Calibration and uncertainty quantification using multivariate simulator output

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A framework for model assessment, prediction and calibration using simulations and experimental data

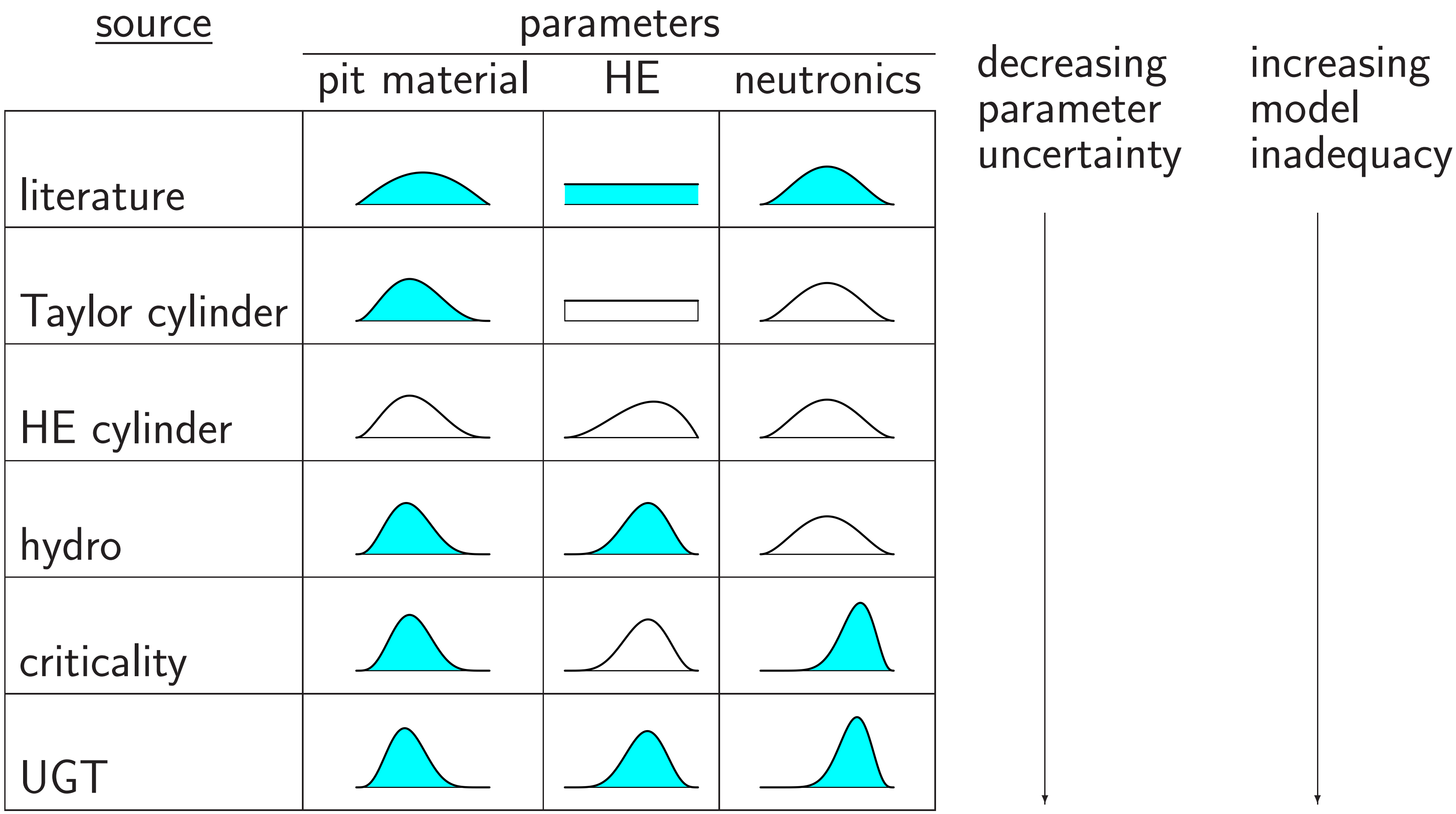
Uncertainty quantification accounts for:

- uncertainty in experimental observations;
- model parameters – first principle and phenomenological parameters;
- inadequacy in physics simulation models;
- multiple sources of data

Byproducts of this approach:

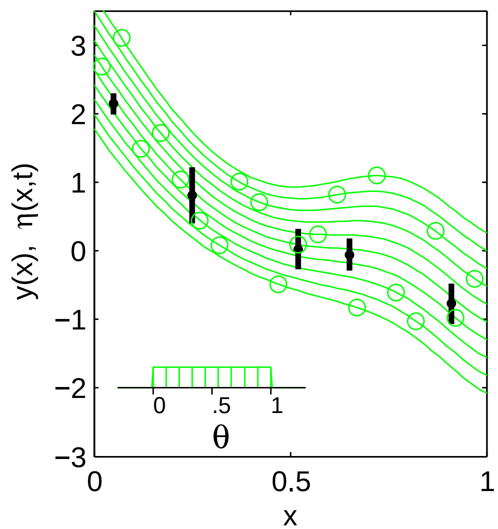
- predictions (with uncertainties);
- can assess value of different sources of experimental data
- determine which parameters are key drivers in uncertainty
- assessment of simulator adequacy.

