Probabilistic Numerics for Ordinary Differential Equations

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Background

- Ordinary differential equations and how to solve them
- State estimation with extended Kalman filtering & smoothing

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Central statement: **ODE solving is state estimation**

- "ODE filters": **How to solve ODEs with extended Kalman filtering and smoothing**
- *Bells and whistles* to make ODE filters work even better
  - Uncertainty calibration
  - Square-root filtering

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Fun with ODE filters

- Generalizing ODE filters to other related problems (higher-order ODEs, DAEs, …)
- Latent force inference: Joint GP regression on both ODEs and data

Background: **Ordinary Differential Equations and how to solve them**

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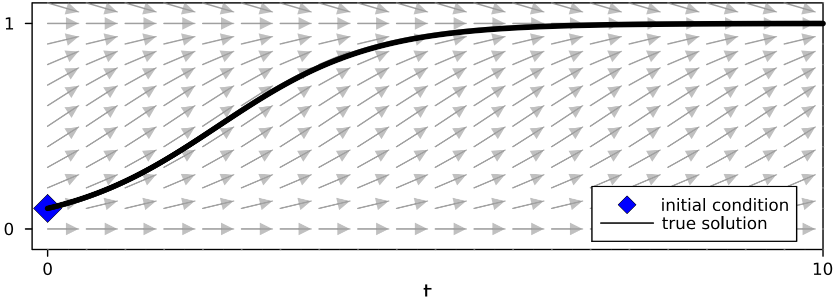
Numerical ODE solvers try to estimate an unknown function by evaluating the vector field

$$\dot{x}(t) = f\left(x(t), t\right)$$

with $t \in [0, T]$, vector field $f : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$, and initial value $x(0) = x_0$. Goal: "Find x".

- **Simple example**: Logistic ODE

$$\dot{x}(t) = x(t)\left(1 - x(t)\right), \qquad t \in [0, 10], \qquad x(0) = 0.1.$$



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  $$\hat{x}(t+h) = \hat{x}(t) + hf(\hat{x}(t), t)$$

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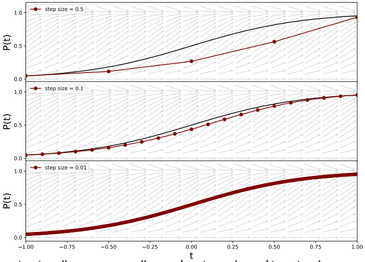
Forward Euler for different step sizes:



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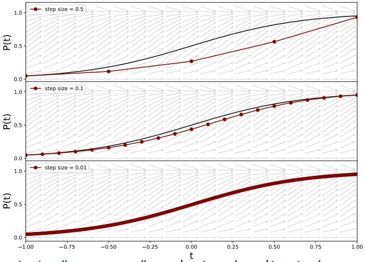

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Numerical ODE solvers **estimate** $x(t)$ *by evaluating f on a discrete set of points.*

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or “How to treat ODEs as the state estimation problem that they really are”

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1. Prior:
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Prior: General Gauss–Markov processes

See also: *Särkkä & Solin, "Applied Stochastic Differential Equations", 2013*

- **Continuous Gauss–Markov prior:** Let $X(t) = [X^{(0)}(t), X^{(1)}(t), \dots, X^{(q)}(t)]^\top$ be the solution of a *linear time-invariant (LTI) stochastic differential equation (SDE)*:

$$\begin{aligned} dX(t) &= FX(t)\,\mathrm{d}t + \Gamma\,\mathrm{d}W(t), \\ X(0) &\sim \mathcal{N}(\mu_0, \Sigma_0), \end{aligned}$$

  with F such that $dX^{(i)}(t) = X^{(i+1)}(t)dt$. Then, *we use $X^{(i)}(t)$ to model the i-th derivative of $x(t)$*.
  Examples: Integrated Wiener process, Integrated Ornstein–Uhlenbeck process, Matérn process.

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- **Discrete transition densities:** $X(t)$ can be described in discrete time with

$$X(t+h) \mid X(t) \sim \mathcal{N}\left(X(t+h); A(h)X(t), Q(h)\right),$$

  where $(A(h), Q(h))$ are given by

$$A(h) = \exp\left(Fh\right), \qquad Q(h) = \int_0^h A(h-\tau)\Gamma\Gamma^\top A(h-\tau)^\top\,\mathrm{d}\tau.$$

  The transition matrices $(A(h), Q(h))$ can be computed with the "matrix fraction decomposition"; see for instance *Särkkä & Solin, "Applied Stochastic Differential Equations", 2013*.

