ENM 540: Data-driven modeling and probabilistic scientific computing

Probabilistic scientific computing with Gaussian processes

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Identification of linear parametrized systems

$$u(x) \longrightarrow \boxed{\mathcal{L}_x^\phi : \phi = ?} \longrightarrow f(x)$$

$$\mathcal{L}_x^\phi u(x) = f(x)$$

$$u(x) \sim \mathcal{GP}(0, k_{uu}(x, x'; \theta)) \longrightarrow \mathcal{L}_x^\phi u(x) = f(x) \sim \mathcal{GP}(0, k_{ff}(x, x'; \theta, \phi))$$

$$k_{ff}(x, x'; \theta, \phi) = \mathcal{L}_x^\phi \mathcal{L}_{x'}^\phi k_{uu}(x, x'; \theta)$$

$$-\log p(\boldsymbol{y}|\phi, \theta, \sigma_{n_u}^2, \sigma_{n_f}^2) = \frac{1}{2}\log|\boldsymbol{K}| + \frac{1}{2}\boldsymbol{y}^T \boldsymbol{K}^{-1}\boldsymbol{y} + \frac{N}{2}\log 2\pi\,,$$

where $\boldsymbol{y} = \begin{bmatrix} \boldsymbol{y}_u \\ \boldsymbol{y}_f \end{bmatrix}$, $p(\boldsymbol{y}|\phi, \theta, \sigma_{n_u}^2, \sigma_{n_f}^2) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{K})$, and $\boldsymbol{K}$ is given by

$$\boldsymbol{K} = \begin{bmatrix} k_{uu}(\boldsymbol{X}_u, \boldsymbol{X}_u; \theta) + \sigma_{n_u}^2 \boldsymbol{I}_{n_u} & k_{uf}(\boldsymbol{X}_u, \boldsymbol{X}_f; \theta, \phi) \\ k_{fu}(\boldsymbol{X}_f, \boldsymbol{X}_u; \theta, \phi) & k_{ff}(\boldsymbol{X}_f, \boldsymbol{X}_f; \theta, \phi) + \sigma_{n_f}^2 \boldsymbol{I}_{n_f} \end{bmatrix}.$$

