Successful Calibration: A Practitioners Guide

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Outline

- Introduction
- Statistical Framework
- Model Calibration
- Simulation Study
- Results
- Summary

Introduction

- Computer Models:
  - Simulate physical phenomena
  - Complex mathematical models
  - Deterministic output
  - Computationally expensive
- Using the computer code:
  - Accurate estimate of the calibration parameter
  - Predictions of the physical system

Available Data

- Computer model, computationally inefficient
- Computer Model Data $y_c = \eta(x, t)$
  - x is controllable inputs in the physical system
  - t uncontrollable calibration parameters
  - m runs performed on the code
- Physical Data $y_f(x) = \zeta(x) + \epsilon(x)$
  - subject to random error
  - x controllable inputs
  - n runs of the physical system

Statistical Model

- Kennedy and O'Hagan (2001) model for calibration
- Statistical Model for Physical Data:

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

- $\eta(x, \theta)$ computer code
- θ true value of the calibration parameter
- $\delta(x)$ discrepancy function
- ϵ is normal random random error
- Model $\eta(x, \theta)$ and $\delta(x)$ as independent Gaussian processes

Statistical Model

- Model the common portion $\eta(x, \theta)$ as a realization of a random function
- Let $\eta(x, \theta) = \mu + Z_\eta(x, \theta)$
  - μ: overall mean
  - $Z_\eta(x^*, t^*)$: Gaussian stochastic process indexed by (x^*, t^*)

Gaussian Stochastic Process

- Assume $Z_\eta(x^*, t^*)$ is normally distributed
  - Mean zero
  - Gaussian Covariance function $\sigma_\eta^2 R_\eta$
  - Where

$$R_\eta((x^*, t^*), (x', t'))$$
$$= \exp\left\{ -\sum_{j=1}^{d} \beta_j |x_j^* - x_j'|^2 - \sum_{j=d+1}^{q} \beta_j |t_j^* - t_j'|^2 \right\}$$

with $\beta_j \geq 0$

Model Discrepancy

- Model $\delta(x)$ as the realization of a random function
  - δ is a Gaussian process (GP) independent of η
  - Mean zero
  - Covariance function $\sigma_\delta^2 R_\delta$

Statistical Model

- Vector of Observations $\mathbf{y} = (\mathbf{y}_F^T, \mathbf{y}_C^T)^T$
- Inputs $(\boldsymbol{x}_1, \boldsymbol{\theta}), \ldots, (\boldsymbol{x}_n, \boldsymbol{\theta})$ and $(\boldsymbol{x}_1^*, \mathbf{t}_1^*), \ldots, (\boldsymbol{x}_m^*, \mathbf{t}_m^*)$
- Likelihood

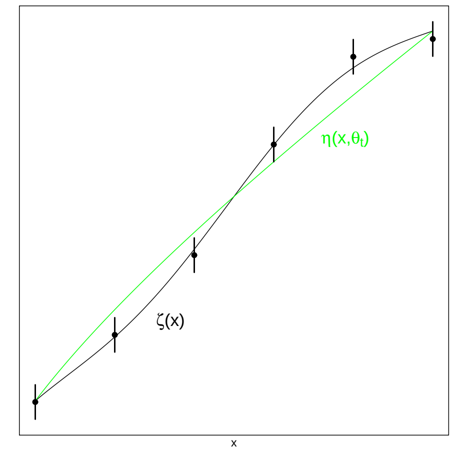
$$L(\mathbf{y}) \propto |\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{y} - \mu\mathbf{1})^T \Sigma^{-1} (\mathbf{y} - \mu\mathbf{1})\right\}$$

where

$$\Sigma = \Sigma_\eta + \begin{pmatrix} \Sigma_\delta + \Sigma_\varepsilon & 0 \\ 0 & 0 \end{pmatrix}$$

- Full MCMC to estimate the parameters

Statistical Framework



- $y_f(x) = \zeta(x) + \epsilon(x)$

$\leftrightarrow$ x: known system inputs

$\leftrightarrow$ $y_f(x)$: experimental data

$\leftarrow$ $\zeta(x)$: unobserved system response

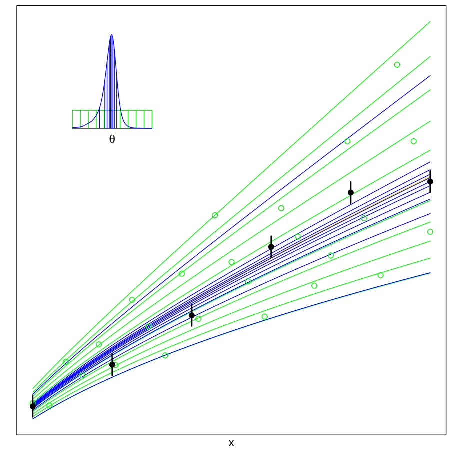
$\leftarrow$ $\epsilon(x)$: experimental error model

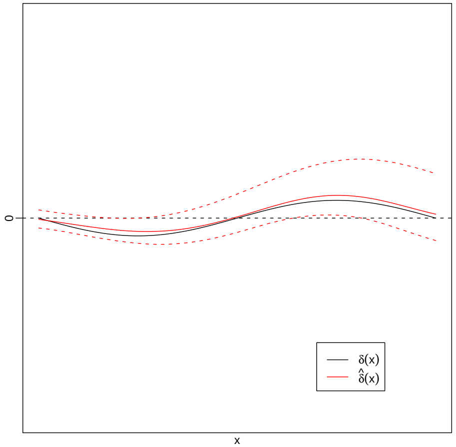
- $\zeta(x) = \eta(x, \theta) + \delta(x)$

$\rightarrow$ θ: unknown calibration inputs

$\rightarrow$ $\eta(x, \theta)$: computer model

$\rightarrow$ $\delta(x)$: model discrepancy

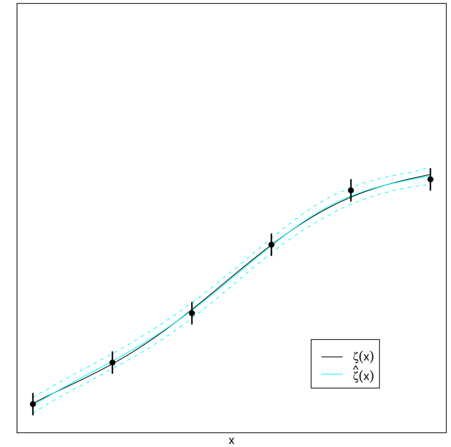




$\leftarrow$ predicted $\delta(x)$

$\rightarrow$ predicted $\zeta(x)$

$\leftrightarrow$ 95/5 uncertainty bounds



Problem

- Estimation of the calibration parameter
  - Estimate of θ may not match the true value
  - Hard to assess if the estimate is correct
  - In some situations accurate estimate is desired
- Goals of the Simulation Study:
  - Develop a test suit of problems to assess the estimation of θ
  - Test suit should cover situations that arise in practice
  - Develop tests that can be used to assess if the true value was estimated.

Test Suite of Problems

- Physical Data: $y_f(x) = \zeta(x) + \epsilon$
  - Scalar response $y_f(x)$
  - One input variable x
  - Added component of random variation
- Computer Data $y_c = \eta(x, \theta)$
  - Scalar response y_c
  - One controllable input x
  - One calibration parameter θ

Outline of Data

- Functions for η, δ and ϵ
  - $\eta(x, \theta)$: unconditional realization of a GP
  - $\delta(x)$: unconditional realization of a GP independent of $\eta(x, \theta)$
  - ϵ is independent Gaussian errors
- Using data that comes from a GP we do not have uncertainty due to using the incorrect model
- Allows a more accurate picture of what factors may affect calibration

Factors to Control

- Factors that may affect calibration
  - Complexity of $\eta(x, \theta)$ and $\delta(x)$
  - Sensitivity of main effects and interaction in $\eta(x, \theta)$
  - Variation of the responses for η, δ and ϵ
  - Ratio of the variability between η and δ
  - Similarity of $\eta(x, \theta)$ and $\delta(x)$
- All of these will be controlled in a systematic manner for the simulation study

Data Generation

- Generation of $\eta(x, \theta)$
  - Generate a mean zero, unit variance GP on a 26×26 grid
  - wee little bit on the diagonal for numerical stability
  - Control the roughness of parameters as $\beta = 0.5$ or 2 in the correlation function

$$\exp\left\{\sum_{i=1}^{d} -\beta_i (x_i - x_i')^2 + \sum_{j=1}^{q} -\beta_{j+d} (t_j - t_j')^2\right\}$$

  - Let $\mathbf{y}_c$ be the vector of $26 \cdot 26 = 676$ responses generated on the grid.

Data Generation, Cont.

- Controlling Sensitivity and Variance of y_c
  - ANOVA decomposition of y_c
  - Compute main effects and interactions
  - Control $Var(\mathbf{y}_c) = 20$
  - Scale x, θ and $x\theta$ to control sensitivity
  - Percentage contribution to the total variance of

