Estimating model-form errors using random field models

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Background

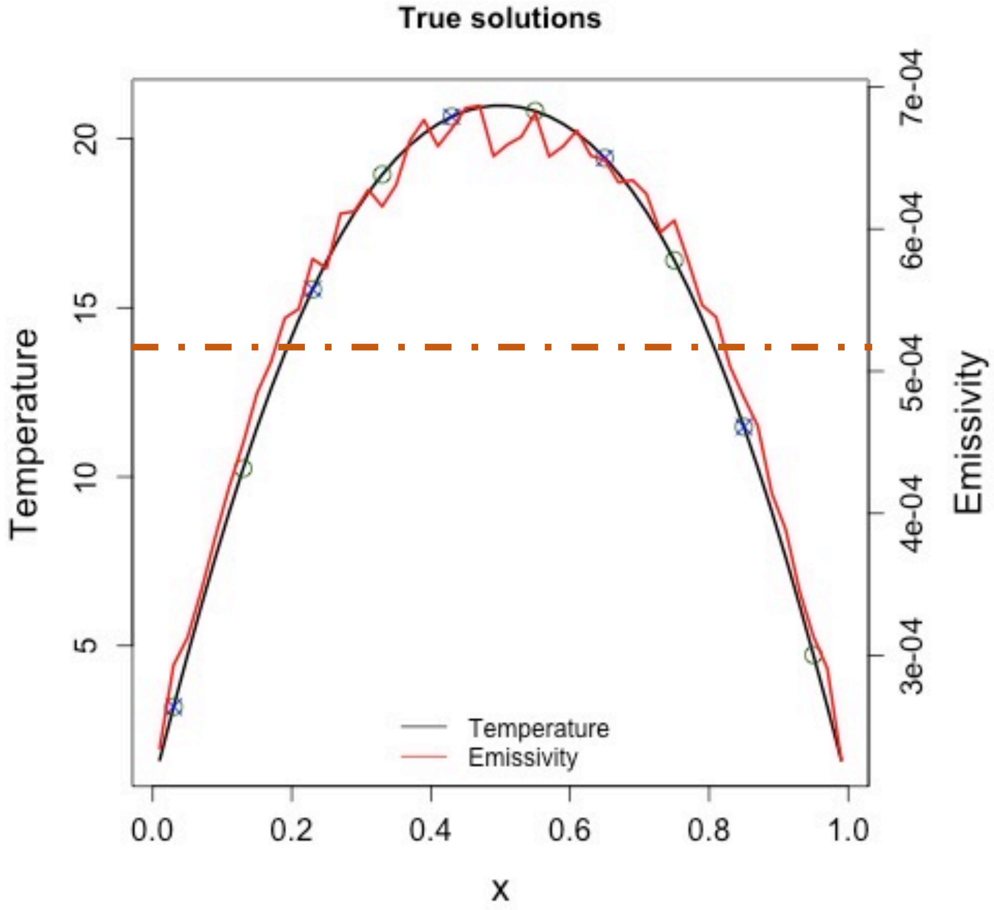
- Model-form error: "Missing physics" in models of scientific phenomena
- Physics models: Usually PDEs in space-time, with terms that approximate some types of physics
    - $U_t + F_x(U) + G_y(U) = \beta(\boldsymbol{x})\,\Xi(U)$
    - $\Xi(U)$ is usually an approximation of a physical process (and source of model-form error)
    - $\beta(\boldsymbol{x})$ is a multiplicative correction that seeks to rectify it & has to be obtained *somehow* ..
- Obtaining $\beta(x)$: Can only be learned from data, $U^{(obs)}$, with all the physics
    - Requires solving an inverse problem for a spatial/spatiotemporal field
    - Challenges: limited $U^{(obs)}$ & high dimensionality
        - Need regularizations or a prior model for $\beta(x)$, e.g., to impose smoothness
        - Plagued by non-uniqueness i.e., $U^{(obs)}$ could imply multiple $\beta_i(x)$, all very different

Introduction

- Aim: Show how $\beta(x)$ could be computed from $U^{(obs)}$
  - What prior info do we need?
  - How much of that can be encoded into random field models (RFM)?
  - How do we deal with non-uniqueness of $\beta(x)$, if RFMs are insufficient?
- Test case: radiative heat transfer, where both the high-fidelity & engineering-fidelity models are available
  - $U^{(obs)}$ are synthetic data, from the high-fidelity model
- Prior information:
  - $\beta(x)$ is smooth in space & can be modeled as a Gaussian Markov random field (GMRF)
  - $\beta(x)$ is known, with uncertainty, at the boundaries of the domain

The model

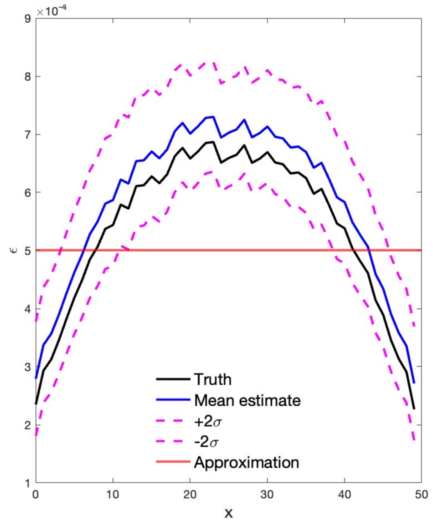
- The equation being solved
  - $\frac{d^2T}{dx^2} = \epsilon(T)(T_\infty^4 - T^4) + h(T_\infty - T)$
  - True: $\epsilon_{true}(T) = (1 + \sin\left(\frac{3\pi}{200}x\right) + \exp(0.02x) + N(0, 0.1^2))\times 10^{-4}$
  - Approximation: $\epsilon(T) = \epsilon_0 = 5 \times 10^{-4}$
  - $\beta_{true}(x) = {\epsilon_{true}(T(x))}/{\epsilon_0}$
- Observations: $T^{(obs)}(x) = T(x_{sensor}) + \gamma, \gamma \sim N(0, \sigma^2)$
- Prior info on $\beta(x)$
  - It is smooth in space & is unimodal (because $\epsilon(x)$ is so)
  - $\beta(x = 0) \sim N(\beta_{l,} \sigma^2), \beta(x = 1) \sim N(\beta_r, \sigma^2)$