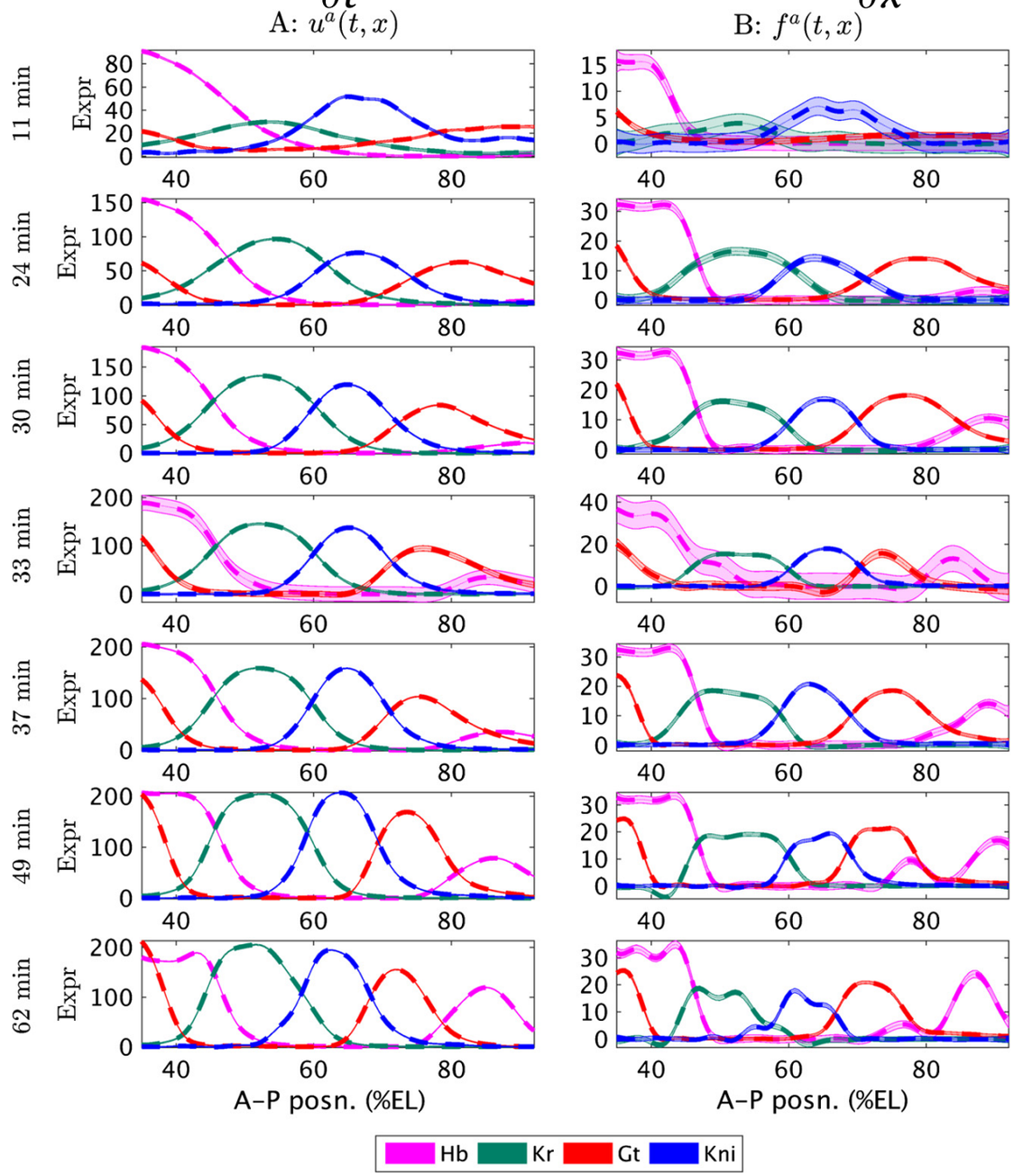
Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2017). Machine learning of linear differential equations using Gaussian processes. Journal of Computational Physics, 348, 683-693.

Identification of linear parametrized systems

Example: Drosophila melanogaster gap gene dynamics

The gap gene dynamics of protein $a \in \{Hb, Kr, Gt, Kni\}$ (see Fig. 5) can be modeled using a reaction-diffusion partial differential equation

$$\mathcal{L}_{(t,x)}^{(\lambda^a, D^a)} u^a(t,x) = \frac{\partial}{\partial t} u^a(t,x) + \lambda^a u^a(t,x) - D^a \frac{\partial^2}{\partial x^2} u^a(t,x) = f^a(t,x),$$



Inferred parameter values for the decay λ^a and diffusion D^a rates of protein a.

Gene	Decay (λ^a)	Diff. (D^a)
Hb	0.1606	0.3669
Kr	0.0797	0.4490
Gt	0.1084	0.4543
Kni	0.0807	0.2683