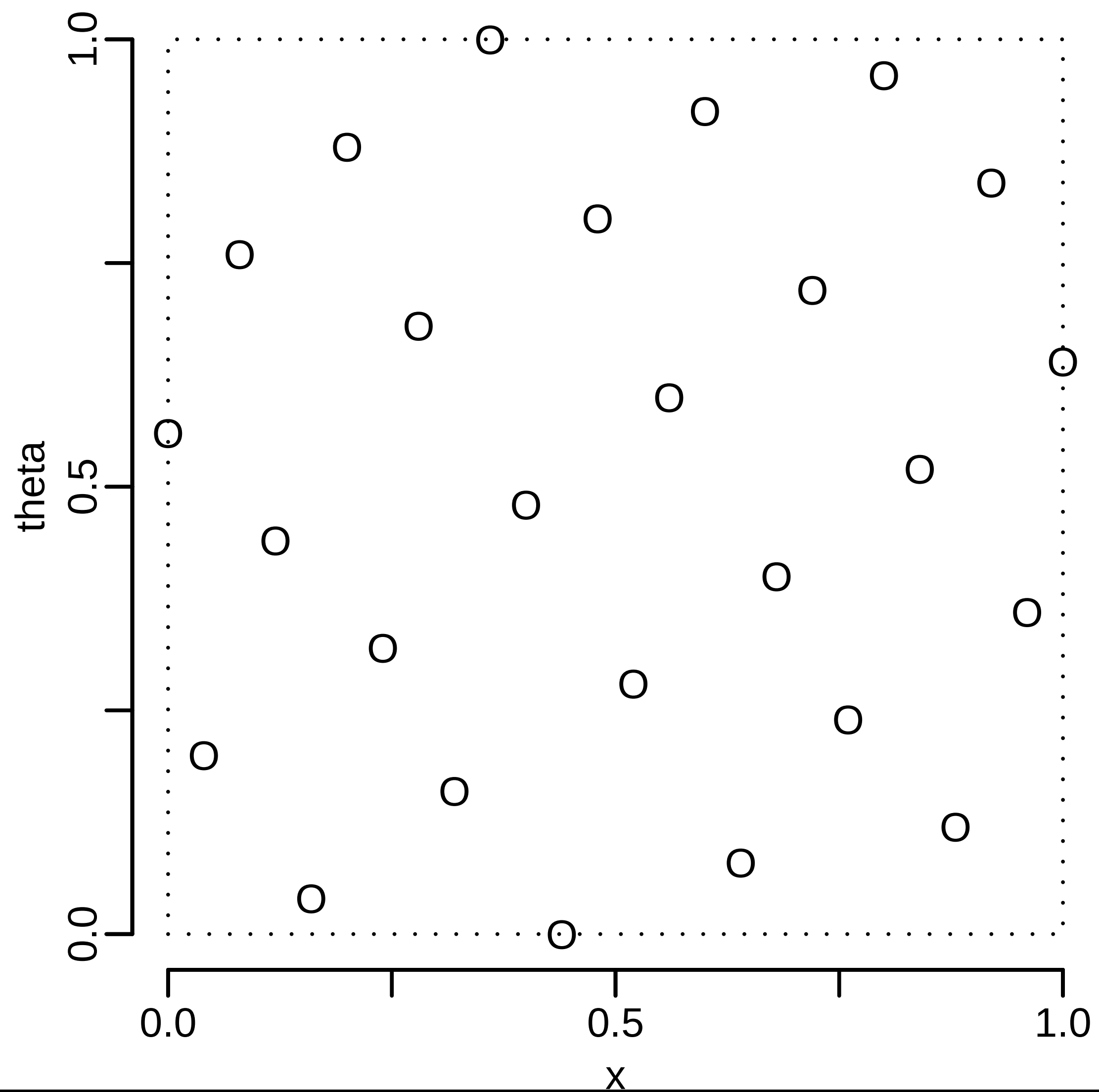
$$(x, \theta, x\theta)$$

    is $(0.6, 0.4, 0)$ and $(0.5, 0.25, 0.25)$
  - Add scaled effects of x, θ and $x\theta$ together

Data Generation, Cont.

- New y_c is sum of the effects of x,θ and $x\theta$
- Allows us to control the properties of y_c
- Code Runs:
  - Obtain a 26-run Maxi-min Latin hypercube
  - Collect y values according to the design
  - Use these values for the computer model data
  - Use remaining observations for assessing prediction accuracy

Design



Data Generation

- Discrepancy Data: $\delta(x)$
  - Generate a mean zero unit variance GP on a grid of 26 x values
  - Control the complexity by adjusting the roughness parameter β
  - Control the similarity measure (discussed below)
- Physical Data: $\zeta(x) + \epsilon(x)$
  - $\zeta(x) = \eta(x, \theta = 0.48) + \delta(x)$
  - $\epsilon \sim N(0, \sigma_\epsilon^2)$, $\sigma_\epsilon^2 = 0.1$ or 1
  - $x = \{0, 0.2, 0.4, 0.6, 0.8, 1.0\}$ used for the physical sites
  - Each point is replicated resulting in 12 runs

Similarity Measure

- For a fixed value of θ in the computer model η is a function of x
- The collection of all functions for any value of θ is the family of computer model curves
- If the discrepancy function is similar to one of these curves calibration may be more challenging
- The angle between the discrepancy and the family of computer model curves measures the similarity

Similarity Measure

- Let δ be the 26×1 vector of discrepancy observations
- Let C be the 26×26 matrix of computer model curves
- Empirically C is not of full rank
- That is the computer model curves do not span the full 26-D space
- Let O be the orthogonal basis vectors for C
- Let $P = OO^T$ be the projection matrix

Similarity Measure

- $P\delta$ is the projection of δ into C
- $(I - P)\delta$ is the orthogonal complement
- Angle between δ and C is given by

$$\cos\phi = \frac{\|P\delta\|}{\|\delta\|}$$

- ϕ is a measure of the similarity between the δ and the computer model curves

Controlling the Similarity

- Let

$$\tilde{\delta} = wP\delta + (1-w)(I-P)\delta$$

changing w will change the angle between δ and the family of computer model curves

- For a new angle φ, $\cos\varphi$ is a quadratic function of w
- Solving the quadratic functions yields

$$w = \frac{\|(I-P)\delta\|\cos\varphi}{\|P\delta\|\sin\varphi + \|(I-P)\delta\|\cos\varphi}$$

Discrepancy, Revisited

- Generate δ and select a value of φ
- Set φ at $0, 30, 60$ and 90 degrees
- Compute w and find $\tilde{\delta}$
- Scale $\tilde{\delta}$ to have the same length as δ
- Scale $\tilde{\delta}$ to have a variance $\sigma_{\delta}^2 = 5$

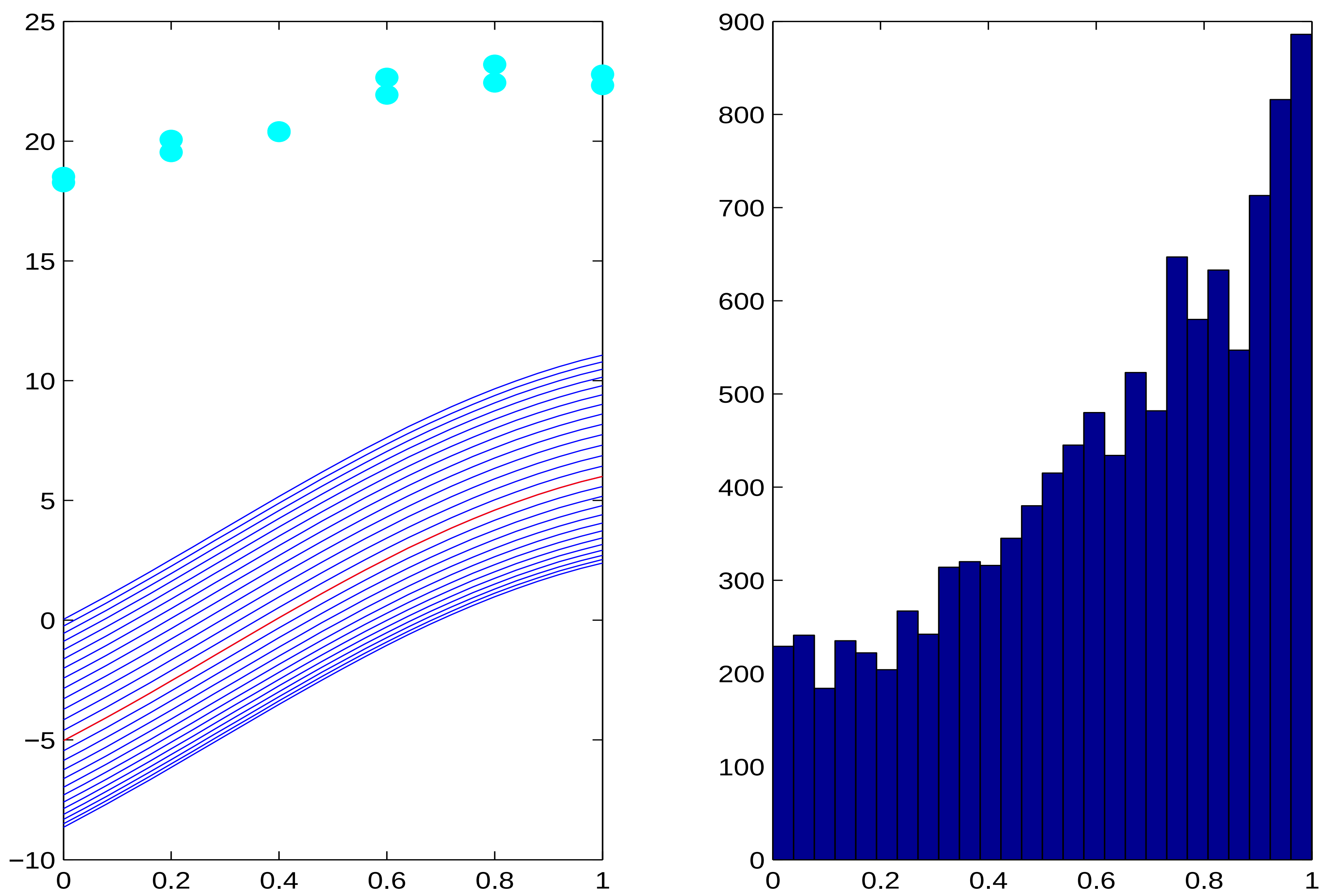
Experimental Setup

- Setup a designed experiment to control the factors above.
  - Factor 1: complexity of the computer model (simple/complex)
  - Factor 2: interaction between x and θ (no/yes)
  - Factor 3: regression component for θ (no/yes)
    - This controls the distance between computer model curves
  - Factor 4: Similarity between η and δ (Angle 0,30,60,90)
- Investigate all possible combinations of the four factors (32 runs)
- Generate 100 realizations for each factor combination