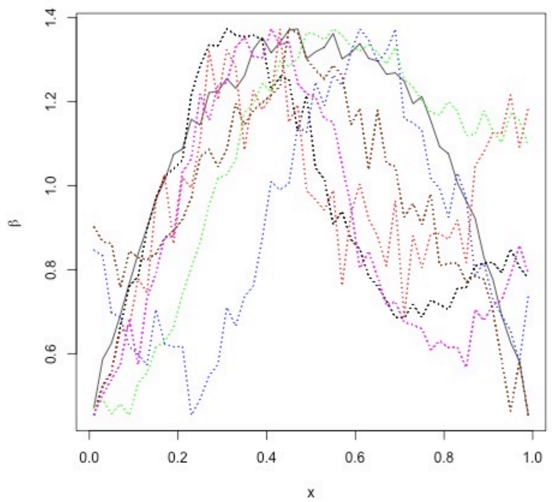
Estimation of β(x)

- $\beta(x)$ is estimated using Ensemble Kalman filters (EnKF)
  - Implication: $\beta(x)$ is modeled as a multivariate Gaussian (Gaussian Markov Random Field)
- Discretization: Uniform mesh, cell-centered, 50 cells
- Observations: $T^{(obs)}(x)$ obtained at M different points in time
  - T is constant in time, but the measurement error changes, so $T^{(obs)}(x, \tau)$ varies in pseudo-time
- Initial ensemble of $\beta(x)$: Drawn from prior
  - General form of prior: $\beta(x) = \beta_0 + \zeta, \zeta \sim N(0, \Gamma)$
  - Will test informative and non-informative priors

Informative prior

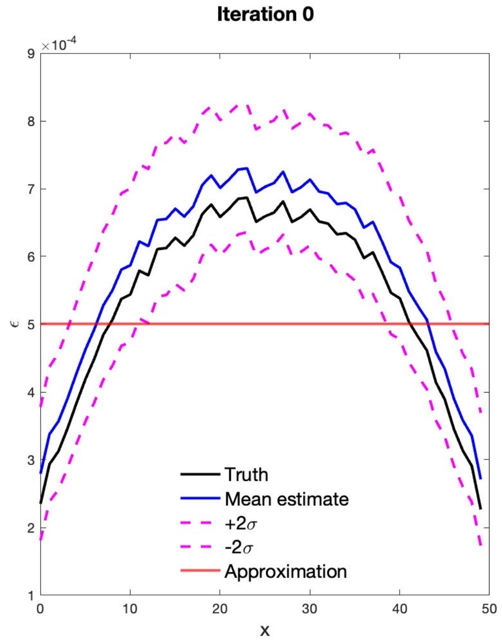


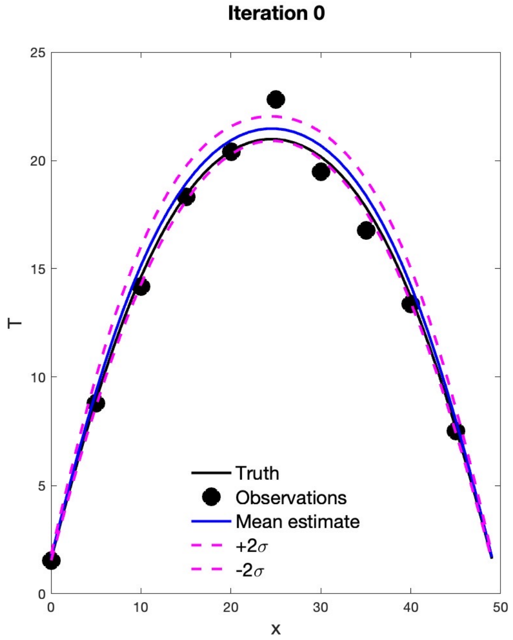
Non-informative prior



Test A – Informative prior

- Prior:
    - $\beta(x) = \beta_{true}(x) + a + b\ \sin(2\pi x + \phi), a, b, \phi \sim N(0, \vartheta^2)$
    - $\epsilon(x) = \beta(x)\epsilon_0$
    - Initial ensemble: Very close to truth
- Observations: 10 observations with 2% noise
- Initial $T^{(pred)}(x)$: Pretty good
- $\beta(x)$ constraints satisfied:
    - Spatially smooth & unimodal
    - Boundary values close to (β_l, β_r)

