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Extending relevance vector machine to resolve overfitting during Bayesian calibration in nonlinear stochastic dynamics

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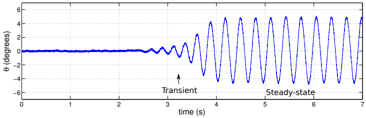
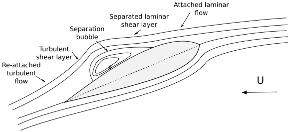
Nonlinear aeroelastic oscillator - overfitting issue

- Aeroelastic limit-cycle oscillation (LCO) (Sandhu et. al, CMAME, 2014; Sandhu et. al, JCP, 2016)





Sandhu et. al, CMAME, 2014; Sandhu et. al, JCP, 2016 (with copyright permission)

- Identify the best model for C_M:

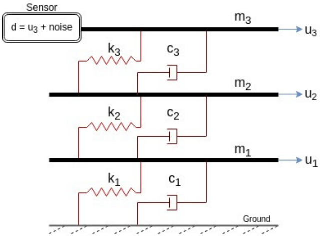
$$\mathcal{M}_1: \quad C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + \sigma\xi(\tau)$$

$$\mathcal{M}_2: \quad \frac{\dot{C}_M}{B} + C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + \frac{c_6}{B}\ddot{\theta} + \sigma\xi(\tau)$$

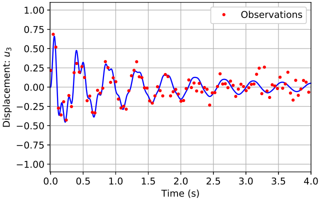
$$\mathcal{M}_3: \quad \frac{\ddot{C}_M}{B_1B_2} + \frac{(B_1+B_2)\dot{C}_M}{B_1B_2} + C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + \frac{(2c_6c_7+0.5)\ddot{\theta}}{B_1B_2} + \frac{c_6\dddot{\theta}}{B_1B_2} + \sigma\xi(\tau)$$

Problem definition: Mass-spring-damper system

- Inverse problem: Estimate a probability density function (pdf) of damping and stiffness parameters while identifying the sparsity in damping parameters. (Sandhu *et al.*, JCP, 2021)



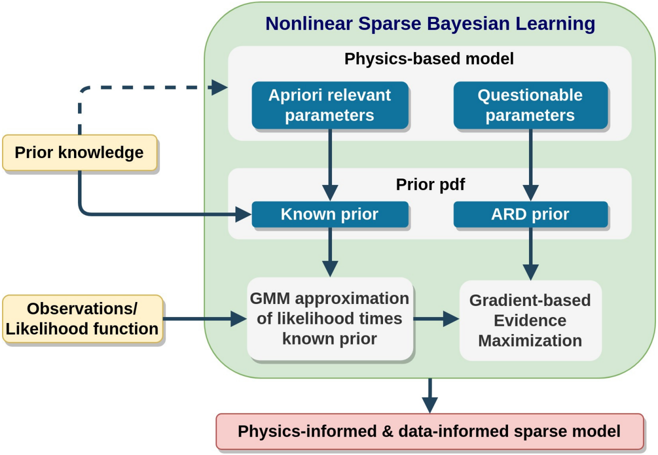
(a) Three-dof mass-spring-damper model.



(b) Measured versus true response.

Sandhu et. al, JCP, 2021 (with copyright permission)

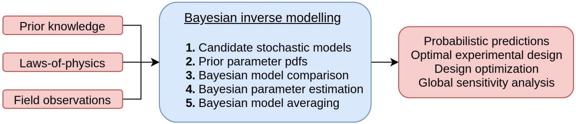
Nonlinear sparse Bayesian learning



Sandhu et. al, JCP, 2021 (with copyright permission)

Bayesian inverse modelling

- Overview of the Bayesian framework



- **Bayesian model comparison**: Ranking of plausible models is based on model evidence,

$$p(\mathcal{D}) = \int p(\mathcal{D}|\phi)p(\phi)d\phi \quad , \quad \underbrace{\ln p(\mathcal{D})}_{\text{Log-evidence}} = \underbrace{E[\ln p(\mathcal{D}|\phi)]}_{\text{Data-fit}} - \underbrace{E\left[\ln \frac{p(\phi|\mathcal{D})}{p(\phi)}\right]}_{\text{Model complexity}}$$