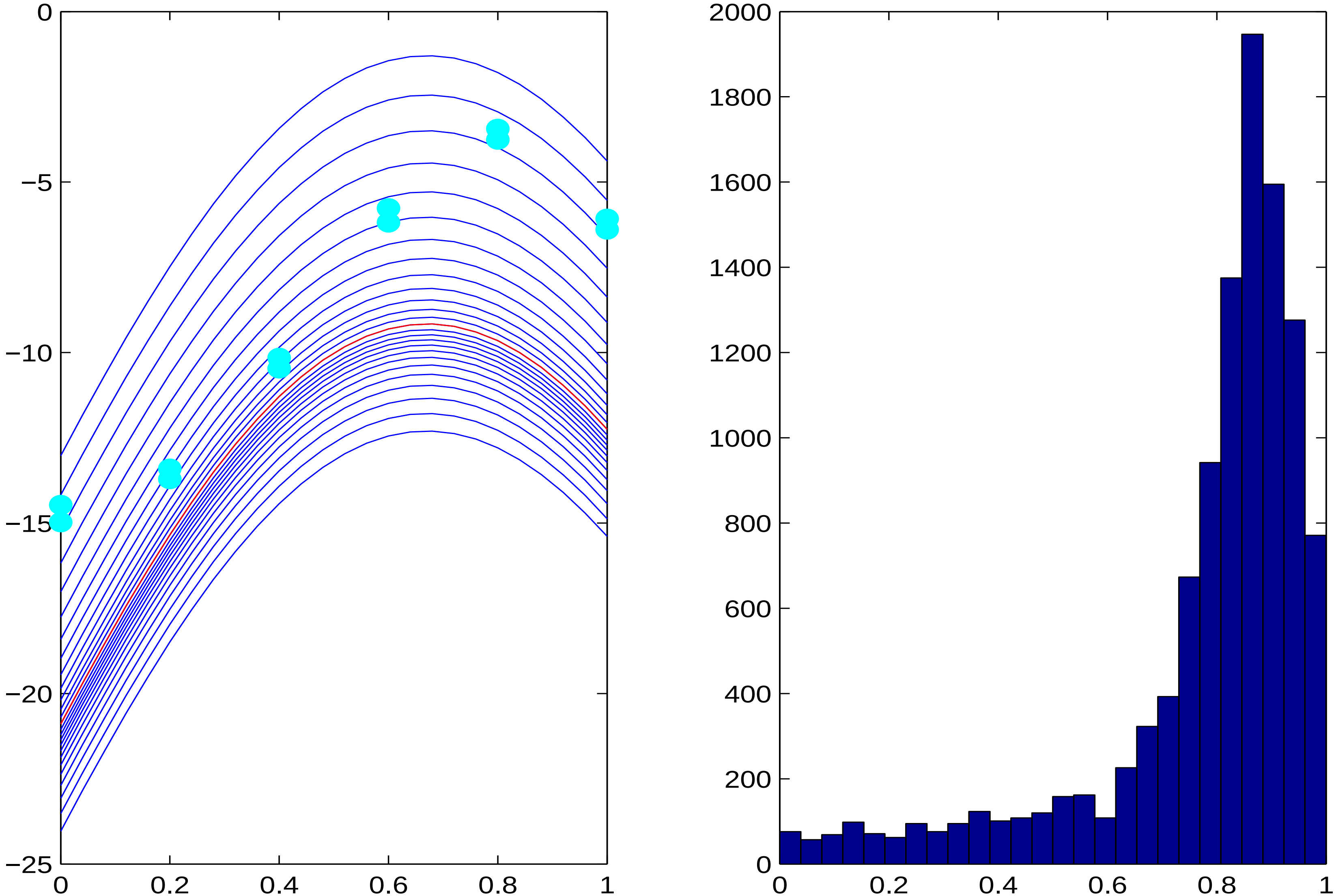
Example 1

- Computer Model:
  - $\beta_\eta = (0.5, 0.5)$
  - Sensitivity to $(x, \theta, x\theta) = (0.6, 0.4, 0)$
  - $Var(y_c) = 20$
  - No regression component
- Discrepancy:
  - $\beta_\delta = 0.5$
  - Angles varied between 0-90 degrees
  - $Var(\delta) = 5$
- Physical Data:
  - $\sigma_\varepsilon^2 = 0.1$

