Uncertainty quantification for neural state-space models

Marco Forgione, Dario Piga

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Motivations

Neural state-space models are widely used for dynamical systems. We have also applied them to the nonlinear benchmarks!

M. Forgione and D.Piga. Continuous-time system identification with neural networks: model structures and fitting criteria. *European Journal of Control, 2021*

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Little focus so far on uncertainty quantification.

- What's our confidence in the model predictions?
- Can we detect model usage outside its validity range?

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`https://github.com/forgi86/sysid-neural-unc`

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Settings

The true system is assumed to have a state-space representation:

$$x^+ = f(x, u)$$
$$y^\circ = g(x),$$

with noisy discrete-time measurements available: $y = y^\circ + e$.

Training dataset $\mathcal{D}$: a single input/output sequence with:

- input samples $\boldsymbol{u} = \{u_1,\ u_1, \ldots,\ u_N\}$
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Objective: estimate a model of the system.

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Neural state-space models

A very generic neural model structure:

$$x^+ = \mathcal{N}_f(x, u;\ \theta)$$
$$y = \mathcal{N}_g(x; \theta)$$

where $\mathcal{N}_f$, $\mathcal{N}_g$ are feed-forward neural networks, e.g.:

$$\mathcal{N}(z) = W_2\sigma\left(W_1 z + b_1\right) + b_2$$
$$\theta = \text{vec}(W_1, b_1, W_2, b_2)$$
$\sigma(\cdot)$ static non-linearity

Can be specialized, according to available system knowledge:

- State fully observed $\Rightarrow$

$$x^+ = \mathcal{N}_f(x, u;\ \theta)$$
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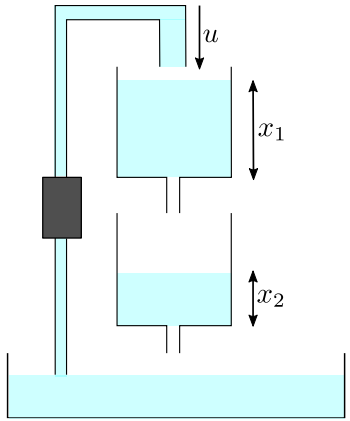
Neural state-space models

Physics-inspired model structures

Two-tank system. Input: flow u in upper tank, output: lower tank level x_2.

- The system has two states: x_1 and x_2
- State x_1 does not depend on x_2
- State x_2 does not depend directly on u
- The state x_2 is measured



These observations are embedded in the physics-inspired neural model:

$$\dot{x}_1 = \mathcal{N}_1(x_1, u;\ \theta)$$
$$\dot{x}_2 = \mathcal{N}_2(x_1, x_2;\ \theta)$$
$$y = x_2$$

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Bayesian Framework

We can frame model learning problem in a Bayesian framework:

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\begin{aligned}
x^+ &= \mathcal{N}_f(x, u; \theta) \\
\hat{y} &= \mathcal{N}_g(x; \theta) \\
y &= \hat{y} + e \\
\theta &\sim \mathcal{N}\left(0, \sigma_\theta^2\right), \quad e \sim \mathcal{N}\left(0, \sigma_e^2\right)
\end{aligned}
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Then, there exist the posterior of θ given observed data $\mathcal{D} = \{\boldsymbol{u}, \boldsymbol{y}\}$ ...

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p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})},
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... and the posterior on a new sequence $\boldsymbol{y}^*$, given input sequence $\boldsymbol{u}^*$:

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p(\boldsymbol{y}^*|\boldsymbol{u}^*, \mathcal{D}) = \int_{\theta \in \Theta} p(\boldsymbol{y}^*|\boldsymbol{u}^*, \theta) p(\theta|\mathcal{D}) \, d\theta
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Challenges

- What are good Bayesian models structures (architecture + priors)?
  - What families of dynamical systems are likely under given assumptions?
- How to obtain the posterior parameter distribution $p(\theta|\mathcal{D})$ and of the posterior predictive distribution $p(\boldsymbol{y}^*|\boldsymbol{u}^*, \mathcal{D})$?
  - $p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$ is accessible up to the denominator constant.
  - $p(\boldsymbol{y}^*|\boldsymbol{u}^*, \mathcal{D}) = \int_{\theta\in\Theta} p(\boldsymbol{y}^*|\boldsymbol{u}^*, \theta)p(\theta|\mathcal{D})\, d\theta$ is a hard multi-dimensional integral anyway...