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Prior: The q-times integrated Wiener process

A very convenient prior with closed-form transition densities

- **q-times integrated Wiener process prior**: $X(t) \sim \mathrm{IWP}(q)$

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\begin{aligned}
\mathrm{d}X^{(i)}(t) &= X^{(i+1)}(t)\,\mathrm{d}t, \qquad i = 0, \dots, q-1, \\
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for any $i, j = 0, \dots, q$. (one-dimensional case).
(proof: [Kersting et al., 2020])

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- **Example**: IWP(2)

$$A(h) = \begin{pmatrix} 1 & h & \frac{h^2}{2} \\ 0 & 1 & h \\ 0 & 0 & 1 \end{pmatrix},$$

$$Q(h) = \begin{pmatrix} \frac{h^5}{20} & \frac{h^4}{8} & \frac{h^3}{6} \\ \frac{h^4}{8} & \frac{h^3}{3} & \frac{h^2}{2} \\ \frac{h^3}{6} & \frac{h^2}{2} & h \end{pmatrix}.$$

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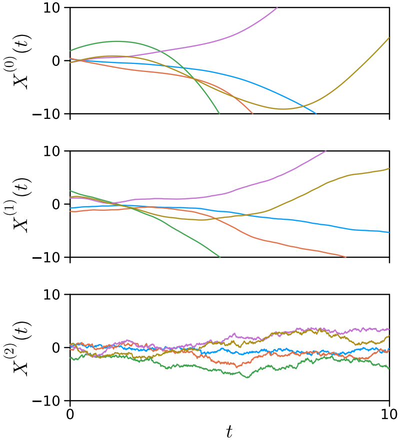

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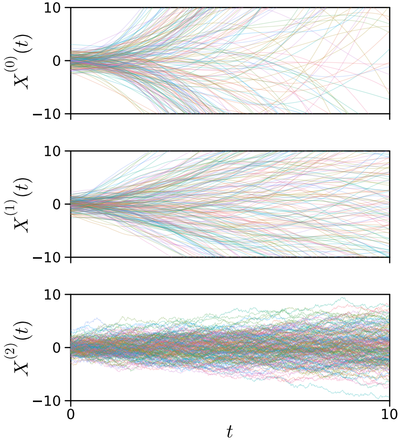

Probabilistic numerical ODE solutions

How to treat ODEs as the state estimation problem that they really are

$$p\left(x(t) \mid x(0) = x_0, \{\dot{x}(t_n) = f\left(x(t_n), t_n\right)\}_{n=1}^{N}\right)$$

To solve an ODE with Gaussian filtering and smoothing, we need:

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The likelihood model and the data

The likelihood and data relate the prior to the desired posterior: the numerical ODE solution

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- **Easier goal:** Satisfy the ODE *on a discrete time grid*

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- This motivates a **measurement model** and **data**:

$$Z(t_i) \mid X(t_i) \sim \mathcal{N}\left(m(X(t_i), t_i), R\right)$$

$$z_i \triangleq 0, \qquad i = 1, \dots, N.$$

where z_i is a realization of $Z(t_i)$.

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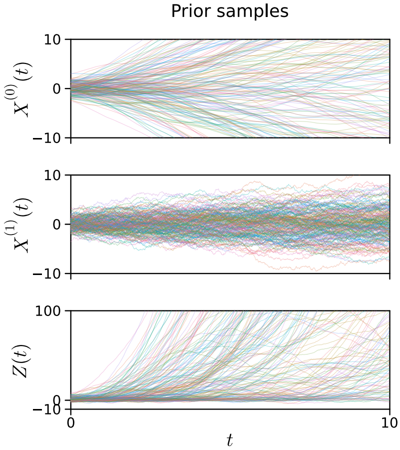

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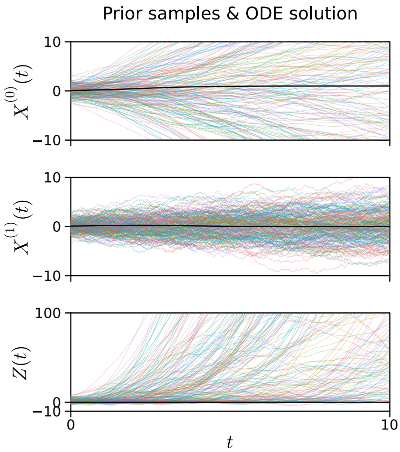

