Numerical Solutions of ODEs by Gaussian (Kalman) Filtering

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joint work with Michael Schober, Philipp Hennig, Tim Sullivan and Han C. Lie

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DFG Deutsche Forschungsgemeinschaft

Contents

Numerical methods such as

- linear algebra (least-squares)
- optimization (training & fitting)
- integration (MCMC, marginalization)
- solving differential equations (RL, control)

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Numerical methods perform inference

an old observation [Poincaré 1896, Diaconis 1988, O'Hagan 1992]

A numerical method
estimates a function's latent property
given the result of computations.

quadrature	estimates $\int_a^b f(x)\,dx$	given $\{f(x_i)\}$
linear algebra	estimates x s.t. $Ax = b$	given $\{As = y\}$
optimization	estimates x s.t. $\nabla f(x) = 0$	given $\{\nabla f(x_i)\}$
analysis	estimates $x(t)$ s.t. $x' = f(x,t)$,	given $\{f(x_i, t_i)\}$

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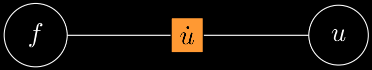
Probabilistic numerics uses this link between statistics and numerics to

(i) perform numerical computation in a statistically interpretable framework, and

(ii) enable an all–inclusive uncertainty quantification (for computations which include both numerical and statistical parts).

ODEs: Initial Value Problems (IVP)

$$\frac{\partial u}{\partial t}(t) = f(u(t), t), \quad u(0) = u_0 \in \mathbb{R}^n$$



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II. In AI, for example:

1. Nesterov's Accelerated Gradient Descent
2. dynamically changing data, and
3. demand forecasting.

Challenge in AI: Most quantities involving the ODE can be uncertain:

1. initial value,
2. partial knowledge of vector field f
3. imprecise function evaluations, and
4. accumulated numerical errors.

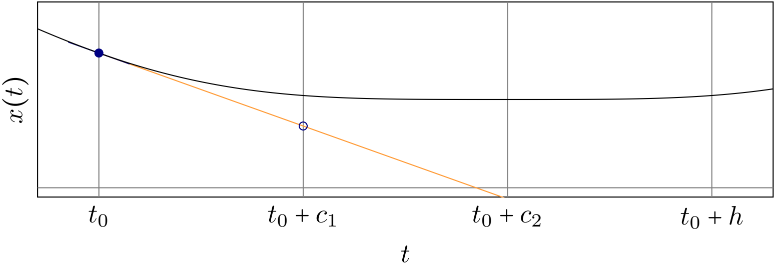
Numerical solutions of IVPs

plots: Runge-Kutta of order 3

How classical solvers extrapolate forward from time t_0 to $t_0 + h$:

- Estimate $\dot{x}(t_i)$, $t_0 \leq t_1 \leq \cdots \leq t_n \leq t_0 + h$ by evaluating $y_i \approx f(t, \hat{x}(t_i))$, where $\hat{x}(t)$ is itself an estimate for $x(t)$
- Use this data $y_i := \dot{x}(t_i)$ to estimate $x(t_0 + h)$, i.e.

$$\hat{x}(t_0 + h) \approx x(t_0) + h \sum_{i=1}^{b} w_i y_i.$$



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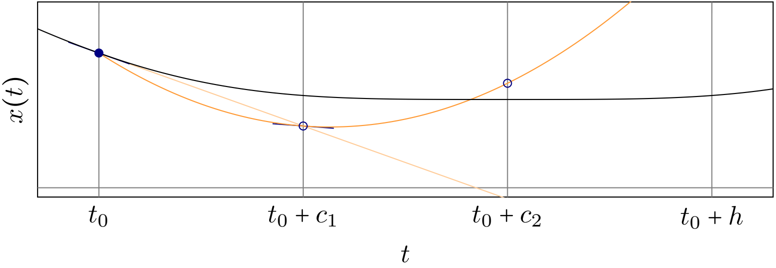

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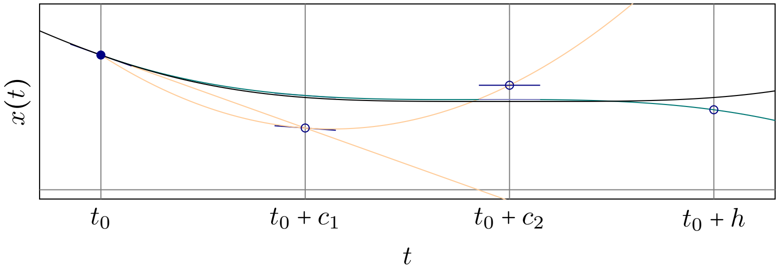

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Uncertainty in these calculations:

- We can only observe x indirectly via $\hat{x}$.
- The observations of $\dot{x}(t) = f(t, \hat{x}(t))$ is inaccurate, since $\hat{x}(t) \approx x(t)$.
- There is uncertainty on our source of information $\hat{x}$, since it is both partial (i.e. discrete) and 'noisy'.
- The quantification of uncertainty on $\hat{x}$ is crucial to quantify uncertainty on x.