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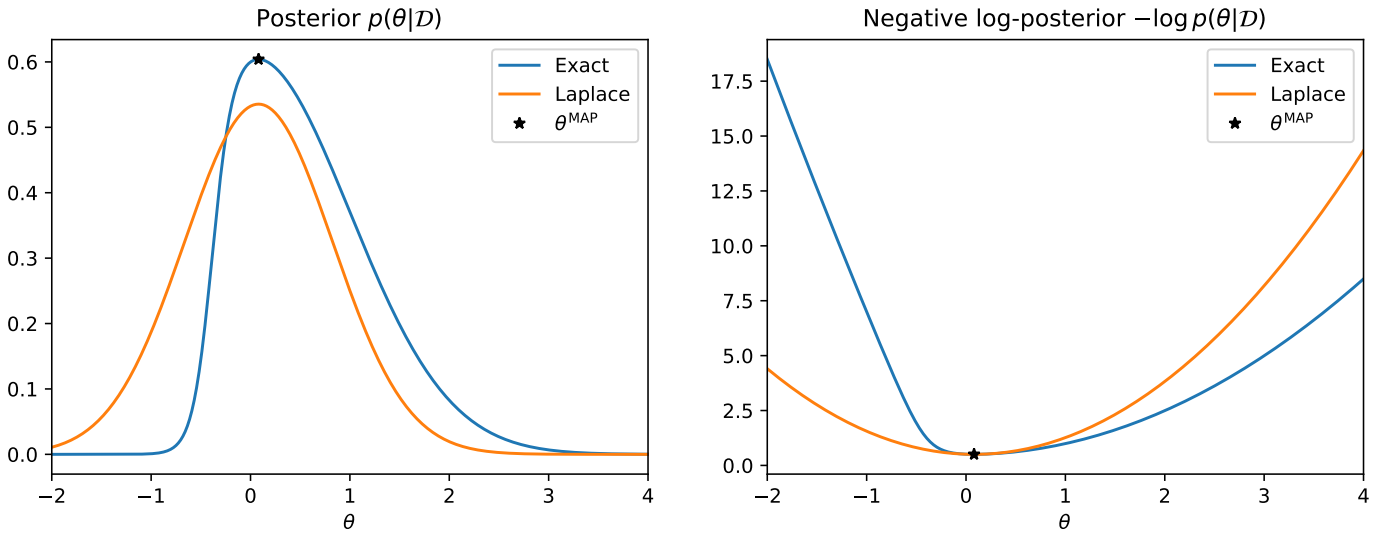
Laplace approximation

Quadratic approximation of the (negative) log-posterior around a *mode*, leading to a Gaussian parameter posterior approximation.



Requires computation of:

