Probabilistic Exponential Integrators

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Probabilistic ODE Solvers

Initial value problem:

$$\dot{y}(t) = f(t, y(t)), \quad t \in [t_0, T], \quad y(t_0) = y_0$$

Classical numerical ODE solvers compute $\hat{y}(t) \approx y(t)$.

***Probabilistic numerical* ODE solution:**

$$p\left(y(t) \mid y(t_0) = y_0, \{\dot{y}(t_n) - f(y(t_n)) = 0\}_{n=1}^N\right)$$

for some time grid $\{t_n\}_{n=1}^N \subset [t_0, T]$.

ODEs as Bayesian State Estimation

Prior: Gauss–Markov process $Y(t) := [y(t), \dot{y}(t), \dots, y^{(q)}(t)]$,

$$\mathrm{d}Y(t) = AY(t)\,\mathrm{d}t + B\,\mathrm{d}W(t), \qquad Y(t_0) \sim \mathcal{N}(\mu_o, \Sigma_0).$$

Equivalent in discrete time:

$$Y(t+h) \mid Y(t) \sim \mathcal{N}\left(\Phi(h)Y(t), Q(h)\right)$$

Likelihood: $Z_n := E_0 Y(t_n) - f\left(E_1 Y(t_n), t\right) \triangleq 0$,

with E_0, E_1 selection matrices.

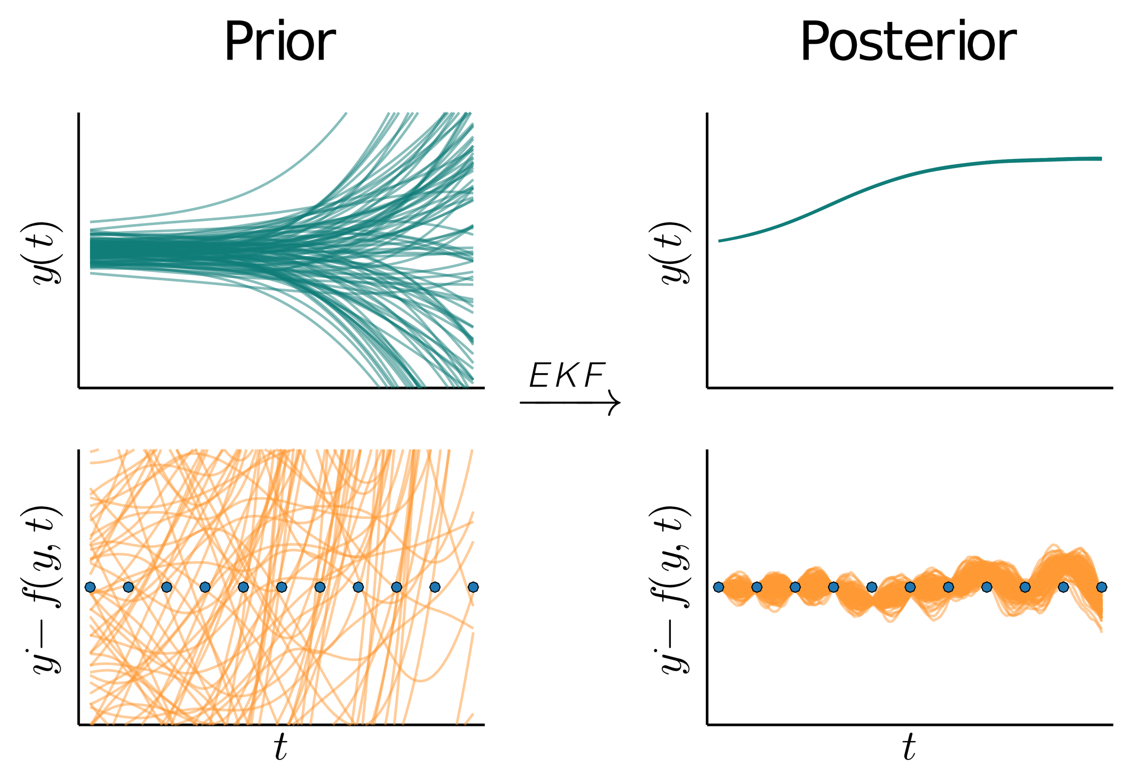
$\Rightarrow$ $p(Y(t) \mid Z_{1:N})$ *is a Bayesian state estimation problem!*

Efficient approximate inference

Extended Kalman filtering and smoothing gives

$$p\big(Y(t) \mid E_0 Y(t_0) = y_0, \{Z_n = 0\}_{n=1}^N\big) \approx \mathcal{N}\left(\mu(t), \Sigma(t)\right)$$

Visualization of probabilistic ODE solvers:



Simulation *is* inference!

For better *stability*, encode some problem structure in the *prior*!