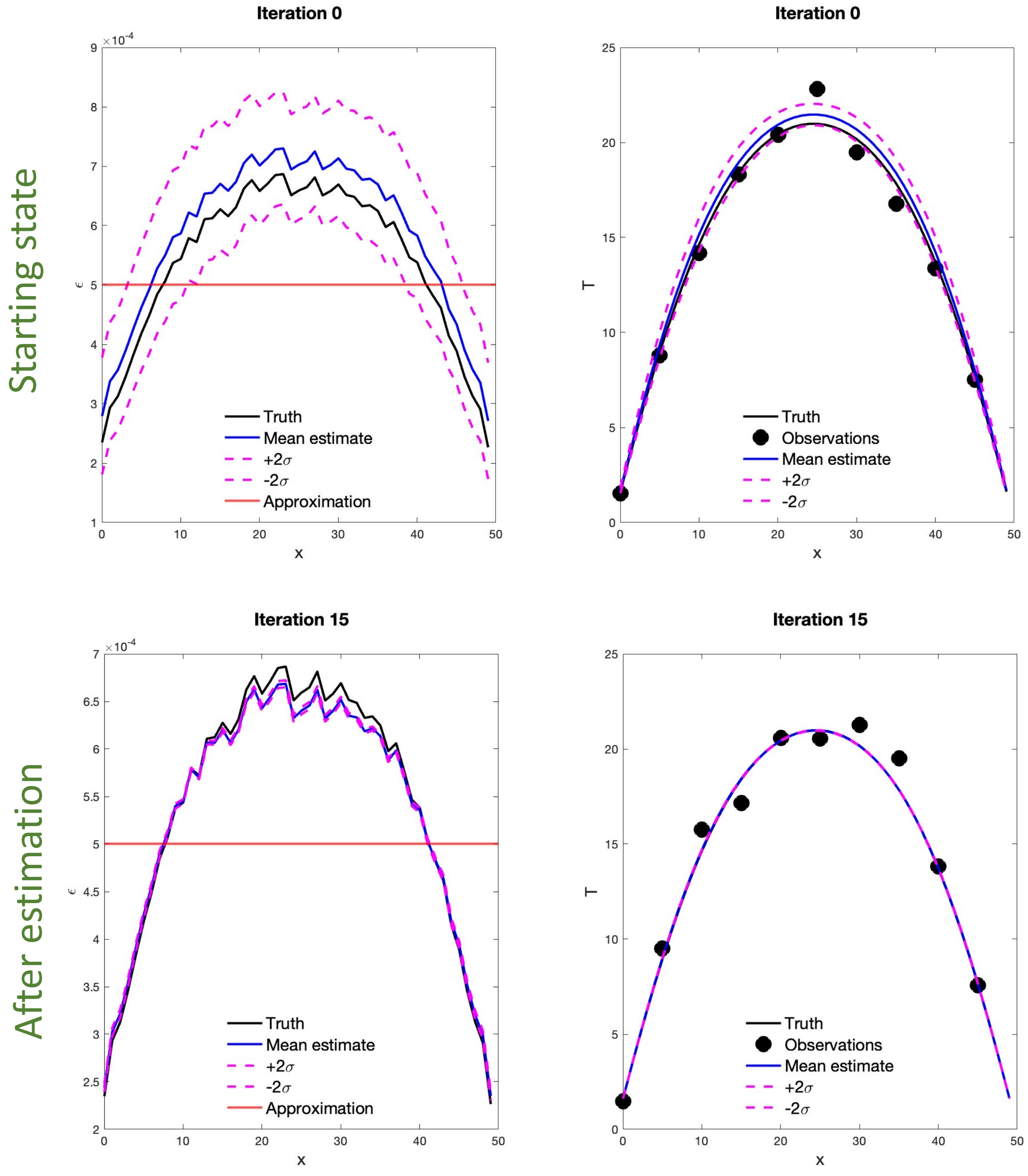




Test A - results

- Posterior:
  - $\widehat{\epsilon(x)}$ close to truth
  - $T^{(pred)}(x)$ is close to observations
  - Uncertainty in $\widehat{\epsilon(x)}$ and $T^{(pred)}(x)$ are small (spurious)
- Numerical method
  - Extracts info from $T^{(obs)}(x)$ to obtain an estimate of β(x) (and therefore ε(x))
  - Stable

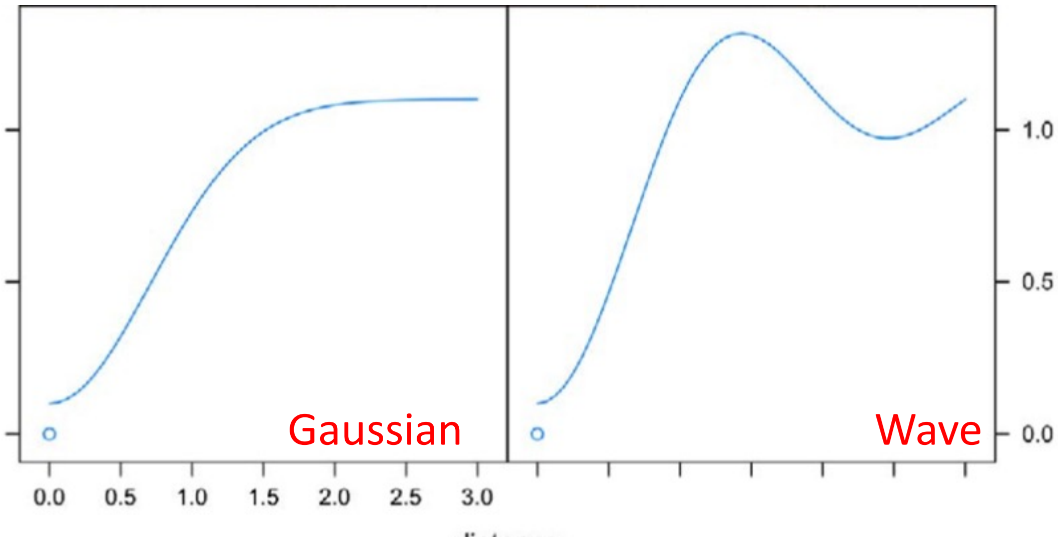
Takeaway: *Estimation of $\beta(x)$ feasible but uncertainties should not be trusted*