- A point estimate $\Rightarrow$ maximimum θ^{MAP} of $\log p(\theta|\mathcal{D})$
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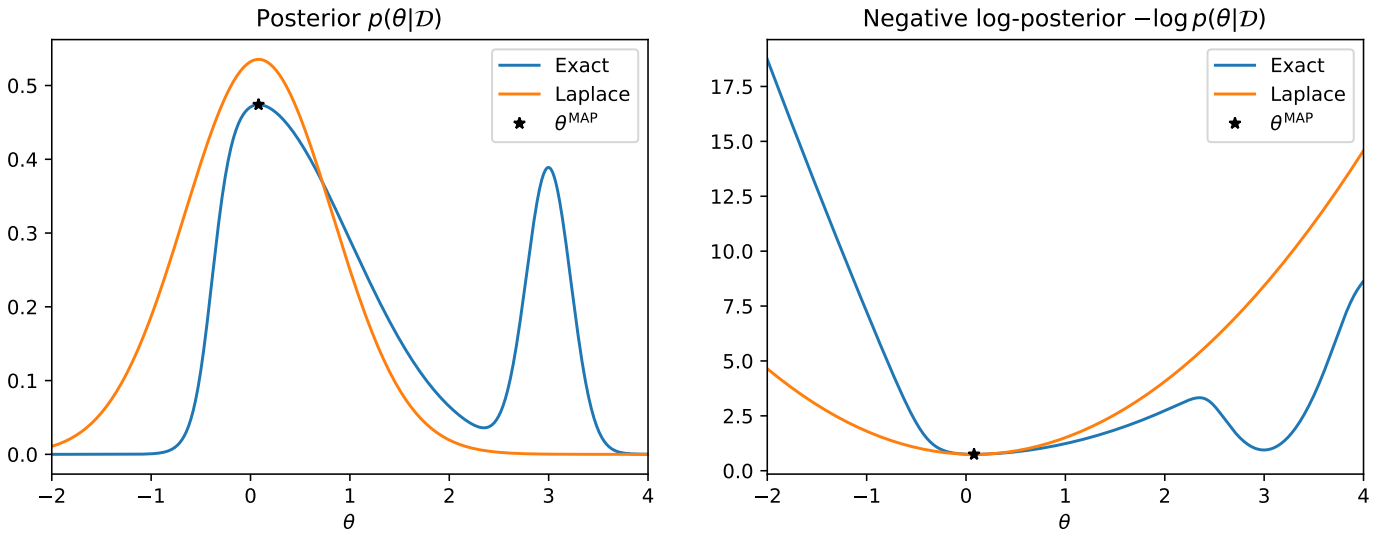

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Laplace method + Linearization

Tested for small ($\approx$ 400 params) neural state-space models:

- Posterior parameter distribution approximated with Laplace's method. $p(\theta|\mathcal{D})$ Gaussian with covariance:

$$P_\theta^{-1} = H = \frac{I}{\sigma_\theta^2} + \frac{1}{\sigma_e^2} \sum_{k=0}^{N-1} \frac{\partial y_k}{\partial \theta} \frac{\partial y_k}{\partial \theta}^\top .$$

  - Gauss-Newton (GN) approximation for the log-likelihood Hessian H
  - Could also be seen as the Fisher matrix in a frequentist setting

- Posterior predictive distribution $p(\boldsymbol{y}^*|\boldsymbol{u}, \mathcal{D})$ based on linearization
  Predictions also Gaussian, centered about nominal $\hat{\boldsymbol{y}}^*$, covariance:

$$\Sigma_{\boldsymbol{y}^*} = J^* P_\theta J^{*\top}$$

Technical challenge: fast computation of the Hessian extending methods recently developed in another work.

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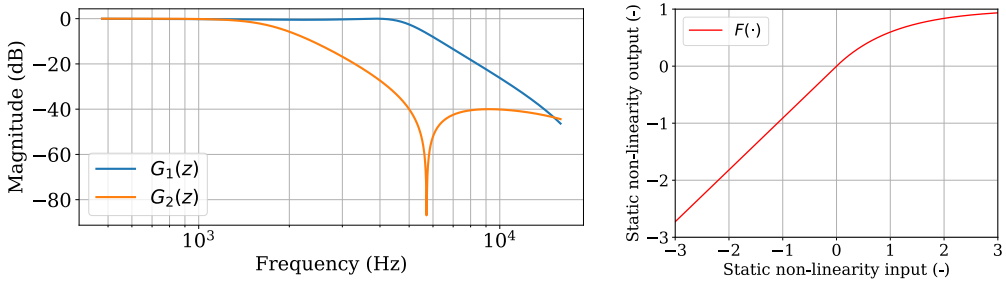
Results: synthetic WH benchmark

Methodology tested on a simulated Wiener-Hammerstein system

model:

$$x^+ = \mathcal{N}_f(x, u; \theta)$$
$$\hat{y} = \mathcal{N}_g(x; \theta)$$

system: $G_1(z) \Rightarrow F(\cdot) \Rightarrow G_2(z)$



$\mathcal{N}_f, \mathcal{N}_g$: 1 hidden layer, 15 neurons + linear term, as in previous literature

Training on a multisine with std 0.4, bandwidth [0 2] kHz, 10K samples.