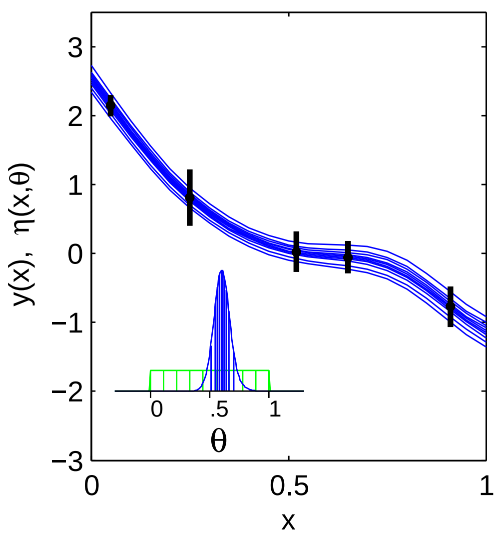
Calibrating to multiple sources of data



- conditioning on more experiments $\Rightarrow$ less parametric uncertainty
- prediction uncertainty becomes more affected by model inadequacies

Statistical formulation for combining simulations and experimental data for forecasting, calibration and uncertainty quantification





x	model or system inputs
θ	model 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 Gaussian process to model $\eta(\cdot,\cdot)$
$y(x)$	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

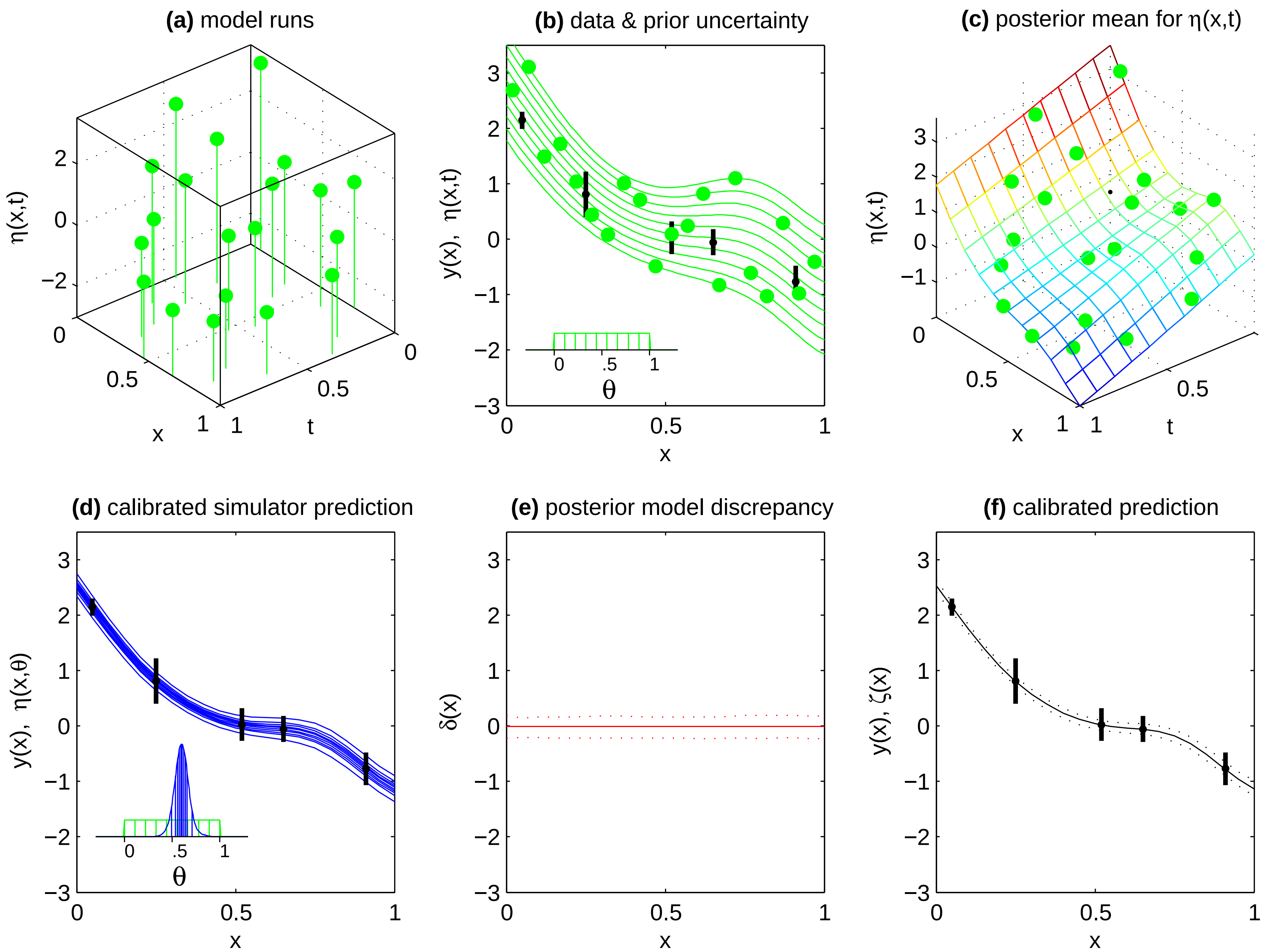
$$\begin{aligned} y(x) &= \zeta(x) + e(x) \\ y(x) &= \eta(x,\theta) + \delta(x) + e(x) \end{aligned}$$

θ, $\eta(\cdot,\cdot)$, and $\delta(\cdot)$ unknowns to be estimated.