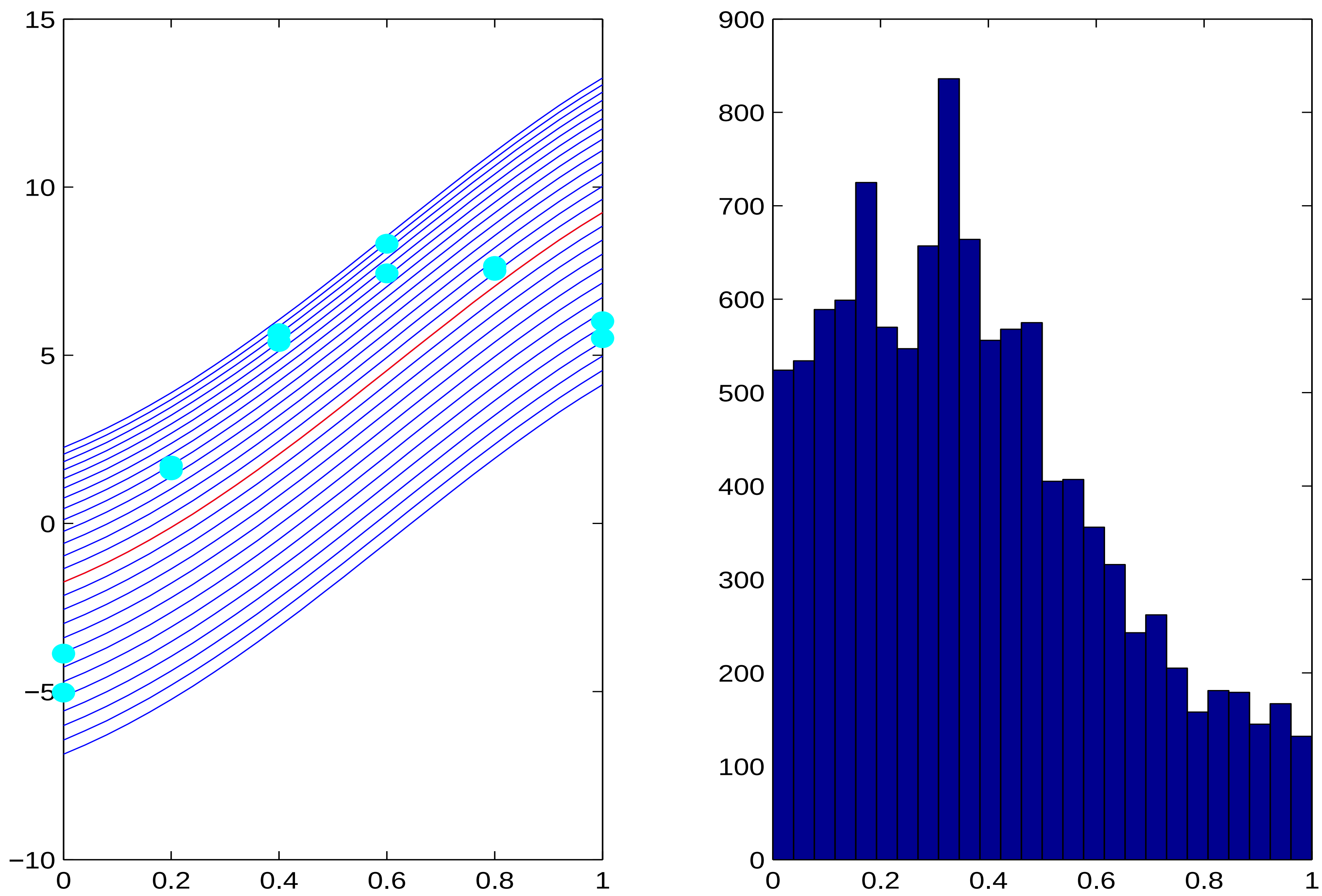
Angle: 0 degrees



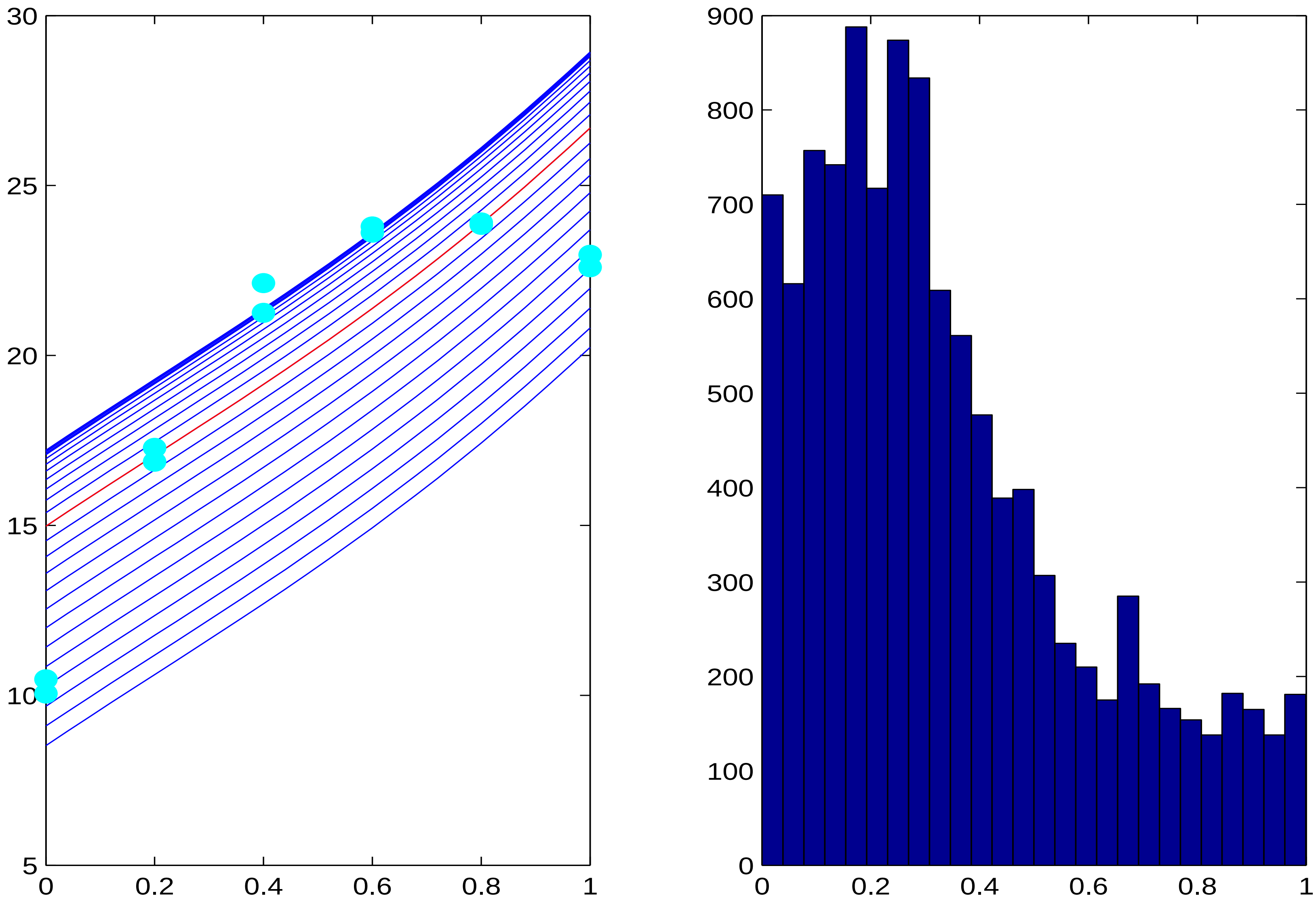
Angle: 30 degrees



Angle: 60 degrees



Angle: 90 degrees

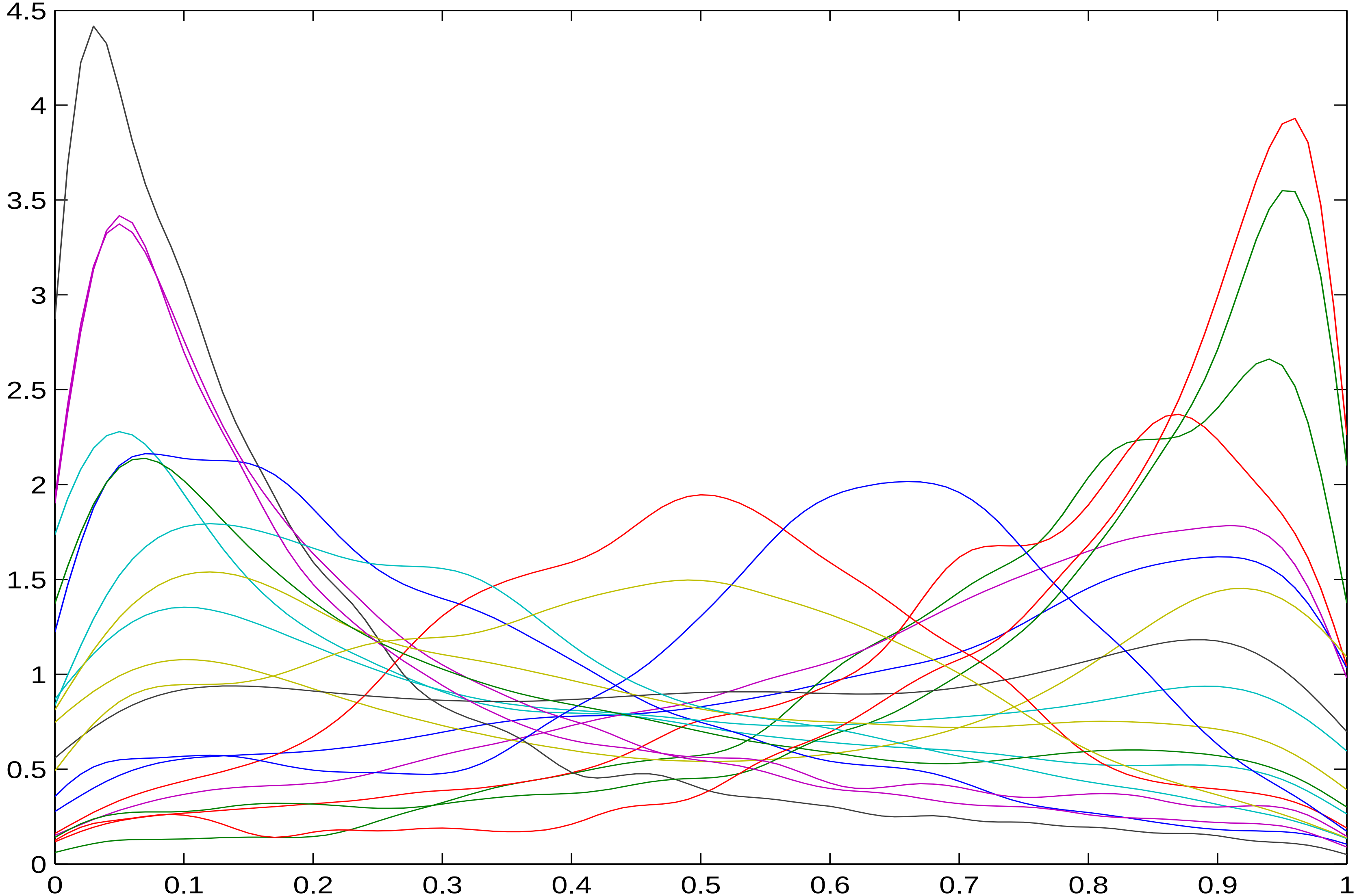


Example Continued

- Based on the above plots calibration has been unsuccessful
  - This is only one realization what about others?
  - Plot the Kernel density estimate of the posterior for various realizations
- Even if calibration is unsuccessful what about prediction
  - Predict the field mean using the Bayesian posterior (adjusted for bias)
  - Predict the field mean using $\theta = 0.48$ and adjust for the bias using the posterior distribution
  - compute the root mean squared error since we know the true field mean.

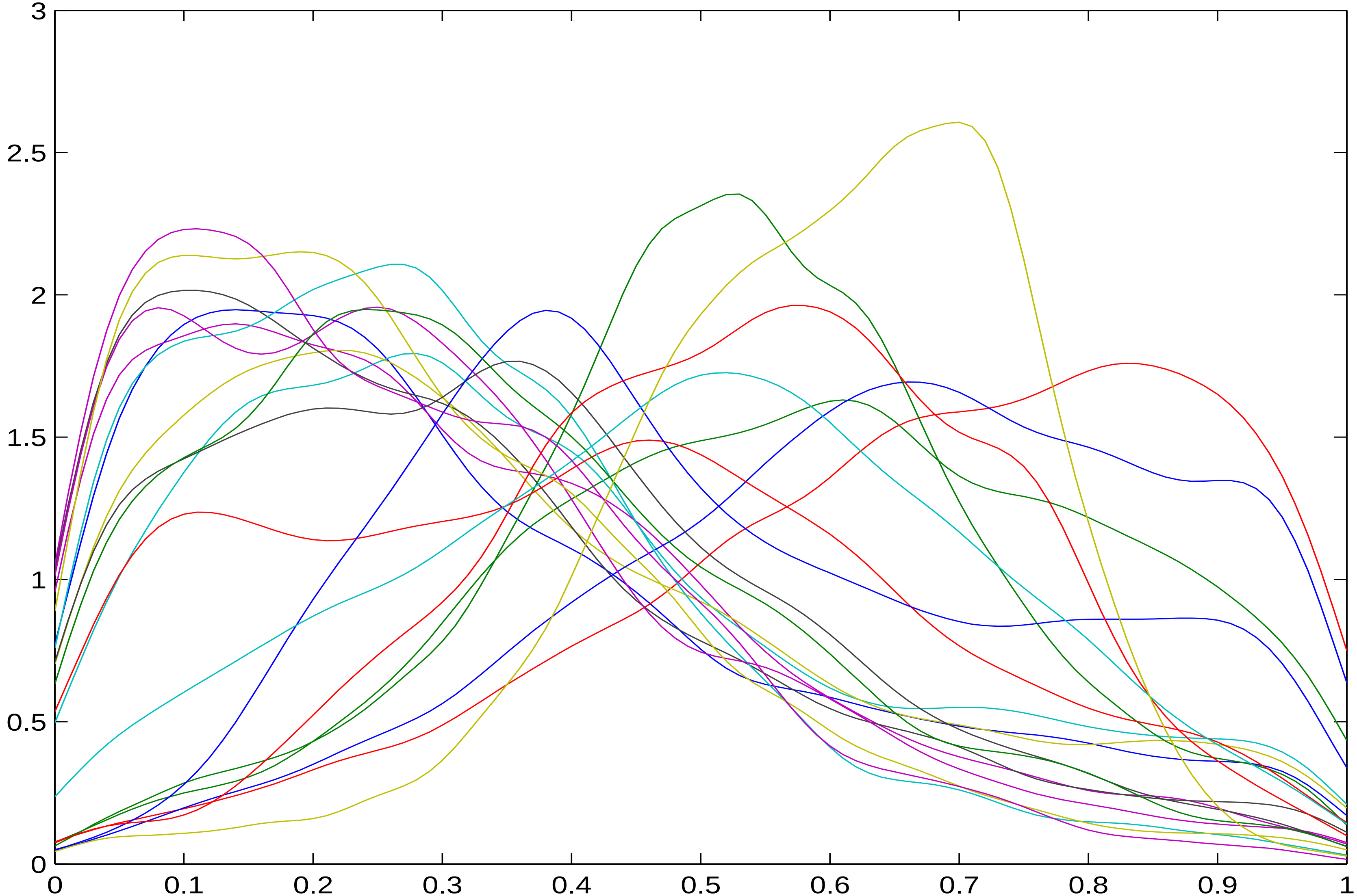
Angle: 0 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



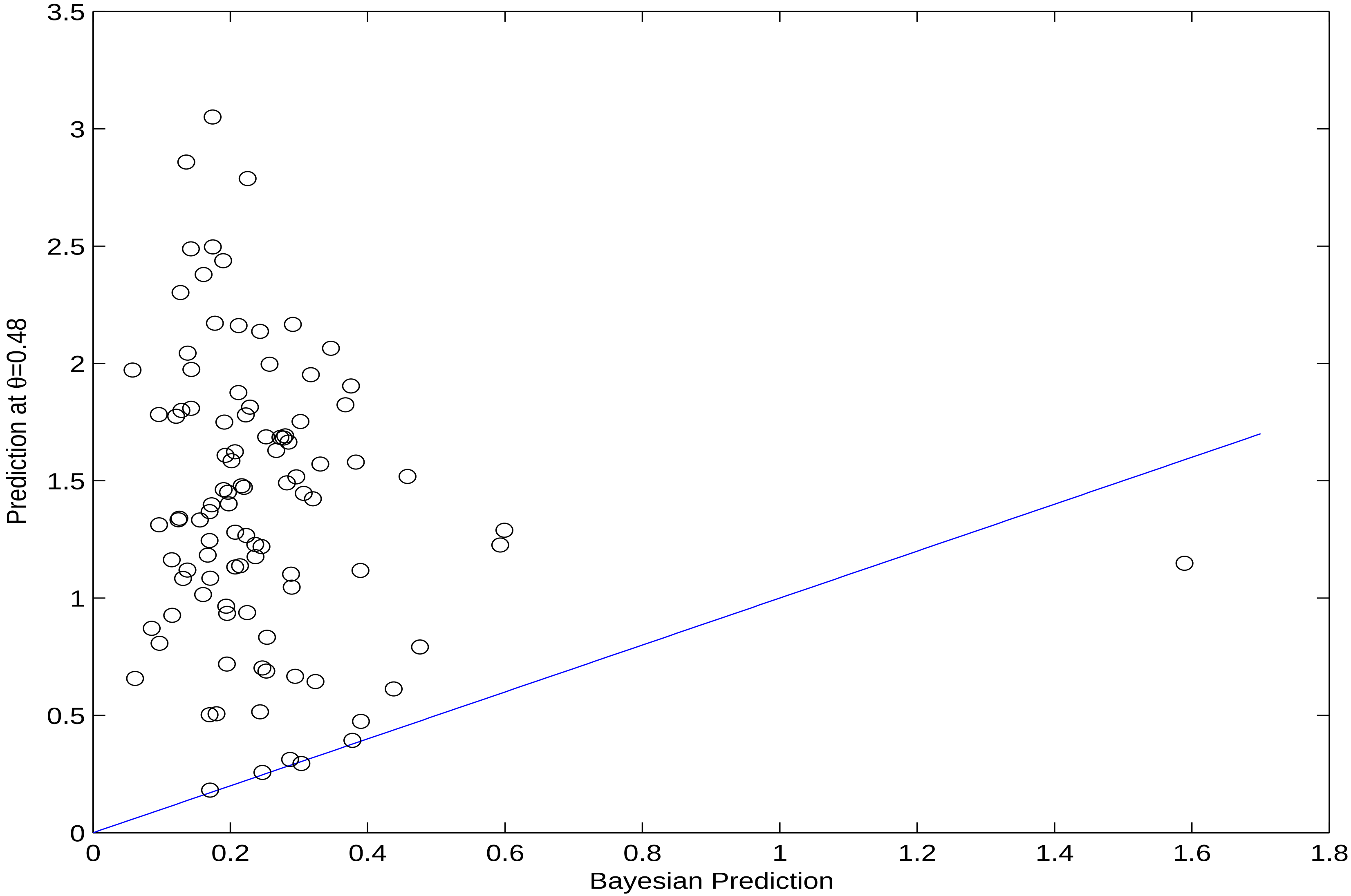
Angle: 90 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