Testing on:

1. A multisine with std 0.4, bandwidth [0 2] kHz
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We expect lower performance and higher uncertainty on signals 3 and 4.

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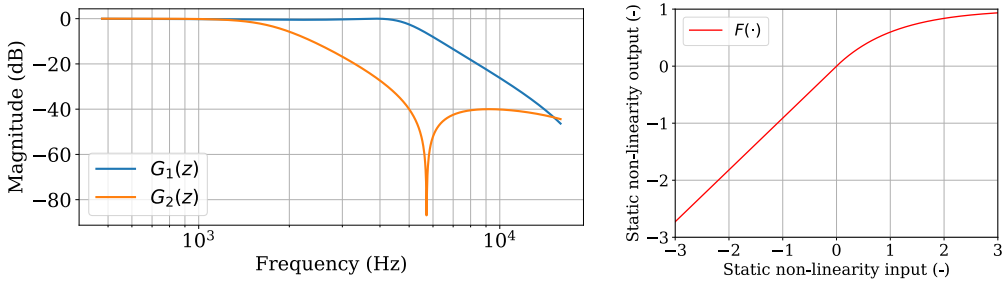

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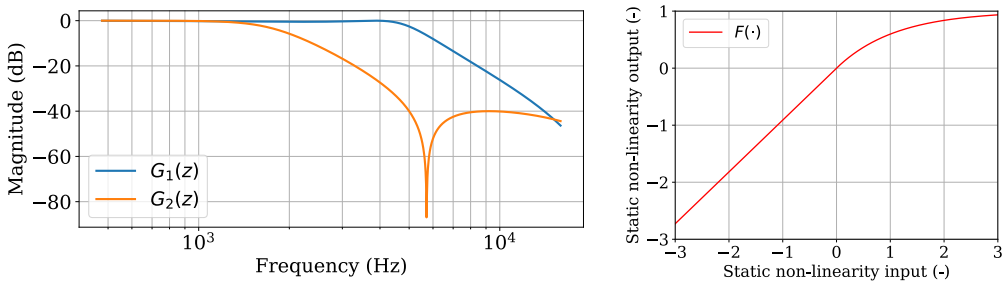

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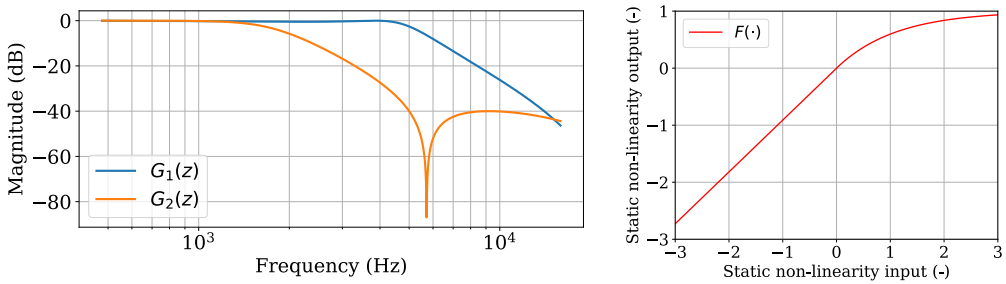