Nonlinear sparse Bayesian learning (NSBL): Methodology

- Stochastic state-space model structure:

$$\text{Model equation}: \quad \mathbf{u}_{k+1} = \mathbf{g}_k(\mathbf{u}_k, \mathbf{f}_k, \mathbf{q}_k; \phi)$$
$$\text{Measurement equation}: \quad \mathbf{d}_k = \mathbf{h}_k(\mathbf{u}_k, \epsilon_k; \phi)$$

- Parameter prior pdf: hybrid assignment ($\boldsymbol{\alpha}$: Hyper-parameters)

$$\phi = \{\phi_\alpha, \phi_{\text{-}\alpha}\} \;\; ; \;\; p(\phi|\boldsymbol{\alpha}) = p(\phi_{\text{-}\alpha})p(\phi_\alpha|\boldsymbol{\alpha}) = \underbrace{p(\phi_{\text{-}\alpha})}_{\text{Known prior}} \underbrace{\prod \mathcal{N}\left(\phi_i|0, \alpha_i^{-1}\right)}_{\text{ARD prior}}$$

- Entity $p(\mathcal{D}|\phi)\, p(\phi_{\text{-}\alpha})$ remains unchanged during sparse learning!

$$p(\phi|\mathcal{D}, \boldsymbol{\alpha}) = \frac{p(\mathcal{D}|\phi)p(\phi|\boldsymbol{\alpha})}{p(\mathcal{D}|\boldsymbol{\alpha})} \propto \underbrace{p(\mathcal{D}|\phi)\, p(\phi_{\text{-}\alpha})}_{\text{Independent of } \boldsymbol{\alpha}} \mathcal{N}(\phi_\alpha|\mathbf{0}, \mathbf{A}^{-1})$$

- Gaussian mixture model (GMM) approximation:

$$p(\mathcal{D}|\phi)p(\phi_{\text{-}\alpha}) \approx \sum_{k=1}^{K} a^{(k)} \mathcal{N}(\phi|\boldsymbol{\mu}^{(k)}, \boldsymbol{\Sigma}^{(k)}),$$

NSBL: Semi-analytical Bayesian framework

Entity	Solution
Parameter decomposition	$\phi = \{\phi_{\alpha}, \phi_{\text{-}\alpha}\}$
Likelihood + known prior	$p(\mathcal{D}\,\vert\,\phi)p(\phi_{\text{-}\alpha}) \approx \sum_{k=1}^{K} a^{(k)} \mathcal{N}(\phi\,\vert\,\boldsymbol{\mu}^{(k)}, \boldsymbol{\Sigma}^{(k)})$
ARD prior	$p(\phi_{\alpha}\,\vert\,\boldsymbol{\alpha}) = \mathcal{N}(\phi_{\alpha}\,\vert\,\mathbf{0}, \mathbf{A}^{-1})$
Hyper-parameter prior	$p(\boldsymbol{\alpha}) = \prod_{i=1}^{N_{\alpha}} \mathcal{G}(\alpha_i\,\vert\,r_i, s_i)$
Model evidence	$\hat{p}(\mathcal{D}\,\vert\,\boldsymbol{\alpha}) = \sum_{k=1}^{K} a^{(k)} \mathcal{N}(\boldsymbol{\mu}_{\alpha}^{(k)}\,\vert\,\mathbf{0}, \mathbf{B}_{\alpha}^{(k)})$; $\mathbf{B}_{\alpha}^{(k)} = \boldsymbol{\Sigma}^{(k)} + \mathbf{A}^{-1}$
Parameter posterior PDF	$\hat{p}(\phi\,\vert\,\mathcal{D}, \boldsymbol{\alpha}) = \sum_{k=1}^{K} w^{(k)} \mathcal{N}(\phi\,\vert\,\mathbf{m}^{(k)}, \mathbf{P}^{(k)})$; $w^{(k)} = \dfrac{a^{(k)} \mathcal{N}(\boldsymbol{\mu}_{\alpha}^{(k)}\,\vert\,\mathbf{0}, \mathbf{B}_{\alpha}^{(k)})}{\hat{p}(\mathcal{D}\,\vert\,\log \boldsymbol{\alpha})}$
Objective function	$\mathcal{L}(\log \boldsymbol{\alpha}) = \log \hat{p}(\mathcal{D}\,\vert\,\log \boldsymbol{\alpha}) + \sum_{i=1}^{N_{\alpha}} (r_i \log \alpha_i - s_i \alpha_i)$
Gradient of $\mathcal{L}(\log \boldsymbol{\alpha})$	$g_i(\log \boldsymbol{\alpha}) = \sum_{k=1}^{K} w^{(k)} v_i^{(k)} + r_i - s_i \alpha_i = \bar{v}_i + r_i - s_i \alpha_i$ $v_i^{(k)} = (\gamma_i^{(k)} - \alpha_i (m_i^{(k)})^2)/2$; $\gamma_i^{(k)} = 1 - \alpha_i P_{ii}^{(k)}$
Hessian of $\mathcal{L}(\log \boldsymbol{\alpha})$	$H_{ij}(\log \boldsymbol{\alpha}) = \sum_{k=1}^{K} w^{(k)} \left[\alpha_i \alpha_j \left(\dfrac{(P_{ij}^{(k)})^2}{2} + m_i^{(k)} m_j^{(k)} P_{ij}^{(k)} \right) + v_i^{(k)} v_j^{(k)} - \bar{v}_i \bar{v}_j \right] + \delta_{ij} \left[\bar{v}_i - \dfrac{1}{2} - s_i \alpha_i \right]$