Angle: 90 degrees

- Prediction comparison for 100 realizations



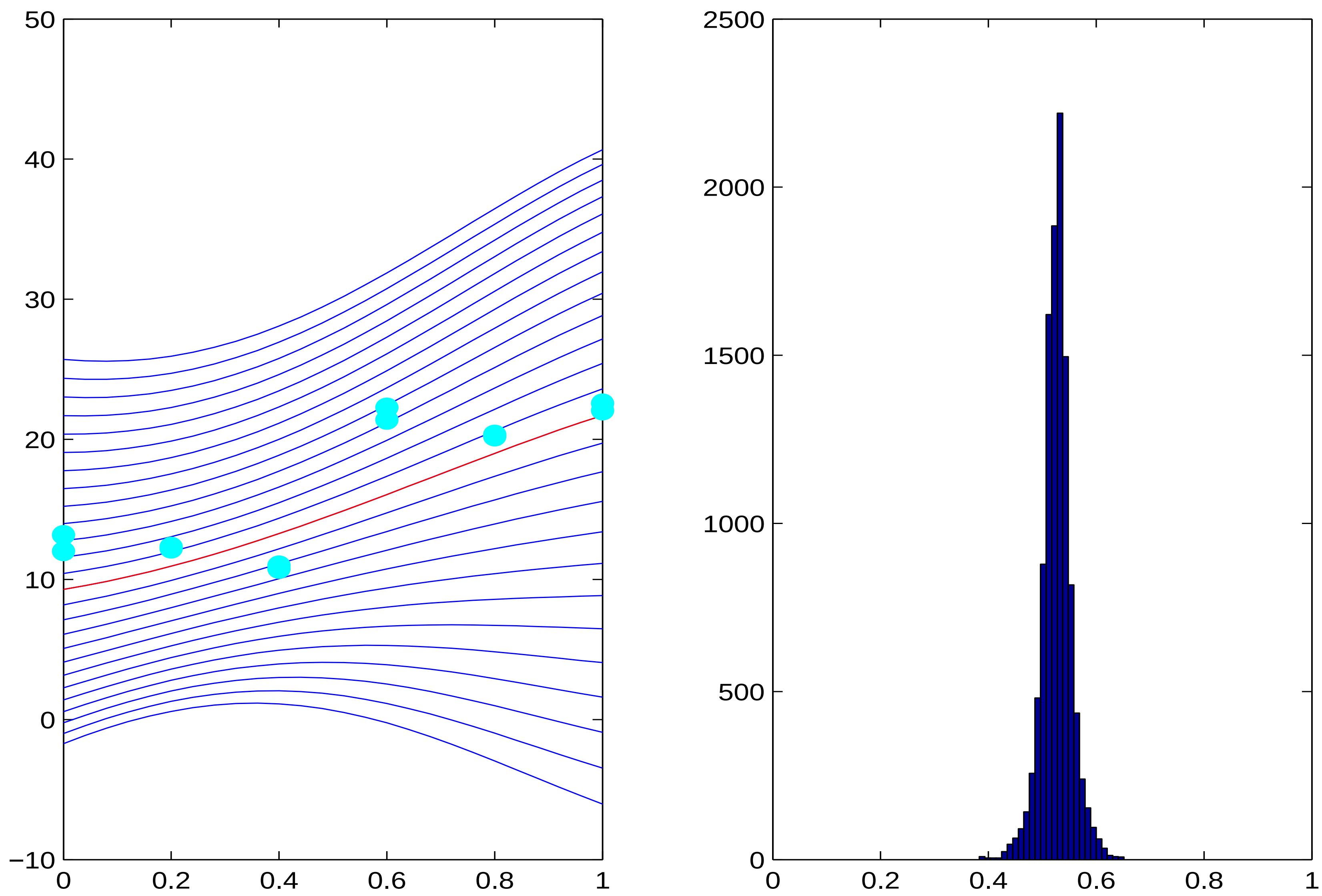
Example 2

- Computer Model:
  - $\beta_\eta = (0.5, 0.5)$
  - Sensitivity to $(x, \theta, x\theta) = (0.5, 0.25, 0.25)$
  - $Var(y_c) = 20$
  - Regression component
- Discrepancy:
  - $\beta_\delta = 0.5$
  - Angles varied between 0-90 degrees
  - $Var(\delta) = 5$
- Physical Data:
  - $\sigma_\varepsilon^2 = 0.1$

Example 2

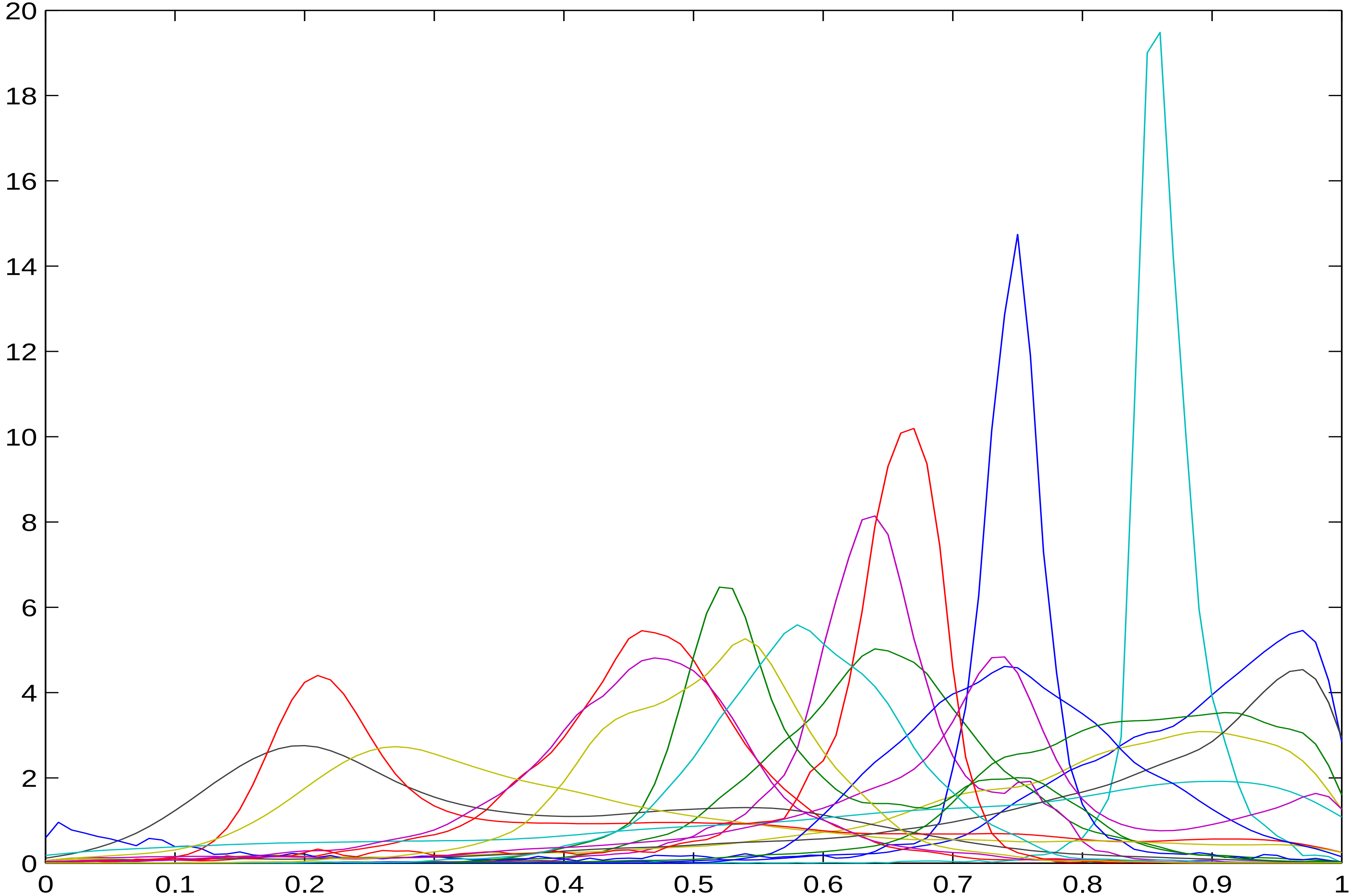
- Same setup as Example 1
- Except there is an interaction between x and θ
- Added a separation between the computer model curves
- Examine one realization
- Look at various realizations for each angle (0, 30,60 90)