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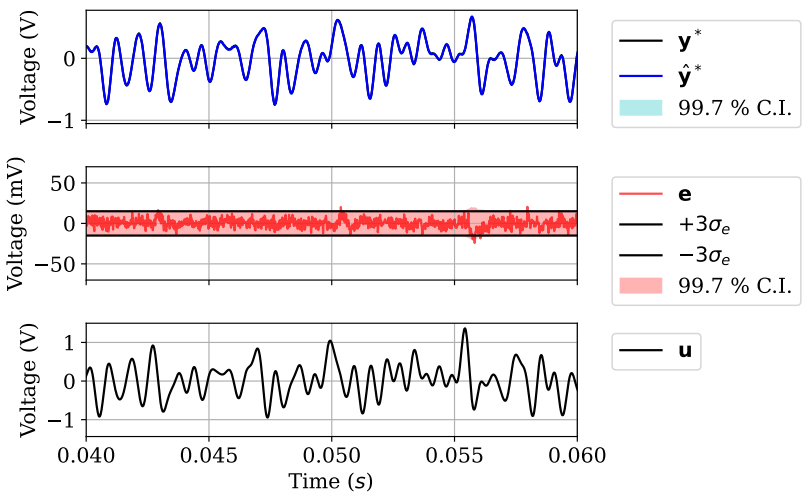
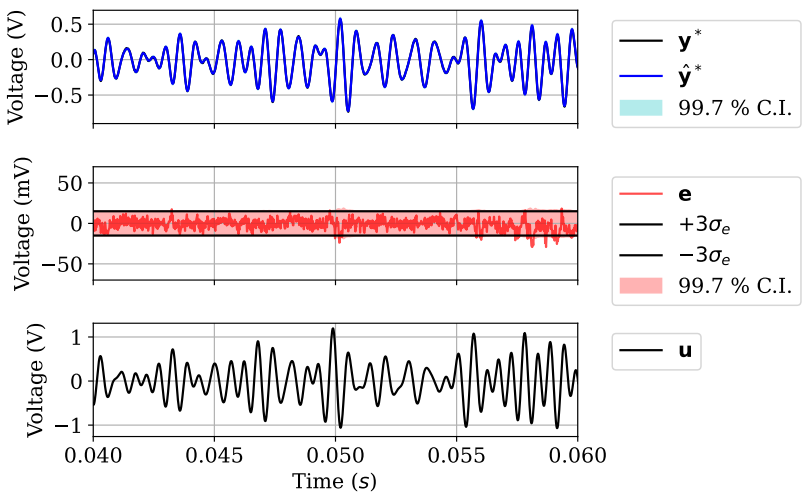
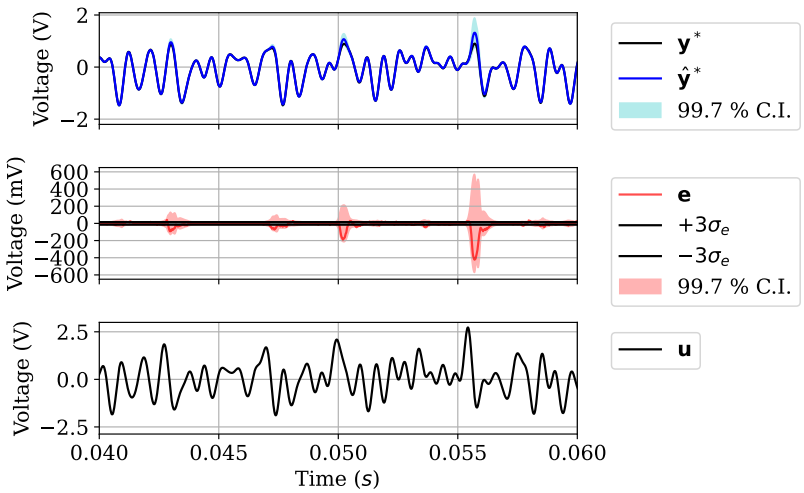