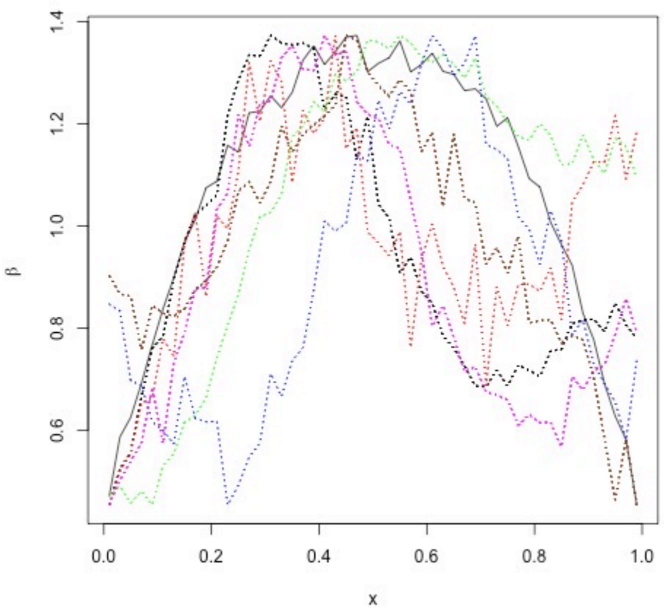
Test B - non-informative prior

- Prior model
  - $\beta^{(prior)}(x) = 1 + \zeta, \zeta \sim N(0, \Gamma)$
  - Γ is modeled using a variogram
- Variogram model
  - Obtained by fitting a Wave and Gaussian variogram to $\beta_{true}(x)$
    - Chose Wave
- $\beta(x)$ constraints satisfied
  - Not spatially smooth
  - Not unimodal
  - Boundary values not close to (β_l, β_r)