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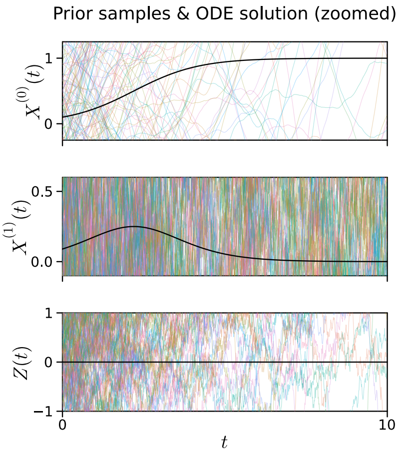

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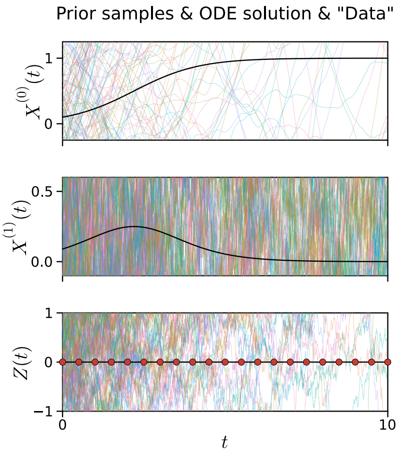

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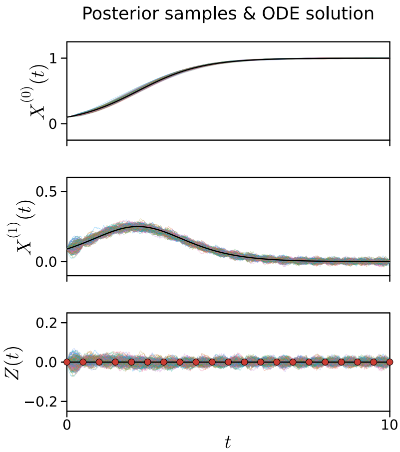

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Spoiler: **This is the thing we want!**

Probabilistic numerical ODE solutions

How to treat ODEs as the state estimation problem that they really are

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$$p\left(x(t) \mid x(0) = x_0, \{\dot{x}(t_n) = f\left(x(t_n), t_n\right)\}_{n=1}^{N}\right)$$

To solve an ODE with Gaussian filtering and smoothing, we need:

1. Prior: q-times integrated Wiener process prior:

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This describes a state estimation problem $\Rightarrow$ solve with EKF/EKS!

The extended Kalman ODE filter – the state-space model

Bringing the last slides all together

For a given initial value problem $\dot{x}(t) = f(x(t), t)$ on $[0, T]$ with $x(0) = x_0$, we have:

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One thing is still missing: **What about the initial value??**

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One thing is still missing: **What about the initial value??** Just add another measurement at $t = 0$:

$$Z^{\text{init}} \mid X(0) \sim \delta\left(Z^{\text{init}}; X^{(0)}(0)\right), \qquad z^{\text{init}} \triangleq x_0.$$

The extended Kalman ODE filter

We can solve ODEs with basically just an extended Kalman filter

Algorithm The extended Kalman ODE filter

procedure EXTENDED KALMAN ODE FILTER($(\mu_0^-, \Sigma_0^-), (A, Q), (f, x_0), \{t_i\}_{i=1}^N$)
    $\mu_0, \Sigma_0 \leftarrow$ KF_UPDATE($\mu_0^-, \Sigma_0^-, E_0, 0_{d\times d}, x_0$) // Initial update to fit the initial value
    for $k \in \{1, \dots, N\}$ **do**
        $h_k \leftarrow t_k - t_{k-1}$ // Step size
        $\mu_k^-, \Sigma_k^- \leftarrow$ KF_PREDICT($\mu_{k-1}, \Sigma_{k-1}, A(h_k), Q(h_k)$) // Kalman filter prediction
        $m_k(X) := E_1 X - f(E_0 X, t_k)$ // Define the non-linear observation model
        $\mu_k, \Sigma_k \leftarrow$ EKF_UPDATE($\mu_k^-, \Sigma_k^-, m_k, 0_{d\times d}, \mathbf{0}_d$) // Extended Kalman filter update
    end for
    return $(\mu_k, \Sigma_k)_{k=1}^N$
end procedure

Recall: The *state* $X(t)$ is a stack of q derivatives $X = \left[X^{(0)}, X^{(1)}, \dots, X^{(q)}\right]^T$.
For convenience, define projection matrices E_i to map to the i-th derivative: $E_i X = X^{(i)}$.

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EXTENDED KALMAN ODE SMOOTHER: Just run a RTS smoother after the filter!