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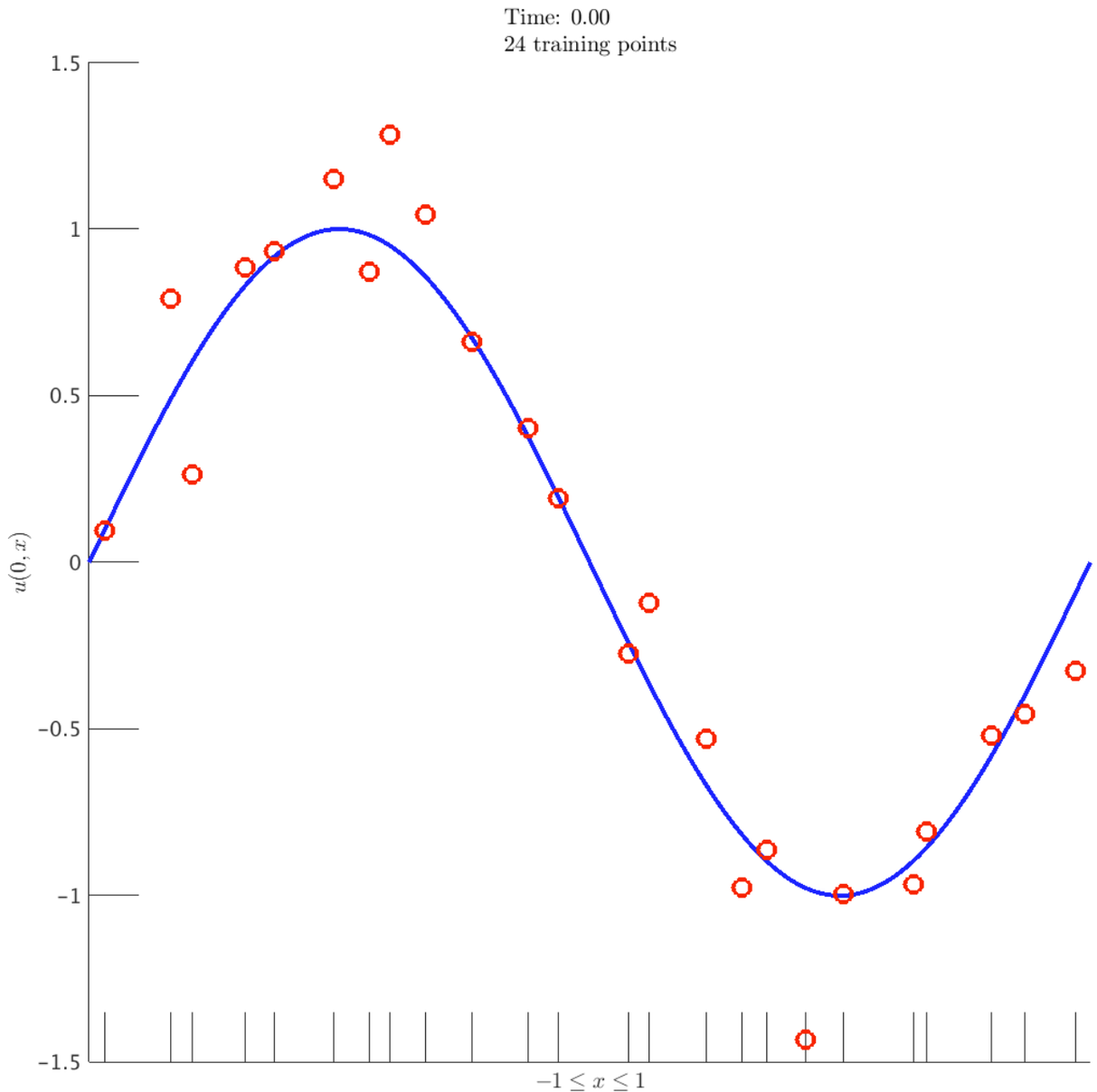
Extension to non-linear equations

Example: 1D viscous Burgers —> *The equation, along with the choice of a time-stepping scheme define a GP prior!*

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}, \quad x \in [-1, 1], \quad t \in [0, 1],$$
$$u(0, x) = u^0(x)$$
$$u(t, 0) = u(t, 1) = 0. \quad \nu = \pi/100$$

$$+ \quad \mathcal{L}_x u^{n+1}(x) := u^{n+1}(x) + \Delta t \; u^n(x) \; \frac{du^{n+1}(x)}{dx} - \Delta t \; \nu \frac{d^2 u^{n+1}(x)}{dx^2} = u^n(x)$$

e.g., Backward Euler time-stepping



Remarks:

- Despite starting from a stationary prior:

  $$u^{n+1,n+1}(x) \sim \mathcal{GP}(0, k^{n+1,n+1}(x, x'; \theta))$$

  the structure of the of the kernel:

  $$k^{n,n}(x, x'; \theta) = \mathcal{L}_x \mathcal{L}_{x'} k^{n+1,n+1}(x, x'; \theta)$$

  can generate discontinuous solutions!
- This is a general approach applicable to any nonlinear equation and any time-stepping scheme.
- We only need to derive the kernel $k^{n,n}(x, x'; \theta)$
- Under this setup, fully implicit time-stepping schemes have the same complexity as their explicit counterparts. Hence, one can obtain highly accurate and stable schemes at no extra cost.