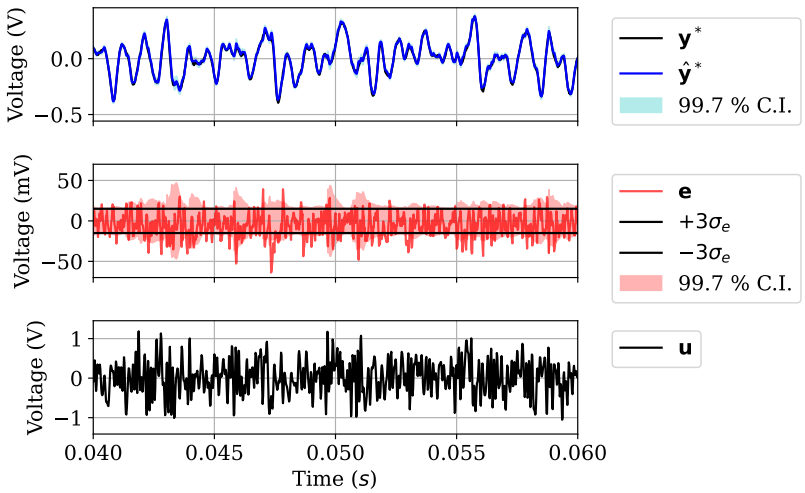
Test signal 2



Test signal 3



Test signal 4

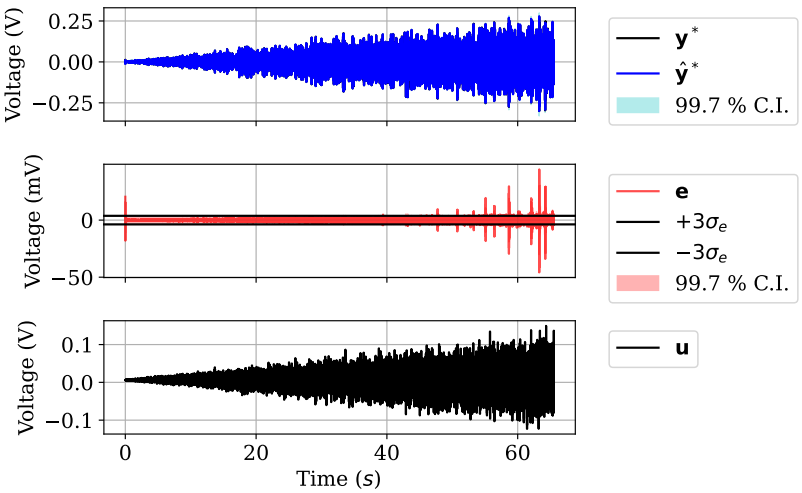


Credible intervals get indeed wider for test signals 3 and 4!

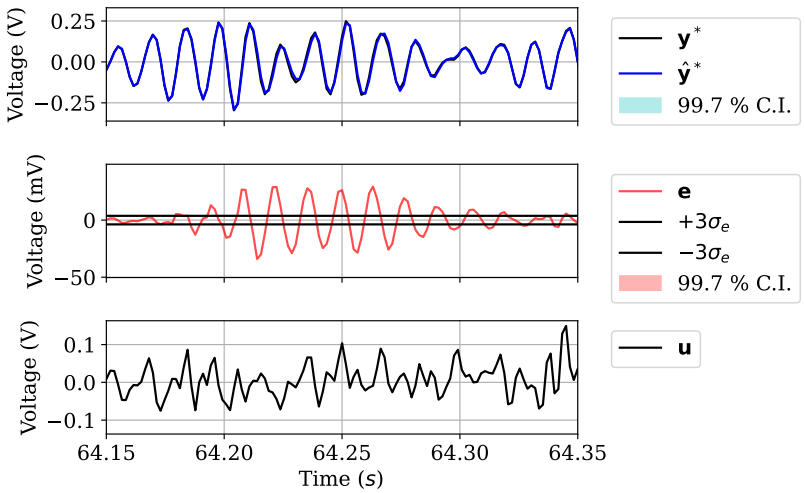
Results: Silverbox benchmark

Methodology also tested on the original Silverbox dataset

Test set (full)



Test set (zoom)



- Large errors towards the end of the ramp test signal (left plot)
- Credible intervals useful, though not calibrated (right plot)

Large values not seen in training, therefore high uncertainty towards the end of the ramp.