Semi-variograms



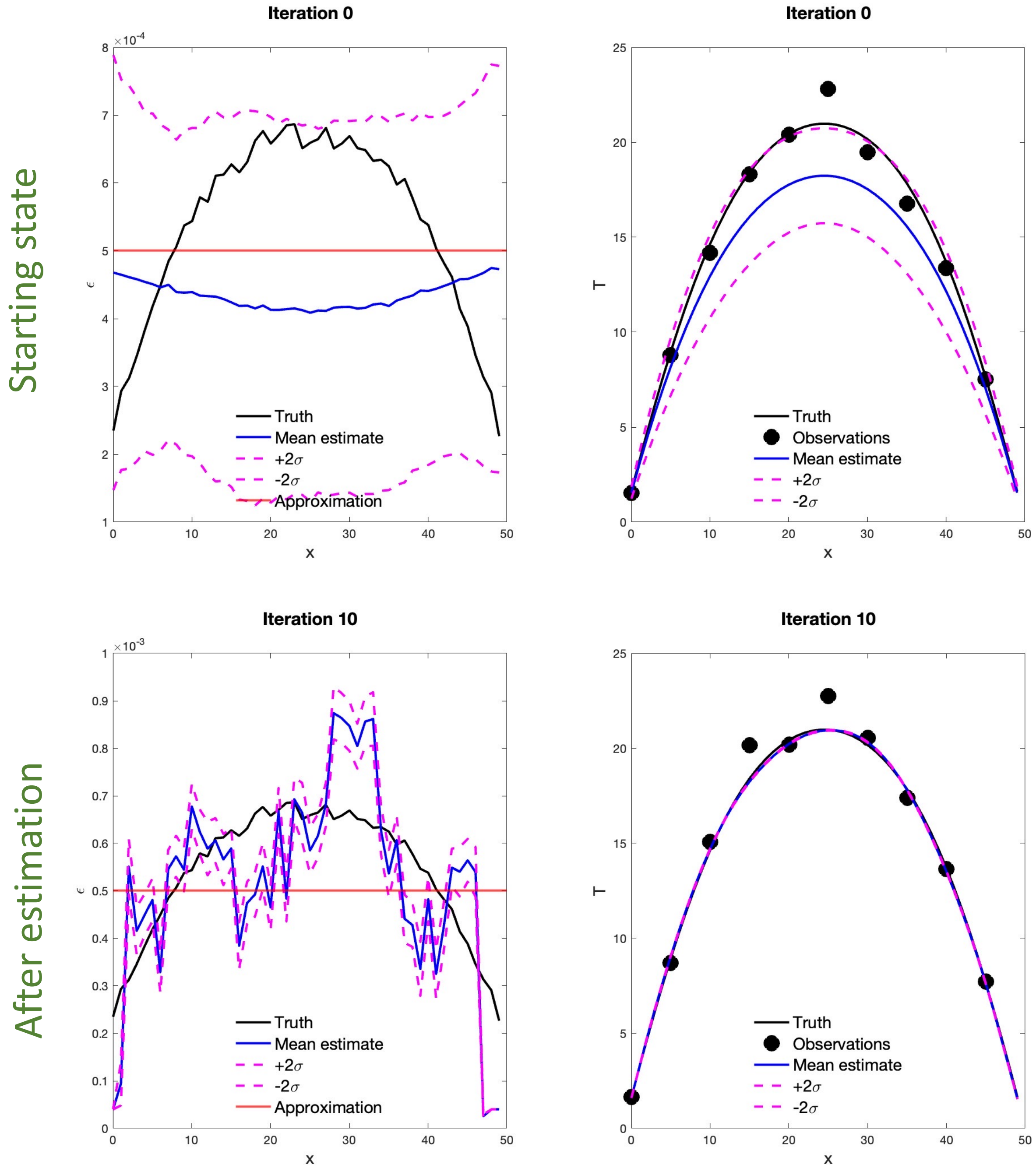
Given and simulated fields



Test B - results

- Prior: Huge variability in $\beta(x)$ ensemble
  - $\epsilon(x) = \beta(x)\epsilon_0$
- Posterior:
  - $\widehat{\epsilon(x)}$ nowhere near truth – multimodal!
  - $T^{(pred)}(x)$ is close to observations!
- What happened? Non-uniqueness of $\epsilon(x)$
  - $T^{(obs)}(x)$ could not constrain $\epsilon(x)$ into a unimodal shape
  - Unimodality was never enforced

Takeaway: *All prior constraints must be enforced during data assimilation*



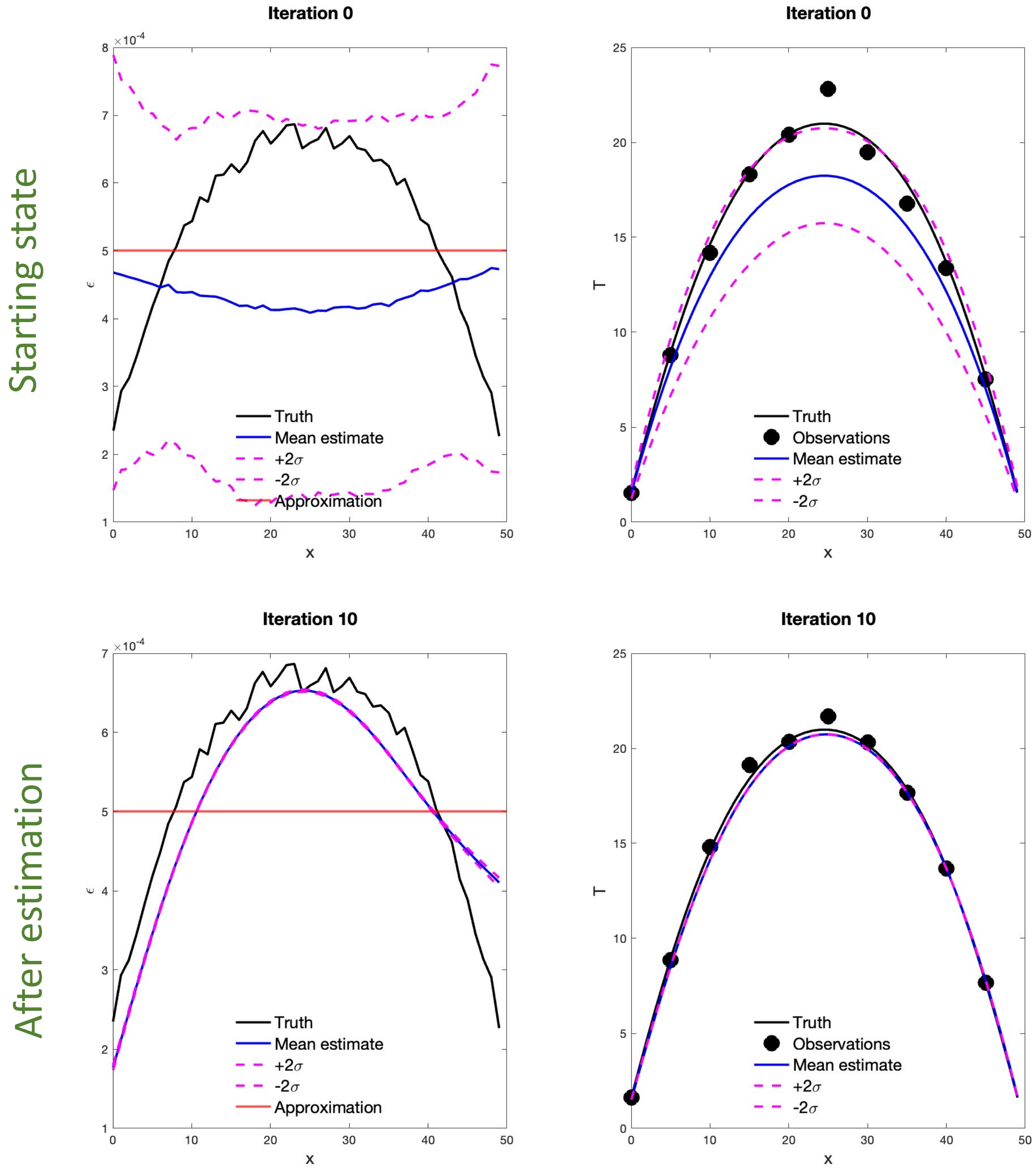
Test C – imposing prior constraints

- Aim: Ensure unimodality
- Hypothesis: Smoothing the (partially) estimated $\beta(x)$ at each step of the data assimilation process will "nudge" solution towards truth
- Recollect: $T^{(obs)}(x)$ obtained at M different points in time
  - Data assimilation is done over these M steps in (pseudo-) time
- Approach: Smooth $\beta(x)$ using the heat equation
  - $\beta_\tau = \nabla^2 \beta, \beta_\tau = 0$ at $x = (0, 1)$
  - Apply heat-equation smoother before assimilating $T^{(obs)}(x, \tau)$ at each of M time-steps
  - Integrate over $0 < \tau < \tau_{end}, \tau_{end} \approx 2\Delta x^2$

