Backward and Inverse
Opportunities for Probnum in Machine Learning

Philipp Hennig

Heilbronn Workshop – 27 March 2022

Eberhard Karls Universität Tübingen

Faculty of Science
Department of Computer Science
Chair for the Methods of Machine Learning

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The Men in Black

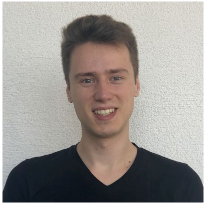
This talk contains work by many people, including many in the room today

Filip Tronarp

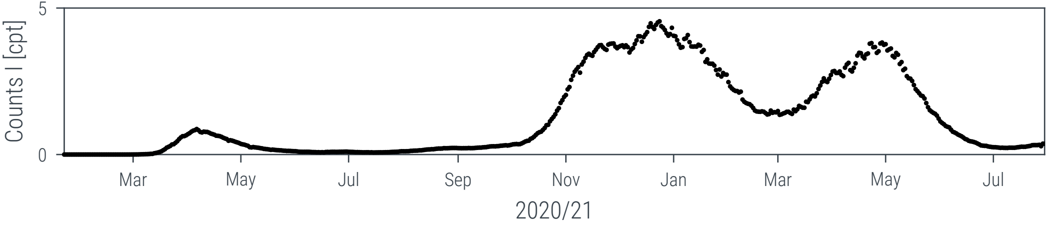
Nico Krämer

Nathanael Bosch

Jonathan Schmidt



Marvin Pförtner



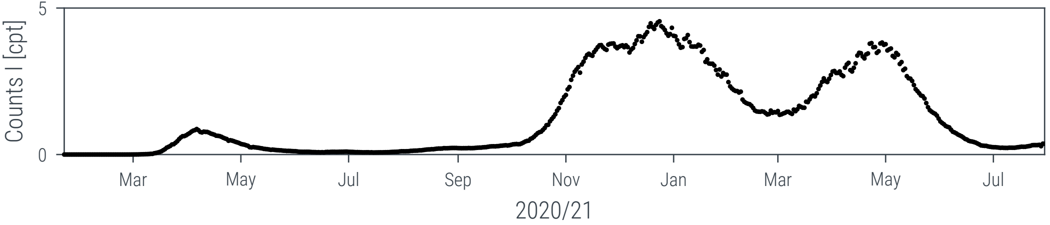
Is this

- a machine learning task? (regress on $I(t)$)
  doesn't work withouth mechanistic knowledge

A very 2021 inference task

Mixed Information Sources

Schmidt, Krämer, Hennig, 2021, NeurIPS 2021



Is this

- a machine learning task? (regress on $I(t)$)
  doesn't work withouth mechanistic knowledge
- a simulation problem? (solve SIRD ODE)
  we don't know β, though!
- an *inverse* problem (estimate β)
  we really care about $I(t)$, though!

$$\frac{d}{dt}\begin{bmatrix} S(t) \\ I(t) \\ R(t) \\ V(t) \\ D(t) \end{bmatrix} = \begin{bmatrix} -\beta(t)S(t)I(t)/P - v(t) \\ \beta(t)S(t)I(t)/P - \gamma I(t) - \eta I(t) \\ \gamma I(t) \\ v(t) \\ \eta I(t) \end{bmatrix}$$

What is an Inverse Problem?

Mechanistic Knowledge and mixed information sources

$$x'(t) = f(x(t), u(t)), \quad p(\mathbf{y} \mid x) = \prod_n^N \mathcal{N}(y_n; H(x(t_n)), \Sigma_n), \quad p(x) = \mathcal{GP}(m_x, k_x), \quad p(u) = \mathcal{GP}(m_u, k_u)$$

An *inverse problem* seems to be

- another word for an *inference* problem (inferring latent quantities from observations) (wikipedia).
- about inferring the objext x in $y = D(x)$, where D is a known operator (here: the ODE integral) from data y.

In both cases, it seems the tough part, arguably, is the ill-posedness. But the data y is already probabilistic, too!