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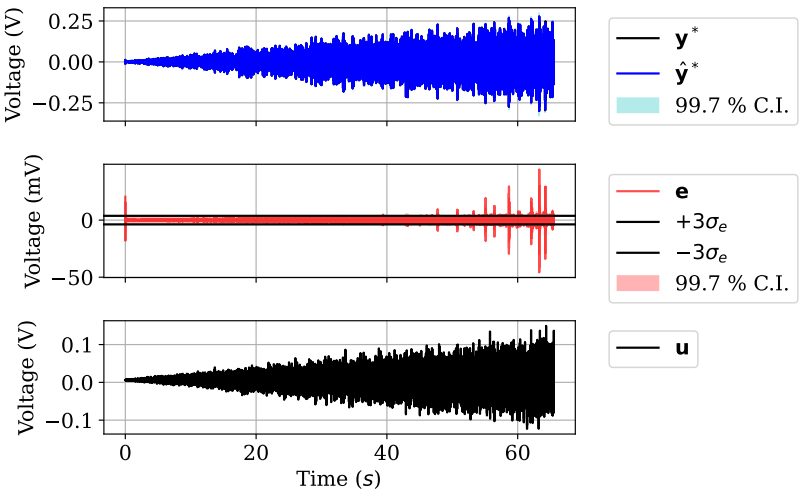
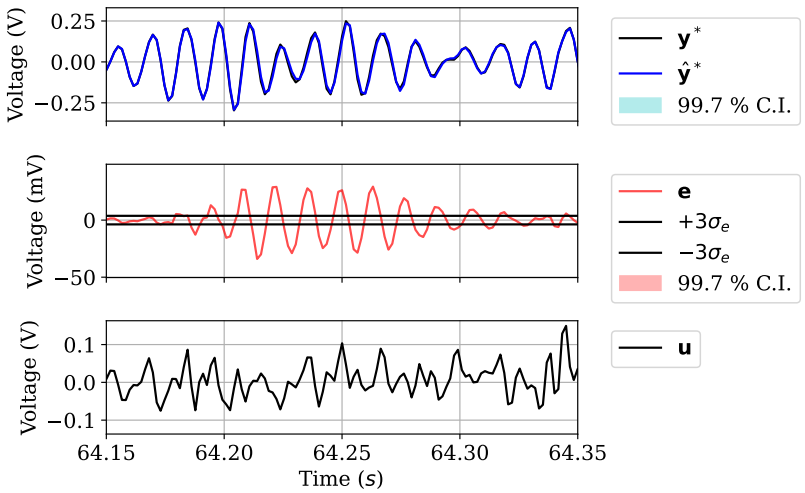


Test set (zoom)



- Large errors towards the end of the ramp test signal (left plot)
- Credible intervals useful, though not calibrated (right plot)

Large values not seen in training, therefore high uncertainty towards the end of the ramp.

Conclusions

Preliminary uncertainty quantification for neural state-space models.

- In a Bayesian Framework
- Using the simplest inference techniques

Obtained credible intervals not well calibrated, but allow one to detect out-of-distribution regimes.

Large room for improvement, both in the theoretical framework and in the approximate inference engine. Benchmarks and metrics also to be devised!

Open opportunity: to exploit the uncertainty for Experiment Design!

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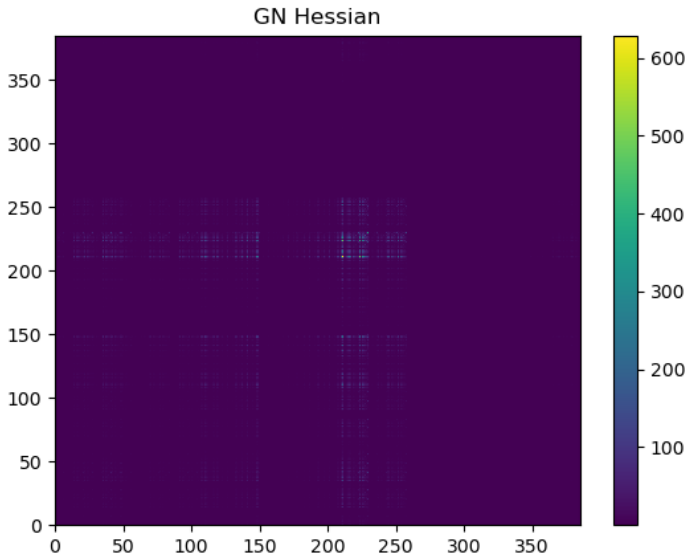
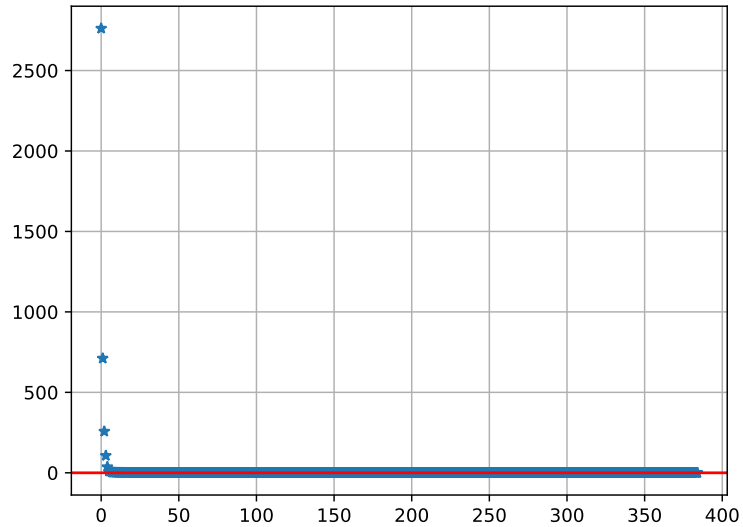
Bonus topic: Hessian Matrix Analysis

