Differentiable Likelihoods for Fast Inversion of ‘Likelihood-Free’ Dynamical Systems

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TL;DR Summary

ODE Forward Problem: Given θ, estimate $x : [0, T] \to \mathbb{R}^d$ which satisfies the

ODE $\dot{x}(t) = f(x(t), \theta)$ on $t \in [0, T]$, under initial condition $x(0) = x_0 \in \mathbb{R}^d$.

ODE Inverse Problems:

Given data $z(t_{1:M}) = x_\theta(t_{1:M}) + \varepsilon \in \mathbb{R}^d$, $\varepsilon \sim \mathcal{N}(0, \Sigma)$, estimate θ.

Question: Are ODE inverse problems really likelihood-free inference?

Answer: No! If we use probabilistic numerics to account for the numerical forward error, there is a differentiable likelihood!

Practical Benefit: New gradient-based methods are now available.

Inverse Problems...

...are defined by their forward map F

[Cranmer et al., 2020]

Forward Map (likelihood): $\theta \mapsto F(\theta)$

Parameter $\theta \in \Theta$ $\xrightarrow{\quad}$ Simulation $F(\theta) \in \mathbb{R}^d$

Inverse Problem: $F(\theta_{\text{true}})$ + 'noise' $\mapsto \theta_{\text{true}}$

- The forward problem is **well-posed**. (Numerical Analysis)
- The inverse problem is **ill-posed**. (Statistics, Machine Learning)
- The mix of numerical and statistical estimation invites a treatment by **probabilistic numerics**.

Inverse problems are called **likelihood-free** if their **forward map** is **too expensive** to approximate exactly.

ODE Inverse Problems...

...are only likelihood-free because they have a numerical forward map

[Cranmer et al., 2020]

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ODE $\dot{x}(t) = f(x(t), \theta)$ on $t \in [0, T]$, under initial condition $x(0) = x_0 \in \mathbb{R}^d$.

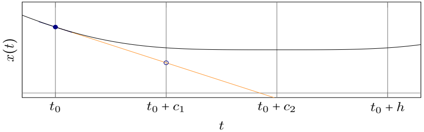
$\forall \theta \in \Theta$, **ODEs** have a **well-defined solution**

$$x_\theta :]0, T] \to \mathbb{R}^d, \qquad t \mapsto x_0 + \int_0^t f(x(s), \theta)\, ds,$$

and hence an **high-fidelity** forward map

$$F : \Theta \to C^1([0, T]; \mathbb{R}^d), \qquad \theta \mapsto x_\theta.$$

- x_θ has to be estimated with **non-zero step size** $h > 0$, i.e. with **low fidelity**!
- With **numerical error**, e.g. **Runge–Kutta**:



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[Cranmer et al., 2020]

Forward Map (likelihood): $\theta \mapsto F(\theta)$

Parameter		Simulation
$\theta \in \Theta$	$\longrightarrow$ / $\longleftarrow$	$F(\theta) \in \mathbb{R}^d$

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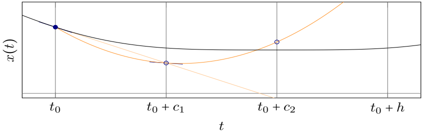

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[Cranmer et al., 2020]

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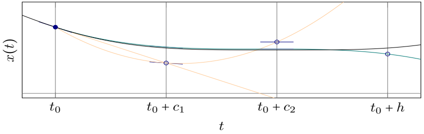

ODE Inverse Problems...

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[Cranmer et al., 2020]

Forward Map (likelihood): $\theta \mapsto F(\theta)$

$$\begin{tikzcd} \begin{array}{c}\text{Parameter}\\ \theta \in \Theta\end{array} \arrow[r, bend left] & \begin{array}{c}\text{Simulation}\\ F(\theta) \in \mathbb{R}^d\end{array} \arrow[l, bend left] \end{tikzcd}$$

Inverse Problem: $F(\theta_{\text{true}})$ + 'noise' $\mapsto \theta_{\text{true}}$

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- x_θ has to be estimated with **non-zero step size** $h > 0$, i.e. with **low fidelity**!
- With **numerical error**, e.g. **Runge–Kutta**:

In classical numerics, ODE inverse problems are likelihood-free!

Probabilistic numerics inserts a likelihood...

...into the 'likelihood-free' ODE inverse problem

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[Hennig et al., 2015]

Forward Map (likelihood): $\theta \mapsto F(\theta)$

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- Inverse problems are called **likelihood-free** if F is **too expensive** to approximate exactly.
- ODE inverse problems are **likelihood-free** if **numerical error** is **unaccounted**.

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Likelihood-free — **Probabilistic Numerics** captures numerical error → Differentiable Likelihood

Gradient-free methods:

- Density estimation methods
- ABC

Gradient-based methods:

- Gradient descent
- Hamiltonian/Langevin MCMC

We propose the following likelihood.

Uncertainty-Aware Likelihood by Gaussian ODE Filtering [Schober et al., 2019, Tronarp et al., 2019, Kersting et al., 2019]

Assume that we observe **noisy data** $\mathbf{z} = z(t_{1:M})$ of the true $\mathbf{x} = x(t_{1:M})$, i.e:

$$p(\mathbf{z} \mid \mathbf{x}) = \mathcal{N}\left(\mathbf{z};\ \mathbf{x}, \sigma^2 I_M\right). \tag{1}$$

For any θ, **Gaussian ODE Filtering**, a probabilistic numerical method, yields

$$p(\mathbf{z} \mid \theta) = \mathcal{N}(\mathbf{z};\ x_0 + J\theta,\ \underbrace{\mathbf{P} + \sigma^2 I_M}_{\text{numerical + statistical var.}}) \tag{2}$$

where J is freely-availabe from the filtering output.