Solving Inverse Problems with Backprop

automatic differentiation in simulation

$$\boldsymbol{u}^{(i)} = \boldsymbol{u}^{(i-1)} + \alpha \nabla_u L(u^{(i)})$$

`while` $L >$ `tol`

$$\hat{x} \leftarrow \texttt{ODEsolve}(f, u^{(i)})$$

$$L(u^{(i)}) = \log p(y \mid \hat{x}(u^{(i)}))$$

- Define some loss $L(u)$, e.g.

$$L(u) := \sum_i - \log p(y_i \mid \hat{x}(u)) = \sum_i (y_i - H(\hat{x}(u)))^2 + \text{const.}.$$

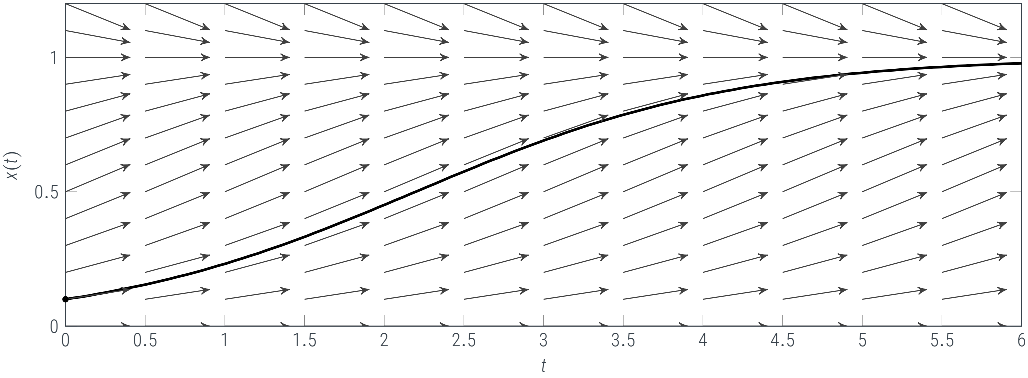
- Compute the gradient $\nabla_u L(u^{(i)})$ with automatic differentiation. Examples:
  - `numppyro` tutorial, using jax's dopri5
  - `Turing.jl` tutorial, using diffeq.jl solvers

Note how the user is discouraged from even thinking about the ODE solver.

The Probabilistic View on ODEs

[Schober, Duvenaud & P.H., 2014. Schober & P.H., 2016. Kersting & P.H., 2016, Tronarp, Kerstin, P.H., 2019, Bosch, Tronarp, P.H., 2021, ...]

$$x'(t) = f(x(t), t), \quad x(t_0) = x_0$$




```
scipy.integrate.solve_ivp(f,t_span,x_0)   ⇒   probnum.diffeq.probsolve_ivp(f,t_span,x_0)
```

The Probabilistic View on ODEs

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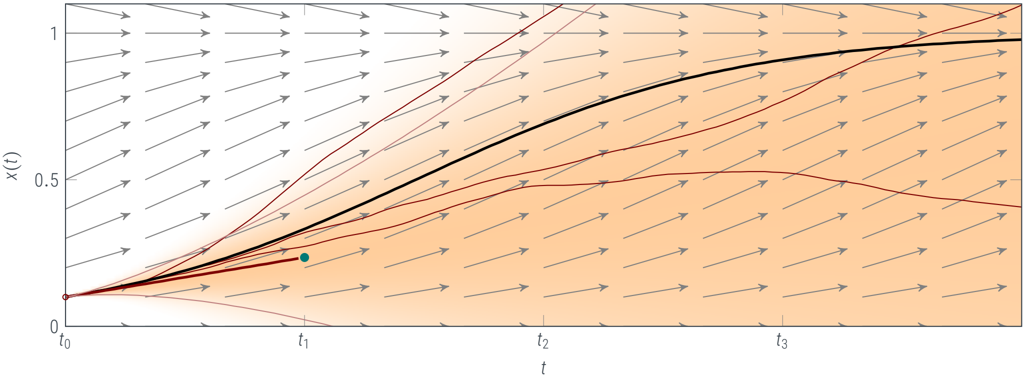

`scipy.integrate.solve_ivp(f,t_span,x_0)` $\Rightarrow$ `probnum.diffeq.probsolve_ivp(f,t_span,x_0)`