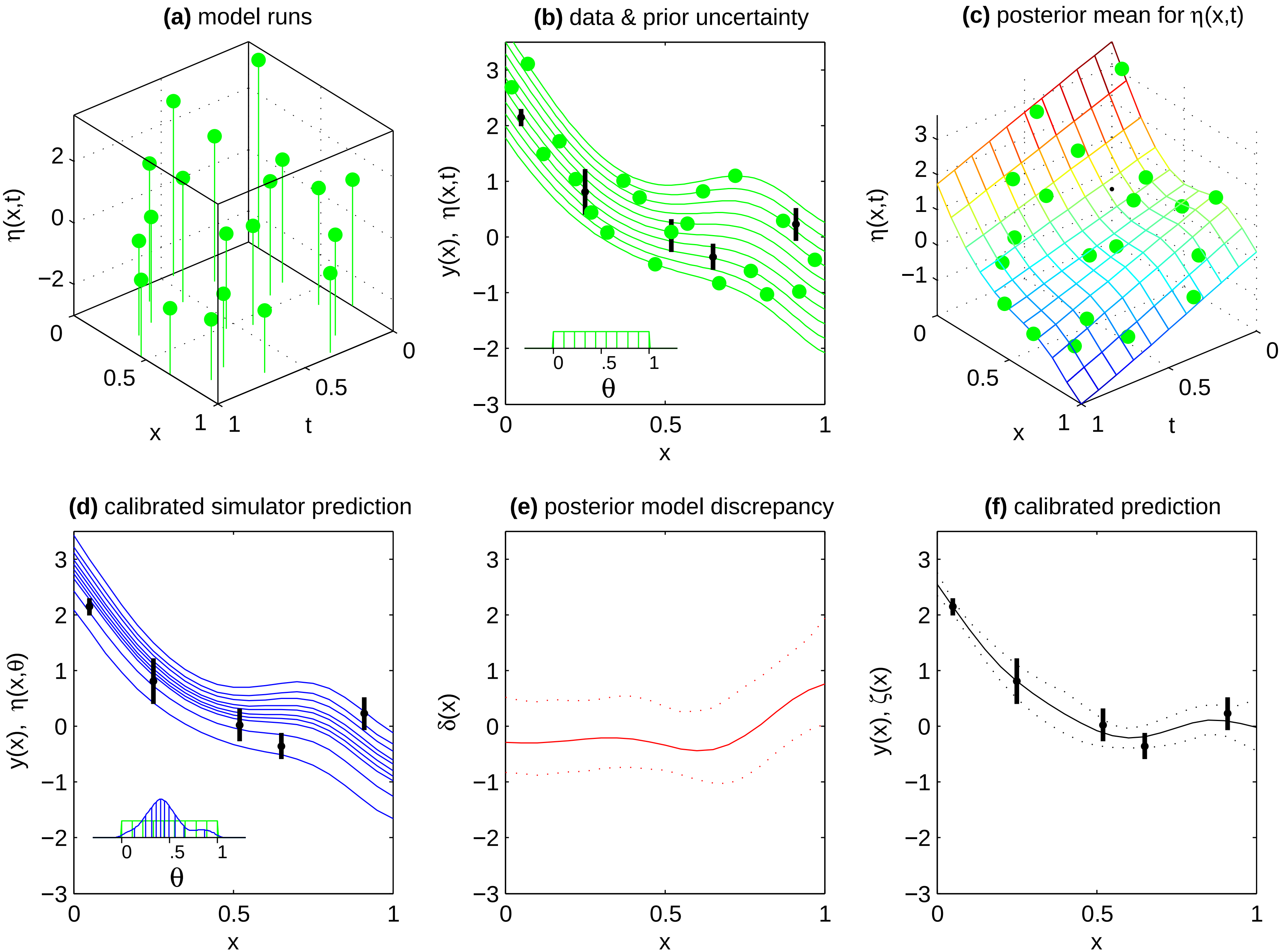
Standard Bayesian estimation gives:

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

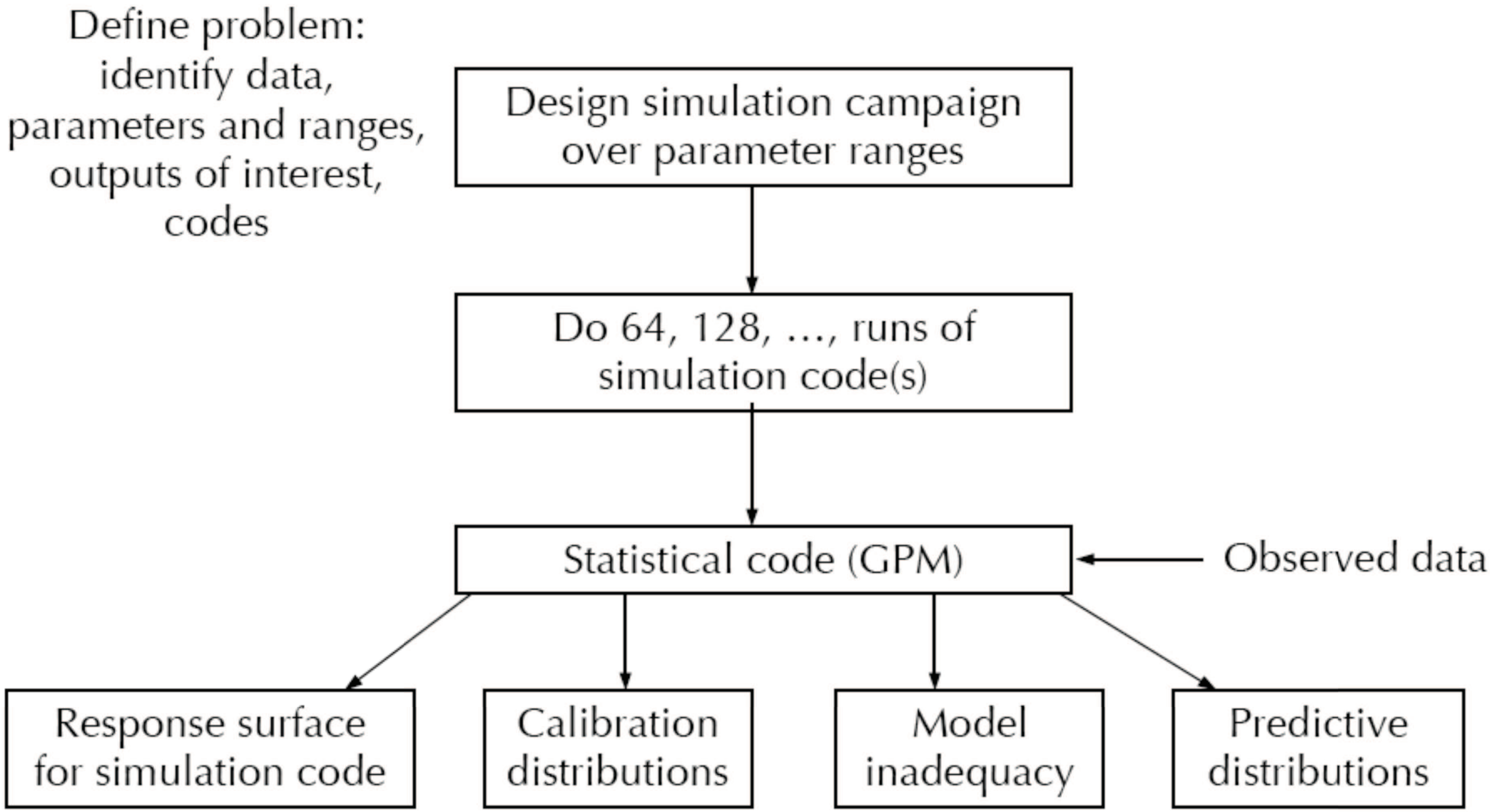
Basic elements of the model and analysis



