ODE Filtering

A Gaussian Decision Agent for Forward Problems

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$$\dot{x}(t) = f(x(t)),\ t \in [0, T] \qquad x(0) = x_0 \in \mathbb{R}^d \tag{1}$$

We model all unkown (even if deterministic) objects, i.e.

- solution $x \in C^1([0, T]; \mathbb{R}^d)$,
- vector field $f \in C^0([0, T]; \mathbb{R}^d)$

by random variables or stochastic processes (**prior information**), and define which information we obtain in the course of the numerical computation of the solution (**measurement model**).

Prior information + measurement model $\longrightarrow$ application of Bayes rule

Choice of Prior information

Prior information on x

For prior information on f see our publications.

We a priori model x and $\dot{x}$ with an arbitrary Gauss-Markov process, i.e. with linear SDE

$$dX_t = FX_t dt + L dB_t,$$

with Gaussian initial condition $X_0 \sim \mathcal{N}(m_0, P_0)$. For an Integrated Brownian motion (Wiener process)

$$\begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix} \sim \begin{pmatrix} \mathrm{d}X_t \\ \mathrm{d}\dot{X}_t \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} X_t \\ \dot{X}_t \end{pmatrix} \mathrm{d}t + \begin{pmatrix} 0 \\ \sigma \end{pmatrix} \mathrm{d}B_t, \tag{2}$$

the ODE filter coincides with Runge-Kutta and Nordsieck methods in a certain sense [SSH18]. An Ornstein Uhlenbeck prior

$$\begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix} \sim \begin{pmatrix} \mathrm{d}X_t \\ \mathrm{d}\dot{X}_t \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & -\theta \end{pmatrix} \begin{pmatrix} X_t \\ \dot{X}_t \end{pmatrix} \mathrm{d}t + \begin{pmatrix} 0 \\ \sigma \end{pmatrix} \mathrm{d}B_t, \tag{3}$$

has also been studied [MKSH17].

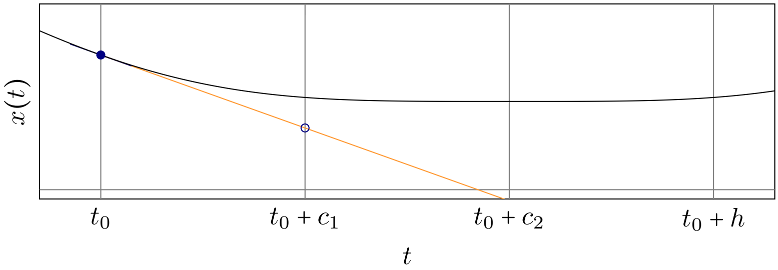
Numerical solutions of IVPs

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 $y_i \approx f(\hat{x}(t_i))$, 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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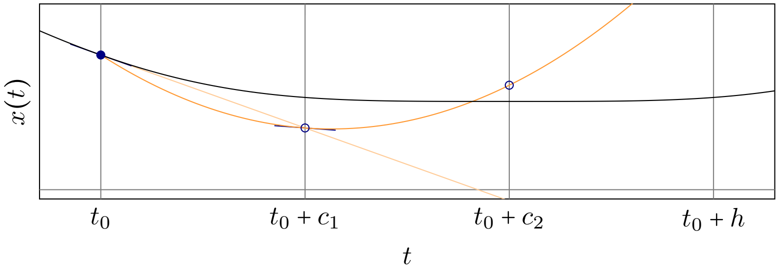

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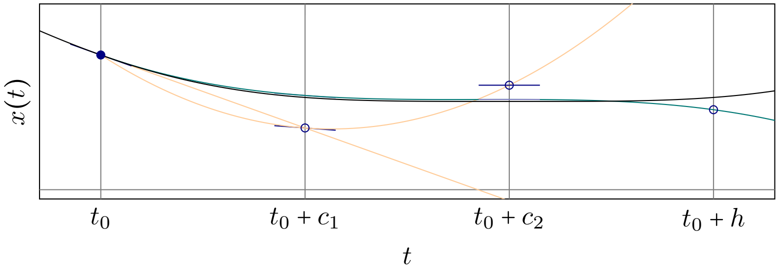

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Information in these calculations:

$$\dot{x}(t) = f(x(t)) \approx f(\hat{x}(t)) \tag{4}$$

For information, f is evaluated at (or around) the current numerical estimate $\hat{x}$ of x.