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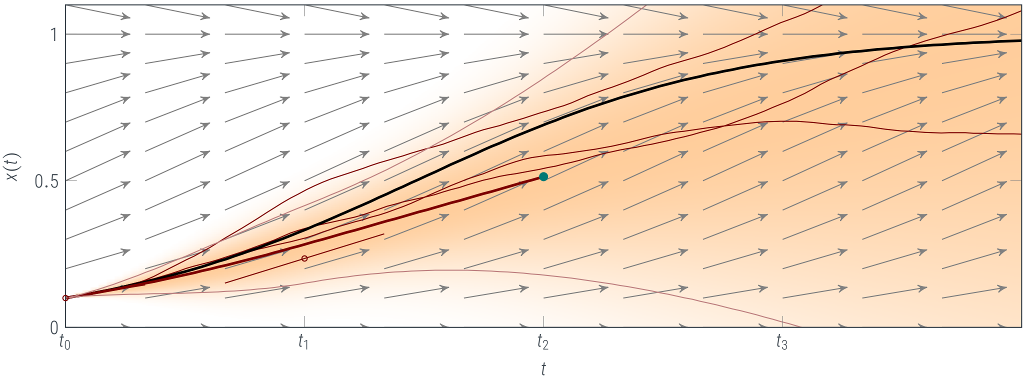

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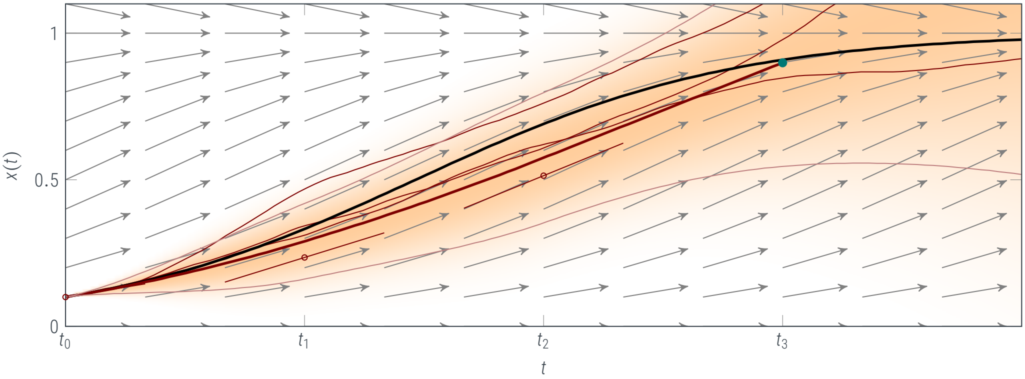

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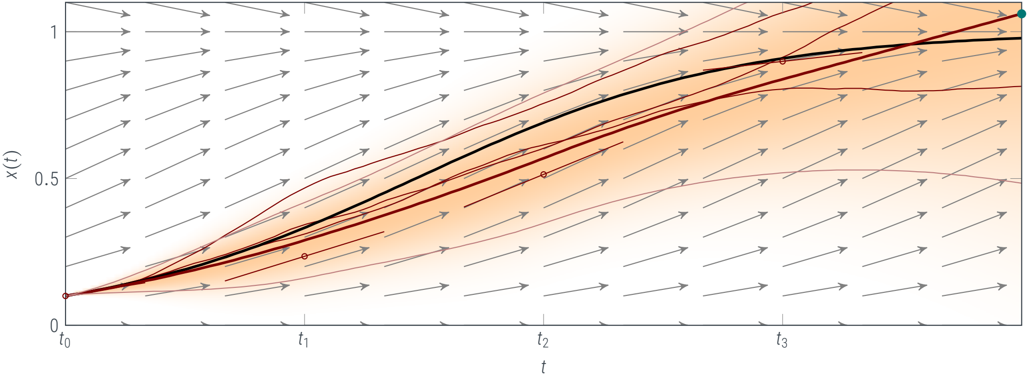