Basic elements of model and analysis



Basic recipe



A simple example

input condition		calibration parameters			exprimental outputs				
x_1	x_2	θ_1	θ_2	θ_3	y_1	y_2	y_3	y_4	y_5

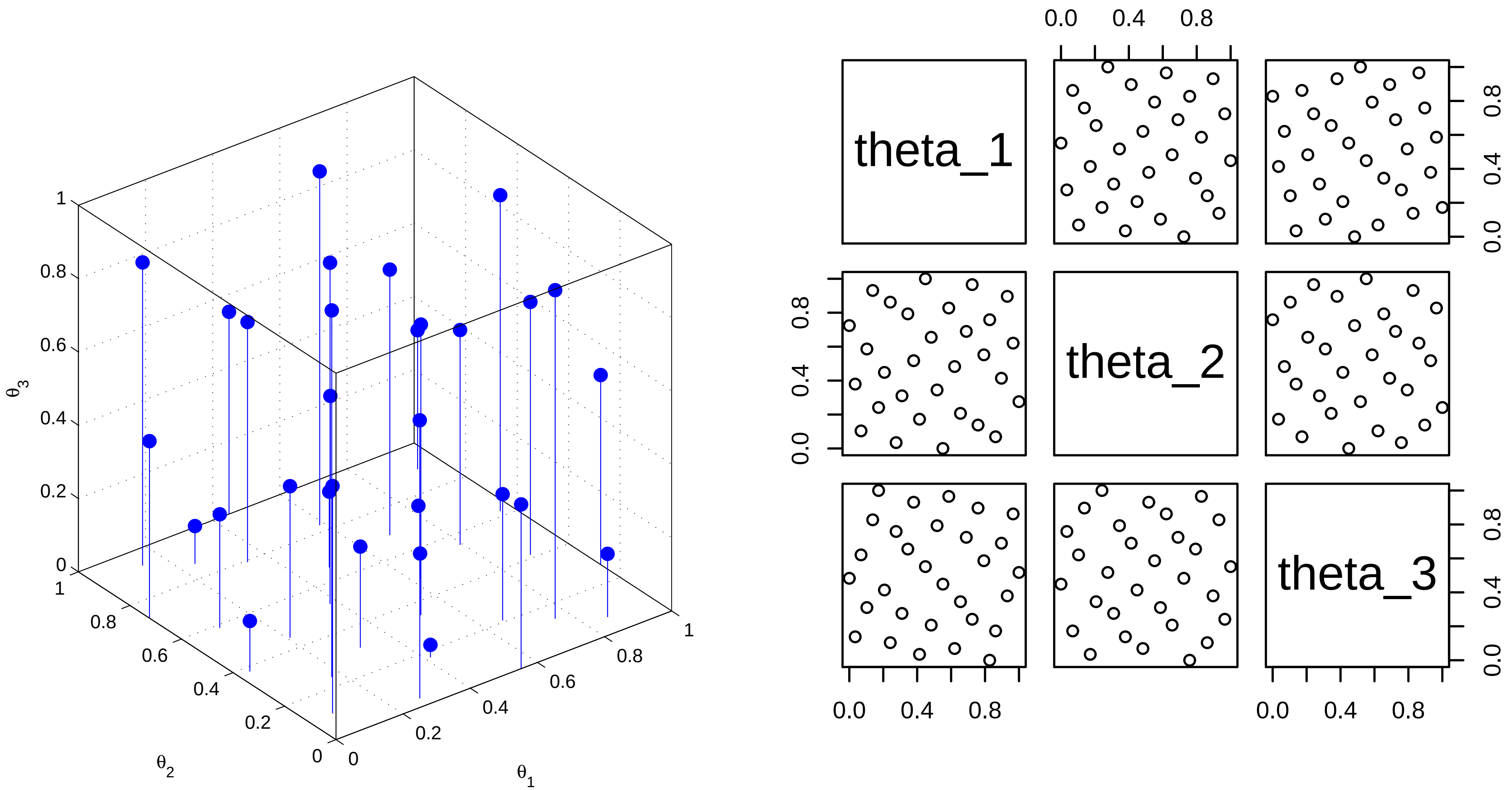
- 6 experiments at $(x_1, x_2) = \{(0,0), (.2,.4), (.4,.4), (.4,.4), (.6,1.0), (1.0,.9)\}$
- Run 30 simulations for each experimental configuration: $\Rightarrow 30 \times 5$ simulations
- Each experimental observation has noise and replicate variability
- Model