Angle: 60 degrees



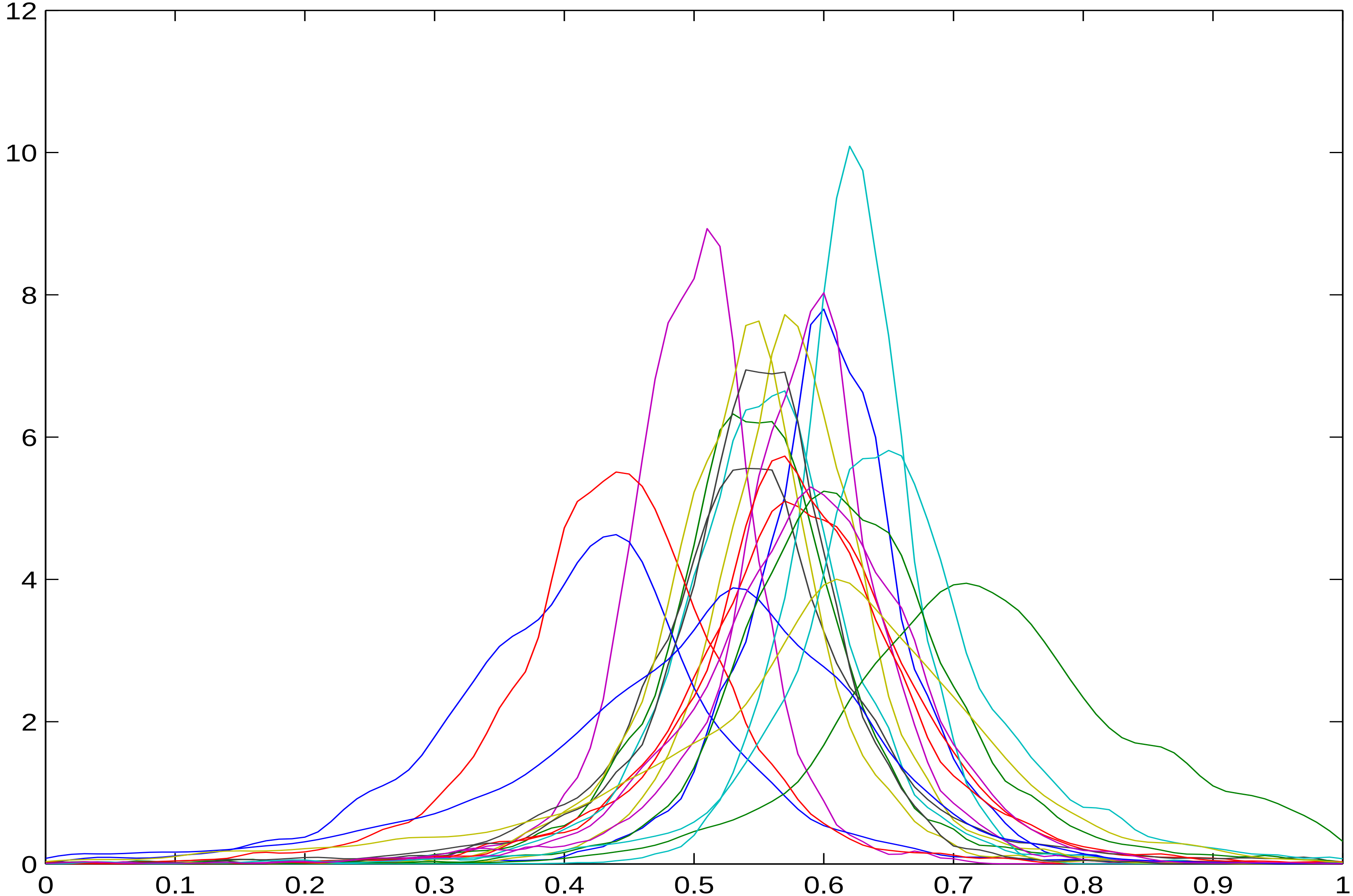
Angle: 0 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



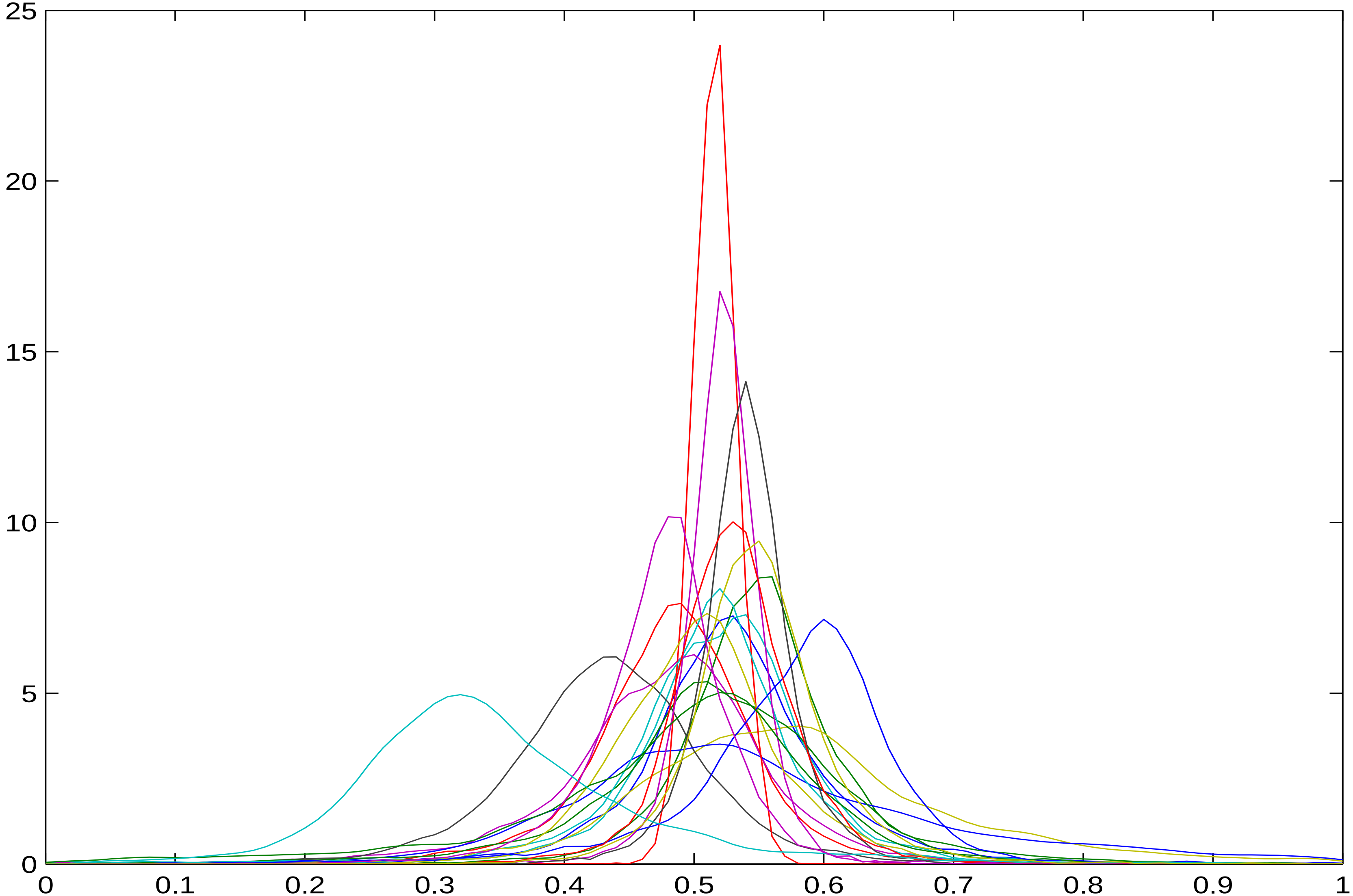
Angle: 30 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



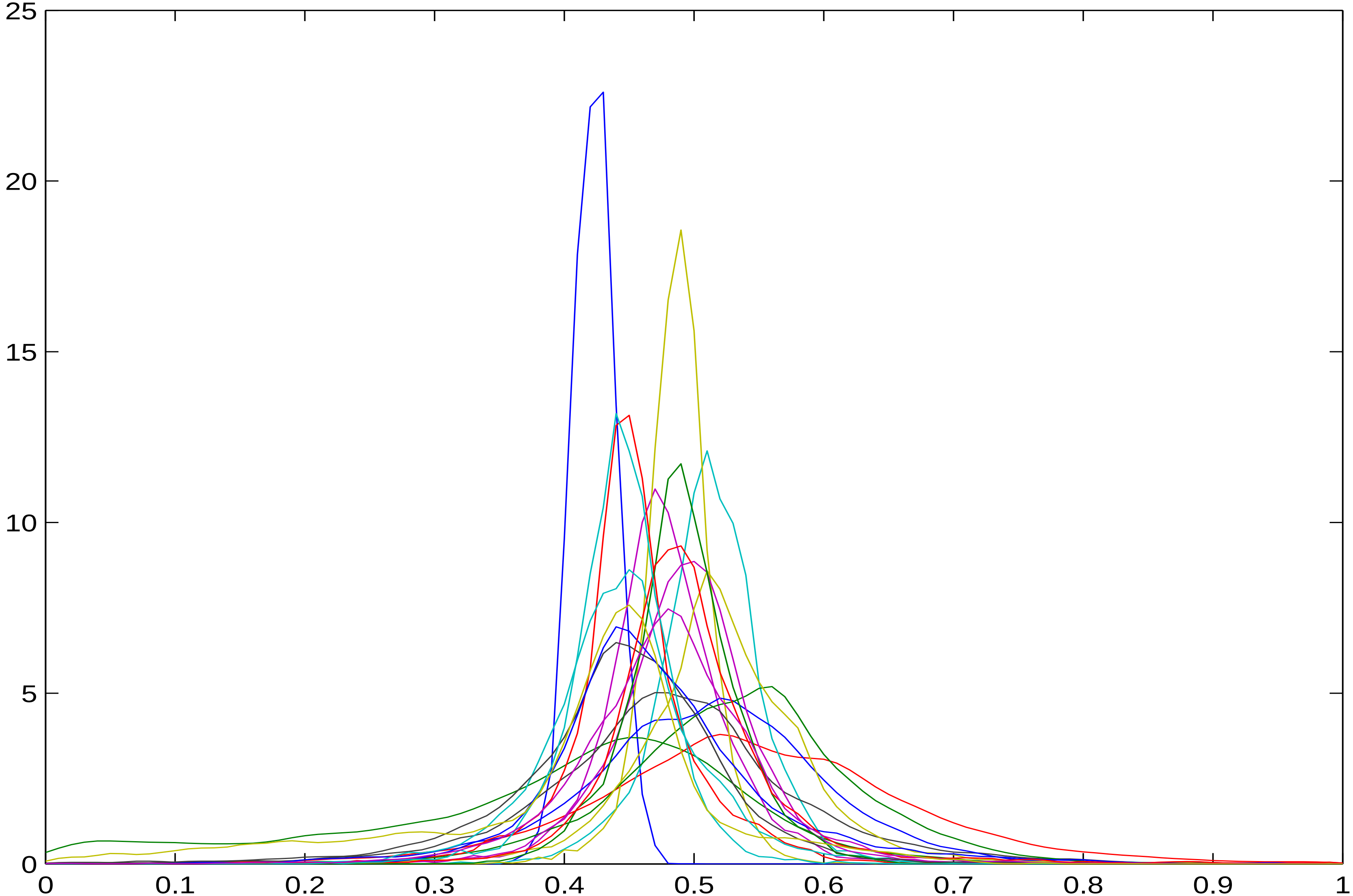
Angle: 60 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