Test C - results

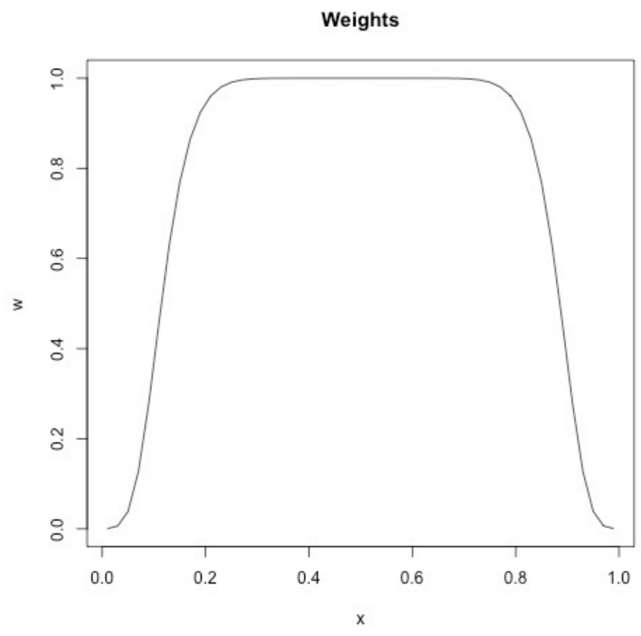
- Prior: Huge variability in $\beta(x)$ ensemble (same as Test B)
- Posterior:
  - $\widehat{\epsilon(x)}$ something like the truth
    - Unimodal and smooth
    - Shape not quite right
  - Wrong value at the boundaries
    - $T^{(obs)}(x)$ has little constraining effect there
  - $T^{(pred)}(x)$ is close to observations!

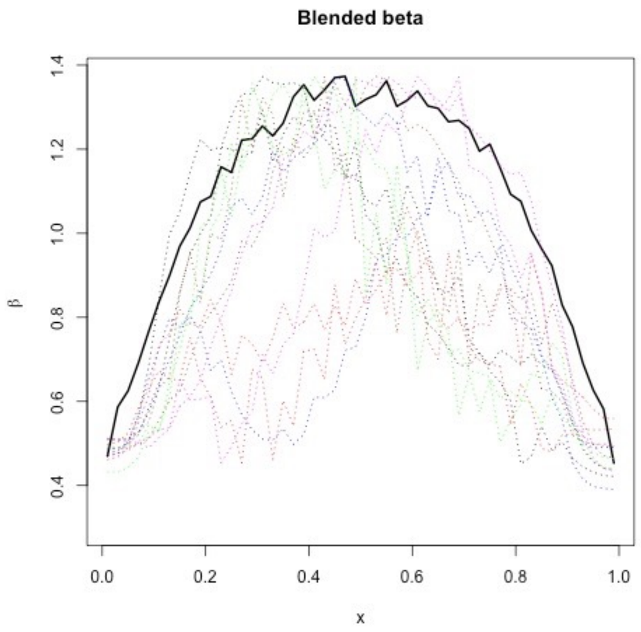
Takeaway:* *Imposing constraints at each step can nudge solution close to physical reality



Test D – impose boundary constraints

- Aim: Get the boundary values of $\widehat{\beta(x)}$ correctly
- Hypothesis: Boundary values could be known with some certainty i.e. $\beta(x = 0\ ) \sim N\left(\beta_l, \alpha^2 \beta_l^2\right)$, α is small
  - If so, this could be enforced in the starting ensemble of β(x)
- Justification: Boundaries could be far from the "action" and model-form errors could be small i.e. β ~ 1
- Approach
  - Generate realizations of (β_l, β_r)
  - Blend with realization of $\beta \sim N(1, \Gamma)$

