Verification and Validation in Scientific Computing - Homework 5

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The source code for this assignment is available at `https://github.com/Steven-Roberts/VVSC-Project`. The Allen–Cahn PDE is a reaction-diffusion PDE governed by equation

$$\begin{aligned} \frac{\partial u(t,x,y)}{\partial t} &= \alpha \nabla^2 u(t,x,y) + \beta \left(u(t,x,y) - u(t,x,y)^3 \right), \\ u(0,x,y) &= \cos(2\pi x) + \cos^2(4\pi y), \\ t,x,y &\in [0,1] \end{aligned} \tag{1}$$

with zero Neumann boundary conditions on all four boundary edges. The parameters α is taken to be 1, and β will be the uncertain model parameter. This PDE is discretized in space on an using second order finite differences on a uniform grid with cells of size $h \times h$. In time, a second order Rosenbrock method is used with a fixed timestep of h. To ensure experiments were sizable, but not too long to run, I selected $h = \frac{1}{64}$. The system response quantity I consider is the average value of u over the spatial domain $[0,1]^2$ at time $t = 1$.

The experimental data for this assignment was generated synthetically. I assumed the reaction rate β is normally distributed with mean 1.25 and standard deviation 0.5. The value of the SRQ for $\beta = 0.75$, which is one standard deviation less than the mean, is 0.7672, and for $\beta = 1.75$, which is one standard deviation above the mean, the SRQ is 0.9534. By selecting points along the line connecting these two data points, two datasets were synthesized. The first dataset has five measurements, and the second has ten.

To propagate the uncertainties through the model, samples of β were generated with Latin hypercube sampling, and for each parameter value, the model was solved to compute the resulting SRQ. Samples sizes of 10, 25, and 100 were used. Figures 1 to 3 plot the results as well as a least-squares polynomial approximation to the system response surface. In all cases, a quadratic polynomial seemed most appropriate and is quite accurate except for very large values of β.

Figures 4 to 6 plot the cumulative distribution functions of the experimental and simulation SRQ values. The corresponding area validation metric (AMV) values are presented in table 1. As the number of samples increase and when the larger synthetic dataset is used, the AMV values decrease. The first synthetic dataset and a sample size of 10 appear insufficient to accurately compute AMV.

Dataset	Sample size	AMV
1	10	0.0885
1	25	0.0852
1	100	0.0788
2	10	0.0574
2	25	0.0541
2	100	0.0477