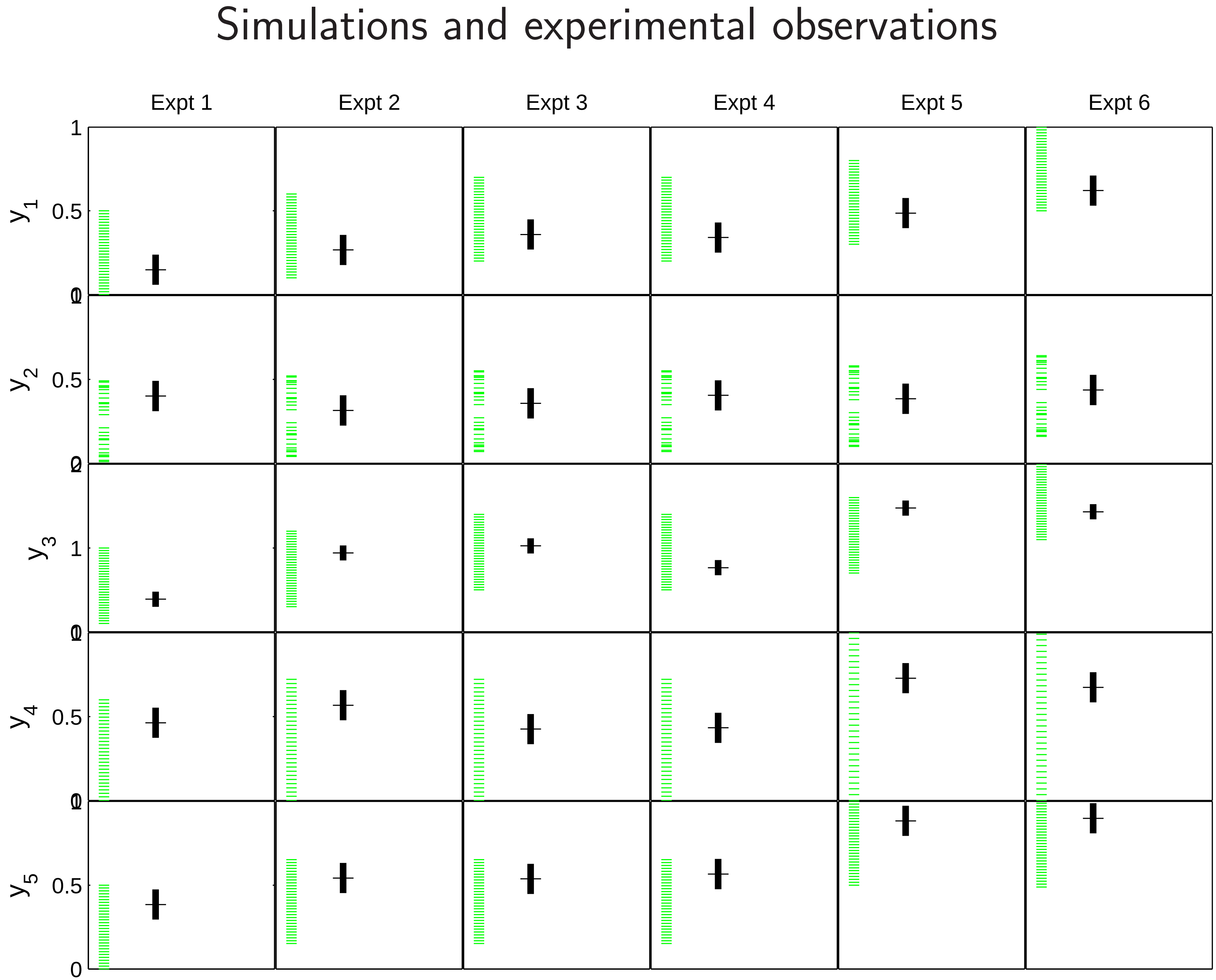
$$y(x) = \eta(x, \theta) + \delta(x) + \epsilon(x)$$

- Calibration: finding range of θ consistent with experimental data
- Prediction: best prediction and uncertainty for new $y(x)$.

Simulation campaign design

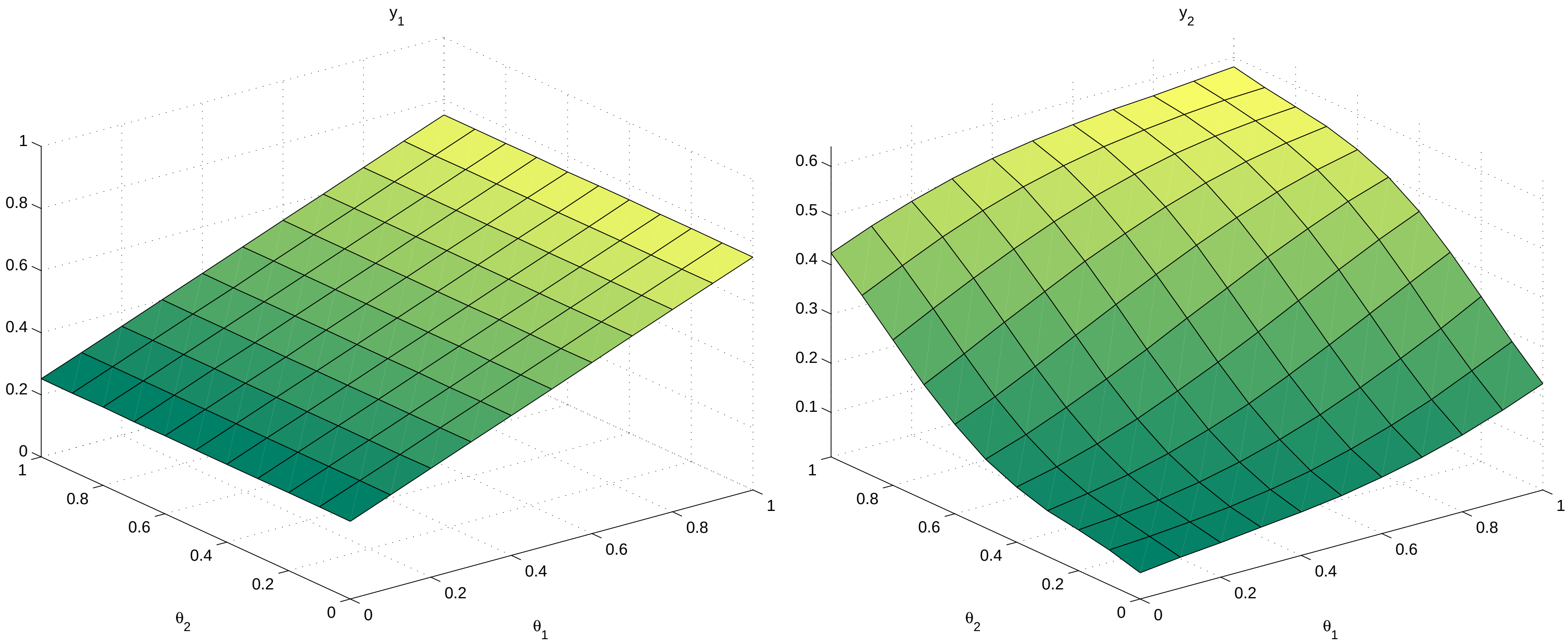
30 point, space-filling, symmetric Latin hypercube design





Simulations and experimental observations
Expt 1
Expt 2
Expt 3
Expt 4
Expt 5
Expt 6
y1
y2
y3
y4
y5
1
0.5
0
2
1
0

Modeling simulator response for experiment 1.