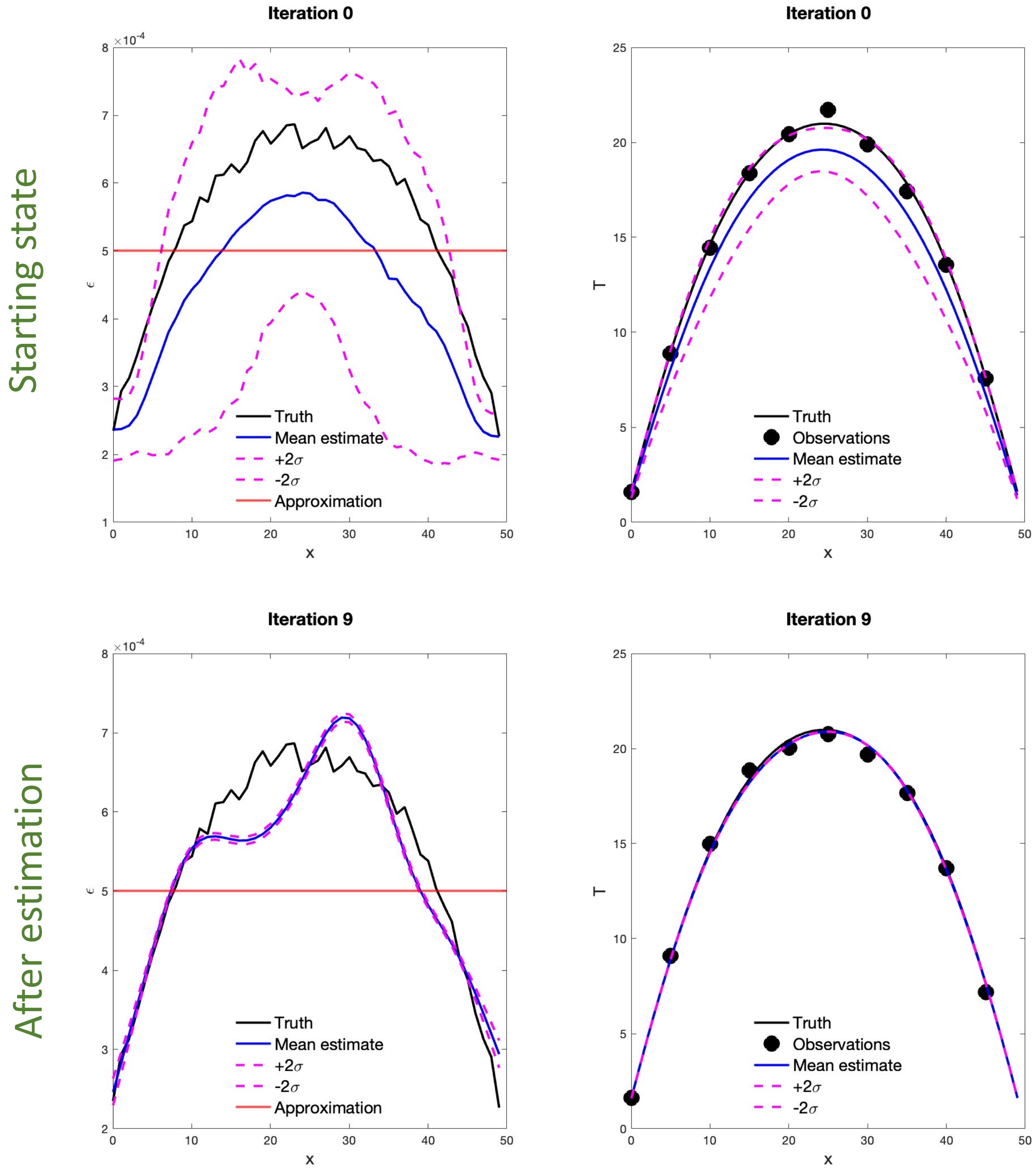




Test D - results

- Prior: Huge variability in $\beta(x)$ ensemble (same as Test B) but not at boundaries
- Posterior:
  - $\widehat{\epsilon(x)}$ something like the truth
    - Smooth, but nearly bimodal
    - Values agree with $\epsilon_{true}(x)$
  - Correct values at the boundaries
  - $T^{(pred)}(x)$ is close to observations!

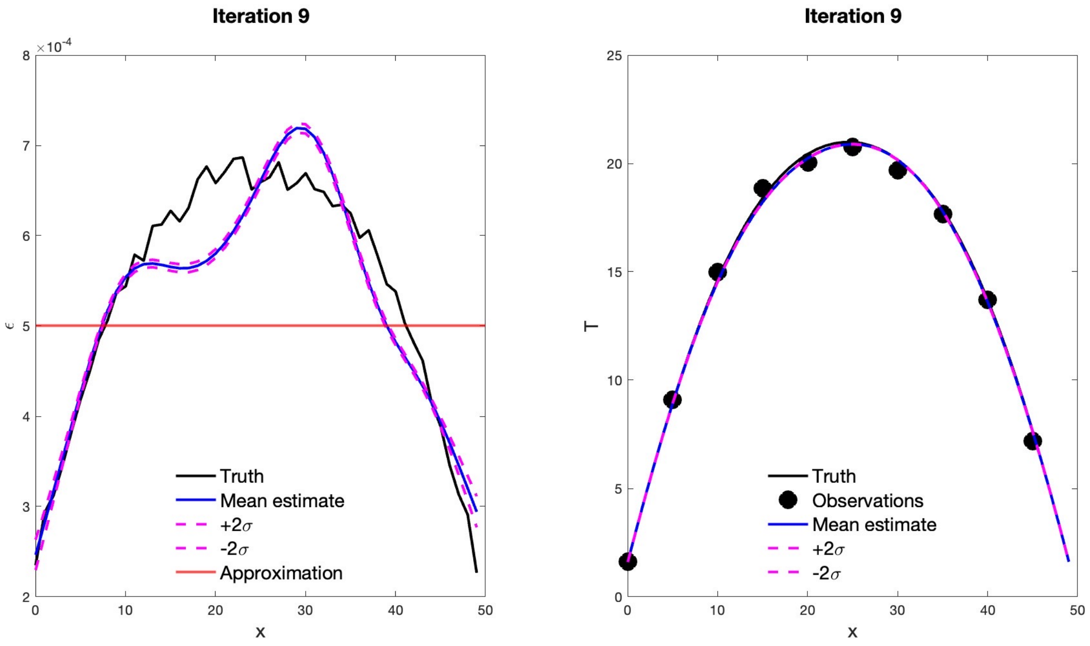
***Takeaway:* Obtaining a good solution requires imposing all the constraints – and it may not be possible in just the starting ensemble**