Table 1: Area validation metric for all datasets and sample sizes

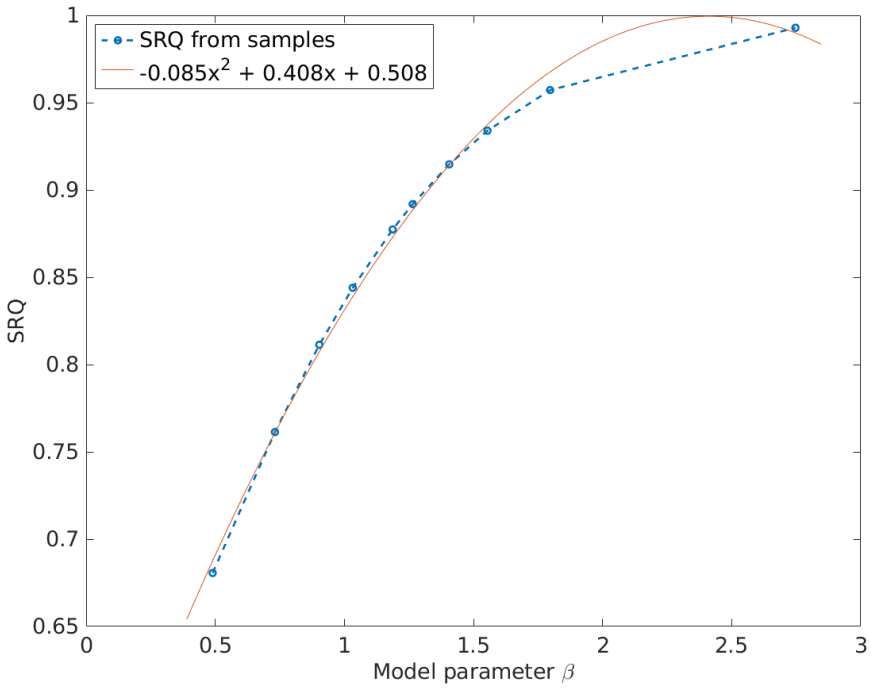


Figure 1: Distribution of SRQ and response surface approximation with 10 samples

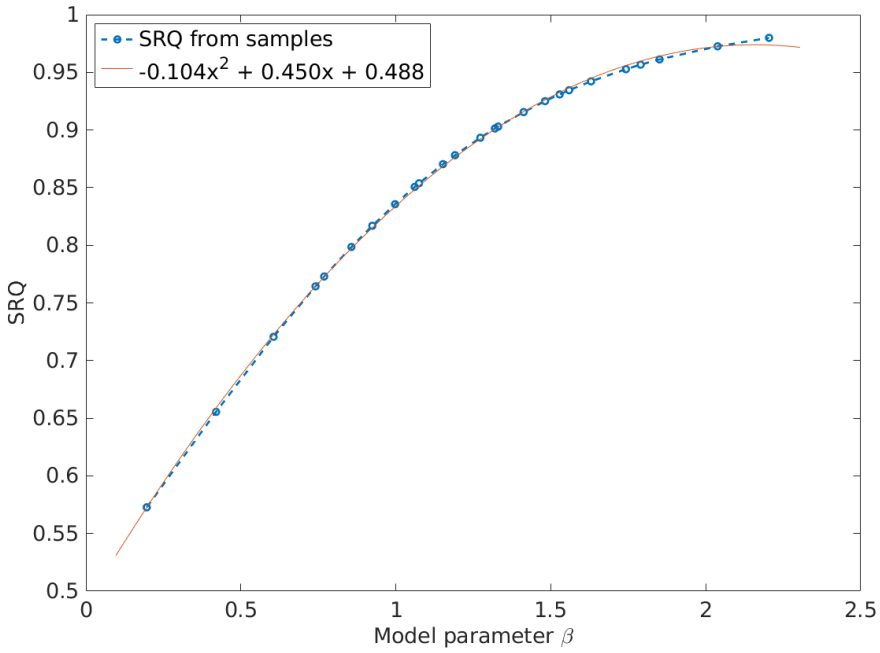


Figure 2: Distribution of SRQ and response surface approximation with 25 samples

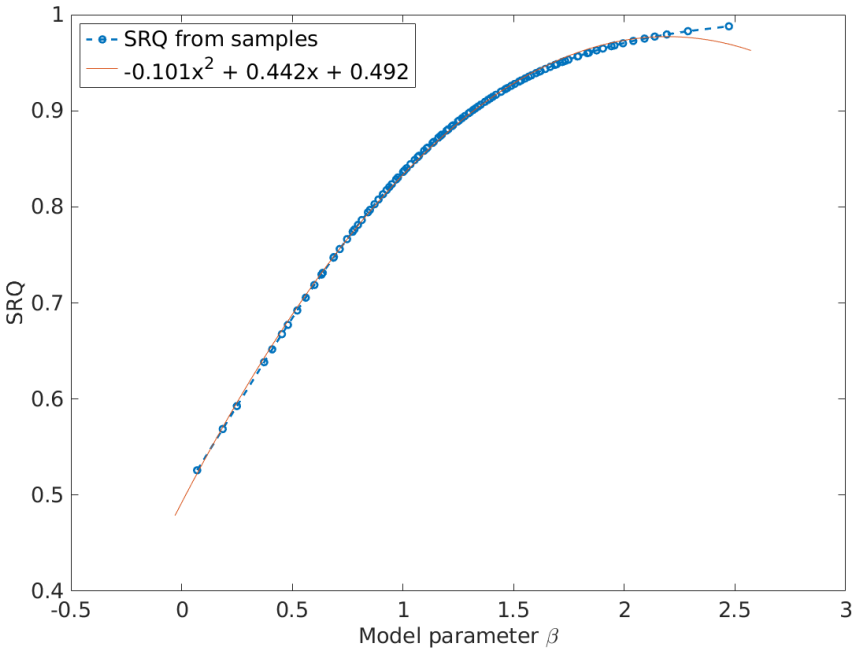
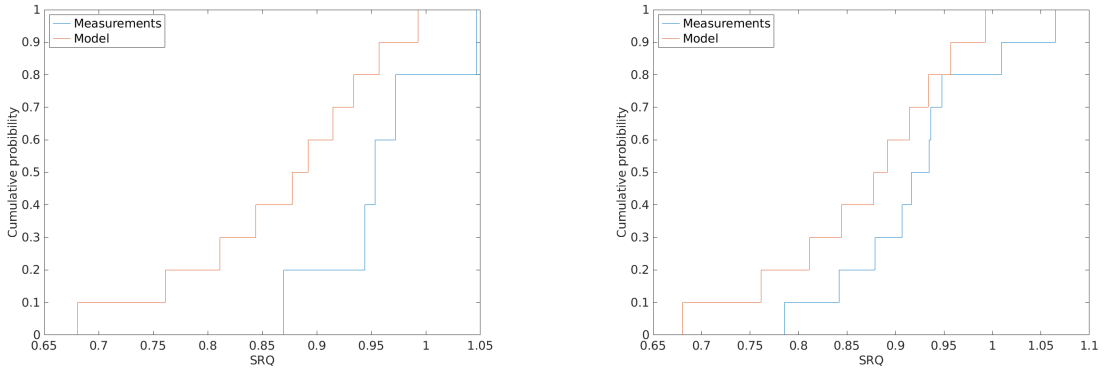