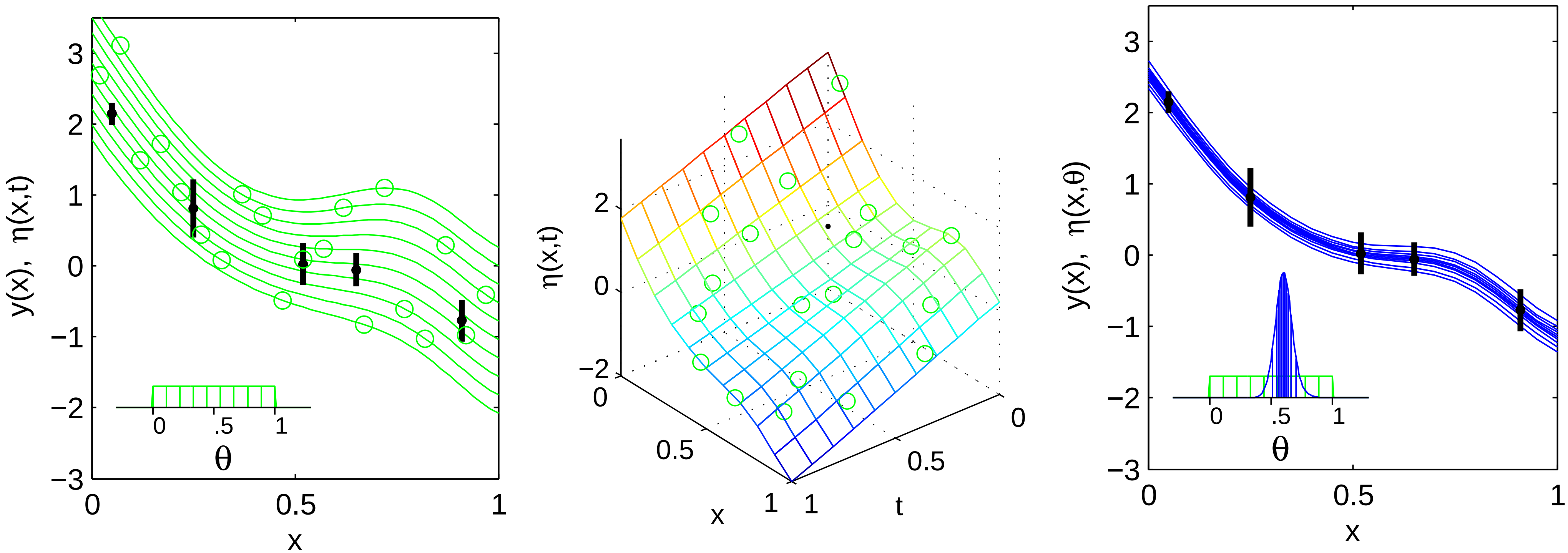


• predicted response of outputs 1 & 2 as a function of θ_1 and θ_2; (x_1, x_2, θ_3) held fixed at .5.

• Smooth and predictable response $\Rightarrow$ fewer sims required.

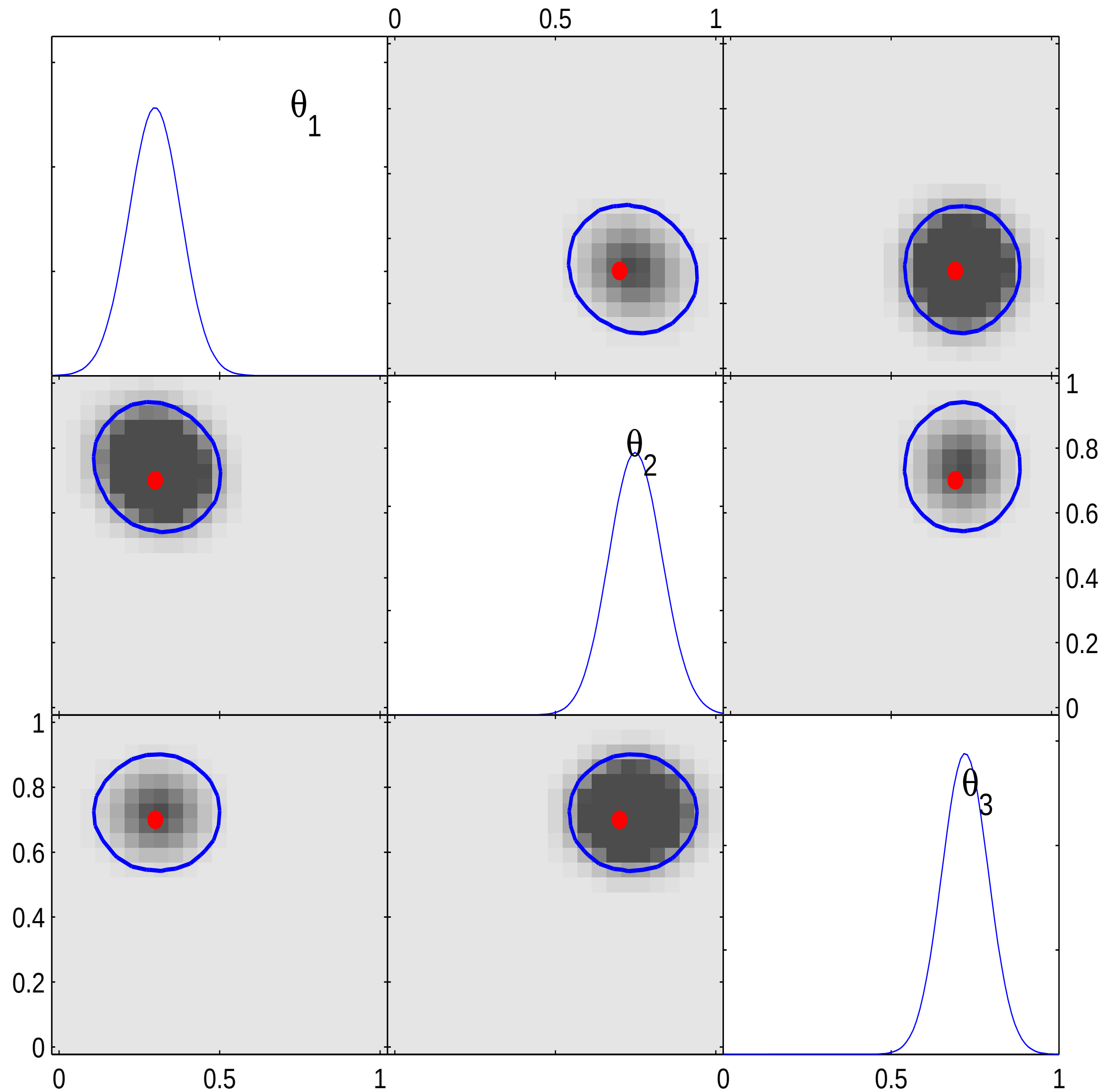
• If response is rough and unpredictable, MC-based approach may be required $\Rightarrow$ many sims will be needed.