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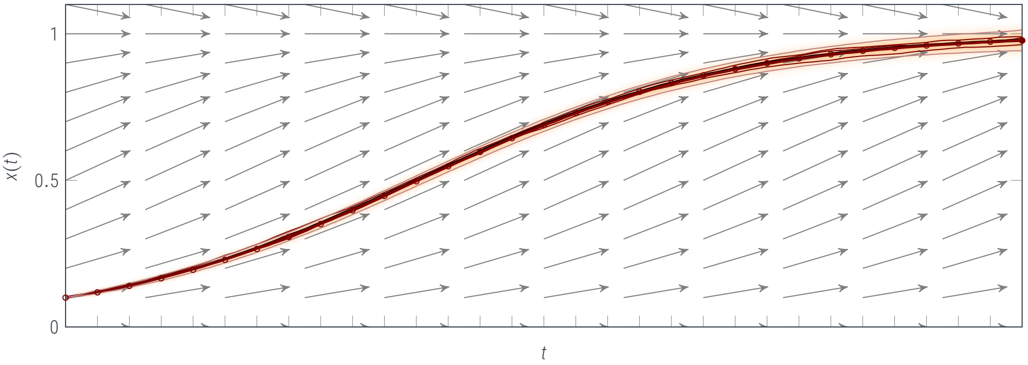

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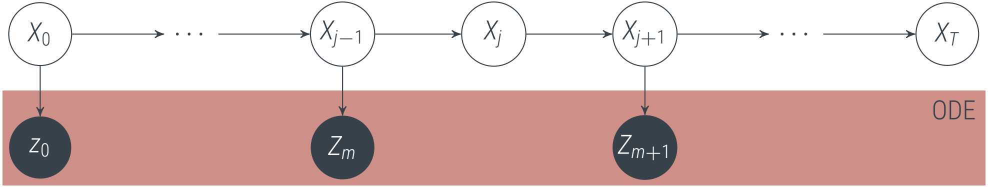
Simulation as Filtering

probabilistic ODE solvers can be realised as Kalman filters

Tronarp, Kersting, Särkkä, PH, Statistics & Computing **29**(6): 1297–1315



$$z_0 \mid X(t_0) \sim \delta(x(t_0) - x_0) \qquad Z_m \mid X(t_m) \sim \delta(X^{(1)}(t_m) - f(X^{(0)}(t_m)))$$

- Use a **tractable** (linear Gaussian) *stochastic* differential equation as a prior for the **intractable** solution of the *nonlinear ordinary* differential equation

$$dX(t) = FX(t)\,dt + L\,dW(t) \qquad \text{with} \qquad X^{(i)}(t) = \frac{d^i}{dt^i}x(t), i = 1, \dots, \nu$$

- Consider *information operators* Z_i to link evaluations of the vector field f to x
- run the *extended Kalman filter (EKF)* to propagate uncertainty through f.

Simulation as Filtering

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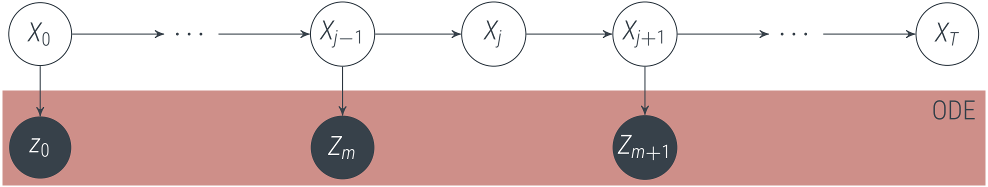


procedure $\textsc{ExtendedFilter}(m_{t-1}, P_{t-1}, A, Q, H, R, y)$

$m_t^- = Am_{t-1}$ // predictive meanm with $A = \int \exp(F(\Delta t))$

$P_t^- = AP_{t-1}A^\intercal + Q$ // predictive covariance, with $Q = \int_0^{\Delta t} e^{F\tau} LL^\intercal e^{F\tau} \, d\tau$

$r = y - Hm_t^-$ // residual, with $y = 0, H = \partial h_{10} / \partial X|_{X=m_t^-}$