The Filtering Problem from Stochastic Calculus

Assume we have an unobservable *state* X_t of a dynamical system given by the SDE:

$$dX_t = b(t, X_t)dt + \sigma(t, X_t)dB_t.$$

We can only observe the *observations process* Z_t, a noisy transform of X_t, given by the SDE:

$$dZ_t = c(t, X_t)dt + \gamma(t, X_t)d\tilde{B}_t, \quad Z_0 = 0.$$

Filtering Problem: What is the L^2-best estimate $\hat{X}_t$ of X_t, based on observations $\{Z_{s_i} | s_i \leq t\}$?

IVPs as Filtering Problems:

- State is the unknown belief over $x(t)$
- Observation process is $\dot{x}(t)$ + 'noise'
- 'noise' process is due to the inaccurate evaluation position $\hat{x}(t)$ in $\dot{x}(t) \approx f(t, \hat{x}(t))$

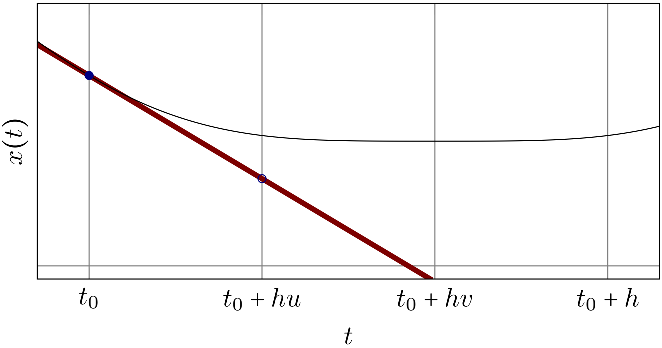
Hence,

(i) IVPs can be recast as Stochastic Filtering Problems,

(ii) and solved by Gaussian (Kalman) filtering.

IVPs by Gaussian filtering

plots by M. Schober



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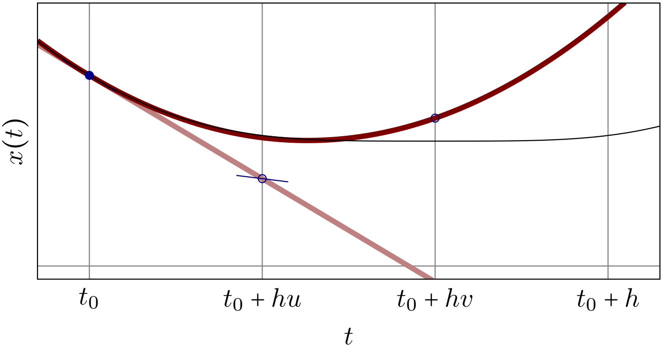

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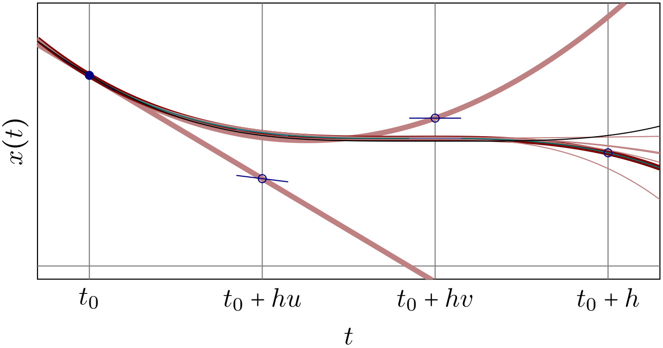
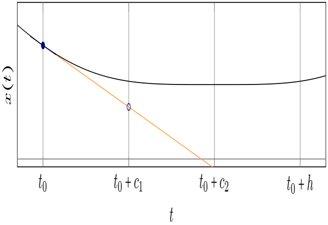
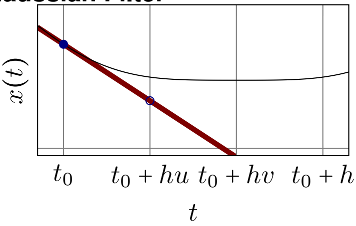


IVPs by Numerical Solver versus Gaussian Filtering

Numerical Solver



Gaussian Filter



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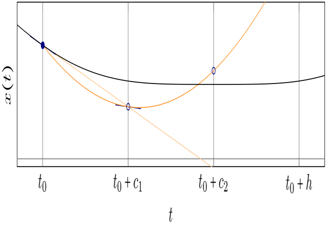

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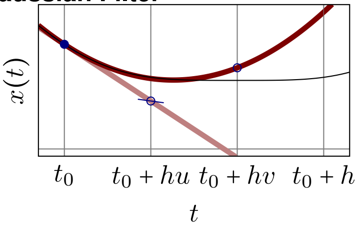