Wiener-Hammerstein: Hessian matrix at optimum:

GN Hessian Matrix abs



GN Hessian Matrix eigenvalues

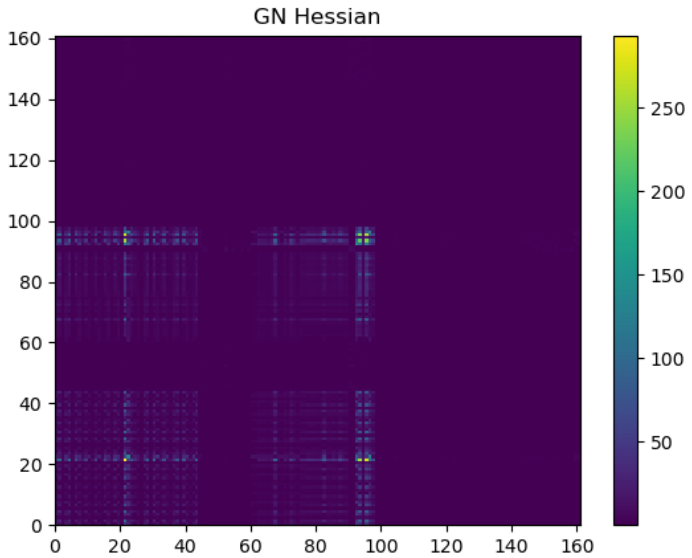


The Hessian is non-degenerate only in ~ 7 directions.

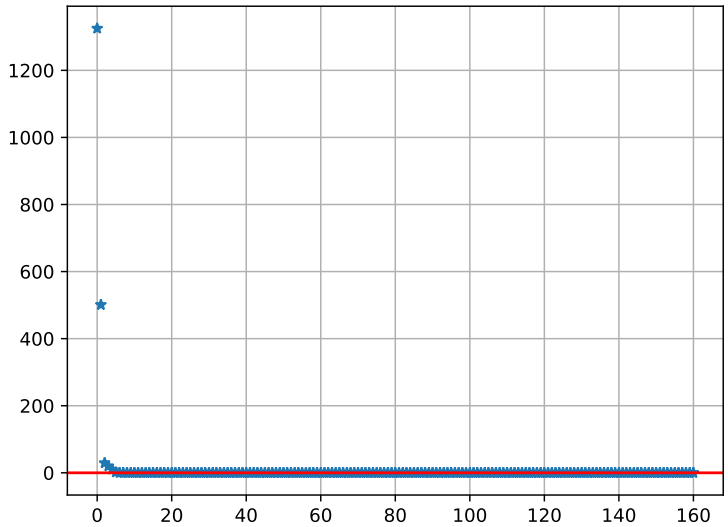
Bonus topic: Hessian Matrix Analysis

Silverbox: Hessian matrix at optimum:

GN Hessian Matrix abs



GN Hessian Matrix eigenvalues



The Hessian is non-degenerate only in $\sim$ 6 directions.

Thank you.
Questions?

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