$S = HP_t^- H^\intercal + R$ // innovation covariance

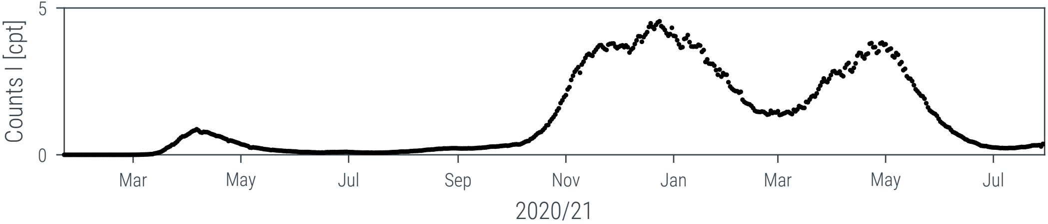
$K = P_t^- H^\intercal S^{-1}$ // gain

$m_t = m_t^- + Kr$ // updated mean

$P_t = (I - KH)P_t^-$ // updated covariance

return $(m_t, P_t), (m_t^-, P_t^-)$

end procedure



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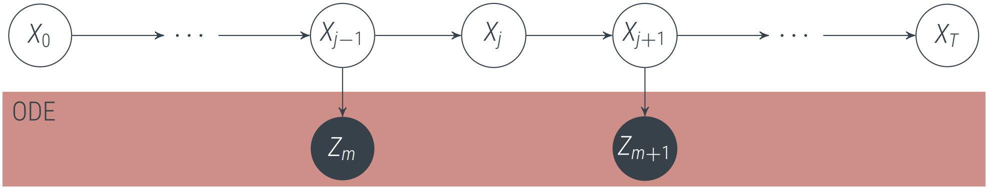
Not forward/inverse, but *mixed information*

blurring the boundaries of the black box

[Tronarp, Kersting, Särkkä, Hennig, 2019; Schmidt, Krämer, Hennig, , NeurIPS 2021]



to solve ODE $\frac{d}{dt}x(t) = f(x(t), t)$, model with SDE $dX(t) = F_X X(t)\,dt + L_X dW_X(t)$ and observation model (information operator)

$$Z_m \mid X(t_m) \sim \delta(E_X^{(1)} X(t_m) - f(E_X^{(0)} X(t_m)))$$

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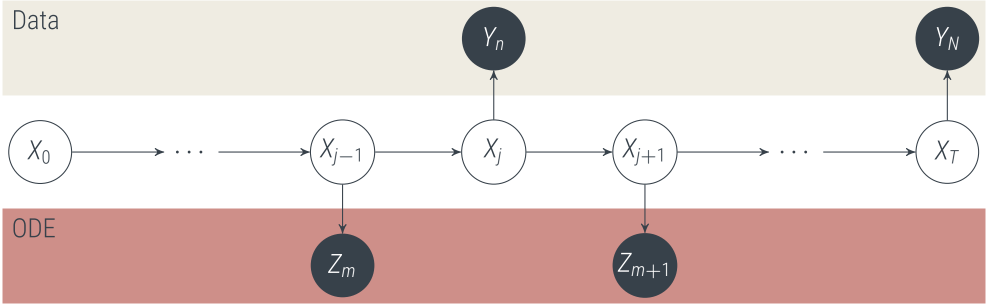


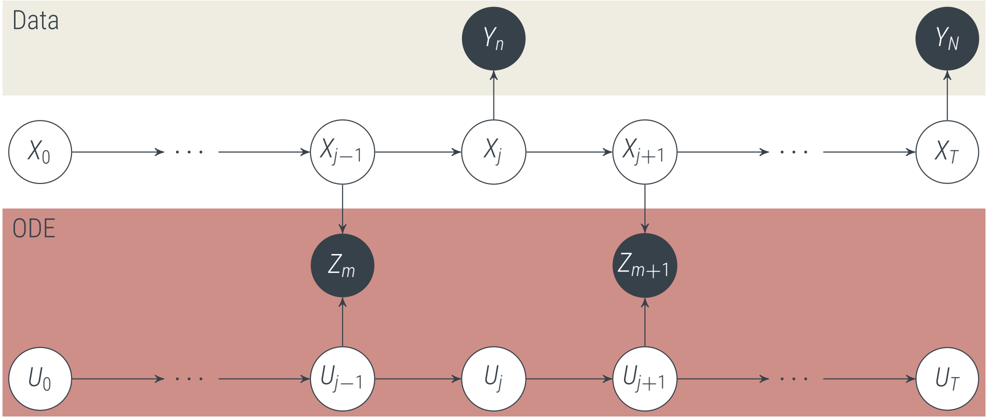
natively (within same "forward" solve) combine with physical observations of the trajectory

$$Y_n \mid X(t_n) \sim \mathcal{N}(HE_X^0 X(t_n), R)$$

Not forward/inverse, but *mixed information*

blurring the boundaries of the black box

[Tronarp, Kersting, Särkkä, Hennig, 2019; Schmidt, Krämer, Hennig, , NeurIPS 2021]



propagate uncertainty about ODE (e.g. from a latent force U) through the extended Kalman filter to solve $\frac{d}{dt}x(t) = f(x(t), u(t), t)$ with $dU(t) = F_U U(t)\, dt + L_U dW_U(t)$.