Two advantages:

- $\mathbf{P}$ accounts for then epistemic (numerical) uncertainty for non-zero step size $h > 0$, and
- $J = J(\hat{\theta})$ is an estimate of the Jacobian of $\theta \mapsto \mathbf{x}_\theta$ at some support point $\hat{\theta}$, and implies gradient and Hessian estimators

$$\hat{\nabla}_\theta E(\mathbf{z}) := -J^\intercal \left[\mathbf{P} + \sigma^2 I_M\right]^{-1} [\mathbf{z} - \mathbf{m}_\theta], \qquad \text{and} \qquad \hat{\nabla}^2_\theta E(\mathbf{z}) := J^\intercal \left[\mathbf{P} + \sigma^2 I_M\right]^{-1} J. \tag{3}$$

The likelihood account for the numerical/epistemic uncertainty!

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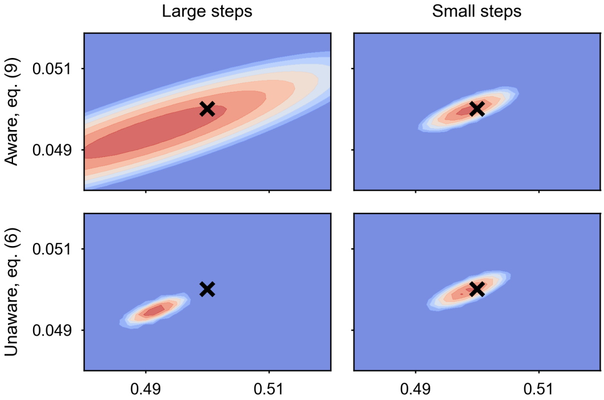
- The **statistical (aleatoric) variance** $\sigma^2 I_M$ is accounted for in any case.
- The **numerical (epistemic) variance** $\mathbf{P}$ makes the implicit forward model tractable.

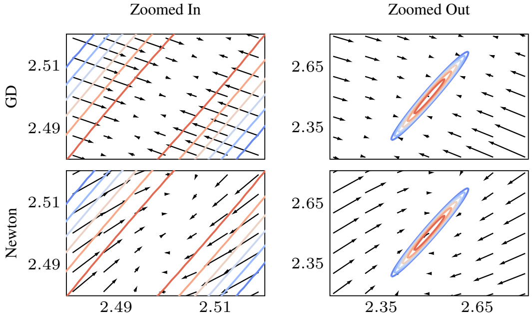


The gradients are accurate enough to point towards modes!

Both the

- **gradient** estimator, and
- the Hessian-precionditioned (**Newton**) gradient estimator

are **useful approximations**.



Insertion of gradients/Hessians unlocks gradient-free methods!

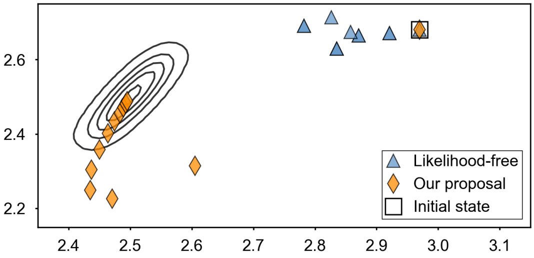
These **gradient-based** methods are more **sample-efficient**.

Sampling:

- Langevin MCMC
- Hamiltonian MCMC

Optimization:

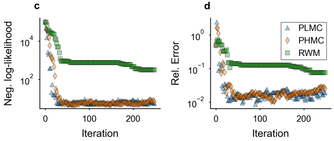
- Gradient descent
- Newton's Method



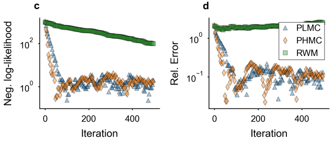
Sampling Experiments

- **Likelihood-free** random-walk **Metropolis** (RWM) **gets lost** in regions of low probability.
- **Gradient-based** sampling quickly finds and covers **regions of high probability**.

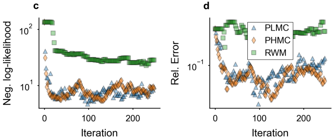
Lotka Volterra



Protein Transduction



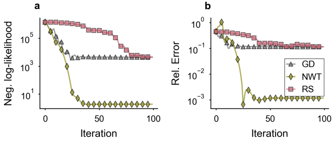
Glucose Uptake in Yeast



Optimization Experiments

- **Likelihood-free** random-search **hardly learns** at all.
- **Gradient-based** optimization **quickly** finds local maxima.

Lotka Volterra



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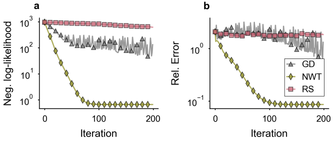

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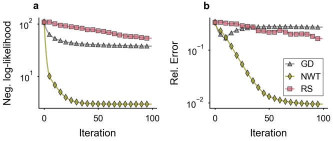

Collaborators

University of Tübingen (top row) and Bosch Center for AI (bottom row)

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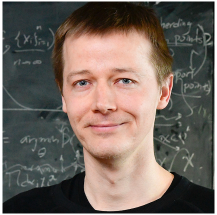
Nicholas Krämer (joint primary author)



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