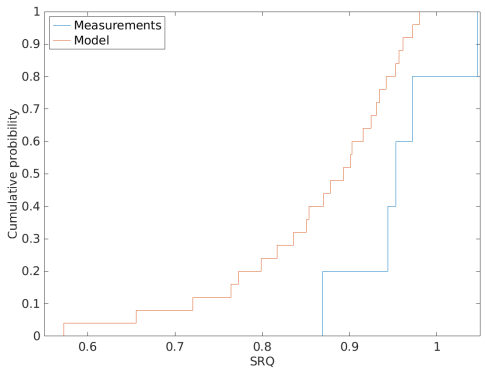
Figure 3: Distribution of SRQ and response surface approximation with 100 samples



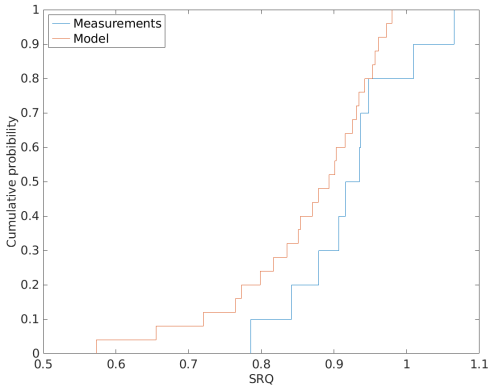
(a) Dataset 1

(b) Dataset 2

Figure 4: CDFs for SRQ with 10 samples

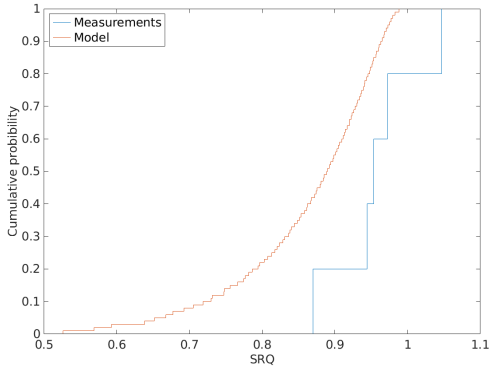


(a) Dataset 1

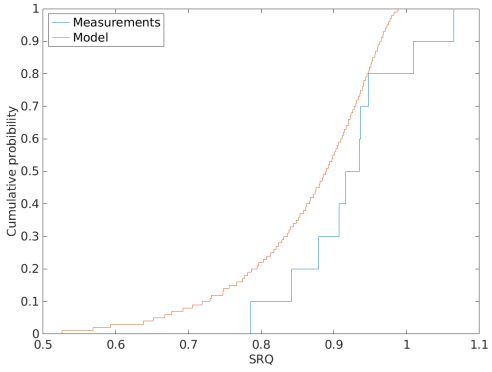


(b) Dataset 2

Figure 5: CDFs for SRQ with 25 samples



(a) Dataset 1



(b) Dataset 2

Figure 6: CDFs for SRQ with 100 samples