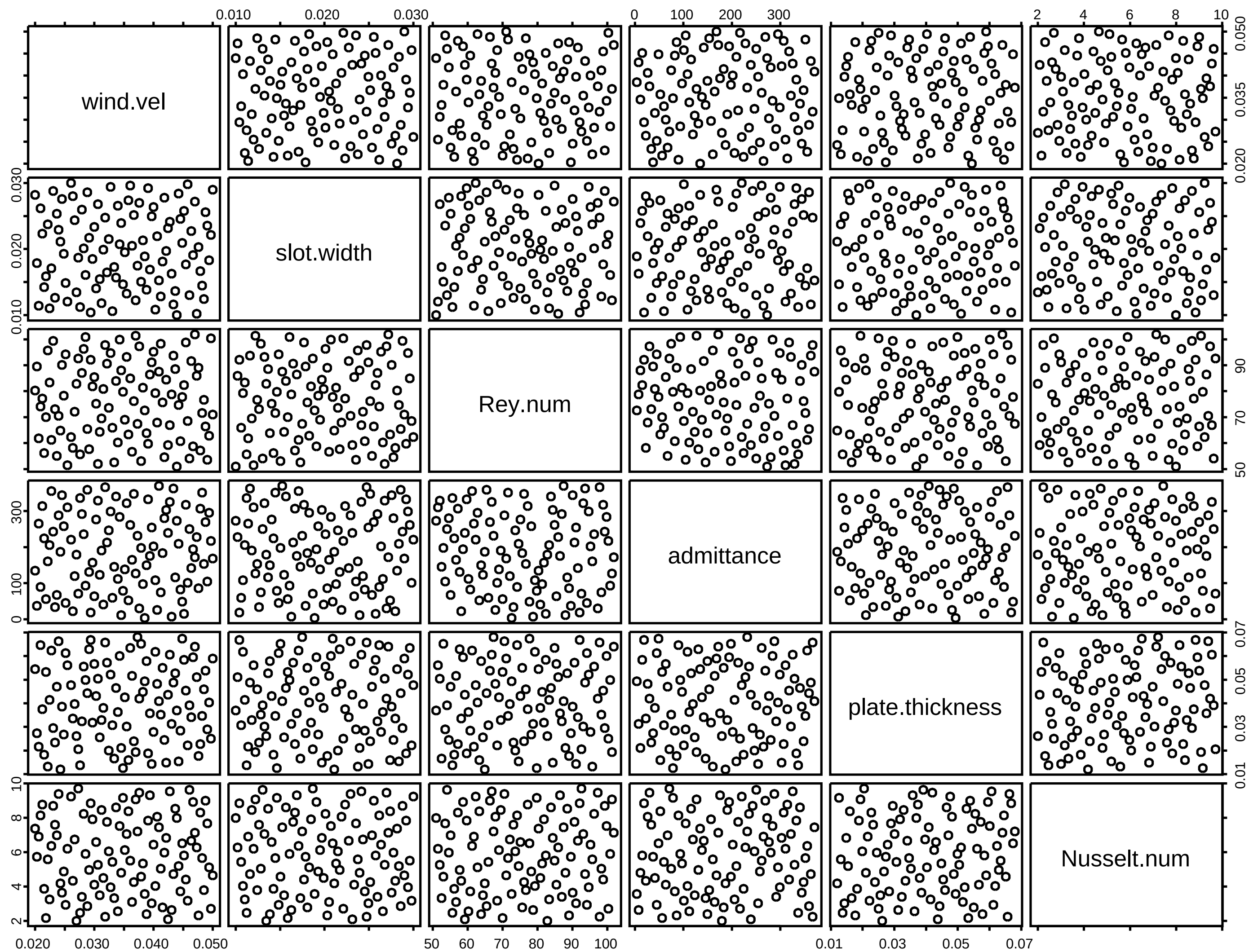
$$\begin{pmatrix} z \\ z^* \end{pmatrix} | \cdots \sim N\left(V \Sigma_y^- \begin{pmatrix} y \\ 0_m \end{pmatrix}, V \right)$$

where

$$\Sigma_y^- = \begin{pmatrix} \lambda_\epsilon I_n & 0 \\ 0 & 0 \end{pmatrix} \text{ and } V^{-1} = \Sigma_y^- + \lambda_z R(\rho, (s, s^*))^{-1}$$

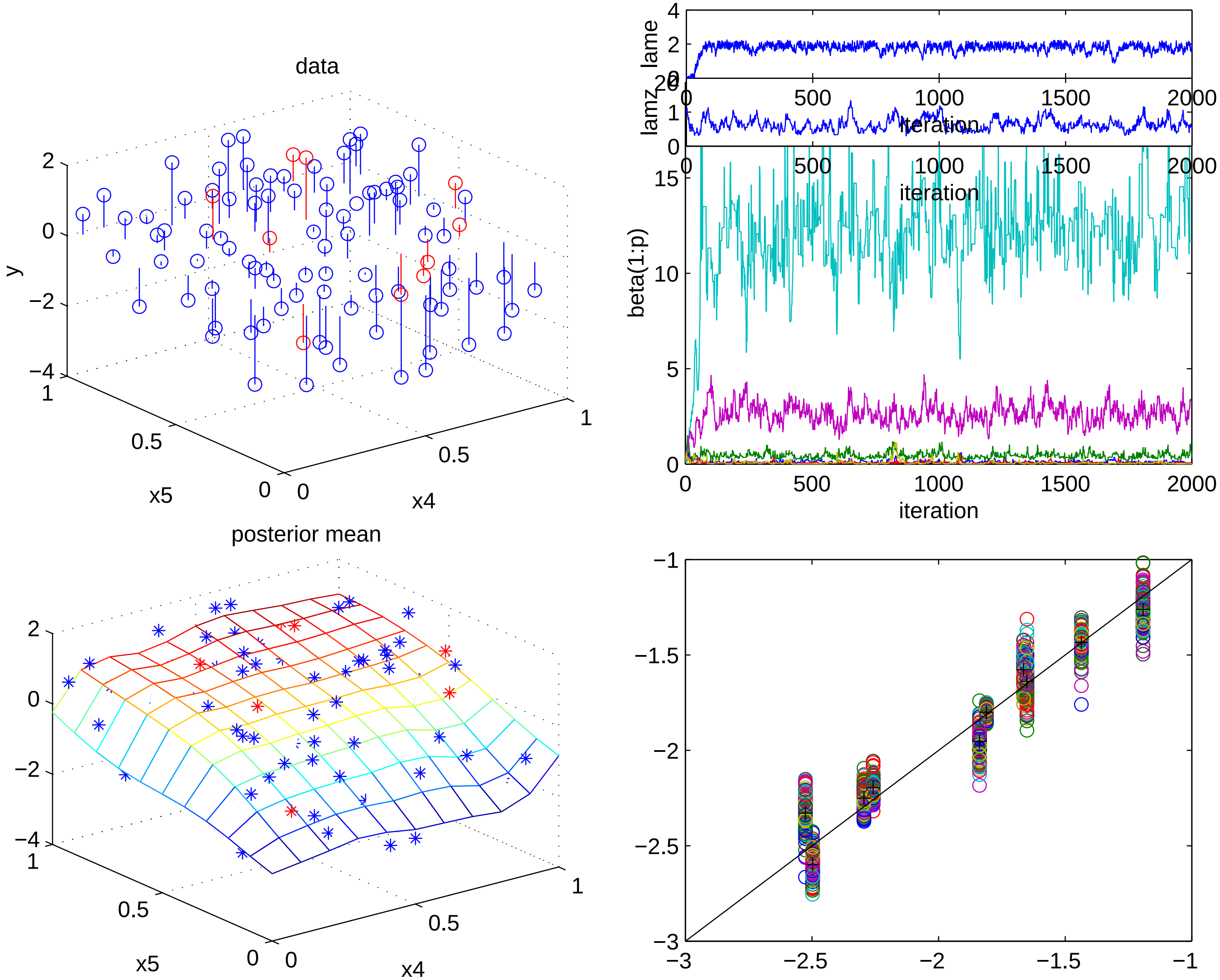
Example: Solar collector Code (Schonlau, Hamada and Welch, 1995)

- $n = 98$ model runs, varying 6 independent variables.
- Response is the increase in heat exchange effectiveness.
- A latin hypercube (LHC) design was used with 2-d space filling.



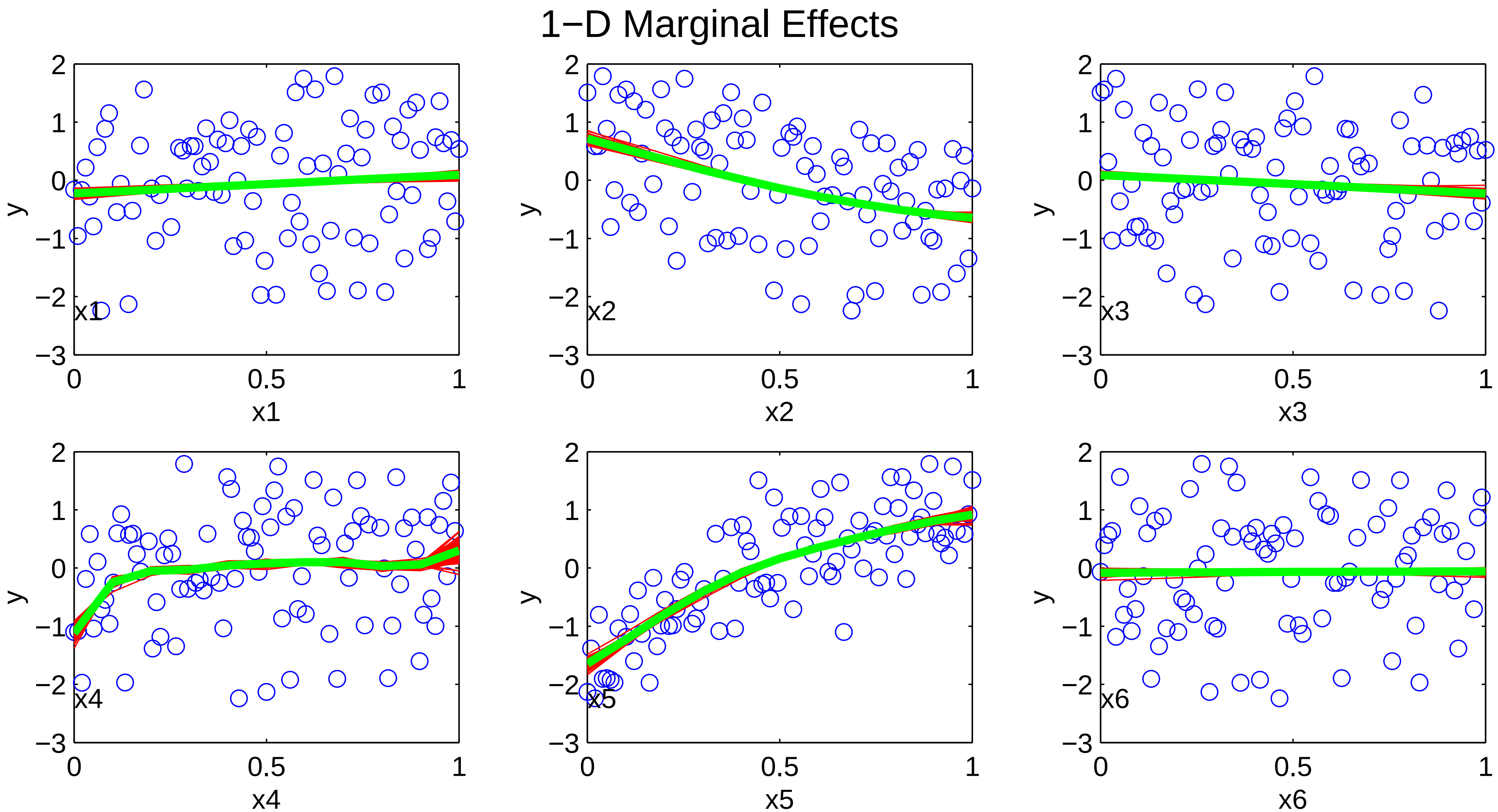
Example: Solar collector Code

- Fit of GASP model and predictions of 10 holdout points
- Two most active covariates are shown here.



Example: Solar collector Code

- Visualizing a 6-d response surface is difficult
- 1-d marginal effects shown here.

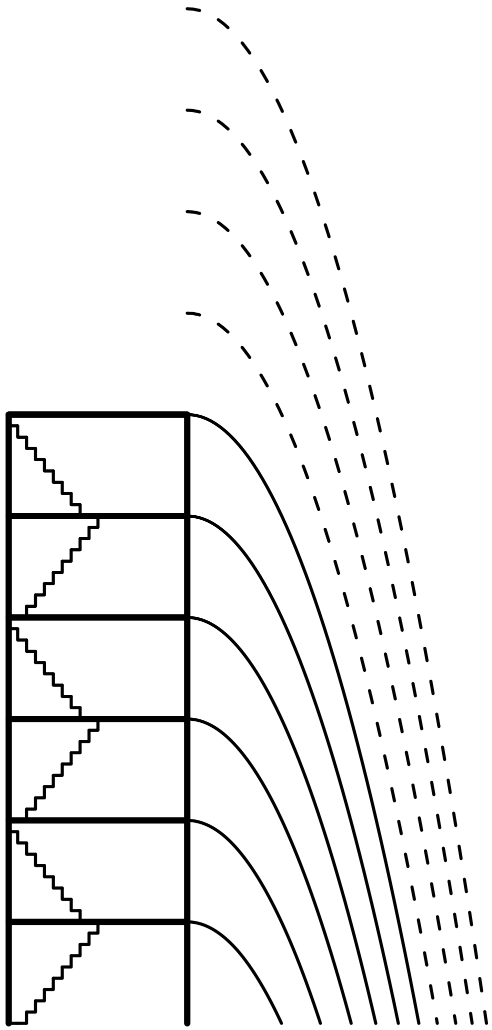


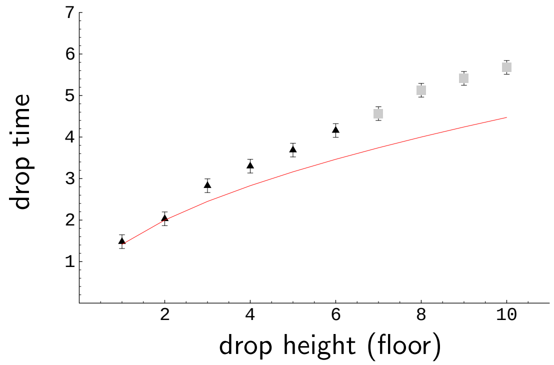
References

- J. Sacks, W. J. Welch, T. J. Mitchell and H. P. Wynn (1989) Design and analysis of comuter experiments *Statistical Science*, 4:409–435.

COMPUTER MODEL CALIBRATION 1

Inference combining a physics model with experimental data



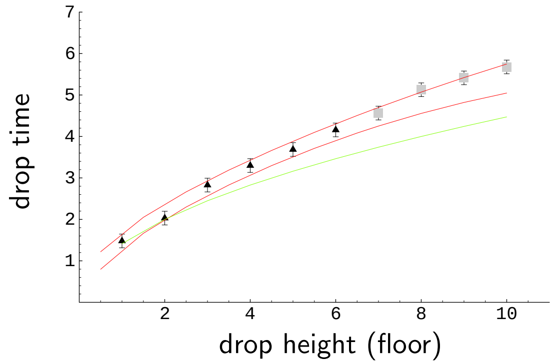


Data generated from model

$$\frac{d^2z}{dt^2} = -1 - .3\frac{dz}{dt} + \epsilon$$

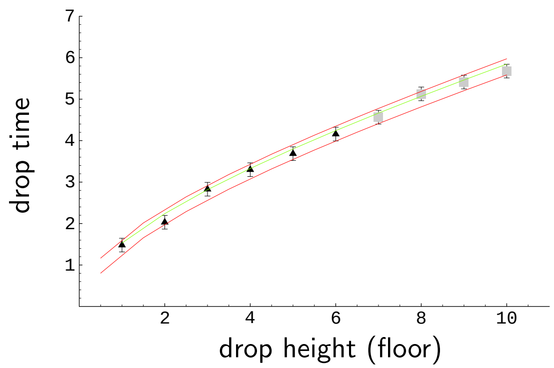
simulation model:

$$\frac{d^2z}{dt^2} = -1$$



statistical model:

$$y(z) = \eta(z) + \delta(z) + \epsilon$$



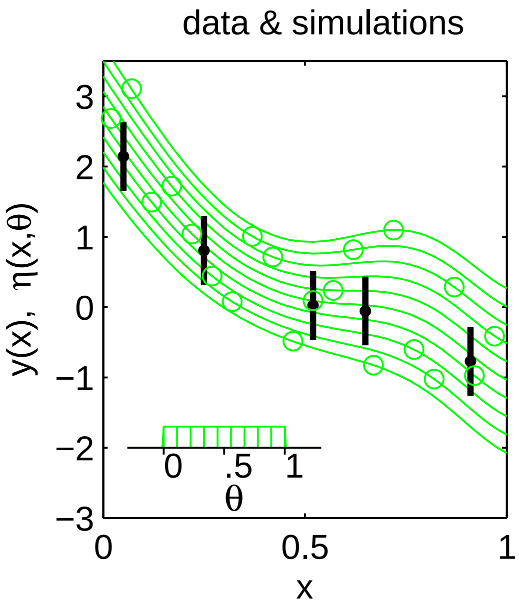
Improved physics model:

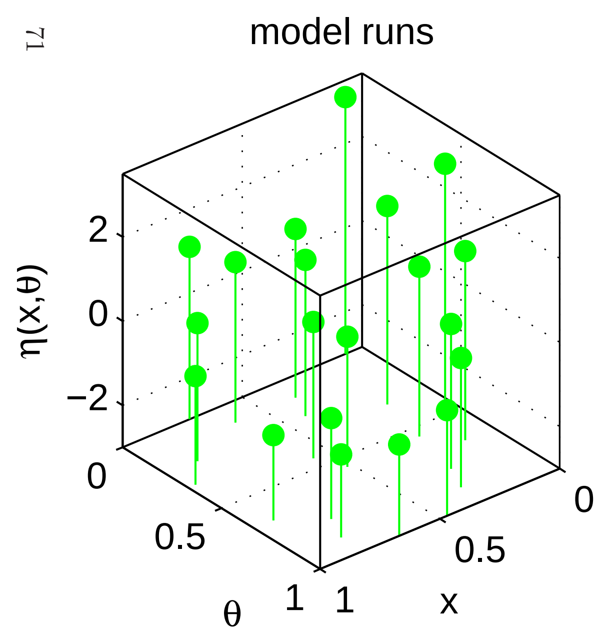
$$\frac{d^2z}{dt^2} = -1 - \theta\frac{dz}{dt} + \epsilon$$

statistical model:

$$y(z) = \eta(z, \theta) + \delta(z) + \epsilon$$

Accounting for limited simulator runs





- Borrows from Kennedy and O'Hagan (2001).