Sandhu et. al, JCP, 2021 (with copyright permission)

NSBL: Numerical Implementation

- Stage 1: GMM construction by sampling $p(\mathcal{D}|\phi)p(\phi_{\text{-}\alpha})$ and then utilizing
  - Kernel density estimation (KDE): Computationally expedient, # of kernels = # of samples (Our choice)
  - Expectation maximization (EM): More involved, smaller # of kernels (Not pursued here)
- Stage 2: Newton's method to maximize model evidence (**non-convex optimization**):

$$\log \boldsymbol{\alpha}_{j+1} = \log \boldsymbol{\alpha}_j + \beta_j \mathbf{p}_j \ , \text{ where } \ \mathbf{H}_j \mathbf{p}_j = -\mathbf{g}_j$$

  - Modified Newton method
  - Trust-region Newton method (Our choice)
- Stage 3: Sparsity identification by exploiting relevance indicator, defined as

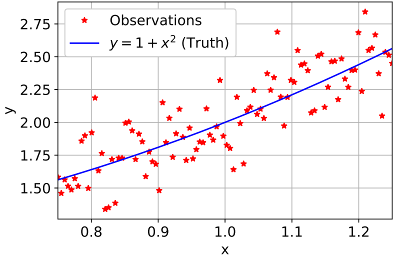
$$\gamma_i^{(k)} = 1 - \frac{\alpha_i}{(P_{ii}^{(k)})^{-1}} = 1 - \frac{\alpha_i}{\alpha_i + \{(\boldsymbol{\Sigma}_\alpha^{(k)})^{-1}\}_{(i,i)}} \in [0, 1], \qquad (1)$$

NSBL: Benefits

- Benefits of NSBL over standard Bayesian model updating
  - Evidence-based pruning of redundant parameters while incorporating prior parametric knowledge
  - Parameter posterior pdf and model evidence available semi-analytically
  - Gradient and Hessian of evidence with respect to hyper-parameters available analytically
  - Can handle non-Gaussian and multimodal pdfs

Example: Polynomial Regression with Multimodal Prior

- Generated observations using $y_i = 1 + x_i^2 + \epsilon_i$, where ϵ_i is a Gaussian white noise process with distribution $\mathcal{N}(\epsilon_i|0, 0.04)$. (Sandhu *et al.*, JCP, 2021)



Sandhu et. al, JCP, 2021 (with copyright permission)

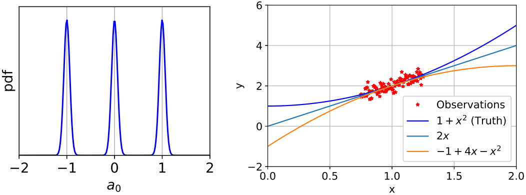
- The observational data consists of 100 noisy samples with equally spaced coordinate x within the domain $x \in [0.75, 1.25]$

Example: Polynomial Regression with Multimodal Prior

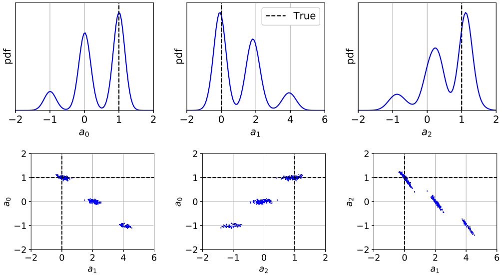
- Inverse problem setup: (Sandhu *et al.*, JCP, 2021, with copyright permission)