Use response surface to determine plausible θ's

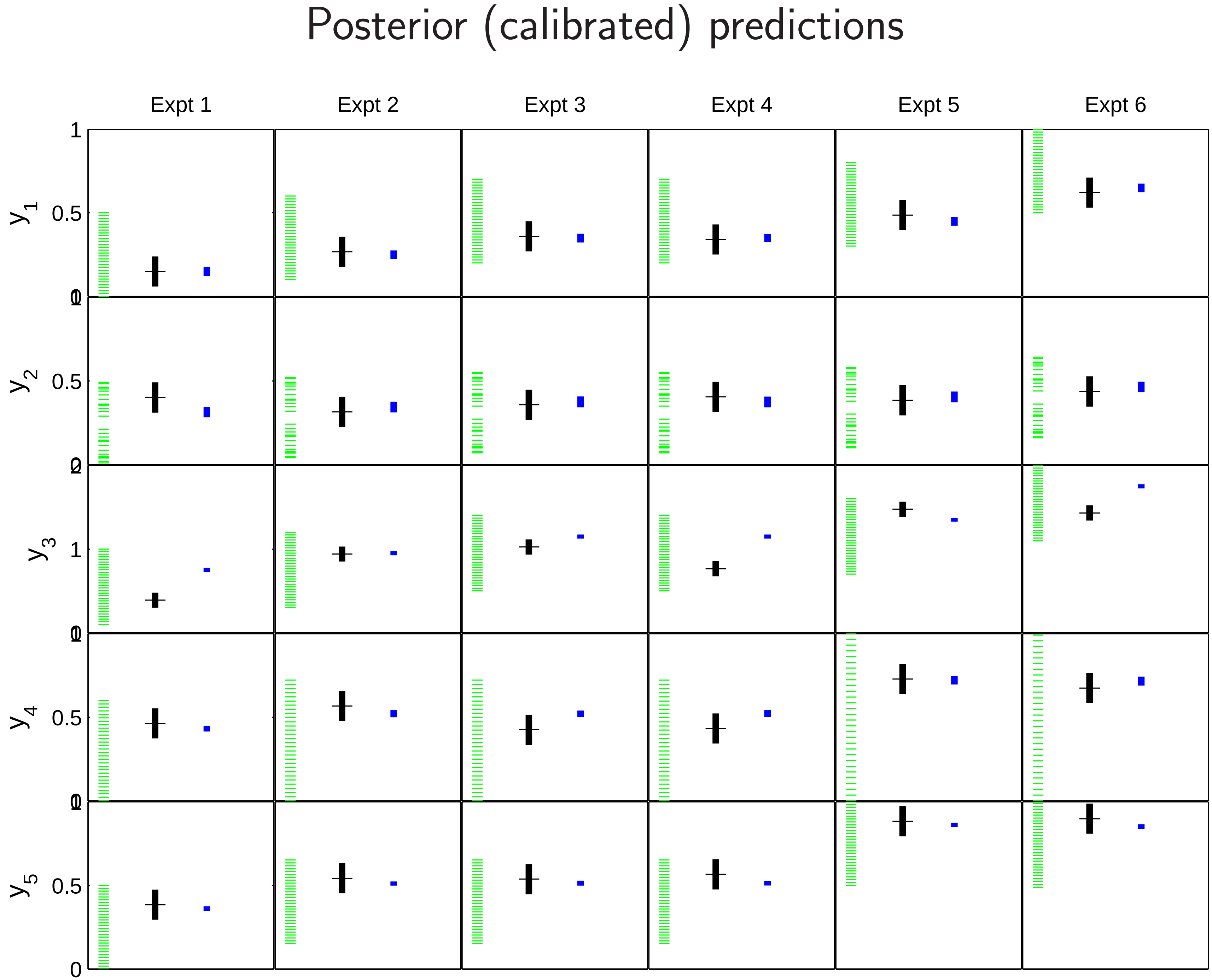


- Response surface allows the posterior distribution for the calibration parameters θ to be estimated.

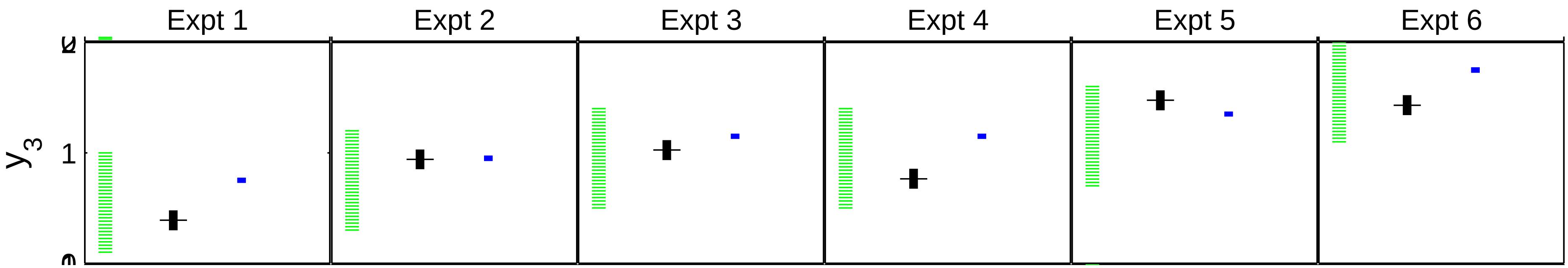
Posterior distribution for calibration parameters



- Posterior distribution gives 3-d description of plausible θ's.
- uncertainty in $\theta \Rightarrow$ some prediction uncertainty (but not all).