Scan the QR code
to check out the paper

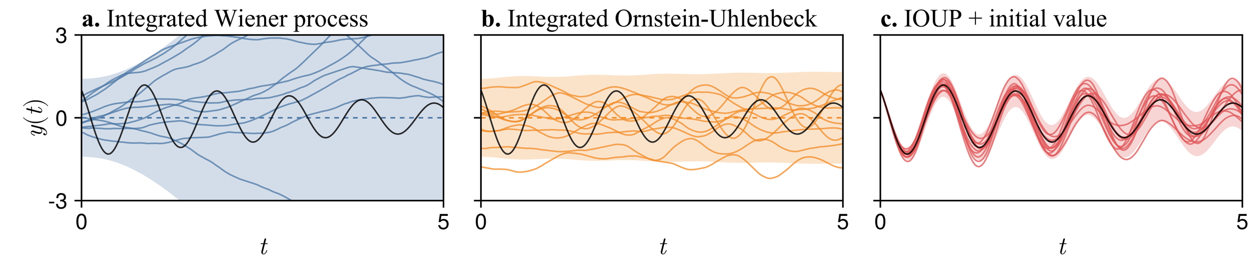
Exponential Integrators

Semi-linear ODE: $\dot{y} = Ly + f(y, t)$,

Goal: Leverage the linearity to improve the method.

Approach: Include it in the prior and solve the linear part exactly.

$\Rightarrow$ *Integrated Ornstein–Uhlenbeck process priors*

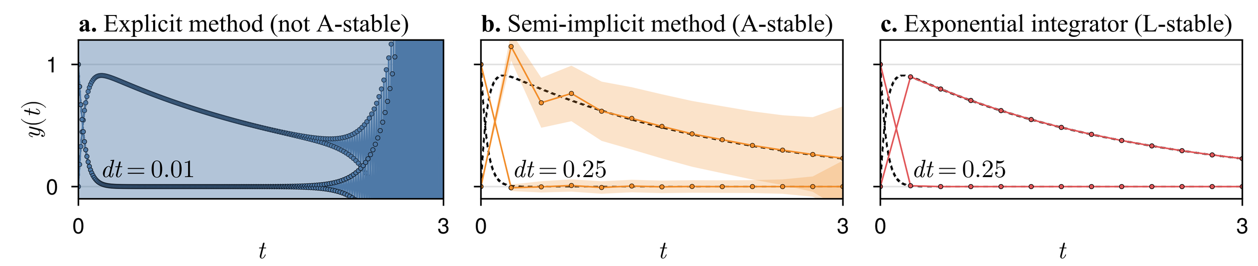


Stability

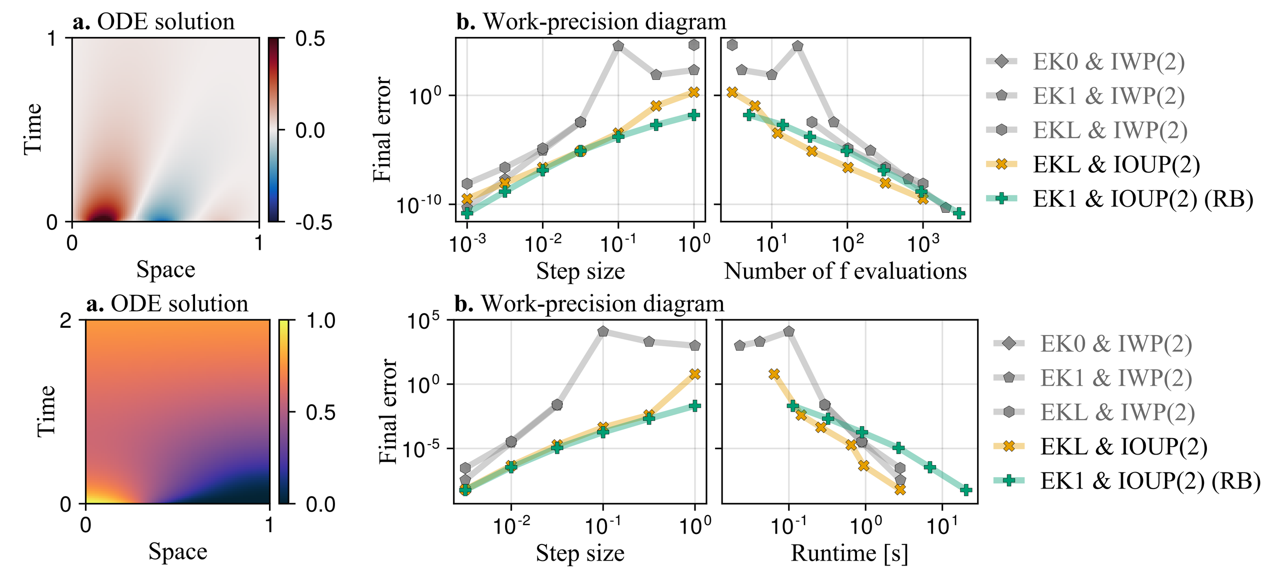
Given the test equation $\dot{y} = \lambda y$ with $\lambda < 0$,

- A-stable: numerical solution decays eventually.
- L-stable: numerical solution decays *at the right rate*.

Probabilistic exponential integrators are "L-stable"!



Experiments



$\Rightarrow$ *Probabilistic exponential integrators can take larger steps than non-exponential methods!*

Software Library

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] add ProbNumDiffEq
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