Proposed model	$y = a_0 + a_1 x + a_2 x^2 + \epsilon \;\; ; \;\; \epsilon \sim \mathcal{N}(0, 0.04)$
ϕ decomposition	$\phi_\alpha = \{a_1, a_2\} \; , \quad \phi_{\text{-}\alpha} = \{a_0\}$
ARD prior, $p(\phi_\alpha \vert \alpha)$	$\mathcal{N}(a_1 \vert 0, \alpha_1^{-1}) \; \mathcal{N}(a_2 \vert 0, \alpha_2^{-1})$
Known prior, $p(\phi_{\text{-}\alpha})$	$\left[\mathcal{N}(a_0 \vert \text{-}1, 0.2^2) + \mathcal{N}(a_0 \vert 0, 0.2^2) + \mathcal{N}(a_0 \vert 1, 0.2^2)\right] / 3$

- Non-Gaussian prior knowledge: (Sandhu *et al.*, JCP, 2021, with copyright permission)



- Stage 1 (GMM construction): 2500 samples distributed according to $p(\mathcal{D}|\phi)p(\phi_{-\alpha})$ or $p(\mathcal{D}|a_0, a_1, a_2)p(a_0)$ using TMCMC, followed by a GMM construction using KDE (Sandhu *et al.*, JCP, 2021, with copyright permission)

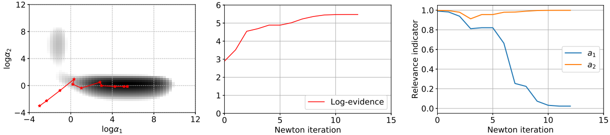


SBL and BCS are not applicable for multimodal/Non-Gaussian posterior pdfs!

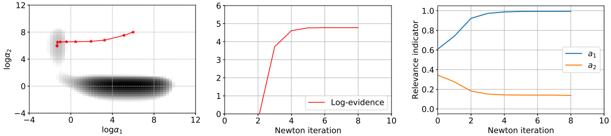
Example: Polynomial Regression with Multimodal Prior

Stage 2: Sparsification (Sandhu *et al.*, JCP, 2021, with copyright permission)

- Initialized at $\log \boldsymbol{\alpha} = \{-3, -3\}$, NSBL suggests a_1 is irrelevant and a_2 is relevant.



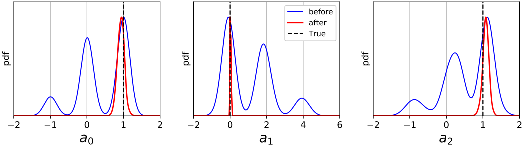
- Iteration initialized at $\log \boldsymbol{\alpha} = \{6, 8\}$, NSBL suggests a_1 is relevant and a_2 is irrelevant.



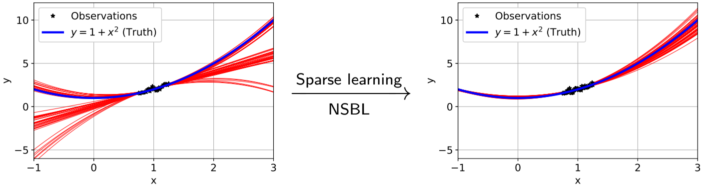
Multistart is necessary!

Example: Polynomial Regression with Multimodal Prior

- Posterior parameter pdf post sparse learning: (Sandhu *et al.*, JCP, 2021, with copyright permission)

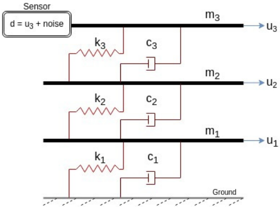


- Predictions before and after sparse learning: (Sandhu *et al.*, JCP, 2021, with copyright permission)

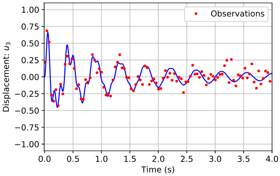


Example: Mass-spring-damper system

- Displacement vector $\mathbf{u} = \{u_1, u_2, u_3\}$; equation-of-motion $\mathbf{M\ddot{u}} + \mathbf{C\dot{u}} + \mathbf{Ku} = 0$ (Sandhu *et al.*, JCP, 2021, with copyright permission)



(c) Three-dof mass-spring-damper model.



(d) Measured versus true response.

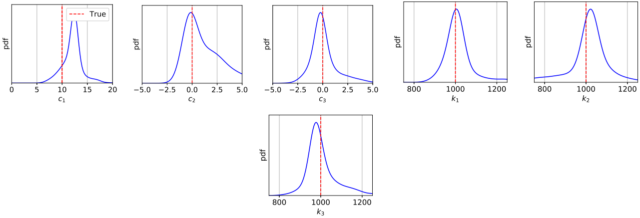
- Parameter true values:
  - Mass: $m_1 = m_2 = m_3 = 1.0$,
  - Stiffness: $k_1 = k_2 = k_3 = 1000.0$,
  - Damping: $c_1 = 10$, $c_2 = 0$, $c_3 = 0$.