Angle: 90 degrees

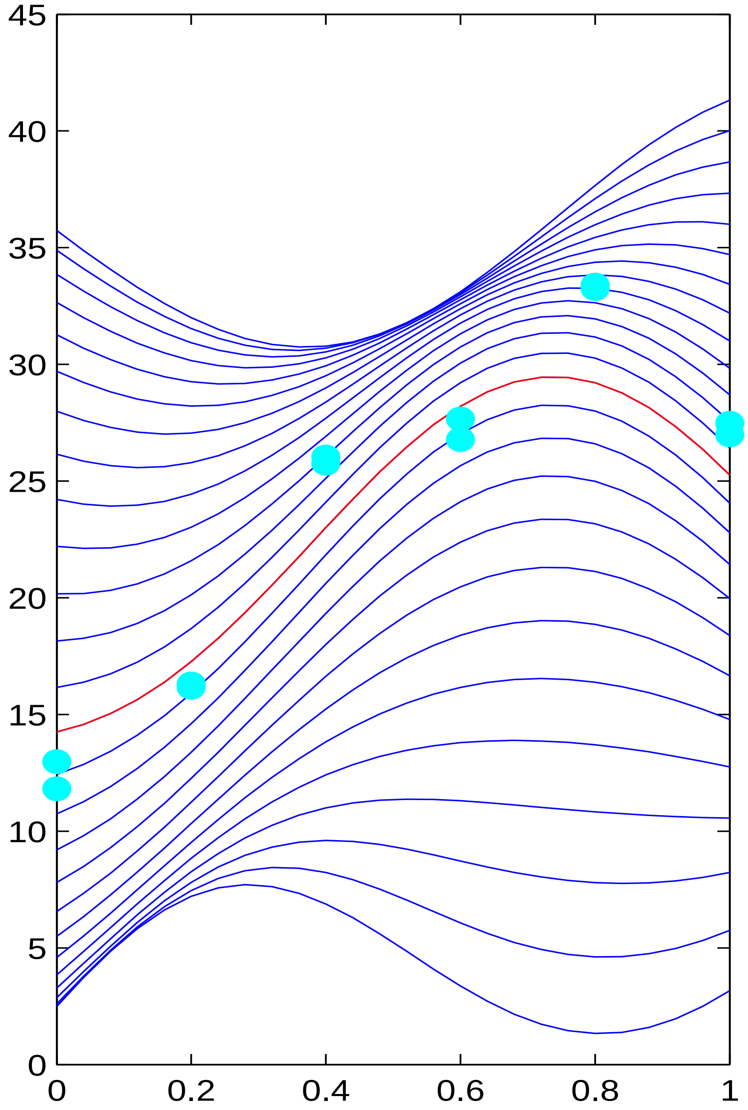
- Kernel Density estimates of posterior of θ for 20 realizations

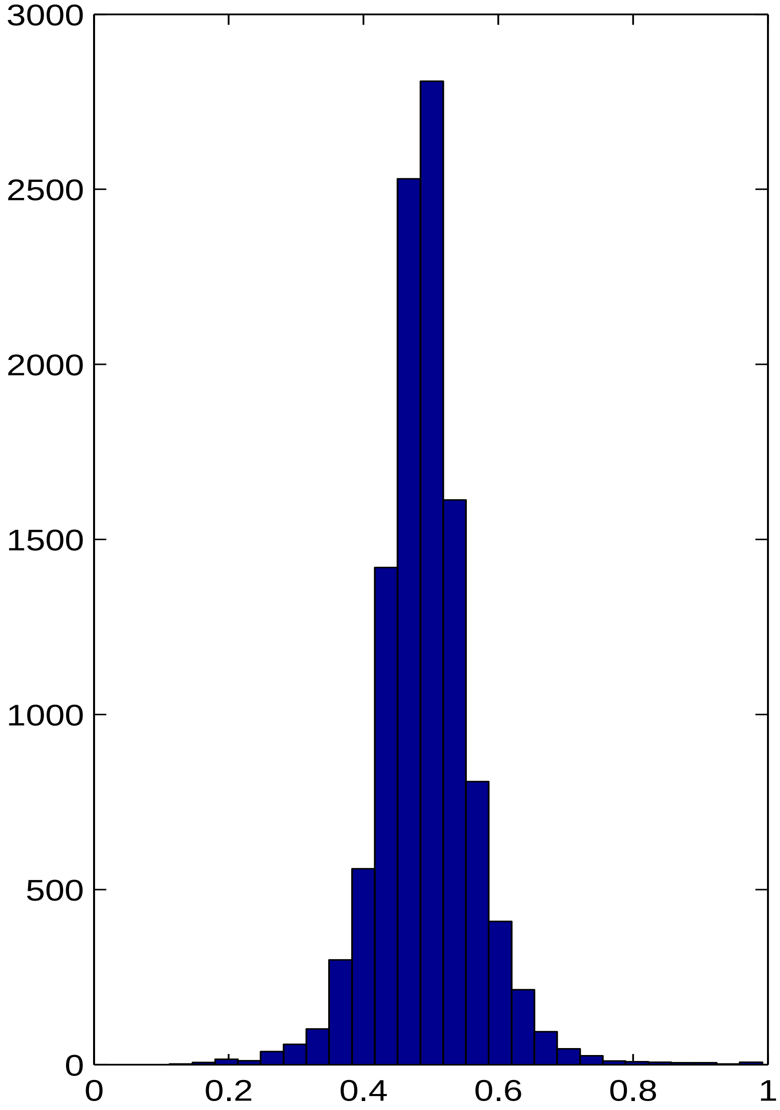


Example 3

- Complex computer model
- Interaction between x and θ
- Added a separation between the computer model curves
- Examine one realization
- Look at various realizations for each angle (0, 30,60 90)