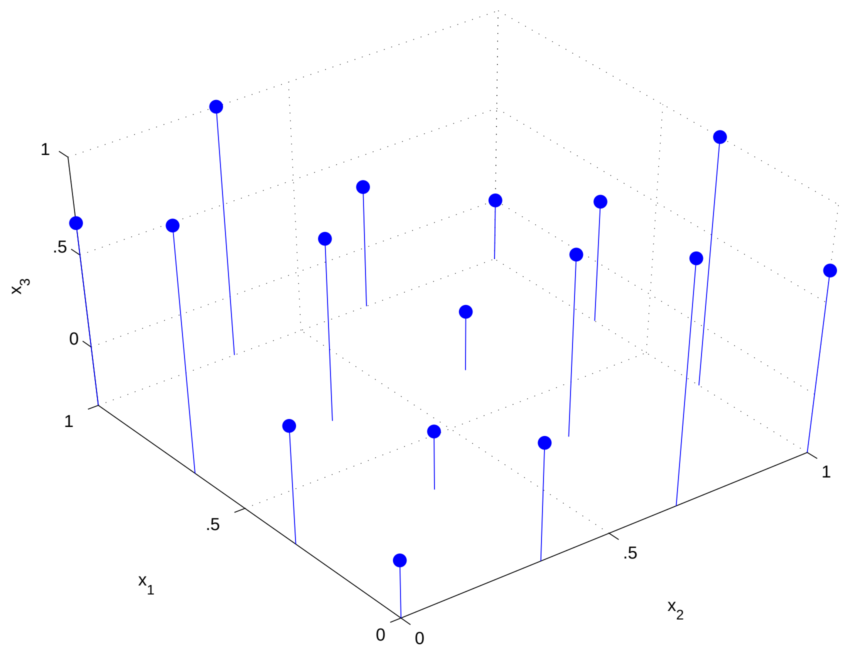
x	model or system inputs
θ	calibration parameters
$\zeta(x)$	true physical system response given inputs x
$\eta(x,\theta)$	simulator response at x and θ.
	simulator run at limited input settings
	$\eta = (\eta(x_1^*,\theta_1^*),\ldots,\eta(x_m^*,\theta_m^*))^T$
	treat $\eta(\cdot,\cdot)$ as a random function
	use GP prior for $\eta(\cdot,\cdot)$
$y(x)$	experimental observation of the physical system
$e(x)$	observation error of the experimental data

$$y(x) = \zeta(x) + e(x)$$
$$y(x) = \eta(x,\theta) + e(x)$$

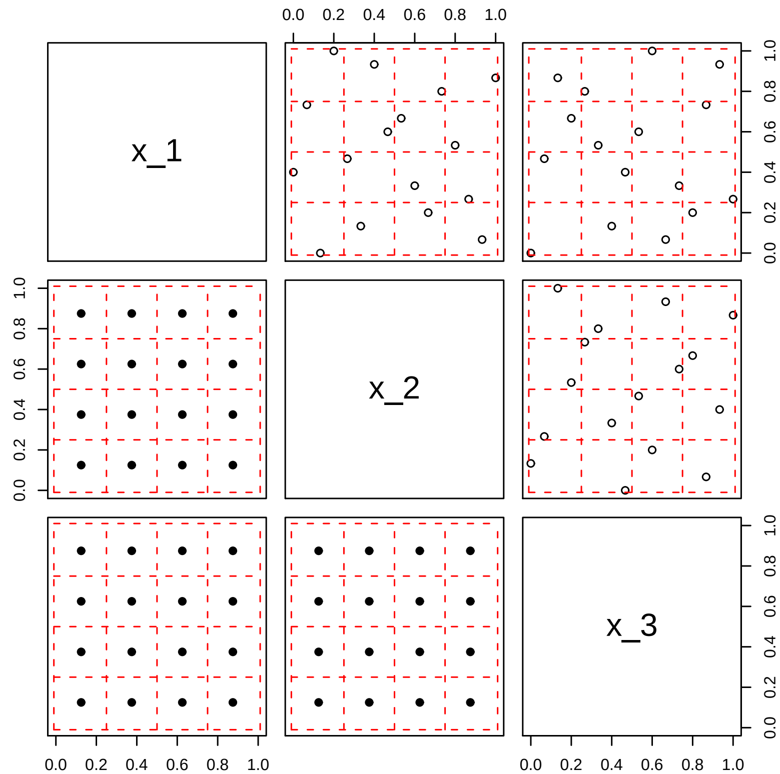
OA designs for simulator runs

Example: $N = 16$, 3 factors each at 4 levels

OA$(16, 4^3)$ design



2-d projections



OA design ensures importance measures R^2 can be accurately estimated for low dimensions

Can spread out design for building a response surface emulator of $\eta(x)$

Gaussian Process models for combining field data and complex computer simulators

field data — input settings (spatial locations)

$$y = \begin{pmatrix} y(x_1) \\ \vdots \\ y(x_n) \end{pmatrix} \qquad \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p_x} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np_x} \end{pmatrix}$$

sim data — input settings x; params θ^*

$$\eta = \begin{pmatrix} \eta(x_1^*, \theta_1^*) \\ \vdots \\ \eta(x_m^*, \theta_m^*) \end{pmatrix} \qquad \begin{pmatrix} x_{11}^* & \cdots & x_{1p_x}^* & \theta_{11}^* & \cdots & \theta_{1p_\theta}^* \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{m1}^* & \cdots & x_{mp_x}^* & \theta_{m1}^* & \cdots & \theta_{mp_\theta}^* \end{pmatrix}$$

Model sim response $\eta(x, \theta)$ as a Gaussian process

$$\begin{aligned} y(x) &= \eta(x, \theta) + \epsilon \\ \eta(x, \theta) &\sim GP\left(0, C^\eta(x, \theta)\right) \\ \epsilon &\sim \text{iid} N(0, 1/\lambda_\epsilon) \end{aligned}$$

$C^\eta(x, \theta)$ depends on $p_x + p_\theta$-vector ρ_η and λ_η

Vector form – restricting to n field obs and m simulation runs

$$\begin{aligned} y &= \eta(\theta) + \epsilon \\ \eta &\sim N_m(0_m, C^\eta(\rho_\eta, \lambda_\eta)) \\ \Rightarrow \begin{pmatrix} y \\ \eta \end{pmatrix} &\sim N_{n+m}\left(\begin{pmatrix} 0_n \\ 0_m \end{pmatrix}, C_{y\eta} = C^\eta + \begin{pmatrix} 1/\lambda_\epsilon I_n & 0 \\ 0 & 1/\lambda_s I_m \end{pmatrix} \right) \end{aligned}$$

where

$$C^\eta = 1/\lambda_\eta R^\eta\left(\begin{pmatrix} x \\ x^* \end{pmatrix}, \begin{pmatrix} \mathbf{1}\theta \\ \theta^* \end{pmatrix}; \rho_\eta \right)$$

and the correlation matrix R^η is given by

$$R^\eta((x,\theta),(x',\theta');\rho_\eta) = \prod_{k=1}^{p_x} \rho_{\eta k}^{4(x_k - x'_k)^2} \times \prod_{k=1}^{p_\theta} \rho_{\eta(k+p_x)}^{4(\theta_k - \theta'_k)^2}$$

74

λ_s is typically set to something large like 10^6 to stabalize matrix computations and allow for numerical fluctuation in $\eta(x,\theta)$.

note: the covariance matrix C^η depends on θ through its "distance"-based correlation function $R^\eta((x,\theta),(x',\theta');\rho_\eta)$.

We use a 0 mean for $\eta(x,\theta)$; an alternative is to use a linear regression mean model.

Likelihood

$$L(y,\eta|\lambda_\epsilon,\rho_\eta,\lambda_\eta,\lambda_s,\theta) \propto$$
$$|C_{y\eta}|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1}\begin{pmatrix} y \\ \eta \end{pmatrix}\right\}$$

Priors

$$\begin{aligned}
\pi(\lambda_\epsilon) &\propto \lambda_\epsilon^{a_\epsilon-1}e^{-b_\epsilon\lambda_\epsilon} \qquad \text{perhaps well known from observation process} \\
\pi(\rho_{\eta k}) &\propto \prod_{k=1}^{p_x+p_\theta}(1-\rho_{\eta k})^{-.5}, \text{ where } \rho_{\eta k}=e^{-.5^2\beta_k^\eta} \text{ correlation at dist} = .5 \sim \beta(1,.5). \\
\pi(\lambda_\eta) &\propto \lambda_\eta^{a_\eta-1}e^{-b_\eta\lambda_\eta} \\
\pi(\lambda_s) &\propto \lambda_s^{a_s-1}e^{-b_s\lambda_s} \\
\pi(\theta) &\propto I[\theta\in C]
\end{aligned}$$

- could fix ρ_η,λ_η from prior GASP run on model output.
- Many prefer to reparameterize ρ as $\beta=-\log(\rho)/.5^2$ in the likelihood term

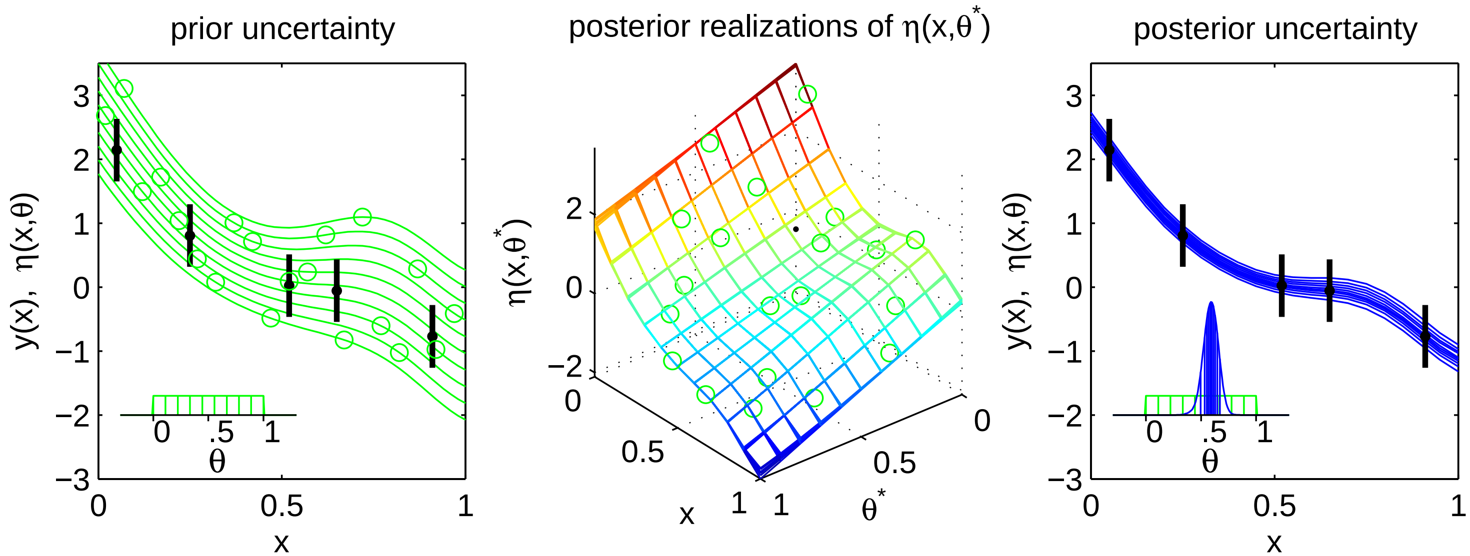
Posterior Density

$$
\begin{aligned}
&\pi(\lambda_\epsilon, \rho_\eta, \lambda_\eta, \lambda_s, \theta | y, \eta) \propto \\
&\quad |C_{y\eta}|^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2} \begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix} \right\} \times \\
&\quad \prod_{k=1}^{p_x+p_\theta} (1-\rho_{\eta k})^{-.5} \times \lambda_\eta^{a_\eta - 1} e^{-b_\eta \lambda_\eta} \times \lambda_s^{a_s - 1} e^{-b_s \lambda_s} \times \\
&\quad \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon} \times I[\theta \in C]
\end{aligned}
$$

If ρ_η, λ_η, and λ_s are fixed from a previous analysis of the simulator data, then

$$
\begin{aligned}
&\pi(\lambda_\epsilon, \theta | y, \eta, \rho_\eta, \lambda_\eta, \lambda_s) \propto \\
&\quad |C_{y\eta}|^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2} \begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix} \right\} \times \\
&\quad \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon} \times I[\theta \in C]
\end{aligned}
$$

Accounting for limited simulation runs



Again, standard Bayesian estimation gives:

$$\pi(\theta, \eta(\cdot,\cdot), \lambda_\epsilon, \rho_\eta, \lambda_\eta | y(x)) \propto L(y(x)|\eta(x,\theta), \lambda_\epsilon) \times \pi(\theta) \times \pi(\eta(\cdot,\cdot)|\lambda_\eta, \rho_\eta) \pi(\lambda_\epsilon) \times \pi(\rho_\eta) \times \pi(\lambda_\eta)$$

- Posterior means and quantiles shown.
- Uncertainty in θ, $\eta(\cdot,\cdot)$, nuisance parameters are incorporated into the forecast.
- Gaussian process models for $\eta(\cdot,\cdot)$.

Predicting a new outcome: $\zeta = \zeta(x') = \eta(x', \theta)$

Given a MCMC realization $(\theta, \lambda_\epsilon, \rho_\eta, \lambda_\eta)$, a realization for $\zeta(x')$ can be produced using Bayes rule.

Data | GP prior for $\eta(x, \theta)(s)$

$$v = \begin{pmatrix} y \\ \eta \\ \zeta \end{pmatrix} \quad \Sigma_v^- = \begin{pmatrix} \lambda_\epsilon I_n & 0 & 0 \\ 0 & \lambda_s I_m & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \mu_z = \begin{pmatrix} 0_n \\ 0_m \\ 0 \end{pmatrix} \quad C_\eta = \lambda_\eta^{-1} R^\eta \left(\begin{pmatrix} x \\ x^* \\ x' \end{pmatrix}, \begin{pmatrix} \mathbf{1}\theta \\ \theta^* \\ \theta \end{pmatrix}; \rho_\eta \right)$$

Now the posterior distribution for $v = (y, \eta, \zeta)^T$ is

$$v|y,\eta \sim N(\mu^{v|y\eta} = V\Sigma_v^- v, V), \quad \text{where } V = (\Sigma_v^- + C_\eta^{-1})^{-1}$$

Restricting to ζ we have

$$\zeta|y,\eta \sim N(\mu^{v|y\eta}_{m+n+1}, V_{n+m+1,n+m+1})$$

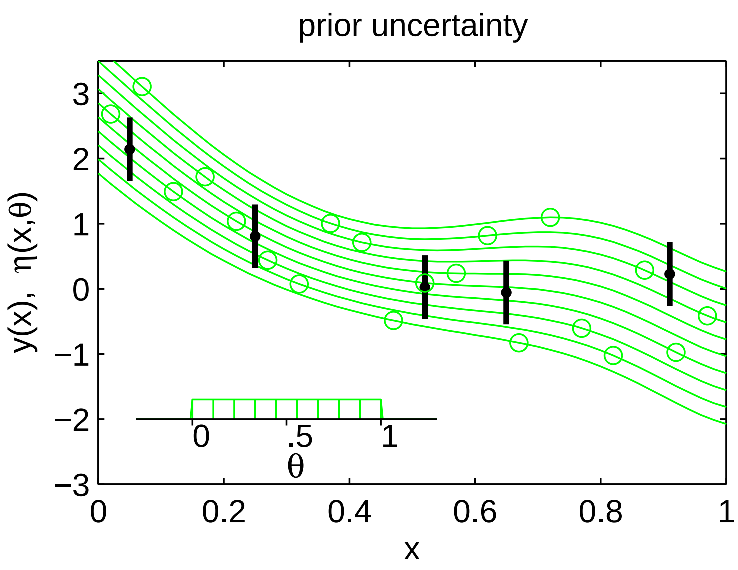
Alternatively, one can apply the conditional normal formula to

$$\begin{pmatrix} y \\ \eta \\ \zeta \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \lambda_\epsilon^{-1} I_n & 0 & 0 \\ 0 & \lambda_s^{-1} I_m & 0 \\ 0 & 0 & 0 \end{pmatrix} + C_\eta \right)$$

so that

$$\zeta|y,\eta \sim N\left(\Sigma_{21}\Sigma_{11}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix}, \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12} \right)$$

Accounting for model discrepancy

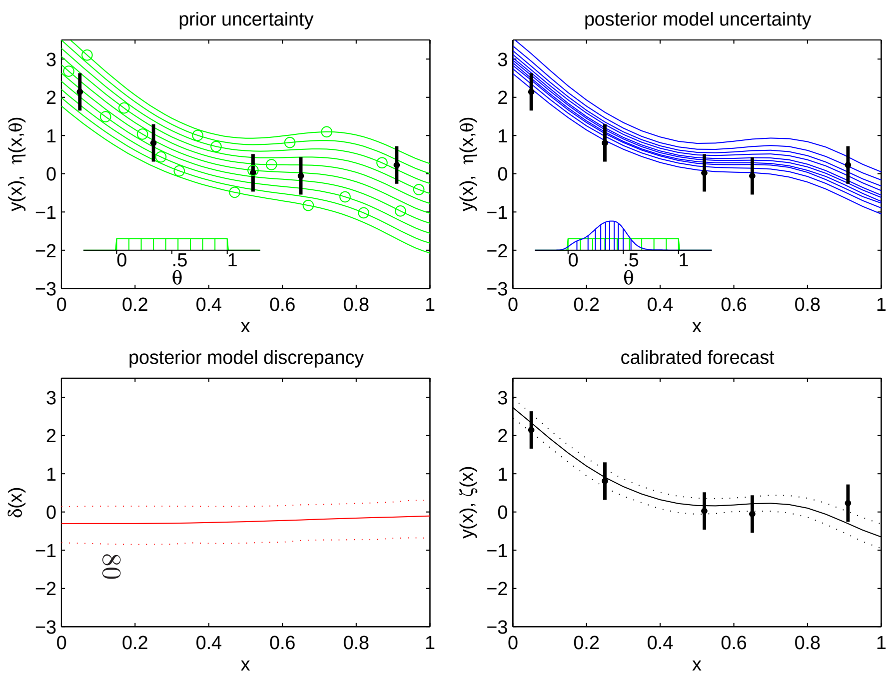


- Borrows from Kennedy and O'Hagan (2001).