No more black box ODE solvers

Example: Covid modelling

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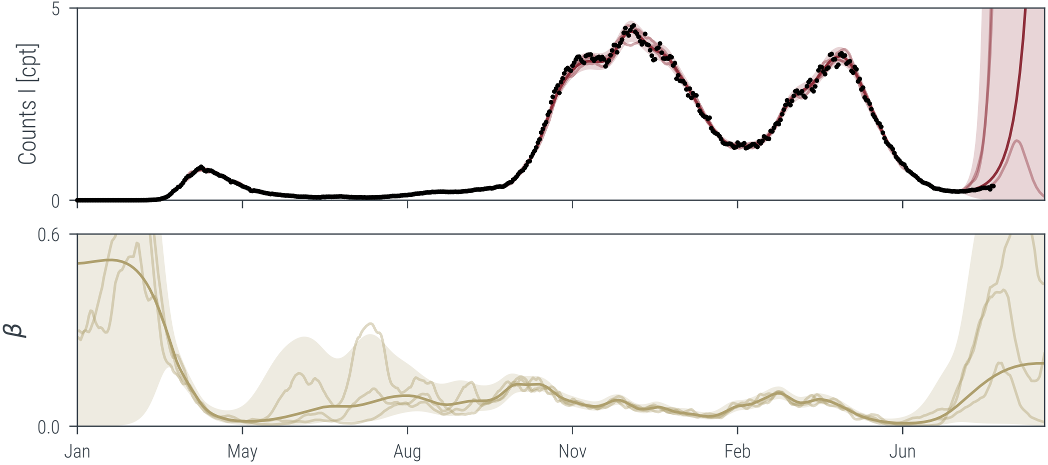
Schmidt, Krämer, Hennig, 2021, NeurIPS 2021



Addiotnal Information can be added, too

Information Operator for Hamiltonians and other conserved quantities

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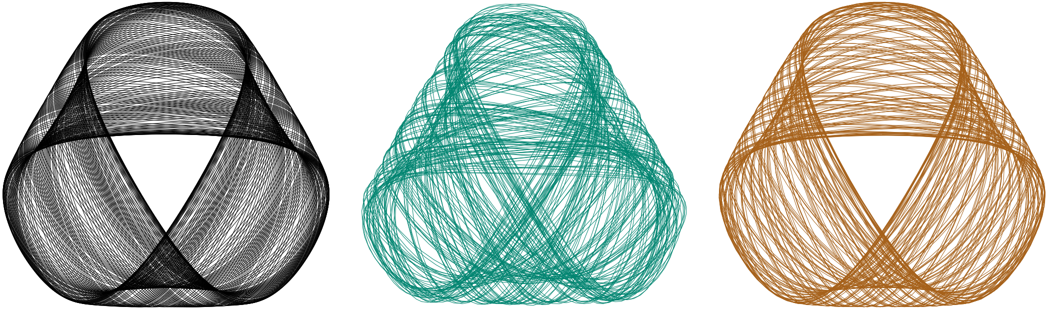
Bosch, Tronarp, PH, AISTATS 2022 (arXiv 2110.10770)



Description	Equation	Information operator
First-order ODE	$\dot{y}(t) = f\left(y(t), t\right)$	$z(t, Y) := Y^{(1)} - f\left(Y^{(0)}, t\right)$
Second-order ODE	$\ddot{y}(t) = f\left(\dot{y}(t), y(t), t\right)$	$z(t, Y) := Y^{(2)} - f\left(Y^{(1)}, Y^{(0)}, t\right)$
Mass matrix DAE	$M\dot{y}(t) = f\left(y(t), t\right)$	$z(t, Y) := MY^{(1)} - f\left(Y^{(0)}, t\right)$
Invariances	$g\left(y(t), \dot{y}(t)\right) = 0$	$z(t, Y) := g\left(Y^{(0)}, Y^{(1)}\right)$
Chain rule	$\ddot{y}(t) = J_f\left(y(t)\right) \cdot \dot{y}(t)$	$z(t, Y) := Y^{(2)} - J_f\left(Y^{(0)}\right) \cdot Y^{(1)}$