- Inverse problem setup: (Sandhu *et al.*, JCP, 2021, with copyright permission)

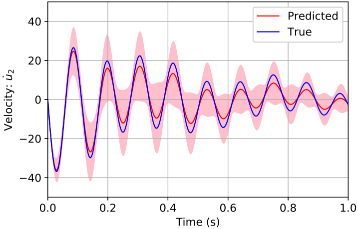
Proposed model	$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{0}$
ϕ decomposition	$\phi_\alpha = \{c_1, c_2, c_3\}$, $\phi_{\text{-}\alpha} = \{k_1, k_2, k_3\}$
Known prior, $p(\phi_{\text{-}\alpha})$	$\mathcal{U}(k_1\|0, 5000)\, \mathcal{U}(k_2\|0, 5000)\, \mathcal{U}(k_3\|0, 5000)$
ARD prior, $p(\phi_\alpha\|\boldsymbol{\alpha})$	$\mathcal{N}(c_1\|0, \alpha_1^{-1})\, \mathcal{N}(c_2\|0, \alpha_2^{-1})\, \mathcal{N}(c_3\|0, \alpha_3^{-1})$
Hyperprior, $p(\boldsymbol{\alpha})$	$\prod_{i=1}^{3} \mathcal{G}(\alpha_i\|r, s)$; $\log r = \log s =$ -10

Example: Mass-spring-damper system

- Bayesian inference with flat priors for questionable parameters: (Sandhu *et al.*, JCP, 2021, with copyright permission)

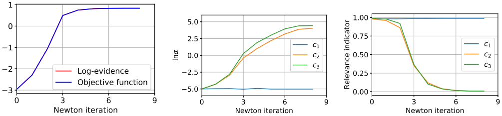


- Predicted versus true time-history of velocity $\dot{u}_2$: (Sandhu *et al.*, JCP, 2021, with copyright permission)

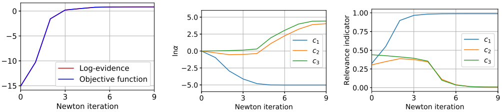


Example: Mass-spring-damper system

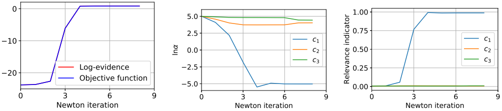
- Stage 2: Sparsification (Sandhu *et al.*, JCP, 2021, with copyright permission)



(e) $\boldsymbol{\alpha}$ initiated at $\{-5, -5, -5\}$



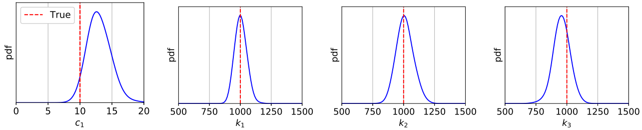
(f) $\boldsymbol{\alpha}$ initiated at $\{0, 0, 0\}$



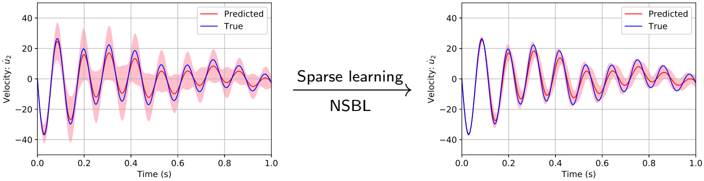
(g) $\boldsymbol{\alpha}$ initiated at $\{5, 5, 5\}$

Example: Mass-spring-damper system

- Bayesian inference post sparse learning, using optimal ARD priors from NSBL: (Sandhu *et al.*, JCP, 2021, with copyright permission)



- Prediction before and after sparse learning of model parameters: (Sandhu *et al.*, JCP, 2021, with copyright permission)