x	model or system inputs
θ	calibration parameters
$\zeta(x)$	true physical system response given inputs x
$\eta(x,\theta)$	simulator response at x and θ.
$y(x)$	experimental observation of the physical system
$\delta(x)$	discrepancy between $\zeta(x)$ and $\eta(x,\theta)$
	may be decomposed into numerical error and bias
$e(x)$	observation error of the experimental data

$$
\begin{aligned}
y(x) &= \zeta(x) + e(x) \\
y(x) &= \eta(x,\theta) + \delta(x) + e(x) \\
y(x) &= \eta(x,\theta) + \delta_n(x) + \delta_b(x) + e(x)
\end{aligned}
$$

Accounting for model discrepancy



Again, standard Bayesian estimation gives:

$$\pi(\theta, \eta, \delta | y(x)) \propto L(y(x)|\eta(x,\theta), \delta(x)) \times \pi(\theta) \times \pi(\eta) \times \pi(\delta)$$

- Posterior means and 90% CI's shown.
- Posterior prediction for $\zeta(x)$ is obtained by computing the posterior distribution for $\eta(x,\theta) + \delta(x)$
- Uncertainty in θ, $\eta(x,t)$, and $\delta(x)$ are incorporated into the forecast.
- Gaussian process models for $\eta(x,t)$ and $\delta(x)$

Gaussian Process models for combining field data and complex computer simulators

field data — input settings (spatial locations)

$$y = \begin{pmatrix} y(x_1) \\ \vdots \\ y(x_n) \end{pmatrix} \qquad \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p_x} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np_x} \end{pmatrix}$$

sim data — input settings x; params θ^*

$$\eta = \begin{pmatrix} \eta(x_1^*, \theta_1^*) \\ \vdots \\ \eta(x_m^*, \theta_m^*) \end{pmatrix} \qquad \begin{pmatrix} x_{11}^* & \cdots & x_{1p_x}^* & \theta_{11}^* & \cdots & \theta_{1p_\theta}^* \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{m1}^* & \cdots & x_{mp_x}^* & \theta_{m1}^* & \cdots & \theta_{mp_\theta}^* \end{pmatrix}$$

Model sim response $\eta(x, \theta)$ as a Gaussian process

$$\begin{aligned} y(x) &= \eta(x,\theta) + \delta(x) + \epsilon \\ \eta(x,\theta) &\sim GP\left(0, C^\eta(x,\theta)\right) \\ \delta(x) &\sim GP\left(0, C^\delta(x)\right) \\ \epsilon &\sim \text{iid} N(0, 1/\lambda_\epsilon) \end{aligned}$$

$C^\eta(x,\theta)$ depends on $p_x + p_\theta$-vector ρ_η and λ_η
$C^\delta(x)$ depends on p_x-vector ρ_δ and λ_δ

Vector form – restricting to n field obs and m simulation runs

$$
\begin{aligned}
y &= \eta(\theta) + \delta + \epsilon \\
\eta &\sim N_m(0_m, C^\eta(\rho_\eta, \lambda_\eta)) \\
\begin{pmatrix} y \\ \eta \end{pmatrix} &\sim N_{n+m}\left(\begin{pmatrix} 0_n \\ 0_m \end{pmatrix}, C_{y\eta} = C^\eta + \begin{pmatrix} C^\delta & 0 \\ 0 & 0 \end{pmatrix} \right)
\end{aligned}
$$

where

$$
\begin{aligned}
C^\eta &= 1/\lambda_\eta R^\eta \left(\begin{pmatrix} x \\ x^* \end{pmatrix}, \begin{pmatrix} \mathbf{1}\theta \\ \theta^* \end{pmatrix}; \rho_\eta \right) + 1/\lambda_s I_{m+n} \\
C^\delta &= 1/\lambda_\delta R^\delta(x; \rho_\delta) + 1/\lambda_\epsilon I_n
\end{aligned}
$$

and the correlation matricies R^η and R^δ are given by

$$
\begin{aligned}
R^\eta((x,\theta),(x',\theta');\rho_\eta) &= \prod_{k=1}^{p_x} \rho_{\eta k}^{4(x_k - x'_k)^2} \times \prod_{k=1}^{p_\theta} \rho_{\eta(k+p_x)}^{4(\theta_k - \theta'_k)^2} \\
R^\delta(x, x'; \rho_\delta) &= \prod_{k=1}^{p_x} \rho_{\delta k}^{4(x_k - x'_k)^2}
\end{aligned}
$$

λ_s is typically set to something large like 10^6 to stabalize matrix computations and allow for numerical fluctuation in $\eta(x,\theta)$.

We use a 0 mean for $\eta(x,\theta)$; an alternative is to use a linear regression mean model.

Likelihood

$$L(y,\eta|\lambda_\epsilon,\rho_\eta,\lambda_\eta,\lambda_s,\rho_\delta,\lambda_\delta,\theta) \propto$$
$$|C_{y\eta}|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix}\right\}$$

Priors

$\pi(\lambda_\epsilon) \propto \lambda_\epsilon^{a_\epsilon-1} e^{-b_\epsilon \lambda_\epsilon}$ perhaps well known from observation process

$\pi(\rho_{\eta k}) \propto \prod_{k=1}^{p_x+p_\theta} (1-\rho_{\eta k})^{-.5}$, where $\rho_{\eta k} = e^{-.5^2 \beta_k^\eta}$ correlation at dist $= .5 \sim \beta(1, .5)$.

$\pi(\lambda_\eta) \propto \lambda_\eta^{a_\eta-1} e^{-b_\eta \lambda_\eta}$

$\pi(\lambda_s) \propto \lambda_s^{a_s-1} e^{-b_s \lambda_s}$

$\pi(\rho_{\delta k}) \propto \prod_{k=1}^{p_x} (1-\rho_{\delta k})^{-.5}$, where $\rho_{\delta k} = e^{-.5^2 \beta_k^\delta}$

$\pi(\lambda_\delta) \propto \lambda_\delta^{a_\delta-1} e^{-b_\delta \lambda_\delta}$,

$\pi(\theta) \propto I[\theta \in C]$

- could fix ρ_η, λ_η from prior GASP run on model output.
- Again, many choose to reparameterize correlation parameters: $\beta = -\log(\rho)/.5^2$ in the likelihood term

Posterior Density

$$
\begin{aligned}
&\pi(\lambda_\epsilon, \rho_\eta, \lambda_\eta, \lambda_s, \rho_\delta, \lambda_\delta, \theta | y, \eta) \propto \\
&\quad |C_{y\eta}|^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2} \begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix} \right\} \times \\
&\quad \prod_{k=1}^{p_x+p_\theta} (1-\rho_{\eta k})^{-.5} \times \lambda_\eta^{a_\eta - 1} e^{-b_\eta \lambda_\eta} \times \lambda_s^{a_s - 1} e^{-b_s \lambda_s} \times \\
&\quad \prod_{k=1}^{p_x} (1-\rho_{\delta k})^{-.5} \times \lambda_\delta^{a_\delta - 1} e^{-b_\delta \lambda_\delta} \times \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon} \times I[\theta \in C]
\end{aligned}
$$

If ρ_η, λ_η, and λ_s are fixed from a previous analysis ofthe simulator data, then

$$
\begin{aligned}
&\pi(\lambda_\epsilon, \rho_\delta, \lambda_\delta, \theta | y, \eta, \rho_\eta, \lambda_\eta, \lambda_s) \propto \\
&\quad |C_{y\eta}|^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2} \begin{pmatrix} y \\ \eta \end{pmatrix}^T C_{y\eta}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix} \right\} \times \\
&\quad \prod_{k=1}^{p_x} (1-\rho_{\delta k})^{-.5} \times \lambda_\delta^{a_\delta - 1} e^{-b_\delta \lambda_\delta} \times \lambda_\epsilon^{a_\epsilon - 1} e^{-b_\epsilon \lambda_\epsilon} \times I[\theta \in C]
\end{aligned}
$$

Predicting a new outcome: $\zeta = \zeta(x') = \eta(x', \theta) + \delta(x')$

$$
\begin{aligned}
y &= \eta(x, \theta) + \delta(x) + \epsilon(x) \\
\eta &= \eta(x^*, \theta^*) + \epsilon_s, \ \ \epsilon_s \text{ small or } 0 \\
\zeta &= \eta(x', \theta) + \delta(x'), \ \ x' \text{ univariate or multivariate}
\end{aligned}
$$

$$
\Rightarrow \begin{pmatrix} y \\ \eta \\ \zeta \end{pmatrix} \sim N_{n+m+1}\left(\begin{pmatrix} 0_n \\ 0_m \\ 0 \end{pmatrix}, \begin{pmatrix} \lambda_\epsilon^{-1} I_n & 0 & 0 \\ 0 & \lambda_s^{-1} I_m & 0 \\ 0 & 0 & 0 \end{pmatrix} + C^\eta + C^\delta \right) \qquad (1)
$$

where

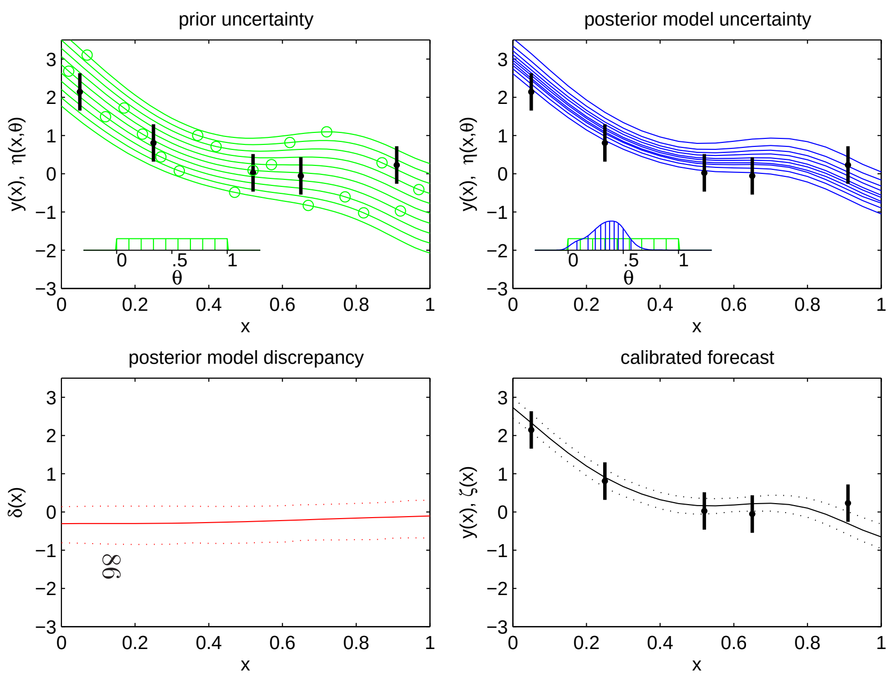
$$
C^\eta = 1/\lambda_\eta R^\eta \left(\begin{pmatrix} x \\ x^* \\ x' \end{pmatrix}, \begin{pmatrix} \mathbf{1}\theta \\ \theta^* \\ \theta \end{pmatrix}; \rho_\eta \right)
$$

$$
C^\delta = 1/\lambda_\delta R^\delta \left(\begin{pmatrix} x \\ x' \end{pmatrix}; \rho_\delta \right), \ \text{on indicies } 1, \ldots, n, n+m+1\text{; zeros elsewhere}
$$

Given a MCMC realization $(\theta, \lambda_\epsilon, \rho_\eta, \lambda_\eta, \rho_\delta, \lambda_\delta)$, a realization for $\zeta(x')$ can be produced using (**??**) and the conditional normal formula:

$$
\zeta | y, \eta \sim N\left(\Sigma_{21} \Sigma_{11}^{-1} \begin{pmatrix} y \\ \eta \end{pmatrix}, \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12} \right)
$$

Accounting for model discrepancy



Again, standard Bayesian estimation gives:

$$\pi(\theta, \eta_n, \delta | y(x)) \propto L(y(x)|\eta(x,\theta), \delta(x)) \times \pi(\theta) \times \pi(\eta) \times \pi(\delta)$$

- Posterior means and 90% CI's shown.
- Posterior prediction for $\zeta(x)$ is obtained by computing the posterior distribution for $\eta(x,\theta) + \delta(x)$
- Uncertainty in θ, $\eta(x,t)$, and $\delta(x)$ are incorporated into the forecast.
- Gaussian process models for $\eta(x,t)$ and $\delta(x)$

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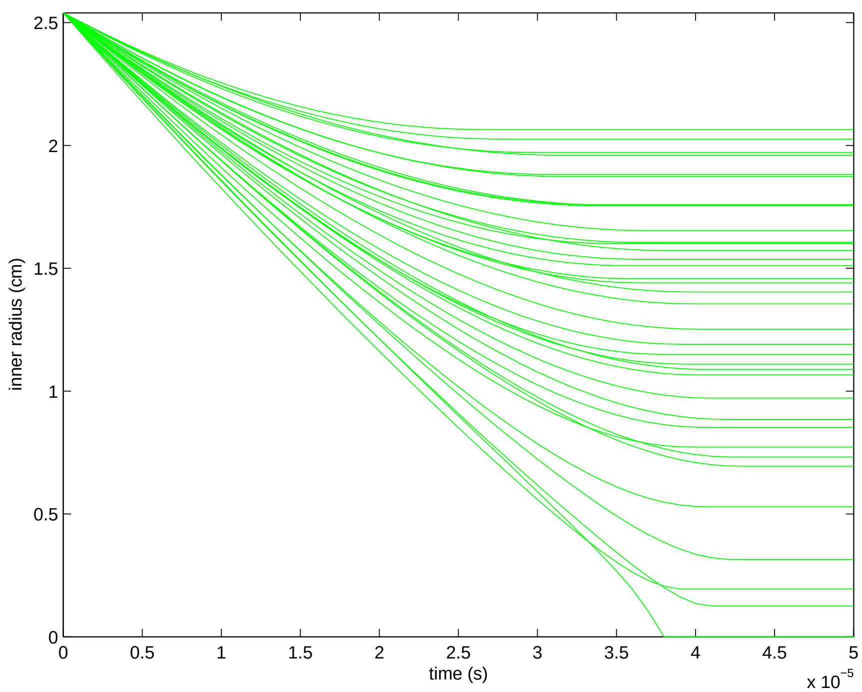
COMPUTER MODEL EMULATION WITH MULTIVARIATE OUTPUT

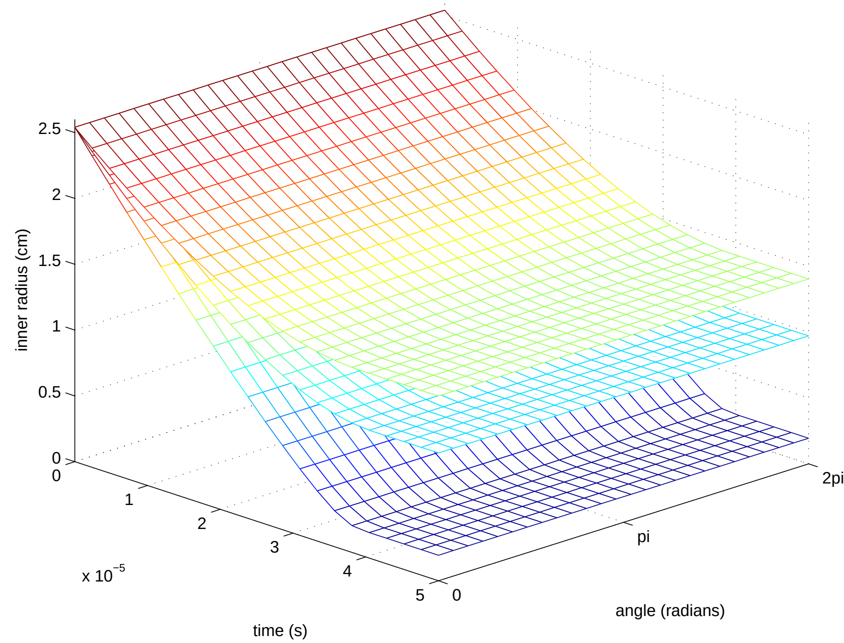
Carry out simulated implosions using Neddermeyer's model

Sequence of runs carried at m input settings $(x^*, \theta_1^*, \theta_2^*) = (m_e/m, s, u_0)$ varying over predefined ranges using an OA$(32, 4^3)$-based LH design.

$$\begin{pmatrix} x_1^* & \theta_{11}^* & \theta_{12}^* \\ \vdots & \vdots & \vdots \\ x_m^* & \theta_{m1}^* & \theta_{m2}^* \end{pmatrix}$$



radius by time



radius by time and angle ϕ.

Each simulation produces a $n_\eta = 22 \cdot 26$ vector of radii for 22 times $\times$ 26 angles.

Kronecker Representation:

model output matrix: $\eta^{\text{matrix}}_{n_\eta \times m} = [\eta_1, \ldots, \eta_m]$

model output vector: $\eta^{\text{vec}}_{n_\eta m \times 1} = [\eta_1; \ldots; \eta_m]$

Index support of the model output with time t (and angle ϕ) and use as additional x's in the GP model – as suggested in Kennedy and O'Hagan (2001).

$$\eta^{\text{vec}} \sim N\left(0_{n_\eta \cdot m}, C^\eta(x^*, \theta^*, t)\right)$$

Use the usual correlation model for these new dimensions.

$$R^\eta((x,\theta,t),(x',\theta',t');\rho_\eta) = \prod_{k=1}^{p_x} \rho_{\eta k}^{4(x_k - x'_k)^2} \times \prod_{k=1}^{p_\theta} \rho_{\eta(k+p_x)}^{4(\theta_k - \theta'_k)^2} \times \rho_{\eta(p_x+p_\theta+1)}^{4(t-t')^2}$$

R^η is a big matrix: $(n_\eta \cdot m) \times (n_\eta \cdot m)$; to big for much computation.