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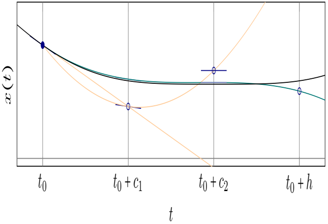

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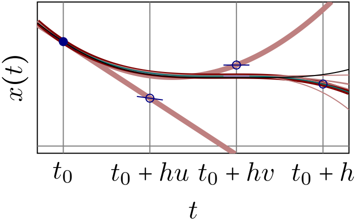

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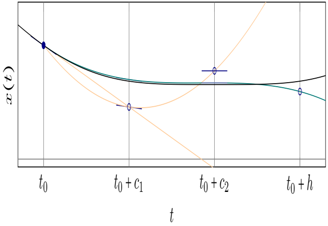

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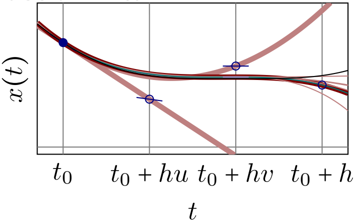

The computation of the numerical mean and the posterior mean of Gaussian filtering share the same analytic structure [Schober et al., 2014]

We interpret $(u, \dot{u}, u^{(2)}, \ldots, u^{(q-1)})$ as a draw from a q-times-integrated Wiener process $(X_t)_{t\in[0,T]} = (X_t^{(1)}, \ldots, X_t^{(q)})^T_{t\in[0,T]}$ given by a linear SDE:

$$dX_t = FX_t dt + QdW_t,$$
$$X_0 = \xi, \quad \xi \sim \mathcal{N}(m(0), P(0))$$
$$\Longrightarrow \; X_t = \mathcal{GP}(A(t)m(0), A(t)P(0)A(t)^\top + Q), \quad A(t) = \exp(hF) \text{ and } Q(t) = \ldots$$

Filtering–based probabilistic ODE solvers

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Vector field y with uncertainty R
main source of uncertainty
cheaply quantified by Bayesian quadrature [Kersting and Hennig, 2016]

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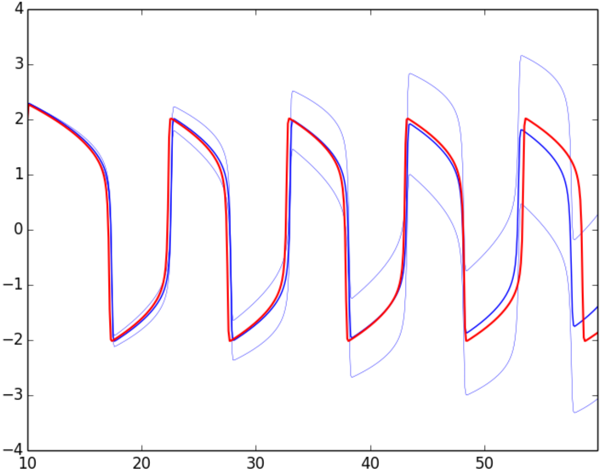
Update step:

$$z = y - e_n^T m^-_{t+h},$$
$$S = e_n^T P^-_{t+h} e_n + R,$$
$$K = P^-_{t+h} e_n S^{-1},$$
$$m_{t+h} = m^-_{t+h} + Kz,$$
$$P_{t+h} = P^-_{t+h} - K e_n^T P^-_{t+h},$$



We can compute a probabilistic output (above 95% confidence interval) at a low computational overhead.

Does this solver live up to classical expectations?

Current project: Theoretical Analysis

For an Integrated Wiener Process prior, we have the following convergence rates for the posterior mean:

Theorem

Under some technical assumptions, we have, for all modeled dimensions $i \in \{0, \dots, q\}$, *globally that*

$$\sup_n \left\| m(nh)_i - x^{(i)}(nh) \right\| \leq K h^{q-i}, \tag{1}$$

and locally that

$$\left\| m(h)_i - x^{(i)}(h) \right\| \leq K h^{q+1-i}, \tag{2}$$

where $K > 0$ *is a constant independent of* h *and* n*.*

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Proof: On arxiv soon!

Summary

The PN perspective on ODEs:

1. Unknown numerical quantities are modeled as random variables
2. uncertainty arises from initial values, imprecise function evaluations, partial knowledge of functions and accumulated numerical errors,
3. modeling these uncertainties yields a stochastic filtering problem.

We have a solver which can

(i) solve IVP at comparable cost of Runge–Kutta,
(ii) performs consistent UQ for all sources of uncertainty
(iii) output a whole probability measures, including confidence intervals,
(iv) filter out higher derivatives of the solution simultaneously, and
(v) learn (e.g. a periodic) vector field, while solving an ODE.

More information at probabilistic-numerics.org.

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Thank you for listening!

Bibliography

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