Likelihood and Parameter Posterior

$$\mathbf{x}_{k+1} = \mathbf{g}_k\left(\mathbf{x}_k, \phi, \mathbf{f}_k, \mathbf{q}_k\right) \tag{2}$$

$$\mathbf{d}_j = \mathbf{h}_j(\mathbf{x}_{d(j)}, \varepsilon_j) \tag{3}$$

$$p(\phi|\mathcal{D}) \propto p(\phi) \underbrace{\prod_{j=1}^{J} \int p(\mathbf{d}_j|\mathbf{x}_{d(j)}, \phi) \underbrace{p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1}, \phi)}_{\text{Non-Gaussian filtering}} d\mathbf{x}_{d(j)}}_{p(\mathcal{D}|\phi)}$$

$$p(\phi|\mathcal{D}) \propto p(\phi)p(\mathcal{D}|\phi)$$

Bisaillon et al., Nonlinear Dynamics, 2015

Likelihood Computation using EKF

$$p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1},\phi) \sim \mathcal{N}(\mathbf{x}_{d(j)}|\mathbf{x}^f_{d(j)},\mathbf{P}^f_{d(j)})$$

$$p(\mathcal{D}|\phi) = \prod_{j=1}^{J} \mathcal{N}(\mathbf{d}_j|\mathbf{h}_j(\mathbf{x}^f_{d(j)},\mathbf{0}),\mathbf{\Sigma}')$$

$$\mathbf{\Sigma}' = \mathbf{C}_j\mathbf{P}^f_{d(j)}\mathbf{C}_j^T + \mathbf{D}_j\mathbf{\Gamma}_j\mathbf{D}_j^T$$

$$\mathbf{C}_j = \left.\frac{\partial \mathbf{h}_j(\mathbf{x}_{d(j)},\varepsilon_j)}{\partial \mathbf{x}_{d(j)}}\right|_{\mathbf{x}_{d(j)}=\mathbf{x}^f_{d(j)},\varepsilon_j=\mathbf{0}} \tag{4}$$

$$\mathbf{D}_j = \left.\frac{\partial \mathbf{h}_j(\mathbf{x}_{d(j)},\varepsilon_j)}{\partial \varepsilon_j}\right|_{\mathbf{x}_{d(j)}=\mathbf{x}^f_{d(j)},\varepsilon_j=\mathbf{0}} \tag{5}$$

Bisaillon et al., Nonlinear Dynamics, 2015

Likelihood Computation using EnKF

$$p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1},\phi) \approx \frac{1}{N}\sum_{s=1}^{N}\delta(\mathbf{x}_{d(j)} - \mathbf{x}^{f}_{d(j),s}).$$

$$\begin{aligned}
p(\mathcal{D}|\phi) &= \prod_{j=1}^{J}\int_{-\infty}^{\infty} p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1},\phi)p(\mathbf{d}_j|\mathbf{x}_{d(j)},\phi)d\mathbf{x}_{d(j)} \\
&\approx \prod_{j=1}^{J}\int_{-\infty}^{\infty} \frac{1}{N}\sum_{s=1}^{N}\delta(\mathbf{x}_{d(j)} - \mathbf{x}^{f}_{d(j),s})p(\mathbf{d}_j|\mathbf{x}_{d(j)},\phi)d\mathbf{x}_{d(j)} \\
&\approx \prod_{j=1}^{J}\left[\frac{1}{N}\sum_{s=1}^{N}p(\mathbf{d}_j|\mathbf{x}^{f}_{d(j),s},\phi)\right]
\end{aligned}$$

Bisaillon et al., Nonlinear Dynamics, 2015

Likelihood Computation using PF

$$p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1},\phi) \approx \sum_{s=1}^{N} w_{d(j),s}\,\delta(\mathbf{x}_{d(j)} - \mathbf{x}^f_{d(j),s})$$

$$\begin{aligned}
p(\mathcal{D}|\phi) &= \prod_{j=1}^{J} \int_{-\infty}^{\infty} p(\mathbf{x}_{d(j)}|\mathbf{x}_{d(j)-1},\phi)\,p(\mathbf{d}_j|\mathbf{x}_{d(j)},\phi)\,d\mathbf{x}_{d(j)} \\
&\approx \prod_{j=1}^{J} \int_{-\infty}^{\infty} \sum_{s=1}^{N} w_{d(j),s}\,\delta(\mathbf{x}_{d(j)} - \mathbf{x}^f_{d(j),s})\,p(\mathbf{d}_j|\mathbf{x}_{d(j)},\phi)\,d\mathbf{x}_{d(j)} \\
&\approx \prod_{j=1}^{J} \sum_{s=1}^{N} w_{d(j),s}\,p(\mathbf{d}_j|\mathbf{x}^f_{d(j),s},\phi)
\end{aligned} \tag{6}$$

$$w_{d(j),i} \propto w_{d(j)-1,i}\,\frac{p(\mathbf{d}_j|\mathbf{x}_{d(j),i})\,p(\mathbf{x}_{d(j),i}|\mathbf{x}_{d(j)-1,i})}{q(\mathbf{x}_{d(j),i}|\mathbf{x}_{d(j)-1,i},\mathbf{d}_j)}$$