R^η has kronecker structure that can be exploited:

$$R^\eta = R^\eta_{m \times m}(x^*, \theta^*) \otimes R^\eta_{n_\eta \times n_\eta}(t)$$

Exploiting Kronecker Structure:

Considering model runs only:

model output matrix: $\eta^{\text{matrix}}_{n_\eta \times m} = [\eta_1, \ldots, \eta_m]$

model output vector: $\eta^{\text{vec}}_{n_\eta m \times 1} = [\eta_1; \ldots; \eta_m]$

$$R^\eta = R^\eta_{m\times m}(x^*, \theta^*) \otimes R^\eta_{n_\eta \times n_\eta}(t)$$

Matrix inverse and Cholesky decompositions maintain kronecker structure.

$$\begin{aligned} R^{-1} &= R^{-1}_{m\times m}(x^*, \theta^*) \otimes R^{-1}_{n_\eta \times n_\eta}(t) \\ R &= U^T U \\ U = \mathsf{chol}(R) &= \mathsf{chol}(R_{m\times m}(x^*, \theta^*)) \otimes \mathsf{chol}(R_{n_\eta\times n_\eta}(t)) = U_1 \otimes U_2 \end{aligned}$$

Likelihood evaluations requires the solve:

$$\begin{aligned} U^{-1}\eta^{\text{vec}} &= (U_1 \otimes U_2)^{-1}\eta^{\text{vec}} \\ &= (U_1^{-1} \otimes U_2^{-1})\eta^{\text{vec}} \\ &= U_1^{-1} \otimes (U_2^{-1}\eta^{\text{matrix}}) \end{aligned}$$

This only involves smaller upper triangular solves:

m solves of a $n_\eta \times n_\eta$ upper triangular matrix $+$

n_η solves of a $m \times m$ upper triangular matrix

COMPUTER MODEL CALIBRATION 2

DEALING WITH MULTIVARIATE OUTPUT

Application: implosions of steel cylinders – Neddermeyer ’43

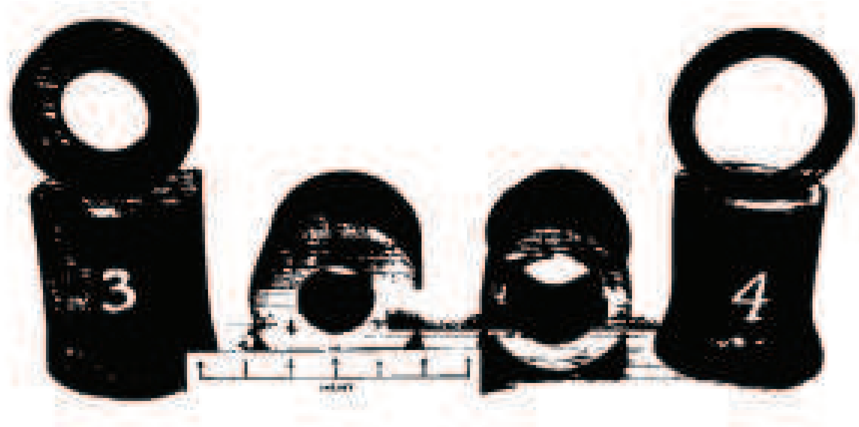
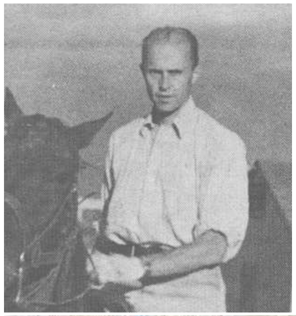


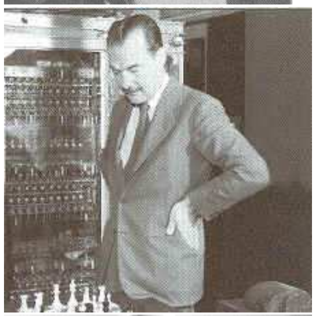
Fig. 13. xp. 3: 4" OD, 1" wall, 8" long
TNT, 1" thick, $7\frac{1}{2}$" long

xp. 4: 4" OD, $\frac{1}{2}$" wall, 8" long
TNT, 1" thick, $7\frac{1}{2}$" long
hearing rupture as shown along lines where detonation waves meet.

- Initial work on implosion for fat man.
- Use high explosive (HE) to crush steel cylindrical shells
- Investigate the feasability of a controlled implosion

Some History





Early work on cylinders called “beer can experiments.”

- Early work not encouraging:

  “...I question Dr. Neddermeyer’s seriousness...” – Deke Parsons.
  “It stinks.” – R. Feynman

  Teller and VonNeumann were quite supportive of the implosion idea

Data on collapsing cylinder from high speed photography.

Symmetrical implosion eventually accomplished using HE lenses by Kistiakowsky.

Implosion played a key role in early computer experiments.

Feynman worked on implosion calculations with IBM accounting machines.

Eventually first computer with addressable memory was developed (MANIAC 1).

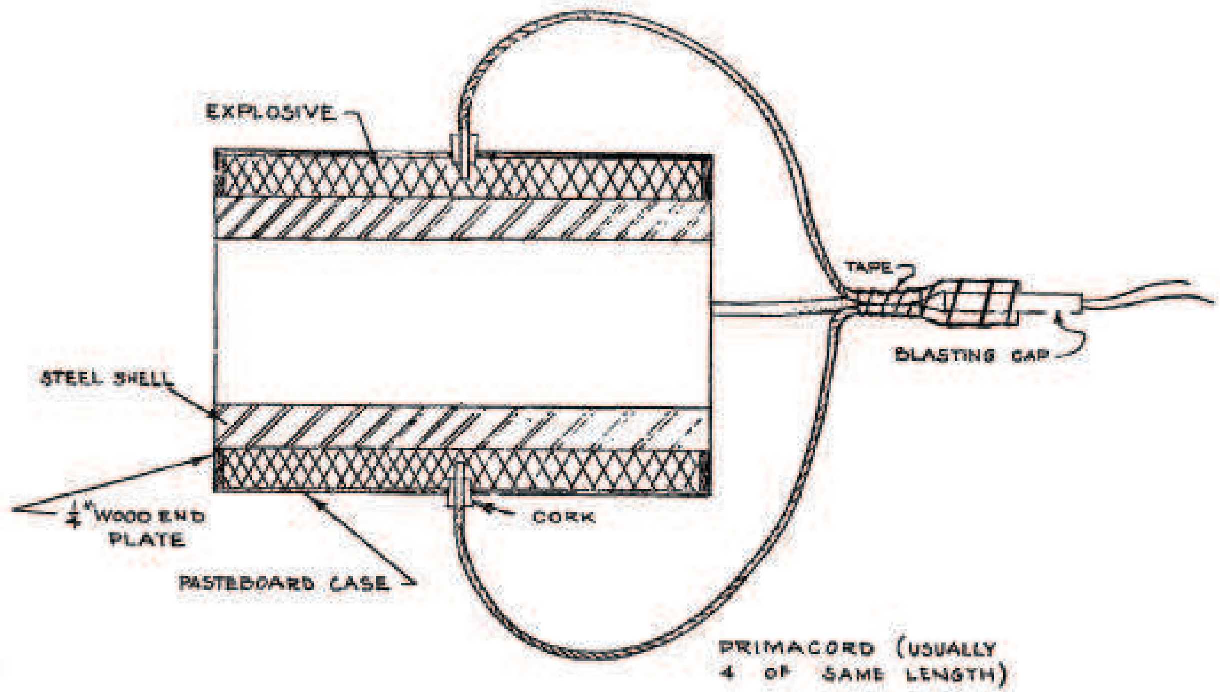
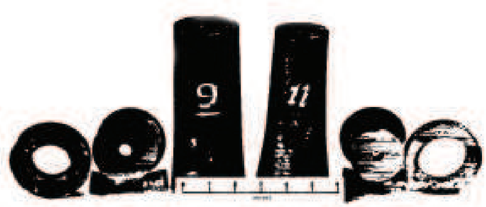


FIG. 10

SECTION OF TYPICAL ASSEMBLY
DRAWN TO SCALE OF EXPERIMENT # 26



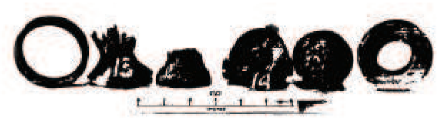


__Fig. 14.__ Exp. 9: 3" OD, $\frac{3}{4}$" wall, 8" long
TNT, $1\frac{1}{2}$" thick, $7\frac{1}{2}$" long

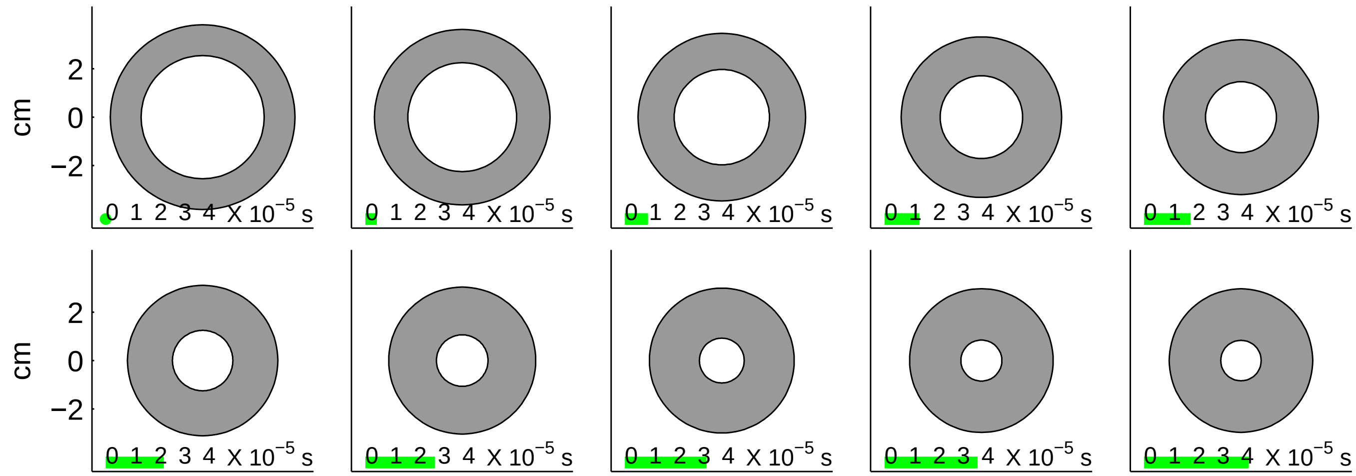
Exp. 11: 3" OD, $\frac{1}{2}$" wall, 8" long, same charge

Both detonated from 4 points at lower end in photograph

__Fig. 15.__ Exp. 13: 3" OD, $\frac{1}{2}$" wall, 8" long
Comp. C, $1\frac{1}{2}$" thick, $7\frac{1}{2}$" long
Cf. Fig. 11, note uniform collapse when excessive charge is used

Exp. 14: 3" OD, $\frac{3}{4}$" wall, 8" long
Comp. C, $1\frac{1}{2}$" thick, $7\frac{1}{2}$" long
Plastic flow can be seen through end of cylinder

Neddermeyer's Model



Energy from HE imparts an initial inward velocity to the cylinder

$$v_0 = \frac{m_e}{m}\sqrt{\frac{2u_0}{1 + m_e/m}}$$

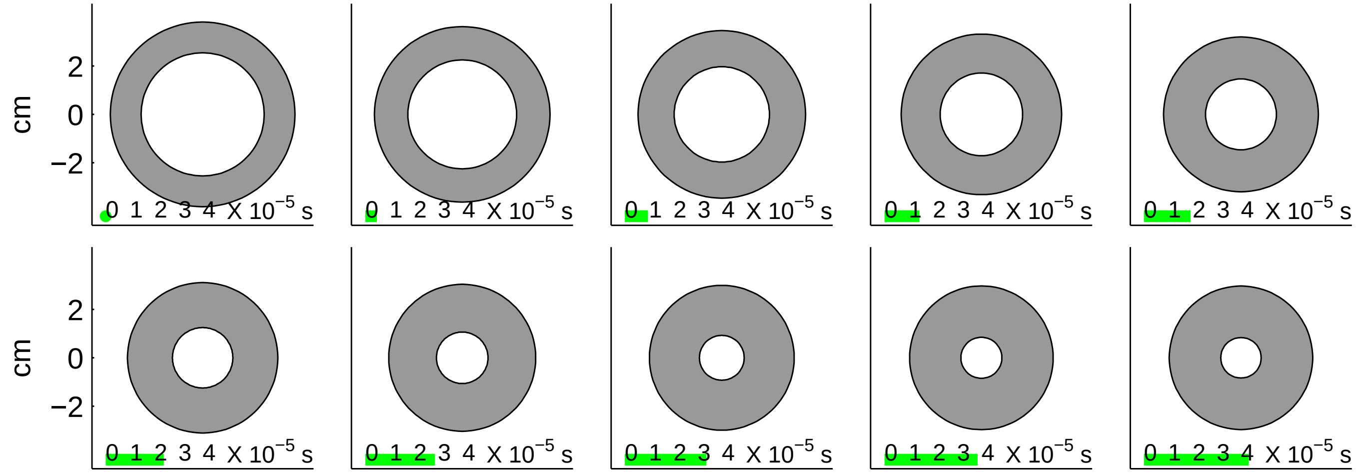
mass ratio m_e/m of HE to steel; u_0 energy per unit mass from HE.

Energy converts to work done on the cylinder:

$$\text{work per unit mass } = w = \frac{s}{2\rho(1-\lambda)}\left\{r_i^2 \log r_i^2 - r_o^2 \log r_o^2 + \lambda^2 \log \lambda^2\right\}$$

r_i = scaled inner radius; r_o = scaled outer radius; λ = initial r_i/r_o; s = steel yielding stress; ρ = density of steel.

Neddermeyer's Model



$$\text{ODE:} \quad \frac{dr}{dt} = \left[\frac{1}{R_1^2 f(r)} \left\{ v_0^2 - \frac{s}{\rho} g(r) \right\} \right]^{\frac{1}{2}}$$

where

r = inner radius of cylinder – varies with time

R_1 = initial outer radius of cylinder

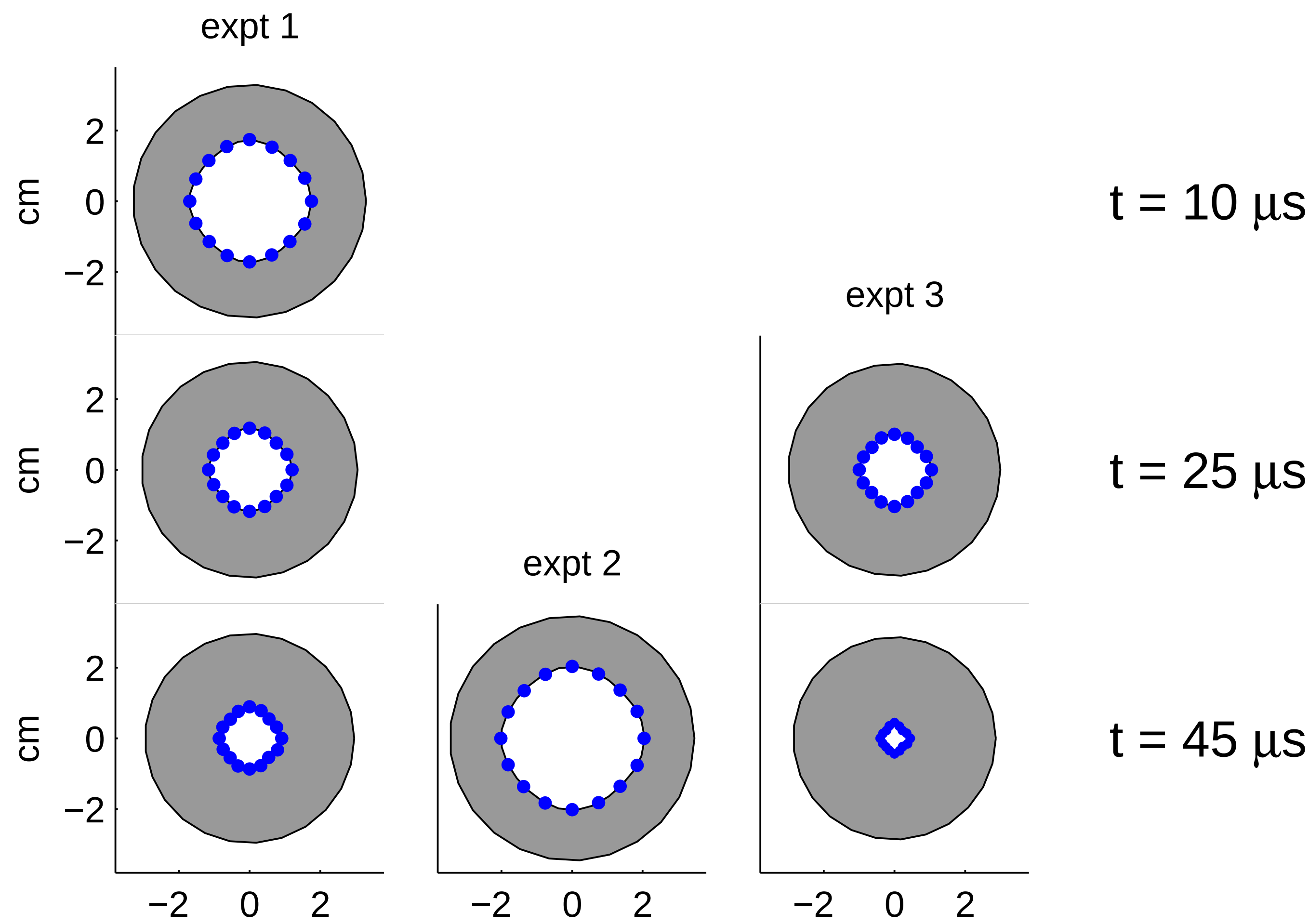
$$f(r) = \frac{r^2}{1-\lambda^2} \ln \left(\frac{r^2 + 1 - \lambda^2}{r^2} \right)$$

$$g(r) = (1-\lambda^2)^{-1} [r^2 \ln r^2 - (r^2 + 1 - \lambda^2) \ln(r^2 + 1 - \lambda^2) - \lambda^2 \ln \lambda^2]$$

λ = initial ratio of cylinder $r(t=0)/R_1$

constant volume condition: $r_{\text{outer}}^2 - r^2 = 1 - \lambda^2$

Goal: use experimental data to calibrate s and u_0; obtain prediction uncertainty for new experiment



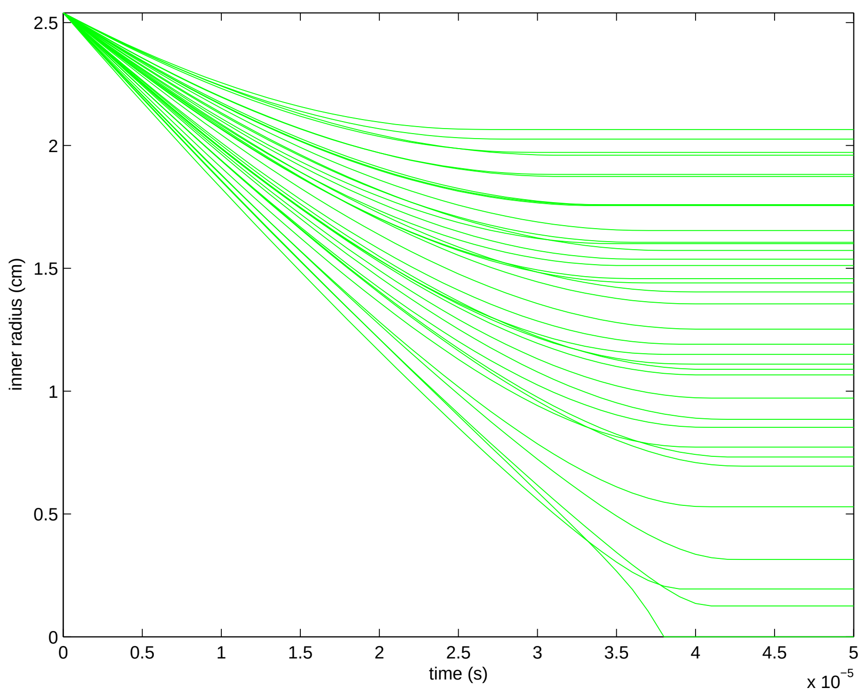
$m_e/m \approx .32$ $m_e/m \approx .17$ $m_e/m \approx .36$

Hypothetical data obtained from photos at different times during the 3 experimental implosions. All cylinders had a 1.5in outer and a 1.0in inner radius. ($\lambda = \frac{2}{3}$).