In principle, given a Gaussian believe

$$\begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m(t) \\ \dot{m}(t) \end{pmatrix}, \begin{pmatrix} P_{00} & P_{01} \\ P_{10} & P_{11} \end{pmatrix} \right), \tag{5}$$

the 'true' information on $\dot{x}(t)$ would be the pushforward measure $f_* \mathcal{N}(\dot{m}(t), P_{00})$. For computational speed, we want a Gaussian, with matched moments

$$y = \int f(\xi) \, \mathrm{d}\mathcal{N}(\xi; m(t), P_{00}), \tag{6}$$

and covariance

$$R = \int f(\xi) f^T(\xi) \, \mathrm{dd}\mathcal{N}(\xi; m(t), P_{00}). \tag{7}$$

Suitable ways to approximate these integrals have been studied in [KH16]. For maximum speed, we can just use $y = f(m(t))$ and $R = 0$ as proposed in [SSH18].

This yields a (Kalman) filtering algorithm for ODEs.

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

$$
\begin{aligned}
dX_t &= FX_t dt + Q dW_t, \\
X_0 &= \xi, \quad \xi \sim \mathcal{N}(m(0), P(0)).
\end{aligned}
$$

Filtering–based probabilistic ODE solvers

Gaussian filtering

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Calculation of Posterior by Gaussian filtering

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

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Calculation of Posterior by Gaussian filtering

Prediction step:

$$
\begin{aligned}
m^-_{t+h} &= A(h)m_t, \\
P^-_{t+h} &= A(h)P_tA(h)^T + Q(h),
\end{aligned}
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Gradient prediction at $t+h$: Approximate

$$\begin{aligned} y &\approx \int f(\xi)\, \mathrm{d}\mathcal{N}\left(\xi; m(t), P_{00}\right), \\ R &\approx \int f(\xi) f^T(\xi)\, \mathrm{d}\mathcal{N}\left(\xi; m(t), P_{00}\right) \end{aligned}$$

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[SDH14]

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Update step:

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

Research Questions

1. worst-case convergence rates vs. average convergence rates (over a measure on $\boldsymbol{f}$),
2. trade-off between computational speed (with Gaussians) and statistical accuracy (with samples),
3. properties of different priors on $\boldsymbol{x}$,
4. in which sense are 'Bayesian' algorithms (like the above) approximations of Bayesian algorithms in the sense of [COSG17],
5. can PN algorithms for ODEs be extended to SDEs?,
6. Bayesian inverse problems—inner loop vs outer loop trade-off like in Bayesian optimization?
7. different filters (particle filter, ensemble Kalman filter)?

Thank you for listening!

Bibliography

- J. Cockayne, C.J. Oates, T. Sullivan, and M.A. Girolami.
  Bayesian probabilistic numerical methods.
  arXiv:1702.03673 [stat.ME], February 2017.
- Hans Kersting and P. Hennig.
  Active Uncertainty Calibration in Bayesian ODE Solvers.
  Uncertainty in Artificial Intelligence (UAI), 2016.
- E. Magnani, H. Kersting, M. Schober, and P. Hennig.
  Bayesian Filtering for ODEs with Bounded Derivatives.
  arXiv:1709.08471 [cs.NA], September 2017.
- M. Schober, D. Duvenaud, and P. Hennig.
  Probabilistic ODE Solvers with Runge–Kutta Means.
  Advances in Neural Information Processing Systems (NIPS), 2014.
- Michael Schober, Simo Särkkä, and Philipp Hennig.
  A probabilistic model for the numerical solution of initial value problems.
  Statistics and Computing, January 2018.