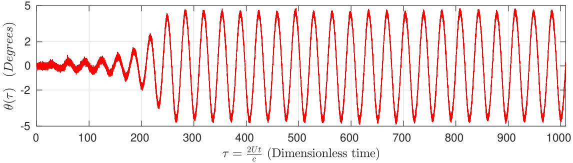
Bisaillon et al., Nonlinear Dynamics, 2015

Single degree-of-freedom aeroelastic system

Data generating model:

$$I\ddot{\theta} + D\dot{\theta} + K\theta + K_{nl}\theta^3 = D_{nl}\,\mathrm{sgn}(\dot{\theta}) + \frac{1}{2}\rho U^2 c^2 s\, C_M(\theta, \dot{\theta}, \ddot{\theta})$$

$$\frac{\dot{C}_M}{B} + C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + \frac{c_6}{B}\ddot{\theta} + \sigma\xi(\tau)$$



Sandhu et. al, CMAME 2017 (with copyright permission)

Case 1: One-dimensional sparse learning problem

1. Aerodynamic parameter e_3 is treated as questionable

$$\frac{\dot{C}_M}{B} + C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + \frac{c_6}{B}\ddot{\theta} + \sigma\xi(\tau)$$

   i. ARD prior, $\mathrm{p}(\phi_\alpha|\alpha)$

$$\mathrm{p}(\phi_\alpha|\alpha) = \mathcal{N}(e_3|0, \alpha^{-1})$$

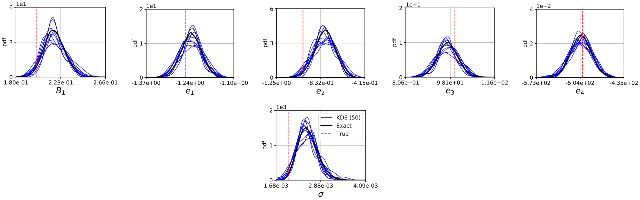
   ii. Known prior, $\mathrm{p}(\phi_{-\alpha})$

$$\mathrm{p}(\phi_{-\alpha}) = \mathcal{L}(B|0.2, 50)\mathcal{U}(e_1|-2, 0)\mathcal{U}(e_2|-2, 0)\mathcal{U}(e_4|-600, 0)\mathcal{L}(\sigma|0.002, 50)$$

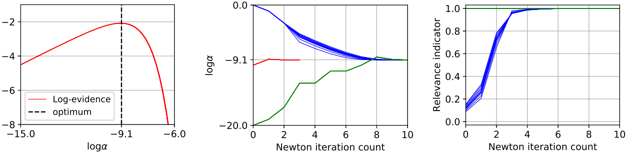
R. Sandhu. Model Comparison and Sparse Learning of Nonlinear Physics-Based Models Using Bayesian Inference. *PhD Thesis*, Carleton University, 2020.

Single degree-of-freedom aeroelastic system

1. Constructing GMM of partial posterior $p(\mathcal{D}|\phi)p(\phi_{-\alpha})$ using KDE



2. Maximizing log evidence with respect to hyperparameter α



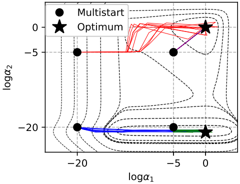
3. Parameter e_3 is correctly identified as relevant

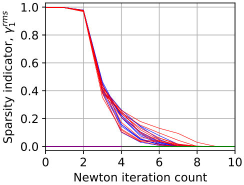
R. Sandhu. Model Comparison and Sparse Learning of Nonlinear Physics-Based Models Using Bayesian Inference. *PhD Thesis*, Carleton University, 2020.

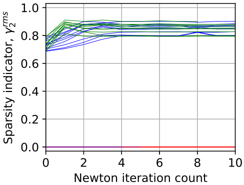
Case 2: Two-dimensional sparse learning problem

1. Aerodynamic parameters e_5 and e_6 are treated as questionable

$$\frac{\dot{C}_M}{B} + C_M = e_1\theta + e_2\dot{\theta} + e_3\theta^3 + e_4\theta^2\dot{\theta} + e_5\theta^5 + e_6\theta^4\dot{\theta} + \frac{c_6}{B}\ddot{\theta} + \sigma\xi(\tau)$$







- (i) One optimum correctly identifies parameters e_5 and e_6 as irrelevant
- (ii) The other finds e_5 to be irrelevant, but e_6 to be relevant

[1] R. Sandhu. Model Comparison and Sparse Learning of Nonlinear Physics-Based Models Using Bayesian Inference. *PhD Thesis*, Carleton University, 2020.