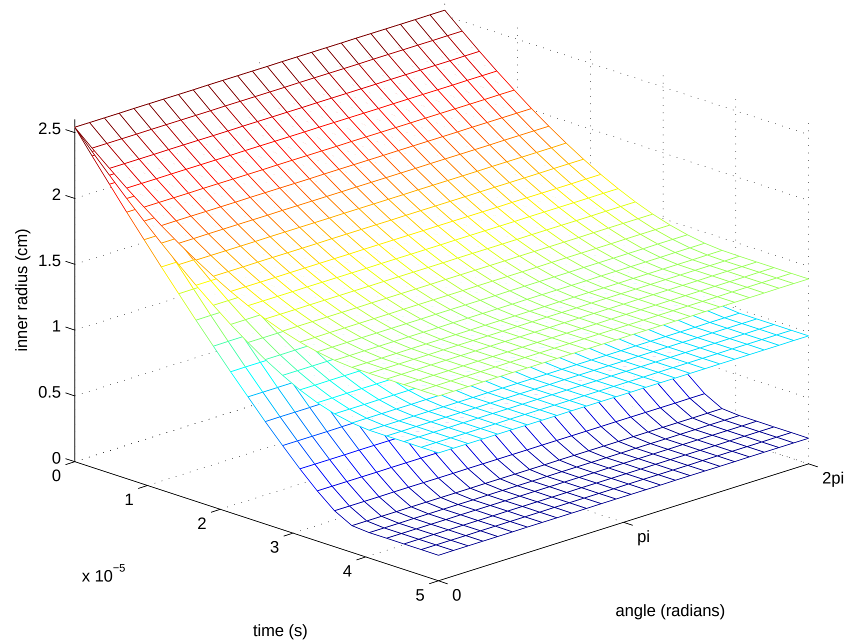
Carry out simulated implosions using Neddermeyer's model

Sequence of runs carried at m input settings $(x^*, \theta_1^*, \theta_2^*) = (m_e/m, s, u_0)$ varying over predefined ranges using an OA$(32, 4^3)$-based LH design.

$$\begin{pmatrix} x_1^* & \theta_{11}^* & \theta_{12}^* \\ \vdots & \vdots & \vdots \\ x_m^* & \theta_{m1}^* & \theta_{m2}^* \end{pmatrix}$$



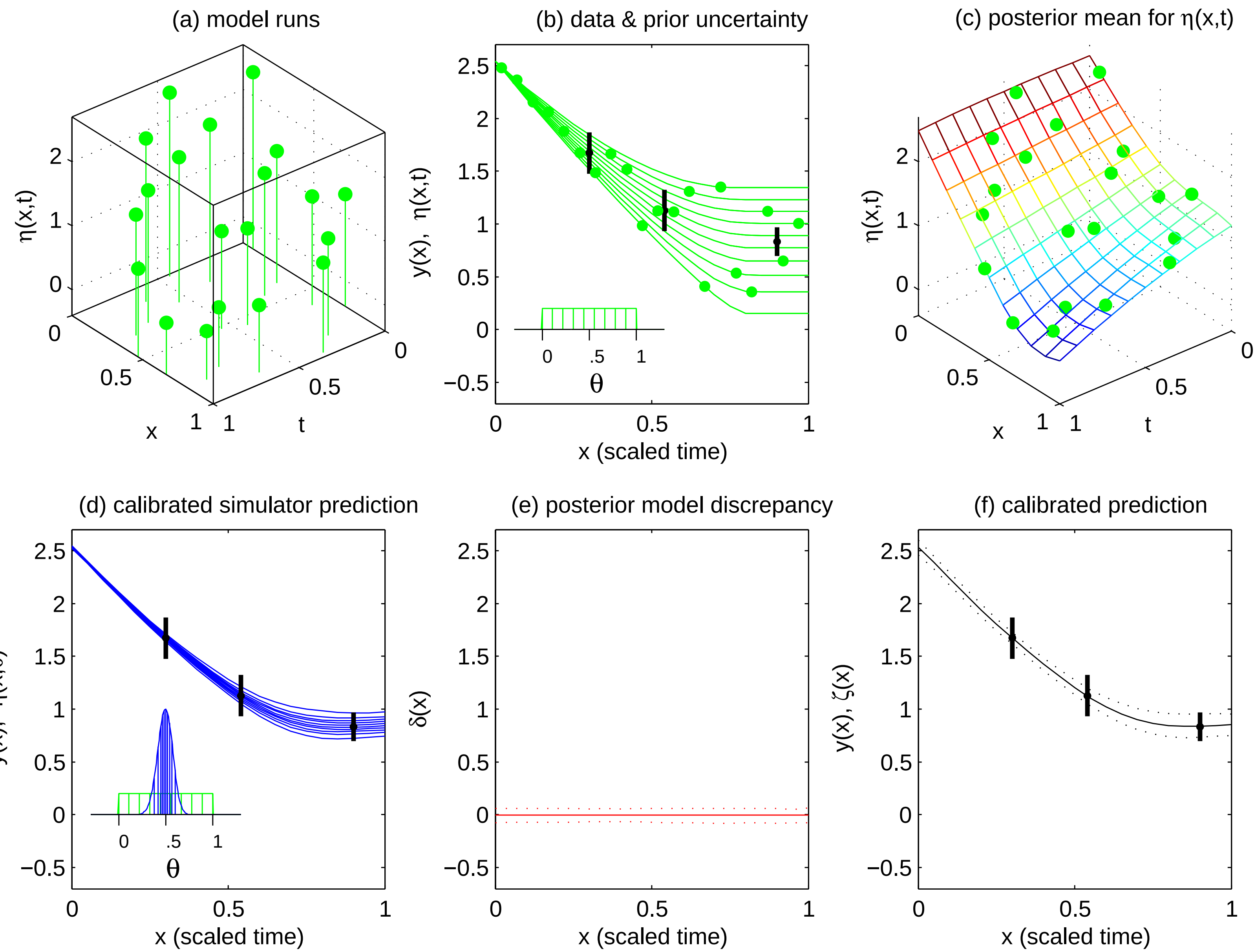
radius by time



radius by time and angle ϕ.

Each simulation produces a $n_\eta = 22 \cdot 26$ vector of radii for 22 times $\times$ 26 angles.

A 1-d implementation of the cylinder application



experimental data are collapsed radially

Features of this basic formulation

- Scales well with the input dimension, dim(x, θ).
- Treats simulation model as "black box" – no need to get inside simulator.
- Can model complicated and indirect observation processes.

Limitations of this basic formulation

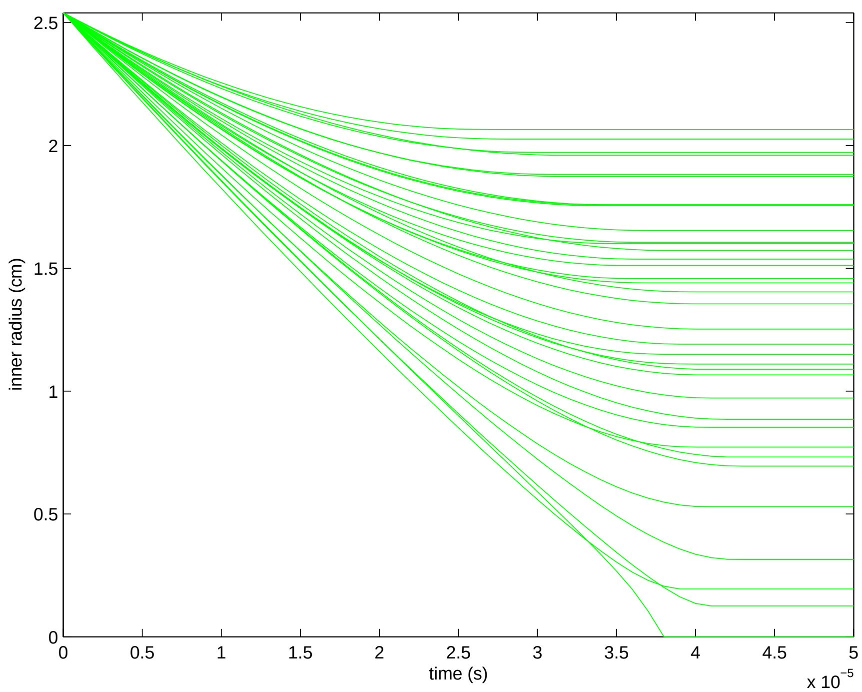
- Does not easily deal with highly multivariate data.
- Inneficient use of multivariate simulation output.

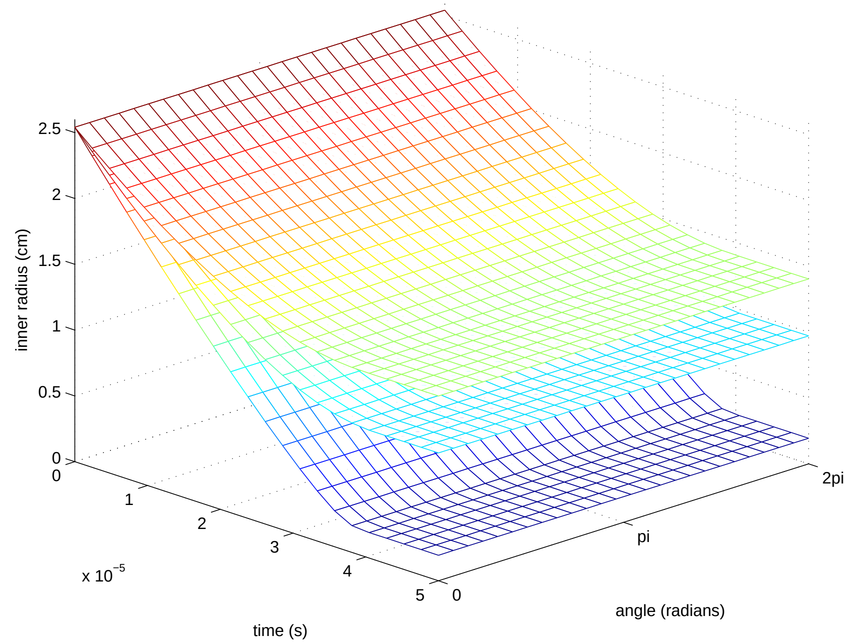
- Can miss important features in the physical process.

Need extension of basic approach to handle multivariate experimental observations and simulation output.

Carry out simulated implosions using Neddermeyer's model

Sequence of runs carried at m input settings $(x^*, \theta_1^*, \theta_2^*) = (m_e/m, s, u_0)$ varying over predefined ranges using an OA$(32, 4^3)$-based LH design.
$$\begin{pmatrix} x_1^* & \theta_{11}^* & \theta_{12}^* \\ \vdots & \vdots & \vdots \\ x_m^* & \theta_{m1}^* & \theta_{m2}^* \end{pmatrix}$$





radius by time

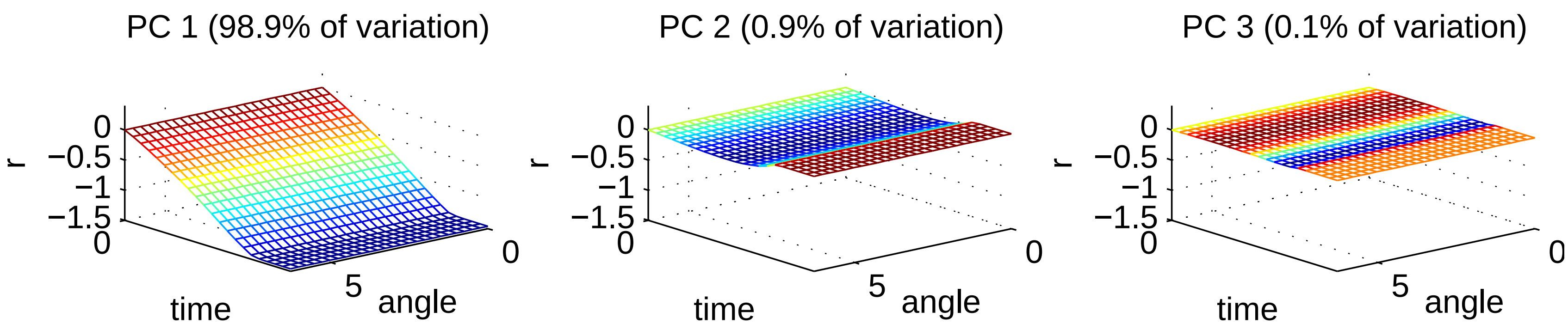
radius by time and angle ϕ.

Each simulation produces a $n_\eta = 22 \cdot 26$ vector of radii for 22 times $\times$ 26 angles.

Basis representation of simulation output

$$\eta(x,\theta) = \sum_{i=1}^{p_\eta} k_i(t,\phi) w_i(x,\theta)$$

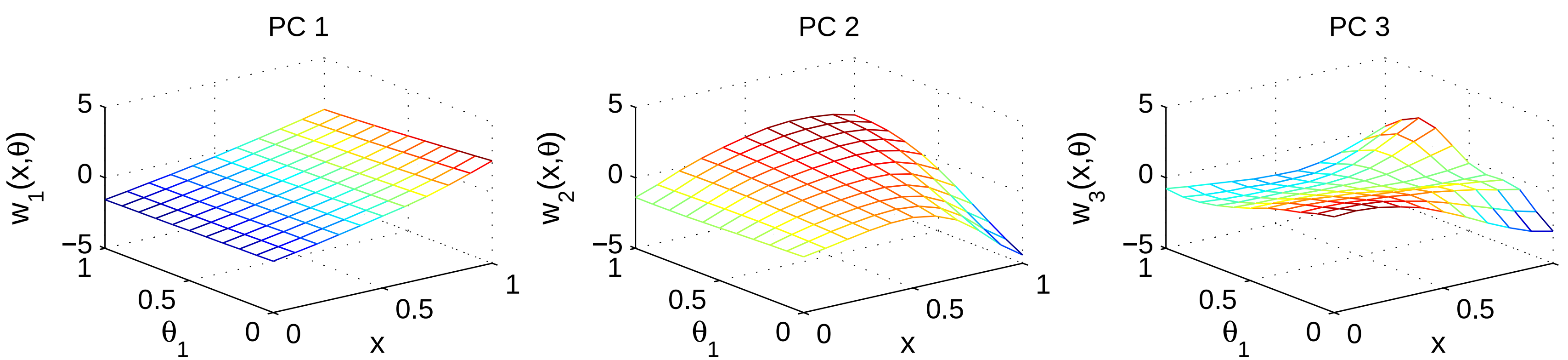
Here we construct bases $k_i(t,\phi)$ via principal components (EOFs):



basis elements do not change with ϕ – from symmetry of Neddermeyer's model.

Model untried settings with a GP model on weights:

$$w_i(x,\theta_1,\theta_2) \sim \mathsf{GP}(0, \lambda_{wi}^{-1} R((x,\theta),(x',\theta');\rho_{wi}))$$



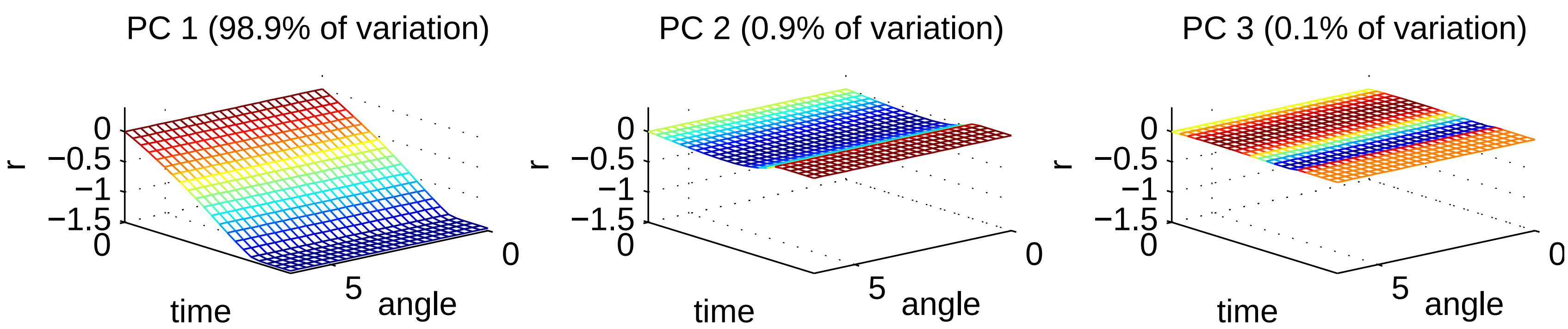
PC representation of simulation output

$\Xi = [\eta_1; \cdots ; \eta_m]$ – a $n_\eta \times m$ matrix that holds output of m simulations

SVD decomposition: $\Xi = UDV^T$

K_η is 1st p_η columns of $[\frac{1}{\sqrt{m}} UD]$ – columns of $[\sqrt{m} V^T]$ have variance 1

Cylinder example:



$p_\eta = 3$ PC's: $K_\eta = [k_1; k_2; k_3]$ – each vector k_i holds trace of PC i.

k_i's do not change with ϕ – from symmetry of Neddermeyer's model.

Simulated trace $\eta(x_i^*, \theta_{i1}^*, \theta_{i2}^*) = K_\eta w(x_i^*, \theta_{i1}^*, \theta_{i2}^*) + \epsilon_i$, ϵ_i's $\stackrel{iid}{\sim}$ N$(0, \lambda_\eta^{-1})$, for any set of tried simulation inputs $(x_i^*, \theta_{i1}^*, \theta_{i2}^*)$.

Gaussian process models for PC weights

Want to evaluate $\eta(x, \theta_1, \theta_2)$ at arbitrary input setting (x, θ_1, θ_2).

Also want analysis to account for uncertainty here.