Stationary Inverse Problems as GP Hyperparameter Inference

Infer the parameters θ of IVP ξ_θ measured with Gaussian noise at solution x

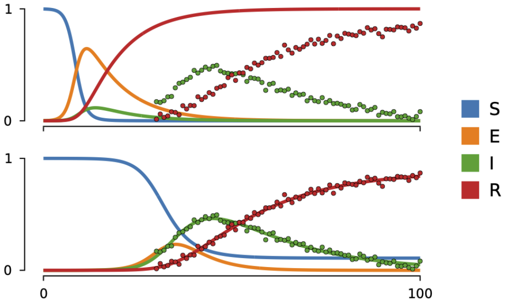
$$\frac{\mathrm{d}}{\mathrm{d}t}\xi_\theta(t) = f_\theta(\xi_\theta(t)), \qquad \phi_\theta(0) = x_0, \qquad p(\boldsymbol{y} \mid x) = \prod_i \mathcal{N}(y_i; H^\intercal x, R_\theta)$$

- We'd like to compute the marginal

$$p(\boldsymbol{y} \mid \theta) = \int p(\boldsymbol{y} \mid x)\delta(x - \xi_\theta)\,\mathrm{d}x$$

- Approximate δ with a Gaussian

$$\hat{p}(\boldsymbol{y} \mid \theta) = \int p(\boldsymbol{y} \mid x)\hat{\delta}_N(x - \xi_\theta)\,\mathrm{d}x$$



Prior Hyperparameters as Regularizers

Tronarp, Bosch, Hennig. *Fenrir: Physics-Enhanced Regression for Initial Value Problems*

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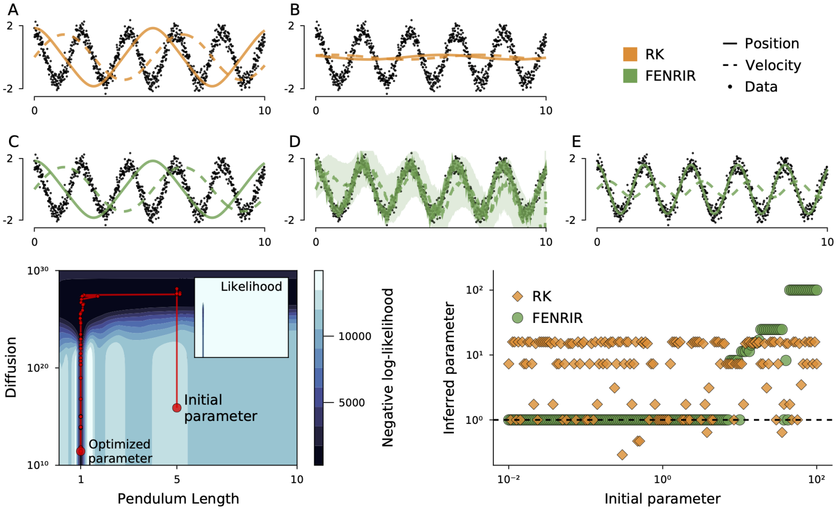
arXiv 2202.01287



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Summary

- *Propagation of Uncertainty* is great, but should not mislead us to keep the rigid structure of classical code
- instead, sometimes, *information* (the opposite of uncertainty) shouldn't be propagated, but *combined* efficiently
- because Probnum methods can deal with imprecise quantities natively, changing the order of the computation does not pose a conceptual problem for them. (That doesn't mean changing the order is always a good idea. But it's also not necessarily a bad idea).
- doing so can break the (artificial) separation between forward and inverse problems.

Re-casting computation as inference allows genuinely new, valuable functionality.

http://mml.inf.uni-tuebingen.de

Probabilistic Numerics – Computation as Machine Learning. P. Hennig, H. Kersting, M.A. Osborne, CUP, 2022

https://www.youtube.com/c/TübingenML

@PhilippHennig5

High-Dimensional ODEs/PDEs

Factorization assumptions allow scaling to millions of dimensions

Krämer, Bosch, Schmidt, PH, arXiv 2110.11812