Conclusion and Future Research

- NSBL is effective for ODE models.
- NSBL for coupled nonlinear ODE and PDE models (bending-bending-torsion-pitch motions) using wind-tunnel data.
- Concurrent selection of physics-based model and model errors.
- Address overfitting using NSBL for Bayesian neural networks.
- Apply to fields outside of aeroelasticity (e.g. epidemiology).

Conclusion

Method	Capabilities			Methodology			Scalability
	Nonlinear models?	Prior knowledge?	Sparse learning?	Prior pdf type	Evidence estimation	Evidence optimization	# of likelihood evaluations
SBL/BCS	×	×	✓	Gaussian ARD (Conjugate prior)	Analytical	Gradient set to zero	N/A
Bayesian model comparison	✓	✓	×	Known pdf	Numerical (MCMC-based)	N/A	$N_{\text{Models}} \times N_{\text{MCMC}}$
ARD (Sampling-based)	✓	✓	✓	Known + Gaussian or Laplace ARD	Numerical (MCMC-based)	Gradient-free	$N_{\text{Iter}} \times N_{\text{MCMC}}$
ARD (NSBL)	✓	✓	✓	Known + Gaussian ARD	Semianalytical (GMM-based)	Gradient and Hessian based	N_{MCMC}

N_{MCMC}: # of MCMC samples needed for computing evidence (for an average model).

N_{Models}: # of candidate models.

N_{Iter}: # of iterations required for optimizing evidence.

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Derivation: Parameter Posterior (closely follows the book by Evensen)

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_k, \phi | \mathbf{d}_1, \ldots, \mathbf{d}_J) = \underbrace{p(\mathbf{x}_1, \ldots, \mathbf{x}_k | \mathbf{d}_1, \ldots, \mathbf{d}_J, \phi)}_{\text{Conditional state pdf}} \; \underbrace{p(\phi | \mathbf{d}_1, \ldots, \mathbf{d}_J)}_{\text{Parameter posterior pdf}}$$

$$\begin{aligned}
& p(\mathbf{x}_1, \ldots, \mathbf{x}_k | \mathbf{d}_1, \ldots, \mathbf{d}_J, \phi) p(\phi | \mathbf{d}_1, \ldots, \mathbf{d}_J) \propto \\
& \quad p(\phi) \left[\prod_{j'=1}^{d(1)-1} p(\mathbf{x}_{j'} | \mathbf{x}_{j'-1}, \phi) \right] p(\mathbf{x}_{d(1)} | \mathbf{x}_{d(1)-1}, \phi) p(\mathbf{d}_1 | \mathbf{x}_{d(1)}, \phi) \\
& \qquad \vdots \\
& \quad \left[\prod_{j'=d(J-1)+1}^{d(J)-1} p(\mathbf{x}_{j'} | \mathbf{x}_{j'-1}, \phi) \right] p(\mathbf{x}_{d(J)} | \mathbf{x}_{d(J)-1}, \phi) p(\mathbf{d}_J | \mathbf{x}_{d(J)}, \phi) \\
& \qquad \vdots \\
& \quad \left[\prod_{j'=d(J)+1}^{k} p(\mathbf{x}_{j'} | \mathbf{x}_{j'-1}, \phi) \right]
\end{aligned}$$

Bisaillon et al., Nonlinear Dynamics, 2015

$$\mathbf{u}_{k+1} = \mathfrak{g}_k \left(\mathbf{u}_k, \phi, \mathbf{f}_k, \mathbf{q}_k^u \right), \tag{7}$$

$$\mathbf{d}_j = \mathfrak{h}_j \left(\mathbf{u}_{d(j)}, \phi, \epsilon_j \right). \tag{8}$$

$$\mathbf{u}_{k+1} = \mathfrak{g}_k \left(\mathbf{u}_k, \phi_k, \mathbf{f}_k, \mathbf{q}_k^u \right), \tag{9}$$

$$\phi_{k+1} = \phi_k + \mathbf{q}_k^{\phi}, \tag{10}$$

$$\mathbf{d}_j = \mathfrak{h}_j \left(\mathbf{u}_{k(j)}, \phi_{k(j)}, \epsilon_j \right) \tag{11}$$

$$\mathbf{x}_k = \begin{Bmatrix} \mathbf{u}_k \\ \phi_k \end{Bmatrix}; \quad \mathbf{q}_k = \begin{Bmatrix} \mathbf{q}_k^u \\ \mathbf{q}_k^{\phi} \end{Bmatrix} \tag{12}$$

Khalil et. al, JSV 2015