Approach: model each PC weight as a Gaussian process:

$$w_i(x, \theta_1, \theta_2) \sim \mathsf{GP}(0, \lambda_{wi}^{-1} R((x, \theta), (x', \theta'); \rho_{wi}))$$

where

$$R((x, \theta), (x', \theta'); \rho_{wi}) = \prod_{k=1}^{p_x} \rho_{wik}^{4(x_k - x'_k)^2} \times \prod_{k=1}^{p_\theta} \rho_{wi(k+p_x)}^{4(\theta_k - \theta'_k)^2} \qquad (1)$$

Restricting to the design settings $\begin{pmatrix} x_1^* & \theta_{11}^* & \theta_{12}^* \\ \vdots & \vdots & \vdots \\ x_m^* & \theta_{m1}^* & \theta_{m2}^* \end{pmatrix}$ and specifying

$$w_i = (w_i(x_1^*, \theta_{11}^*, \theta_{12}^*), \ldots, w_i(x_m^*, \theta_{m1}^*, \theta_{m2}^*))^T$$

gives

$$w_i \overset{iid}{\sim} N\left(0, \lambda_{wi}^{-1} R((x^*, \theta^*); \rho_{wi})\right), \quad i = 1, \ldots, p_\eta$$

where $R((x^*, \theta^*); \rho_{wi})_{m \times m}$ is given by (1).

*note: additional nugget term $w_i \overset{iid}{\sim} N\left(0, \lambda_{wi}^{-1} R((x^*, \theta^*); \rho_{wi}) + \lambda_{\epsilon i}^{-1} I_m\right), \quad i = 1, \ldots, p_\eta$, may be useful.

Gaussian process models for PC weights

At the m simulation input settings the mp_η-vector w has prior disribution

$$w = \begin{pmatrix} w_1 \\ \vdots \\ w_{p_\eta} \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} \lambda_{w1}^{-1} R((x^*, \theta^*); \rho_{w1}) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_{wp_\eta}^{-1} R((x^*, \theta^*); \rho_{wp_\eta}) \end{pmatrix} \right)$$

$$\Rightarrow \; w \sim N(0, \Sigma_w);$$

note $\Sigma_w = I_{p_\eta} \otimes \lambda_w^{-1} R((x^*, \theta^*); \rho_w)$ can break down.

Emulator likelihood: $\eta = \text{vec}([\eta(x_1^*, \theta_{11}^*, \theta_{12}^*); \cdots ; \eta(x_m^*, \theta_{m1}^*, \theta_{m2}^*)])$

$$L(\eta | w, \lambda_\eta) \propto \lambda_\eta^{\frac{mn_\eta}{2}} \exp\left\{ -\tfrac{1}{2} \lambda_\eta (\eta - Kw)^T (\eta - Kw) \right\}, \quad \lambda_\eta \sim \Gamma(a_\eta, b_\eta)$$

where n_η is the number of observations in a simulated trace and

$$K = [I_m \otimes k_1; \cdots ; I_m \otimes k_{p_\eta}].$$

Equivalently

$$\begin{aligned} L(\eta | w, \lambda_\eta) \;\propto\; & \lambda_\eta^{\frac{mp_\eta}{2}} \exp\left\{ -\tfrac{1}{2} \lambda_\eta (w - \hat{w})^T (K^T K)(w - \hat{w}) \right\} \times \\ & \lambda_\eta^{\frac{m(n_\eta - p_\eta)}{2}} \exp\left\{ -\tfrac{1}{2} \lambda_\eta \eta^T (I - K(K^T K)^{-1} K^T) \eta \right\} \\ \propto\; & \lambda_\eta^{\frac{mp_\eta}{2}} \exp\left\{ -\tfrac{1}{2} \lambda_\eta (w - \hat{w})^T (K^T K)(w - \hat{w}) \right\}, \quad \lambda_\eta \sim \Gamma(a'_\eta, b'_\eta) \end{aligned}$$

$a'_\eta = a_\eta + \frac{m(n_\eta - p_\eta)}{2}$, $b'_\eta = b_\eta + \frac{1}{2} \eta^T (I - K(K^T K)^{-1} K^T) \eta$, $\hat{w} = (K^T K)^{-1} K^T \eta$.

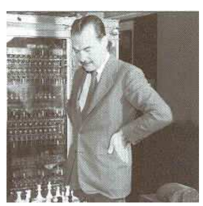
Gaussian process models for PC weights

Resulting posterior can then be based on computed PC weights $\hat{w}$:

$$\begin{aligned} \hat{w}|w,\lambda_\eta &\sim N(w,(\lambda_\eta K^T K)^{-1}) \\ w|\lambda_w,\rho_w &\sim N(0,\Sigma_w) \\ \Rightarrow \hat{w}|\lambda_\eta,\lambda_w,\rho_w &\sim N(0,(\lambda_\eta K^T K)^{-1}+\Sigma_w) \end{aligned}$$

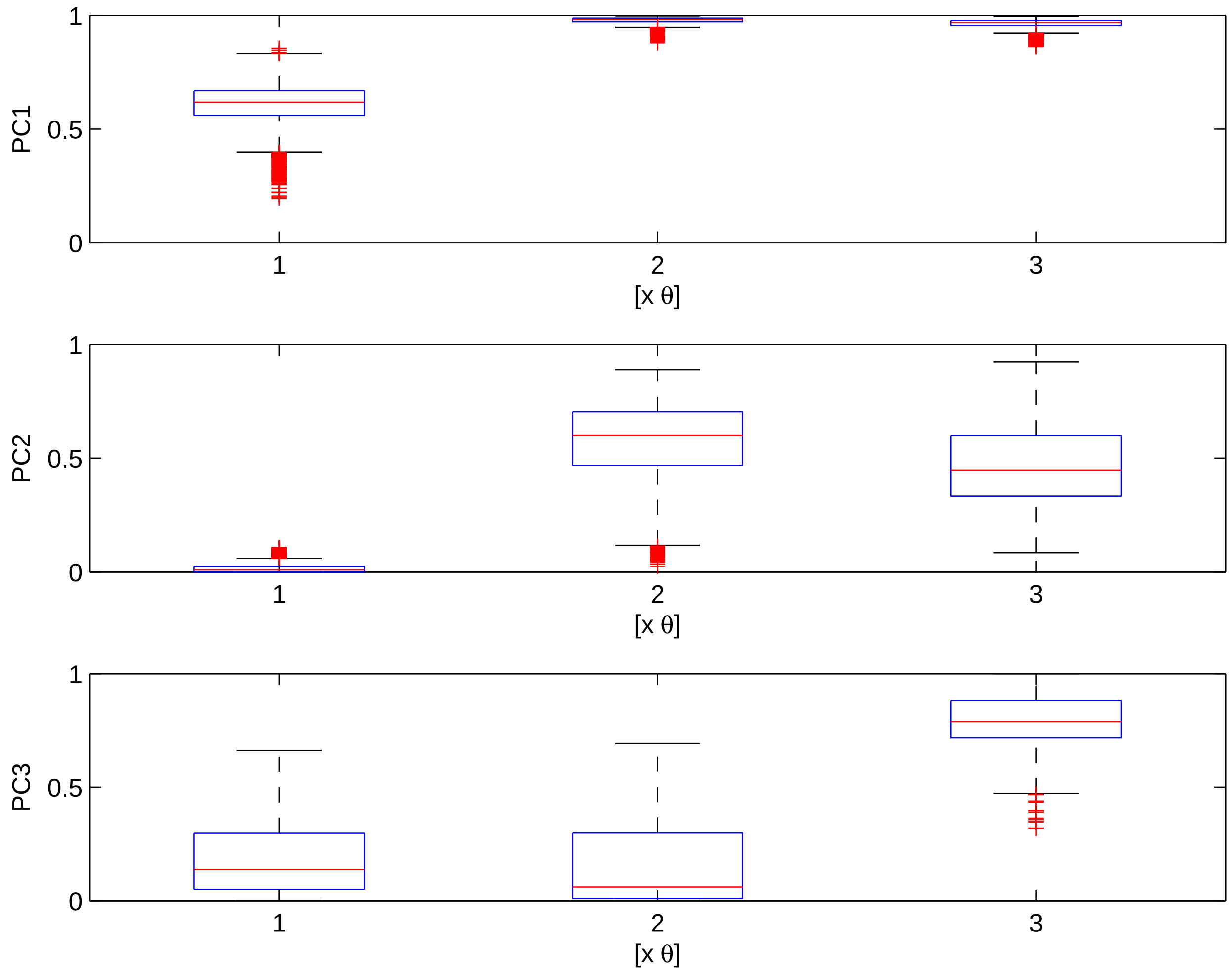
Resulting posterior is then:

$$\begin{aligned} \pi(\lambda_\eta,\lambda_w,\rho_w|\hat{w}) \;\propto\; & \left|(\lambda_\eta K^T K)^{-1}+\Sigma_w\right|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}\hat{w}^T([\lambda_\eta K^T K]^{-1}+\Sigma_w)^{-1}\hat{w}\} \times \\ & \lambda_\eta^{a'_\eta-1} e^{-b'_\eta \lambda_\eta} \times \prod_{i=1}^{p_\eta} \lambda_{wi}^{a_w-1} e^{-b_w \lambda_{wi}} \times \\ & \prod_{i=1}^{p_\eta} \left\{ \prod_{j=1}^{p_x} (1-\rho_{wij})^{b_\rho-1} \prod_{j=1}^{p_\theta} (1-\rho_{wi(j+p_x)})^{b_\rho-1} \right\} \end{aligned}$$

MCMC via Metropolis  works fine here.

Bounded range of ρ_{wij}'s facilitates MCMC.

Posterior distribution of ρ_w



Separate models by PC

More opportunity to take advantage of effect sparsity

Predicting simulator output at untried $(x^\star, \theta_1^\star, \theta_2^\star)$

Want $\eta(x^\star, \theta_1^\star, \theta_2^\star) = Kw(x^\star, \theta_1^\star, \theta_2^\star)$

For a given draw $(\lambda_\eta, \lambda_w, \rho_w)$ a draw of $w^\star$ can be produced:

$$\begin{pmatrix} \hat{w} \\ w^\star \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \left[\begin{pmatrix} (\lambda_\eta K^T K)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \Sigma_{w,w^\star}(\lambda_w, \rho_w) \right] \right)$$

Define

$$V = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \left[\begin{pmatrix} (\lambda_\eta K^T K)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \Sigma_{w,w^\star}(\lambda_w, \rho_w) \right]$$

Then

$$w^\star | \hat{w} \sim N(V_{21} V_{11}^{-1} \hat{w}, V_{22} - V_{21} V_{11}^{-1} V_{12})$$

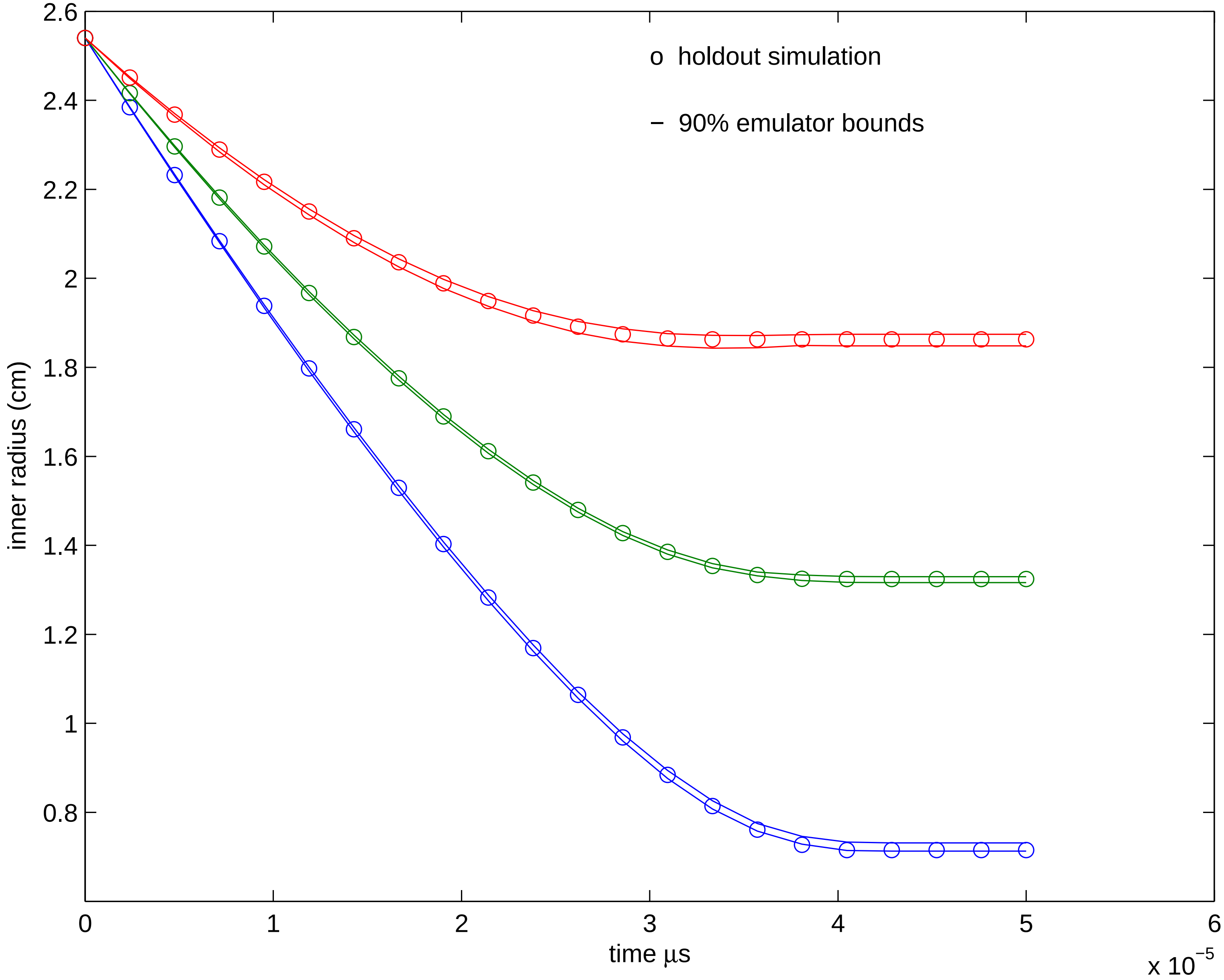
Realizations can be generated from sample of MCMC output.

Lots of info (data?) makes conditioning on point estimate $(\widehat{\lambda}_\eta, \widehat{\lambda}_w, \widehat{\rho}_w)$ a good approximation to the posterior.

Posterior mean or median work well for $(\widehat{\lambda}_\eta, \widehat{\lambda}_w, \widehat{\rho}_w)$

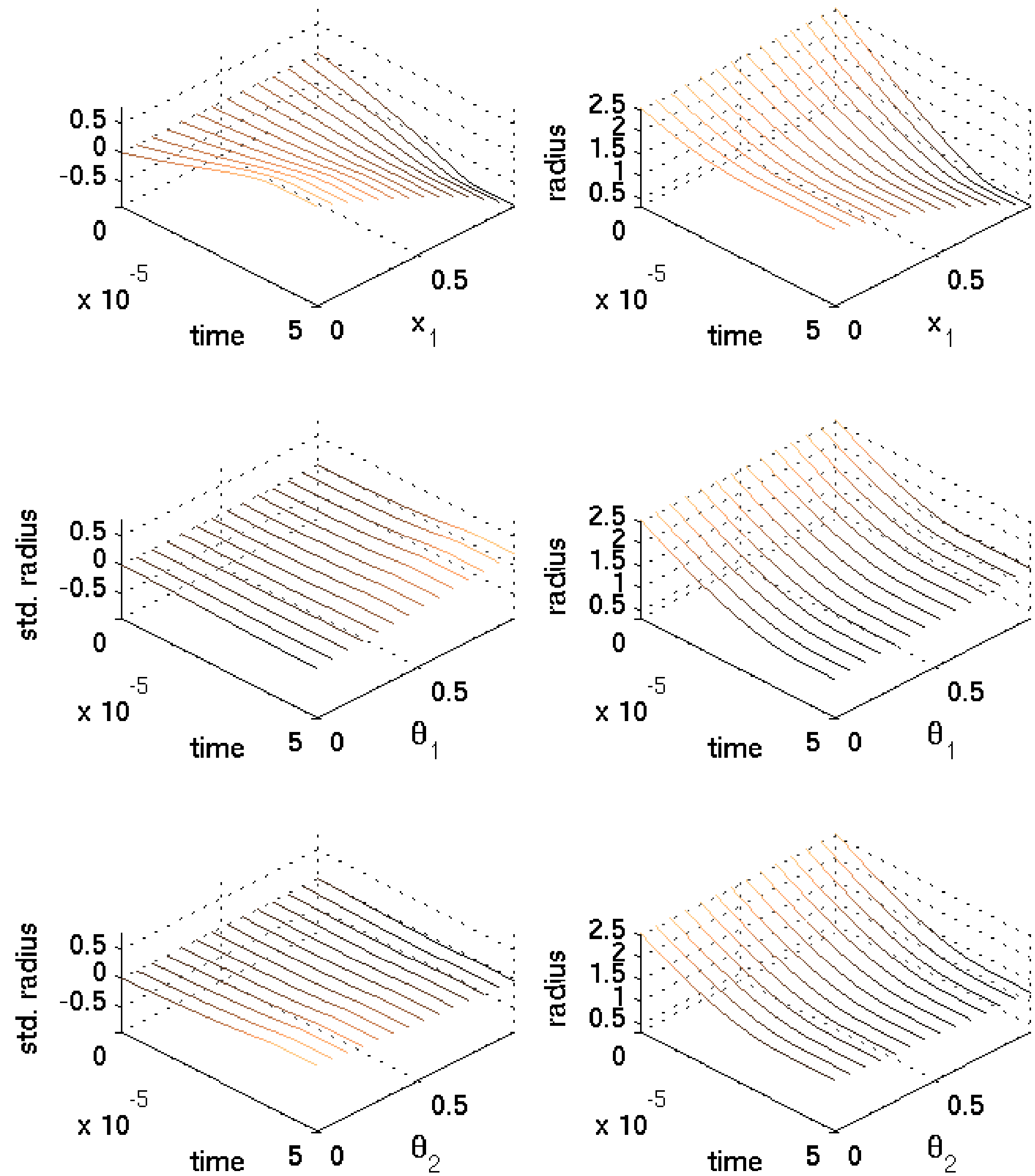
Comparing emulator predictions to holdout simulations

emulator 90% prediction bands and actual (holdout) simulations

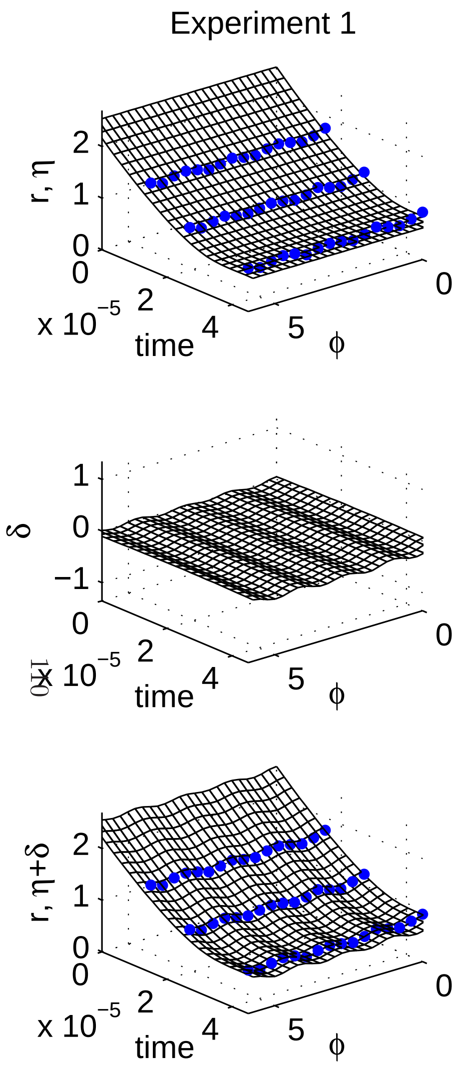


Exploring sensitivity of simulator output to model inputs

Simulator predictions varing 1 input, holding others at nominal



Basic formulation – borrows from Kennedy and O'Hagan (2001)