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2018). Numerical Gaussian Processes for Time-Dependent and Nonlinear Partial Differential Equations. SIAM Journal on Scientific Computing, 40(1), A172-A198.

Identification of non-linear parametrized systems

$$h_t + \mathcal{N}_x^\lambda h = 0,\ x \in \Omega,\ t \in [0, T]$$

Temporal discretization: $h^n + \Delta t \mathcal{N}_x^\lambda h^n = h^{n-1}, \quad h^n(x) \sim \mathcal{GP}(0, k(x, x', \theta))$

$$\downarrow$$

$$\begin{bmatrix} h^n \\ h^{n-1} \end{bmatrix} \sim \mathcal{GP}\left(0, \begin{bmatrix} k^{n,n} & k^{n,n-1} \\ k^{n-1,n} & k^{n-1,n-1} \end{bmatrix}\right)$$

$k^{n,n}(x, x'; \theta)$, $k^{n,n-1}(x, x'; \theta, \lambda)$, $k^{n-1,n}(x, x'; \theta, \lambda)$, $k^{n-1,n-1}(x, x'; \theta, \lambda)$

$\longrightarrow$

$k^{n,n} = k$, $k^{n,n-1} = \mathcal{L}_{x'}^\lambda k$, $k^{n-1,n} = \mathcal{L}_x^\lambda k$, $k^{n-1,n-1} = \mathcal{L}_x^\lambda \mathcal{L}_{x'}^\lambda k$

$$-\log p(\boldsymbol{h}|\theta, \lambda, \sigma^2) = \frac{1}{2}\boldsymbol{h}^T \boldsymbol{K}^{-1}\boldsymbol{h} + \frac{1}{2}\log|\boldsymbol{K}| + \frac{N}{2}\log(2\pi),$$

where $\boldsymbol{h} = \begin{bmatrix} \boldsymbol{h}^n \\ \boldsymbol{h}^{n-1} \end{bmatrix}$, $p(\boldsymbol{h}|\theta, \lambda, \sigma^2) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{K})$, and $\boldsymbol{K}$ is given by

$$\boldsymbol{K} = \begin{bmatrix} k^{n,n}(\boldsymbol{x}^n, \boldsymbol{x}^n) & k^{n,n-1}(\boldsymbol{x}^n, \boldsymbol{x}^{n-1}) \\ k^{n-1,n}(\boldsymbol{x}^{n-1}, \boldsymbol{x}^n) & k^{n-1,n-1}(\boldsymbol{x}^{n-1}, \boldsymbol{x}^{n-1}) \end{bmatrix} + \sigma^2 \boldsymbol{I}.$$