Posterior (calibrated) predictions
Expt 1
Expt 2
Expt 3
Expt 4
Expt 5
Expt 6
y1
y2
y3
y4
y5
1
0.5
0
2
1
0
0.5
0
0.5
0
0.5
0

Accounting for inadequacies in the simulation model



- No value of θ matches the y_3 data.
- Calibration matches all other outputs fairly well.
- Must account for this in calibration and in prediction uncertainty.

– ignoring this leads to overly optimistic prediction uncertainties, and poor calibrations

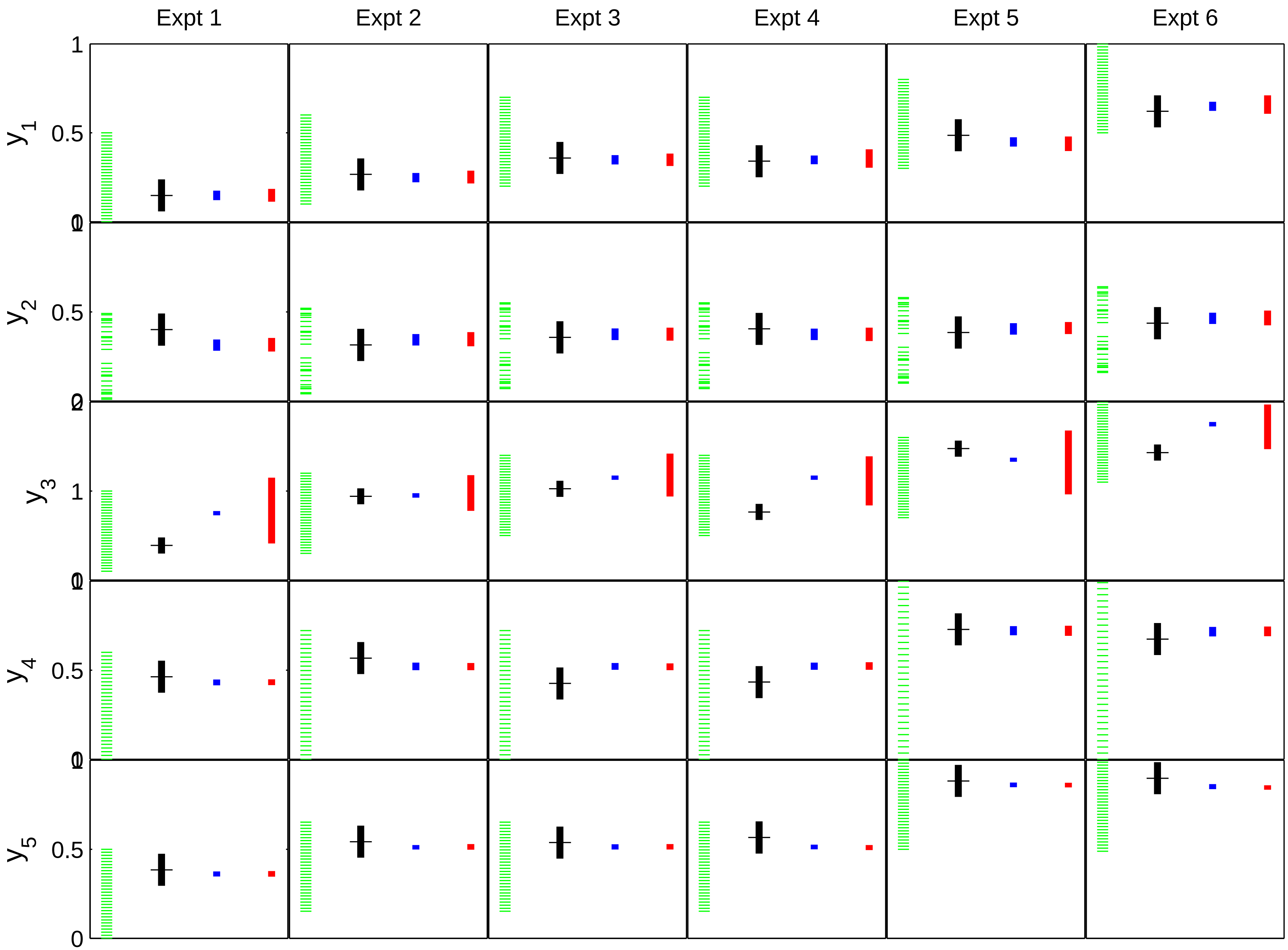
- Potential discrepancy models: Independent terms:

$$\delta_j(x) \sim N(0, \sigma_j^2),\ j = 1, \ldots, 5$$

Discrepancy depends on input conditions (x_1, x_2):

$$\delta_j(x) \sim GP(0, R(\cdot,\cdot))$$

“Holdout” predictions (include model inadequacy)



Some (interim) summary points

- Not V&V – certification is about making the best of current models (results will likely feed back into V&V needs).
- Need a variet of experiments (separate effects, pinshots, core punch, scaled hydros, NTS) to get a robust calibration. This requires a model that can simulate a wide range of experiments.
- Robust calibration may not be enough – some model inadequacy is likely to persist.
- Need carefully chosen hold out data to inform about model discrepancy $\delta(\cdot)$. Holdouts should be extrapolations similar to the extrapolation made in certification.

  $$\text{training/calibration data} \rightarrow \pi(\theta, \delta | y, \eta)$$

  Holdout data to test predictions and refine discrepancy.