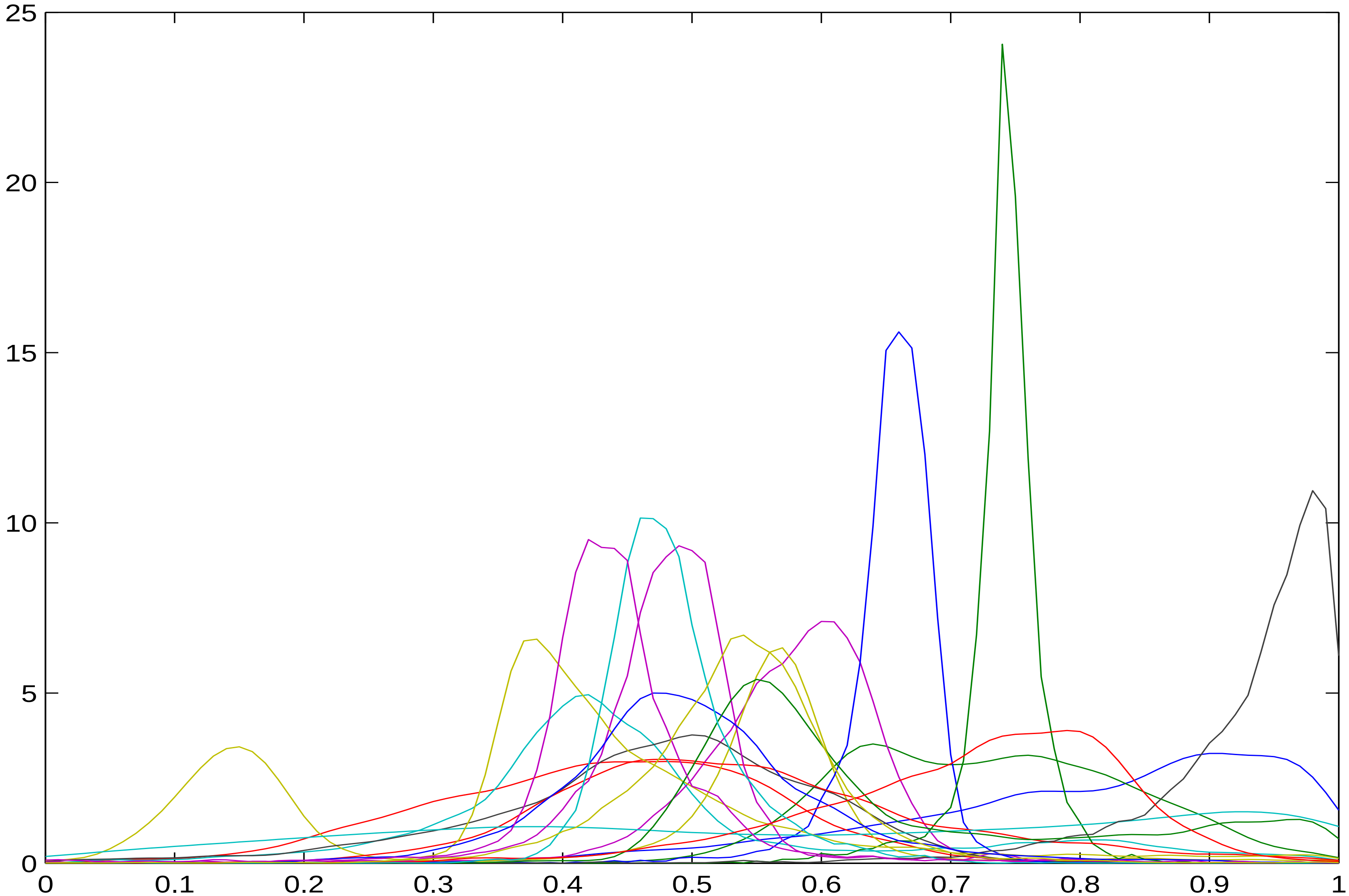
Angle: 60 degrees





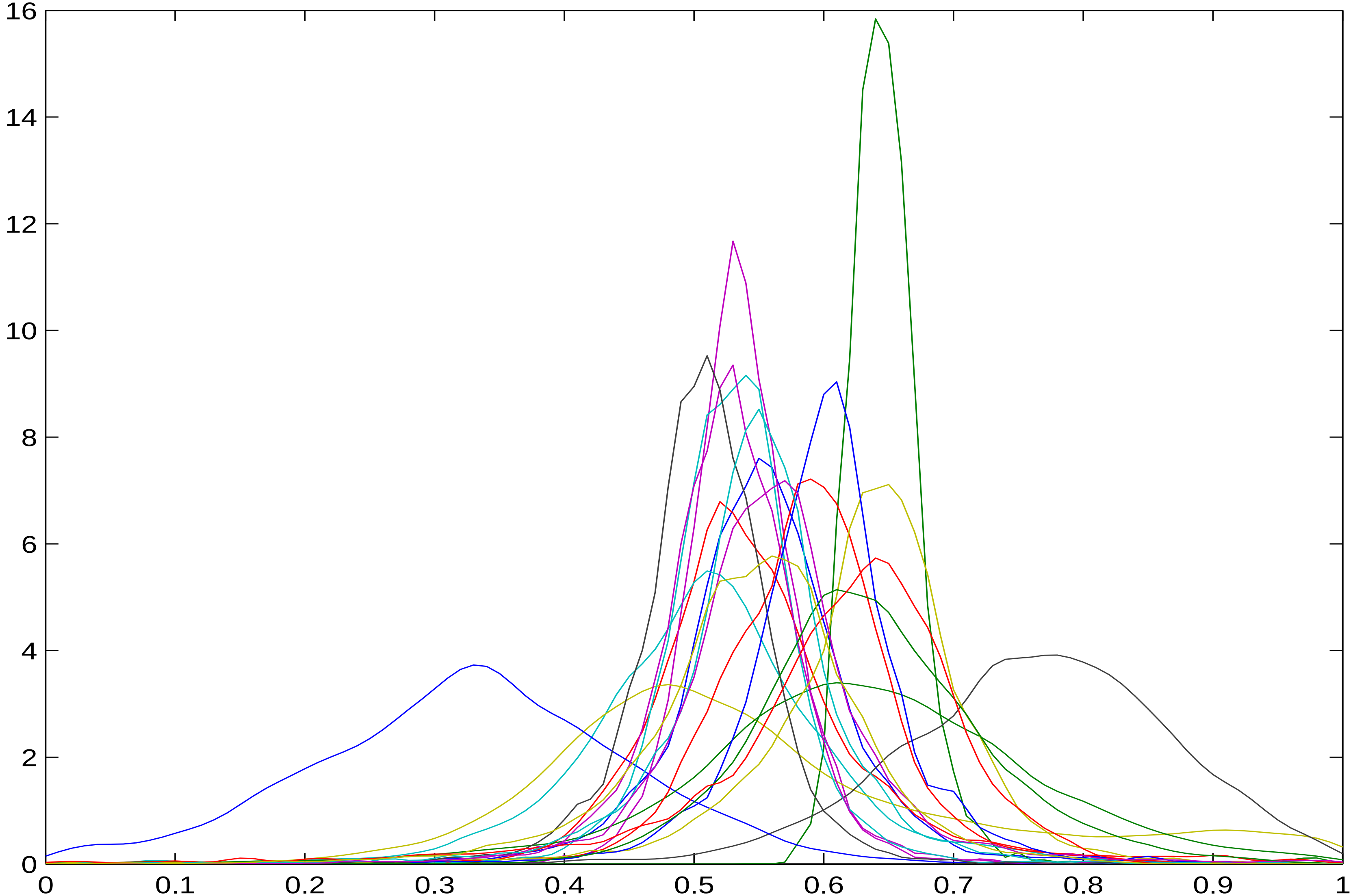
Angle: 0 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



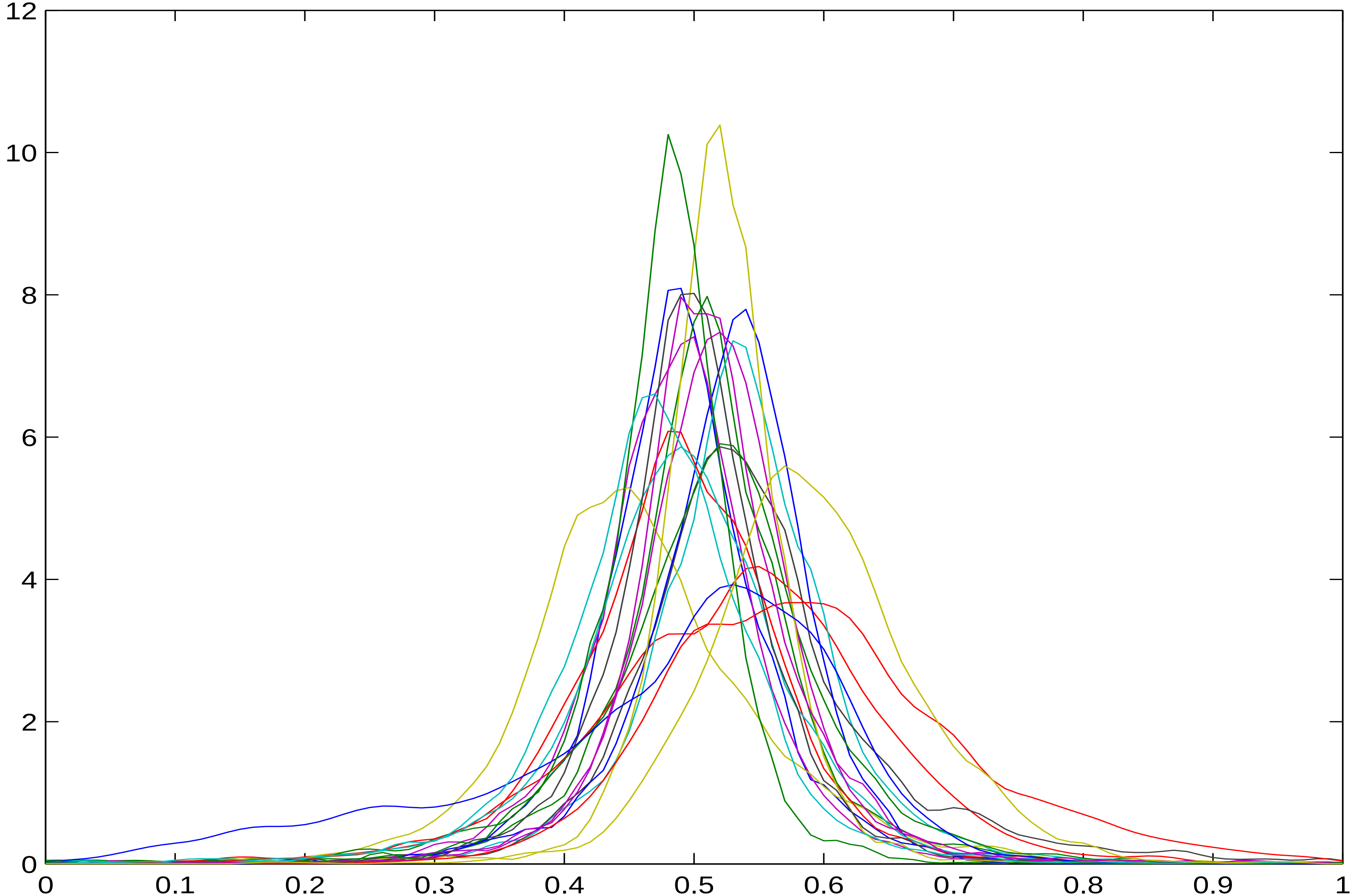
Angle: 30 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



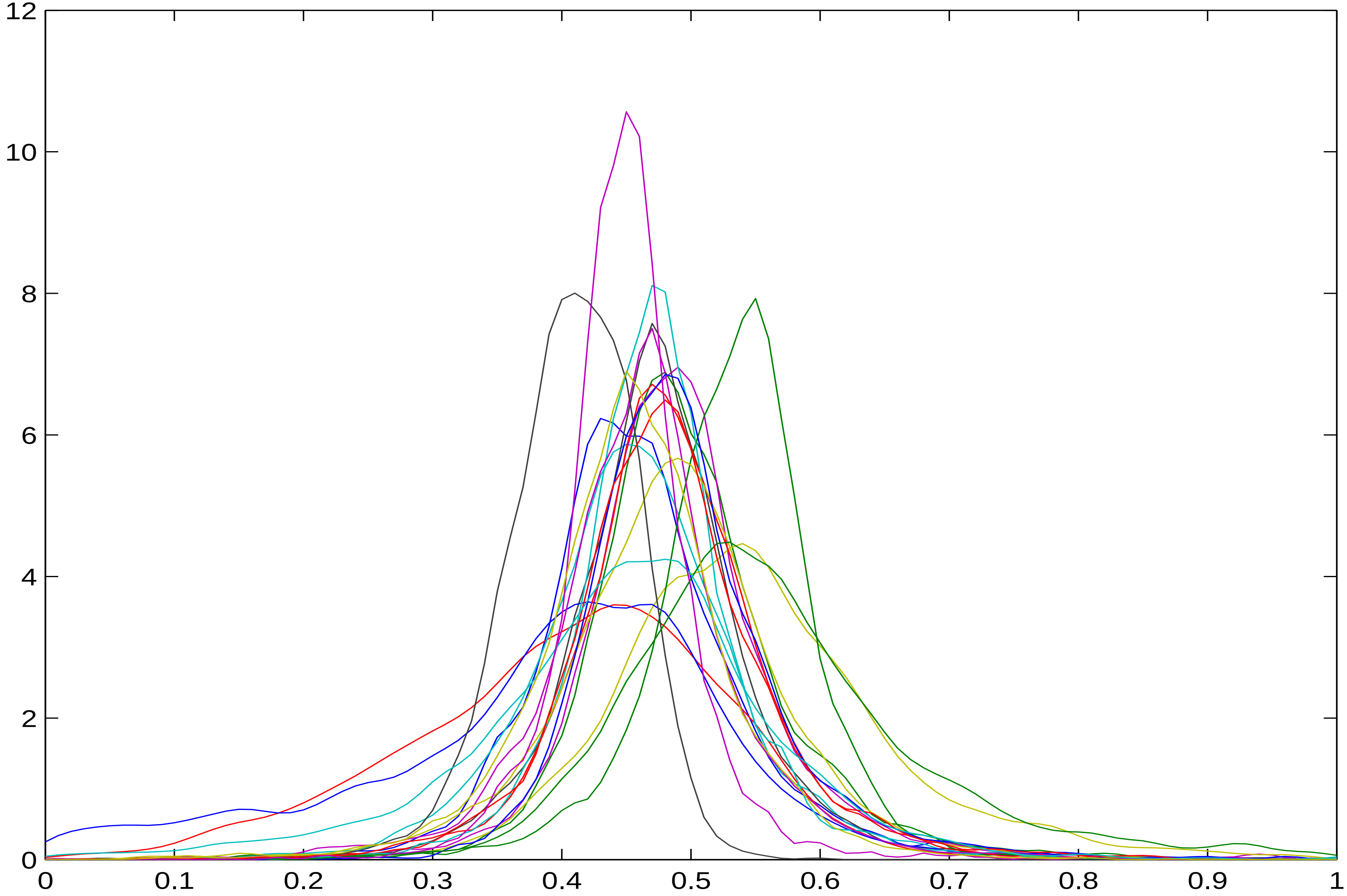
Angle: 60 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



Angle: 90 degrees

- Kernel Density estimates of posterior of θ for 20 realizations



Observations

- Orthogonality helps calibration
- However: orthogonality is rarely the case
- Promising results for angles of 60 degrees
- Orthogonality makes it hard to control the complexity of the discrepancy
- Interaction between x and θ helps calibration
- Complexity of code seems to have a limited effect on the ability to calibrate
- Whatever the situation Calibration is VERY difficult