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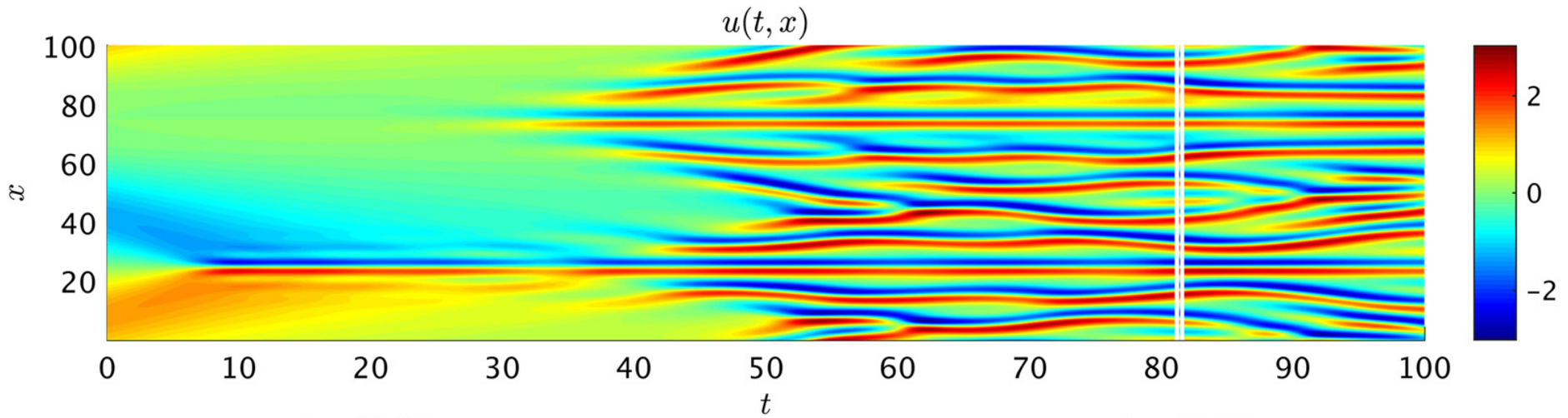
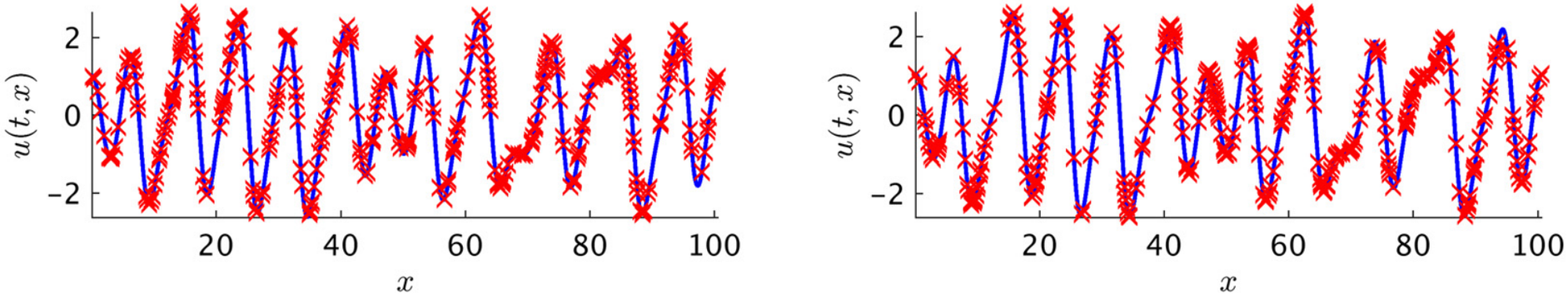
Identification of non-linear parametrized systems

Example: Kuramoto-Sivashinsky equation: $u_t + \lambda_1 u u_x + \lambda_2 u_{xx} + \lambda_3 u_{xxxx} = 0$



$t = 81.20$
301 training data

$t = 81.60$
299 training data



Correct PDE	$u_t + uu_x + u_{xx} + u_{xxxx} = 0$
Identified PDE (clean data)	$u_t + 0.952uu_x + 1.005u_{xx} + 0.980u_{xxxx} = 0$
Identified PDE (1% noise)	$u_t + 0.908uu_x + 0.951u_{xx} + 0.927u_{xxxx} = 0$

Kuramoto–Sivashinsky equation: Resulting statistics for the learned parameter values.

	Clean data			1% noise			5% noise		
	λ_1	λ_2	λ_3	λ_1	λ_2	λ_3	λ_1	λ_2	λ_3
First quartile	0.9603	0.9829	0.9711	0.7871	0.8095	0.5891	−0.0768	0.0834	−0.0887
Median	0.9885	1.0157	0.9970	0.8746	0.9124	0.8798	0.4758	0.5539	0.4086
Third quartile	1.0187	1.0550	1.0314	0.9565	0.9948	0.9553	0.6991	0.7644	0.7009

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