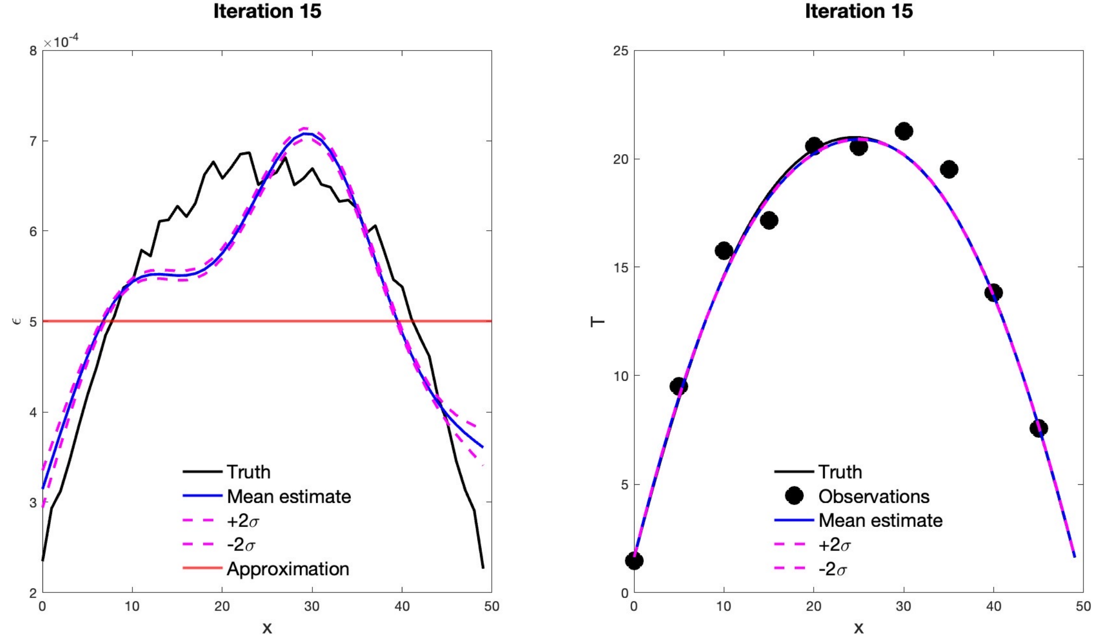
Sensitivity of β(x)

- What if we did this with half the sensors?
  - The estimate is not even symmetric
- Halved the measurement the noise?
  - Not much effect

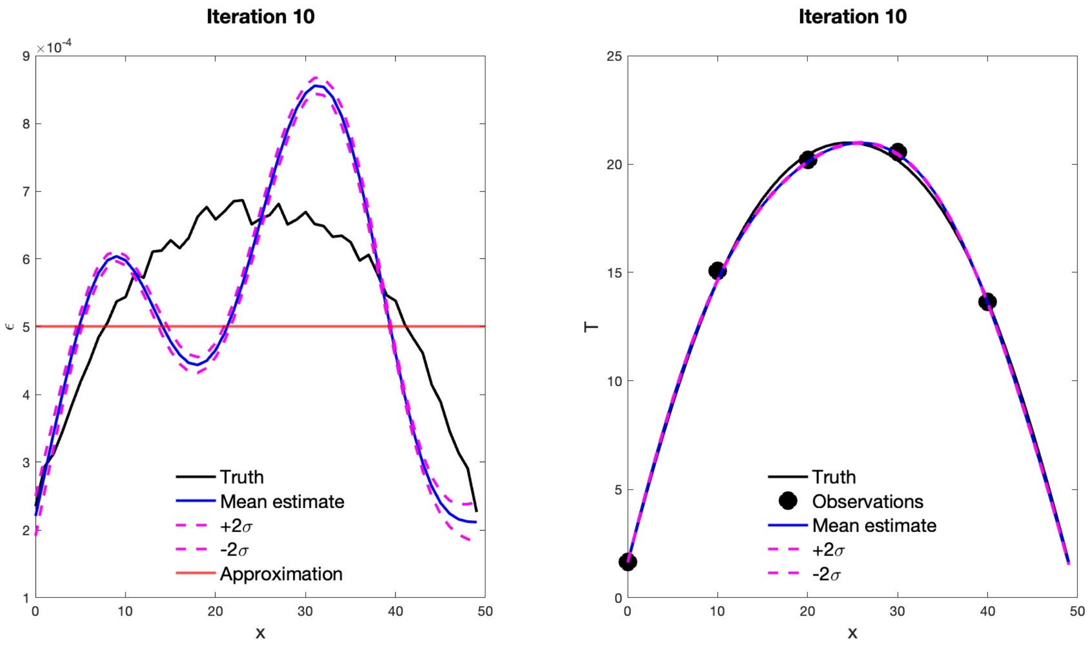
Half the noise



Original run: 10 sensors & 5% noise



5 sensors



Conclusions

- We’ve demonstrated a problem in the estimation of model-form error
  - Requires field estimation
- Method: Field estimation performed iteratively (in pseudo-time)
  - Using iterated ensemble Kalman filters
- Findings:
  - Plagued by non-uniqueness due to low information content in observations
  - Necessary to impose as many physical constraints as possible
    - Not usually hard in iterated EnKF, if they are known
  - Reducing noise did not help much. Increasing sensors helps.
    - Likely because they were too limited in any case

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