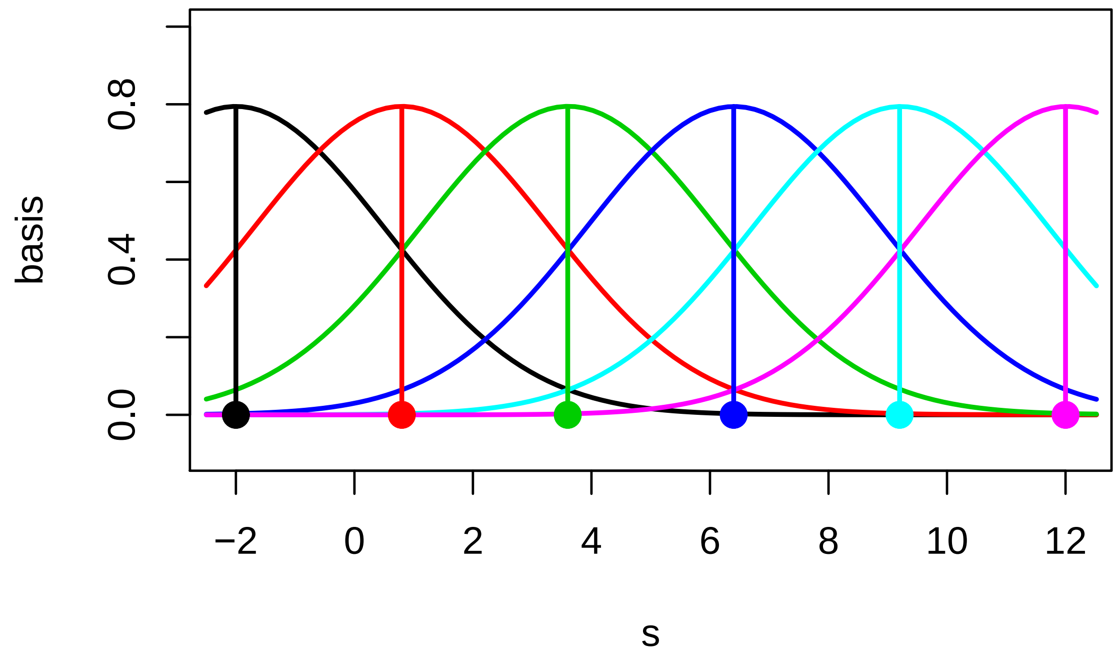
(t, ϕ)	simulation output space
x	experimental conditions
θ	calibration parameters
$\zeta(x)$	true physical system response given conditions x
$\eta(x,\theta)$	simulator response at x and θ.
$y(x)$	experimental observation of the physical system
$\delta(x)$	discrepancy between $\zeta(x)$ and $\eta(x,\theta)$ may be decomposed into numerical error and bias
$e(x)$	observation error of the experimental data

$$y(x) \;=\; \zeta(x) + e(x)$$
$$y(x) \;=\; \eta(x,\theta) + \delta(x) + e(x)$$

$$x = \; m_e/m \approx .32$$
$$\theta_1 = \; s \approx \text{?}$$
$$\theta_2 = \; u_0 \approx \text{?}$$

Kernel basis representation for spatial processes $\delta(s)$

Define p_δ basis functions $d_1(s), \ldots, d_{p_\delta}(s)$.



Here $d_j(s)$ is normal density cetered at spatial location ω_j:

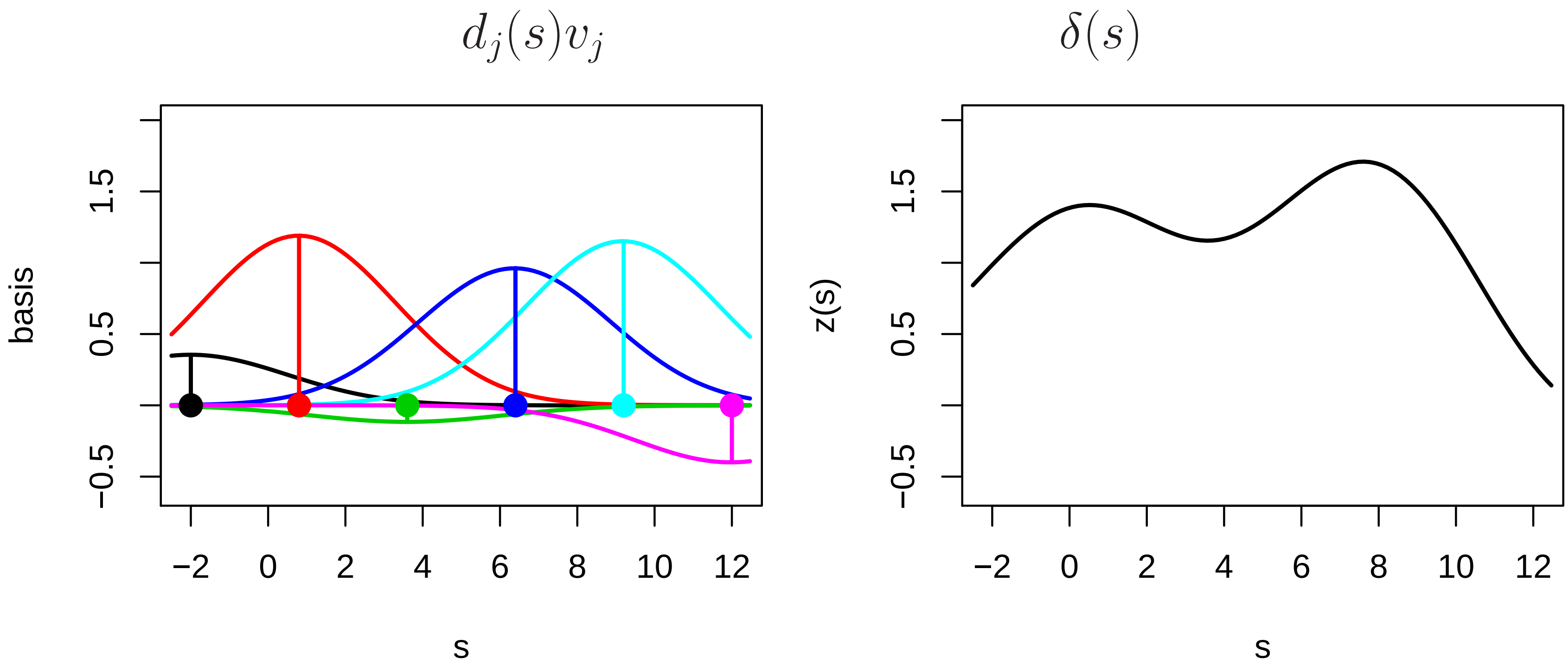
$$d_j(s) = \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2}(s - \omega_j)^2\}$$

$$\text{set } \delta(s) = \sum_{j=1}^{p_\delta} d_j(s) v_j \text{ where } v \sim N(0, \lambda_v^{-1} I_{p_\delta}).$$

Can represent $\delta = (\delta(s_1), \ldots, \delta(s_n))^T$ as $\delta = Dv$ where

$$D_{ij} = d_j(s_i)$$

v and $d(s)$ determine spatial processes $\delta(s)$

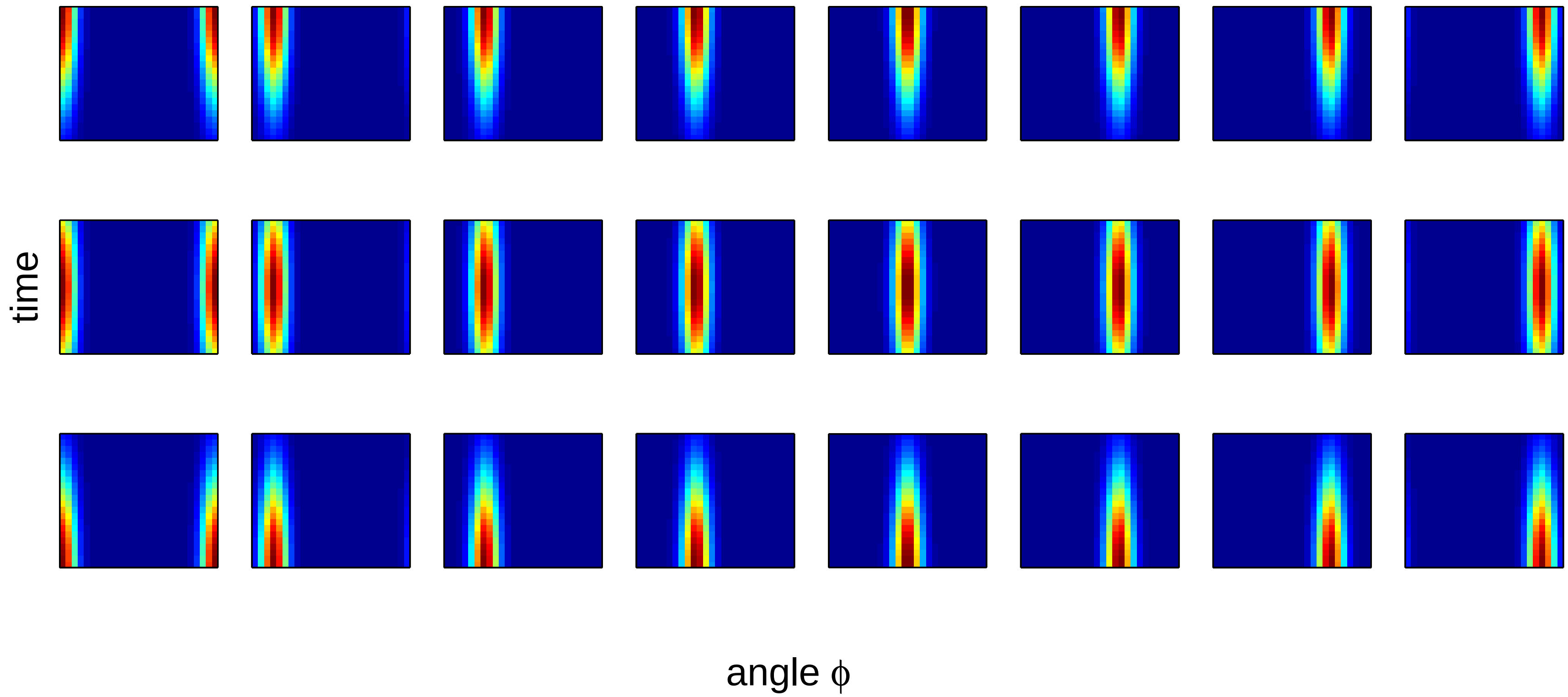


Continuous representation:

$$\delta(s) = \sum_{j=1}^{p_\delta} d_j(s) v_j \text{ where } v \sim N(0, \lambda_v^{-1} I_{p_\delta}).$$

Discrete representation: For $\delta = (\delta(s_1), \ldots, \delta(s_n))^T$, $\delta = Dv$ where $D_{ij} = d_j(s_i)$

Basis representation of discrepancy



Represent discrepancy $\delta(x)$ using basis functions and weights

$p_\delta = 24$ basis functions over (t, ϕ); $D = [d_1; \cdots ; d_{p_\delta}]$; d_k's hold basis.

$$\delta(x) = Dv(x) \text{ where } v(x) \sim \text{GP}\left(0, \lambda_v^{-1} I_{p_\delta} \otimes R(x, x'; \rho_v)\right)$$

with

$$R(x, x'; \rho_v) = \prod_{k=1}^{p_x} \rho_{vk}^{4(x_k - x'_k)^2} \tag{2}$$

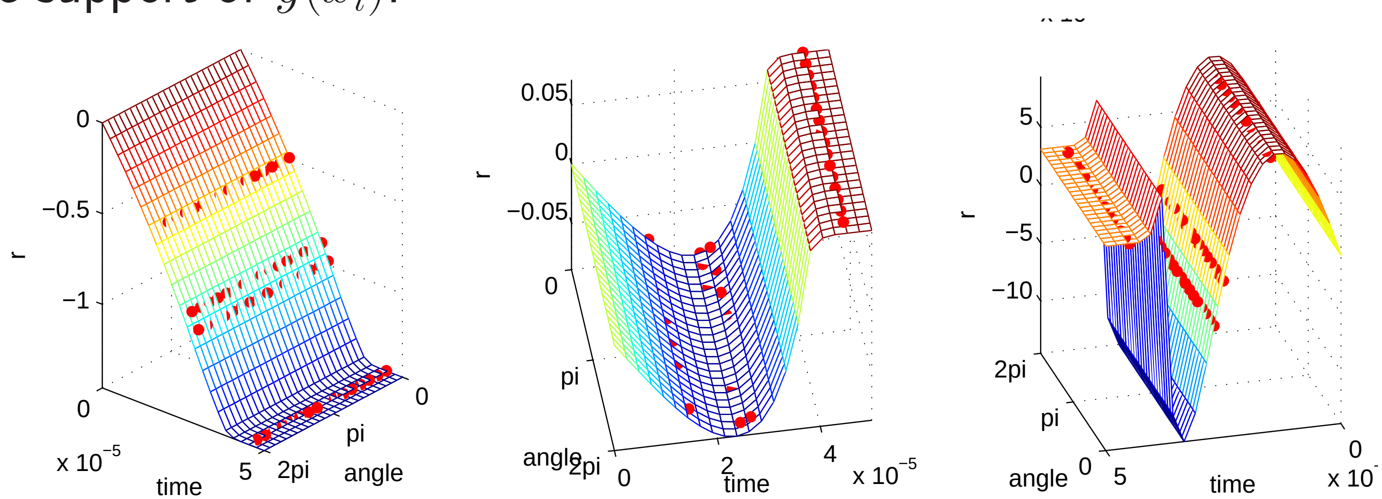
Integrated model formulation

Data $y(x_1), \ldots, y(x_n)$ collected for n experiments at input conditions $x_1, \ldots, x_n$.

Each $y(x_i)$ is a collection of n_{y_i} measurements over points indexed by (t, ϕ).

$$\begin{aligned} y(x_i) &= \eta(x_i, \theta) + \delta(x_i) + e_i \\ &= K_i w(x_i, \theta) + D_i v(x_i) + e_i \\ y(x_i) | w(x_i, \theta), v(x_i), \lambda_y &\sim N\left([D_i; K_i] \begin{pmatrix} v(x_i) \\ w(x_i, \theta) \end{pmatrix}, (\lambda_y W_i)^{-1} \right) \end{aligned}$$

Since support of each $y(x_i)$ varies and doesn't match that of sims, the basis vectors in K_i must be interpolated from K_η; similary, D_i must be computed from the support of $y(x_i)$:



*note: cubic spline interpolation over (time, ϕ) used here.

Integrated model formulation

Define

$n_y = n_{y_1} + \cdots + n_{y_n}$, the total number of experimental data points,

y to be the n_y-vector from concatination of the $y(x_i)$'s,

$v = \text{vec}([v(x_1); \cdots ; v(x_n)]^T)$ and

$u(\theta) = \text{vec}([w(x_1, \theta_1, \theta_2); \cdots ; w(x_n, \theta_1, \theta_2)]^T)$

$$y|v, u(\theta), \lambda_y \sim \mathsf{N}\left(B\begin{pmatrix} v \\ u(\theta) \end{pmatrix}, (\lambda_y W_y)^{-1}\right), \ \lambda_y \sim \Gamma(a_y, b_y) \qquad (3)$$

where

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$W_y = \text{diag}(W_1, \ldots, W_n)$ and

$B = \text{diag}(D_1, \ldots, D_n, K_1, \ldots, K_n)\begin{pmatrix} P_D^T & 0 \\ 0 & P_K^T \end{pmatrix}$

P_D and P_K are permutation matricies whose rows are given by:

$$\begin{aligned} P_D(j + n(i-1); \cdot) &= e^T_{(j-1)p_\delta + i}, \ i = 1, \ldots, p_\delta; \ j = 1, \ldots, n \\ P_K(j + n(i-1); \cdot) &= e^T_{(j-1)p_\eta + i}, \ i = 1, \ldots, p_\eta; \ j = 1, \ldots, n \end{aligned}$$

Integrated model formulation (continued)

Equivalently (3) can be represented

$$\begin{pmatrix}\hat v\\ \hat u\end{pmatrix} \Bigg| \begin{pmatrix} v \\ u(\theta)\end{pmatrix}, \lambda_y \sim \mathsf{N}\left(\begin{pmatrix} v \\ u(\theta)\end{pmatrix}, (\lambda_y B^T W_y B)^{-1}\right), \quad \lambda_y \sim \Gamma(a'_y, b'_y)$$

with

$$\begin{aligned}
n_y &= n_{y_1} + \cdots + n_{y_n}, \quad \text{the total number of experimental data points} \\
\begin{pmatrix}\hat v\\ \hat u\end{pmatrix} &= (B^T W_y B)^{-1} B^T W_y y \\
a'_y &= a_y + \tfrac{1}{2}[n_y - n(p_\delta + p_\eta)] \\
b'_y &= b_y + \frac{1}{2}\left[\left(y - B\begin{pmatrix}\hat v\\ \hat u\end{pmatrix}\right)^T W_y \left(y - B\begin{pmatrix}\hat v\\ \hat u\end{pmatrix}\right)\right]
\end{aligned}$$

	dimension reduction	
model	simulator	data and discrep
standard	$n_\eta \cdot m$	n_y
basis	$p_\eta \cdot m$	$n \cdot (p_\delta + p_\eta)$

Basis approach particularly efficient when n_η and n_y are large.

Marginal likelihood

The (marginal) likelihood $L(\hat{v}, \hat{u}, \hat{w} | \lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta)$ has the form

$$\begin{pmatrix} \hat{v} \\ \hat{u} \\ \hat{w} \end{pmatrix} \sim \mathsf{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Lambda_y^{-1} & & 0 \\ & & 0 \\ 0 & 0 & \Lambda_\eta^{-1} \end{pmatrix} + \begin{pmatrix} \Sigma_v & 0 & 0 \\ 0 & & \\ 0 & \multicolumn{2}{c}{\Sigma_{uw}} \end{pmatrix} \right)$$

where

$$\begin{aligned}
\Lambda_y &= \lambda_y B^T W_y B \\
\Lambda_\eta &= \lambda_\eta K^T K \\
\Sigma_v &= \lambda_v^{-1} I_{p_\eta} \otimes R(x, x; \rho_v) \\
R(x, x; \rho_v) &= n \times n \text{ correlation matrix from applying (2) to the conditions} \\
& \ x_1, \ldots, x_n \text{ corresponding the the } n \text{ experiments.} \\
\Sigma_{uw} &=
\end{aligned}$$

$$\begin{pmatrix}
\lambda_{w1}^{-1} R((x,\theta),(x,\theta);\rho_{w1}) & 0 & 0 & \lambda_{w1}^{-1} R((x,\theta),(x^*,\theta^*);\rho_{w1}) & 0 & 0 \\
0 & \ddots & 0 & 0 & \ddots & 0 \\
0 & 0 & \lambda_{wp_\eta}^{-1} R((x,\theta),(x,\theta);\rho_{wp_\eta}) & 0 & 0 & \lambda_{wp_\eta}^{-1} R((x,\theta),(x^*,\theta^*);\rho_{wp_\eta}) \\
\lambda_{w1}^{-1} R((x^*,\theta^*),(x,\theta);\rho_{w1}) & 0 & 0 & \lambda_{w1}^{-1} R((x^*,\theta^*),(x^*,\theta^*);\rho_{w1}) & 0 & 0 \\
0 & \ddots & 0 & 0 & \ddots & 0 \\
0 & 0 & \lambda_{wp_\eta}^{-1} R((x^*,\theta^*),(x,\theta);\rho_{wp_\eta}) & 0 & 0 & \lambda_{wp_\eta}^{-1} R((x^*,\theta^*),(x^*,\theta^*);\rho_{wp_\eta})
\end{pmatrix}$$

Permutation of Σ_{uw} is block diagonal $\Rightarrow$ can speed up computations.

Only off diagonal blocks of Σ_{uw} depend on θ.

Posterior distribution

Likelihood: $L(\hat{v}, \hat{u}, \hat{w} | \lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta)$

Prior: $\pi(\lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta)$

$\Rightarrow$ Posterior:

$$\begin{aligned}\pi(\lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta | \hat{v}, \hat{u}, \hat{w}) \;\propto\; & L(\hat{v}, \hat{u}, \hat{w} | \lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta) \times \\ & \pi(\lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta)\end{aligned}$$

Posterior exploration via MCMC

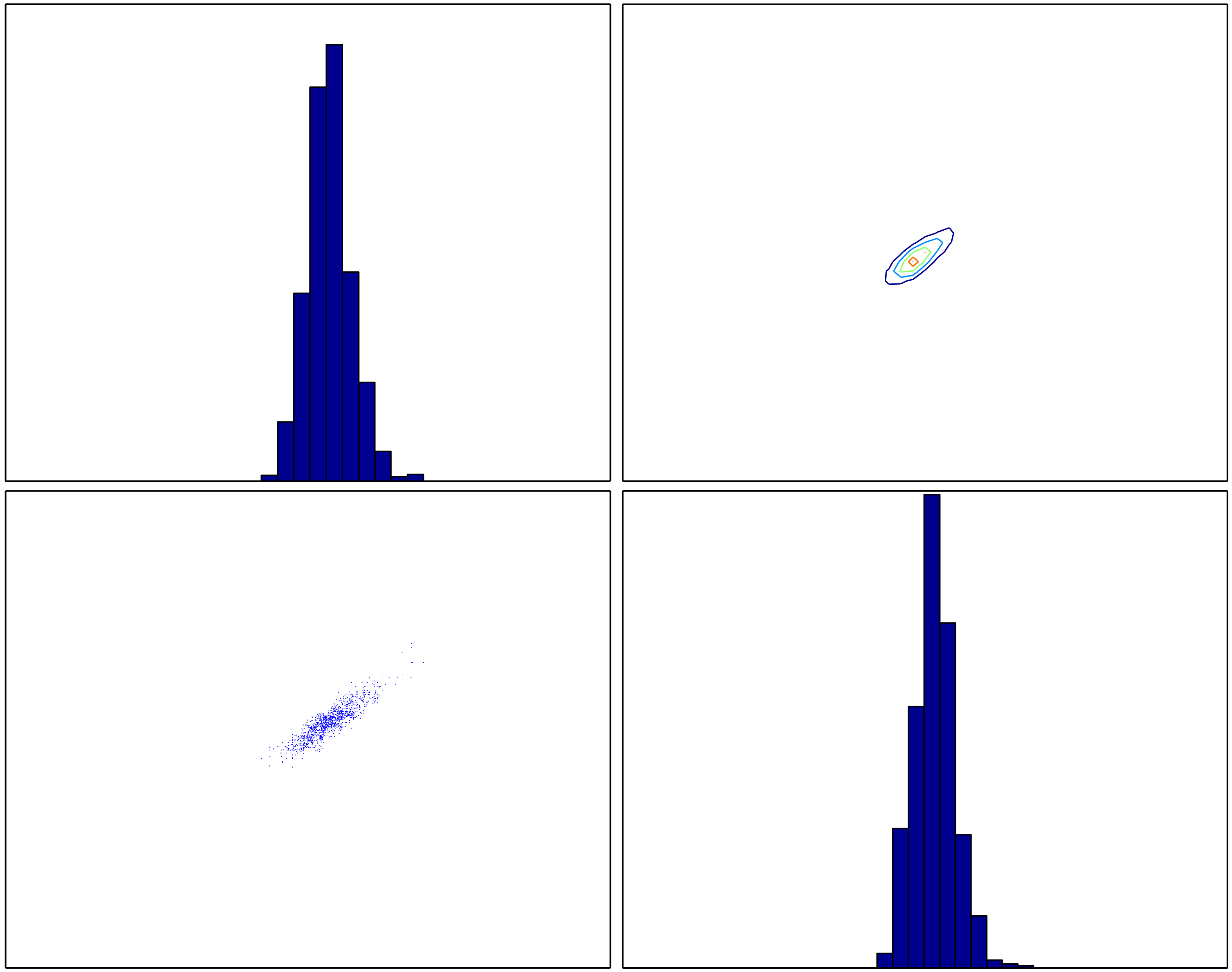
Can take advantage of structure and sparcity to speed up sampling.

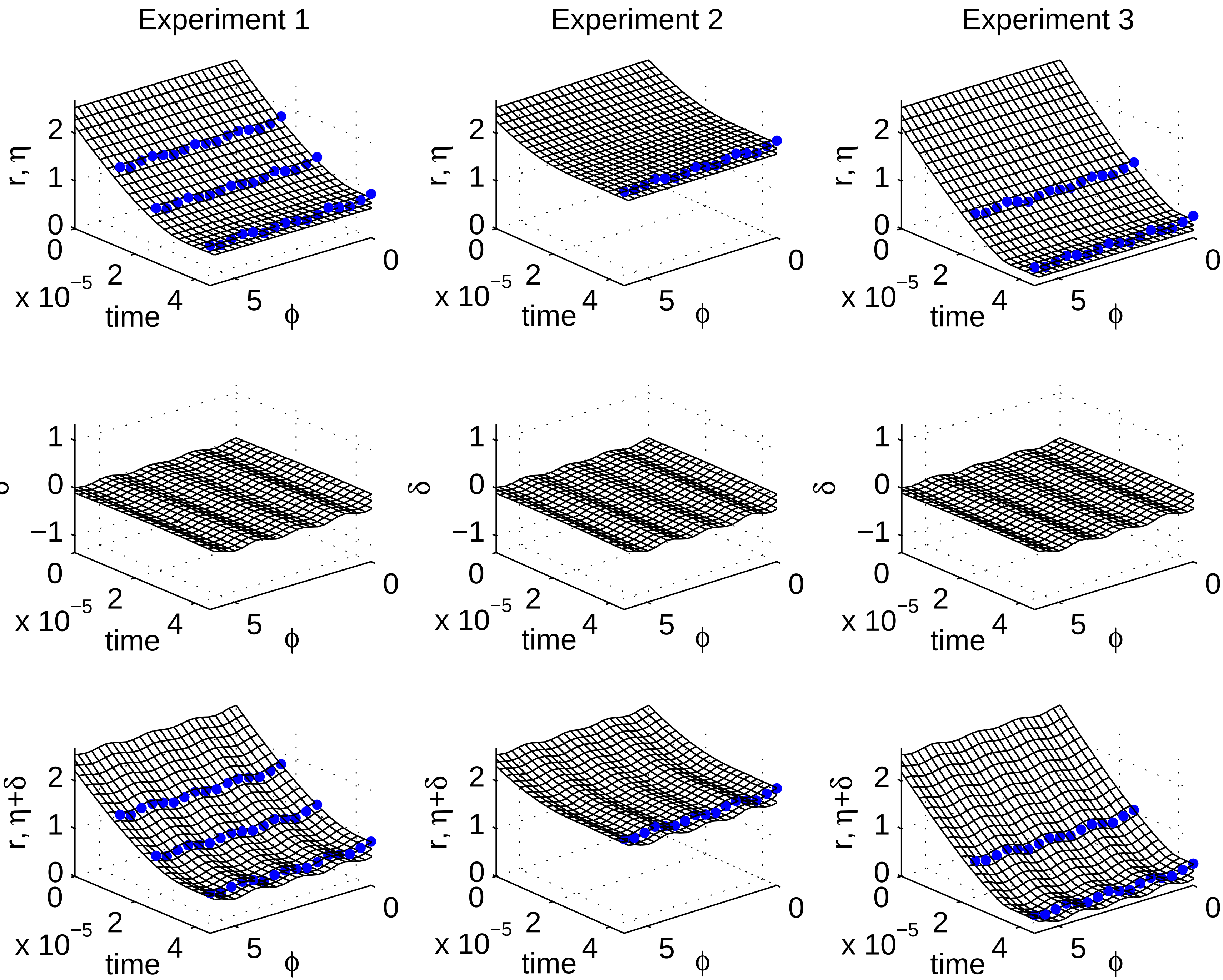
A useful approximation to speed up posterior evaluation:

$$\begin{aligned}&\pi(\lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta | \hat{v}, \hat{u}, \hat{w}) \\ &\propto\; L(\hat{w} | \lambda_\eta, \lambda_w, \rho_w) \times \pi(\lambda_\eta, \lambda_w, \rho_w) \times \\ &\quad\; L(\hat{v}, \hat{u} | \lambda_\eta, \lambda_w, \rho_w, \lambda_y, \lambda_v, \rho_v, \theta) \times \pi(\lambda_y, \lambda_v, \rho_v, \theta)\end{aligned}$$

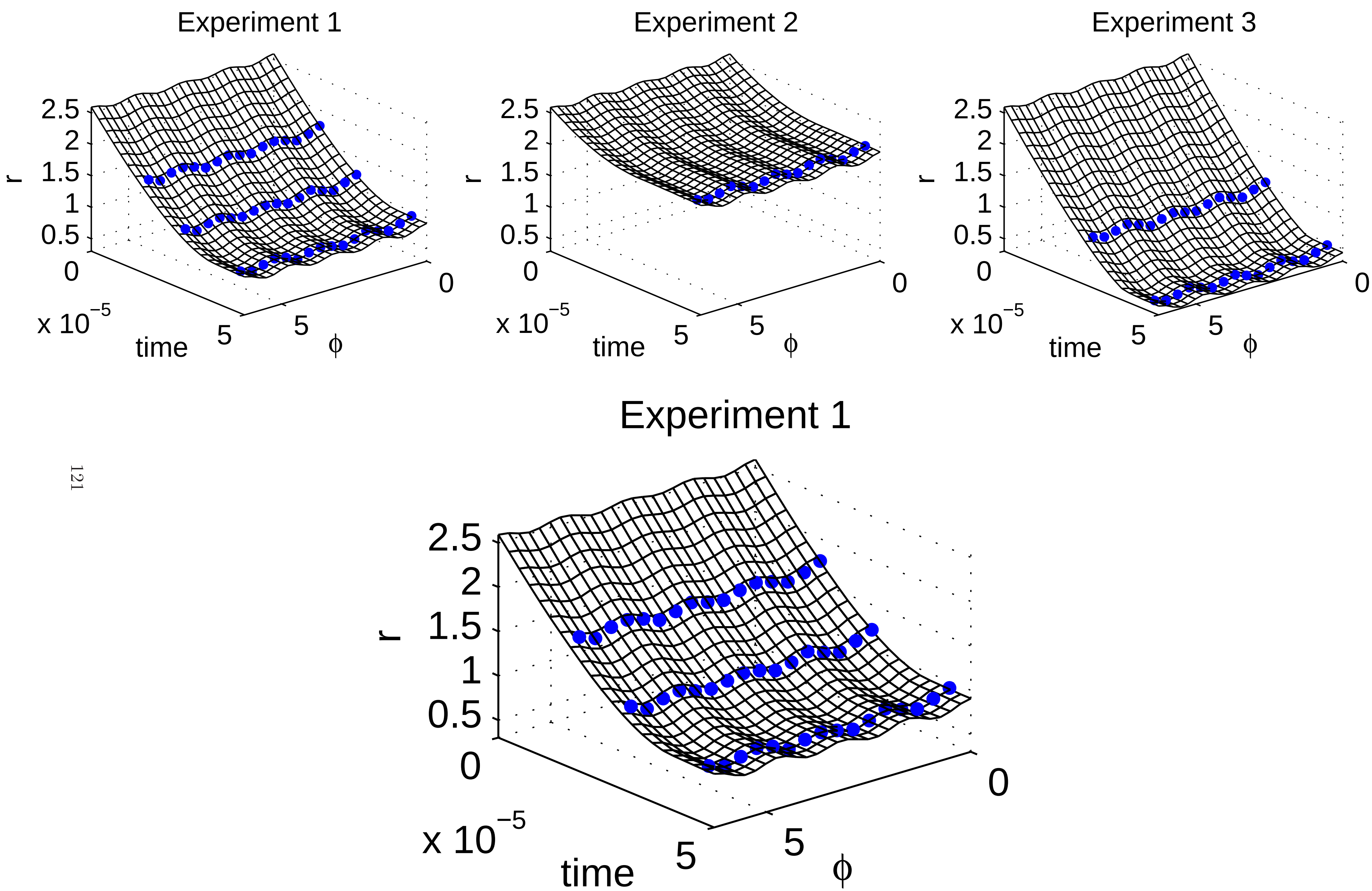
In this approximation, experimental data is not used to inform about parameters λ_η, λ_w, ρ_w which govern the simulator process $\eta(x, \theta)$.

Posterior distribution of model parameters (θ_1, θ_2)

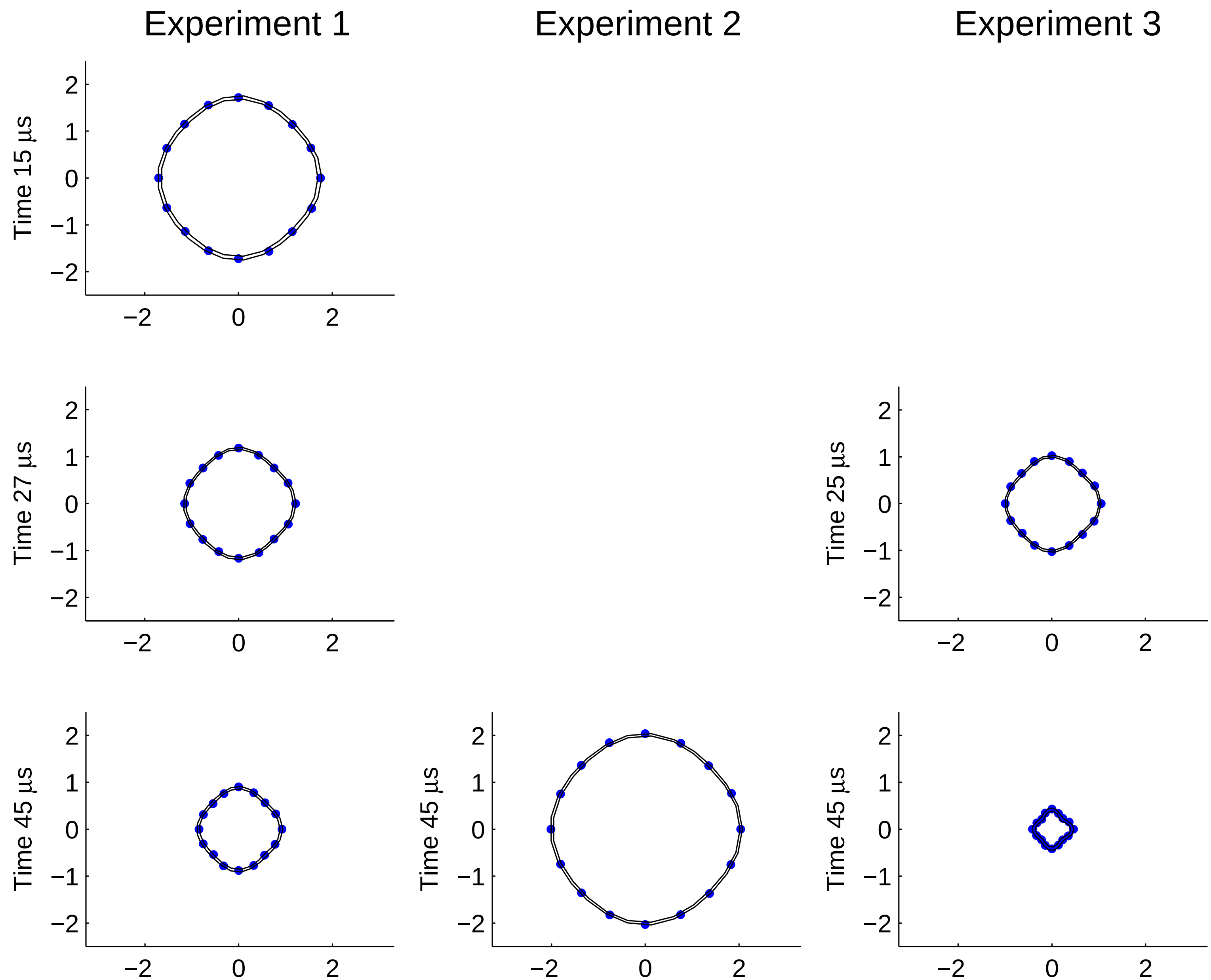



Experiment 1
Experiment 2
Experiment 3
r, η
δ
r, η+δ
time
φ
x 10−5

Posterior prediction for implosion in each experiment



90% prediction intervals for implosions at exposure times



Predictions from separate analyses which hold data from the experiment being predicted.

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