The extended Kalman ODE filter – building blocks

The well-known predict and update steps for (extended) Kalman filtering

Algorithm Kalman filter prediction

```
procedure KF_PREDICT(μ, Σ, A, Q)
    μ^P ← Aμ                      // Predict mean
    Σ^P ← AΣA^⊤ + Q               // Predict covariance
    return μ^P, Σ^P
end procedure
```

Algorithm Extended Kalman filter update

```
procedure EKF_UPDATE(μ, Σ, h, R, y)
    ŷ ← h(μ)                      // evaluate the observation model
    H ← J_h(μ)                    // Jacobian of the observation model
    S ← HΣH^⊤ + R                 // Measurement covariance
    K ← ΣH^⊤ S^{-1}               // Kalman gain
    μ^F ← μ + K(y − ŷ)            // update mean
    Σ^F ← Σ − KSK^⊤               // update covariance
    return μ^F, Σ^F
end procedure
```

(`KF_UPDATE` analog but with affine h)

DEMO TIME: The extended Kalman ODE filter in code

`demo.jl`

Uncertainty calibration or “how to choose prior hyperparameters”

Hyperparameters of the prior have a strong influence on posteriors – so we need to estimate them [Tronarp et al., 2019]

- **Problem**: The prior hyperparameter σ strongly influences covariances. How to choose it?

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[Tronarp et al., 2019]

- **Problem**: The prior hyperparameter σ strongly influences covariances. How to choose it?
- **Standard approach**: Maximize the marginal likelihood:

$$\hat{\sigma} = \arg\max p(\mathcal{D}_{\text{PN}} \mid \sigma) = p(z_{1:N} \mid \sigma) = p(z_1 \mid \sigma) \prod_{k=2}^{N} p(z_k | z_{1:k-1}, \sigma).$$

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- The EKF provides Gaussian estimates $p(z_k \mid z_{1:k-1}) \approx \mathcal{N}(z_k; \hat{z}_k, S_k)$.
  $\Rightarrow$ Quasi-maximum likelihood estimate:

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- **In our specific context** there is a closed-form solution (proof: [Tronarp et al., 2019]):

$$\hat{\sigma}^2 = \frac{1}{Nd} \sum_{i=1}^{N} (z_i - \hat{z}_i)^\top S_i^{-1} (z_i - \hat{z}_i),$$

  and we don't even need to run the filter again! Just adjust the estimated covariances:

$$\Sigma_i \leftarrow \hat{\sigma}^2 \cdot \Sigma_i, \quad \forall i \in \{1, \dots, N\}.$$

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DEMO TIME: Calibrated vs uncalibrated posteriors

`demo.jl`

Numerically stable implementation: Square-root filtering

When steps get small numerical stability suffers — so better work with matrix square-roots directly [Krämer and Hennig, 2020]

- **Problem:** The computed covariances can have negative eigenvalues due to finite precision arithmetic and numerical round-off, in particular with small step sizes. Failure example: `demo.jl`

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- It holds: **A matrix** $M \in \mathbb{R}^{d \times d}$ **is positive semi-definite if and only if there exists a matrix** $B \in \mathbb{R}^{d \times d}$ **such that** $M = BB^\top$**.**

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$$M = ABA^\top + C,$$

$$\Leftrightarrow \qquad M_L(M_L)^\top = AB_L(B_L)^\top A^\top + C_L(C_L)^\top$$

Numerically stable implementation: Square-root filtering

When steps get small numerical stability suffers — so better work with matrix square-roots directly

[Krämer and Hennig, 2020]

- **Problem:** The computed covariances can have negative eigenvalues due to finite precision arithmetic and numerical round-off, in particular with small step sizes. Failure example: `demo.jl`
- It holds: A matrix $M \in \mathbb{R}^{d \times d}$ is positive semi-definite if and only if there exists a matrix $B \in \mathbb{R}^{d \times d}$ such that $M = BB^\top$.
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Numerically stable implementation: Square-root filtering

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$\Rightarrow$ `PREDICT`/`UPDATE`/`SMOOTH` can be formulated directly on square-roots to preserve PSD-ness!

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$\Rightarrow$ `PREDICT`/`UPDATE`/`SMOOTH` can be formulated directly on square-roots to preserve PSD-ness!

$\Rightarrow$ **To solve ODEs in a stable way, use the square-root Kalman filters / smoothers!**

DEMO TIME: Solving on extremely small step sizes with square-root filtering

`demo.jl`

Intermediate summary

- *ODE solving is state estimation*
- *We can estimate ODE solutions with extended Kalman filtering/smoothing,* in a stable and calibrated way

Next: **Extending ODE filters**

1. *Flexible information operators*: The ODE filter formulation extends to other numerical problems
2. *Latent force inference*: Joint GP regression on both ODEs and data

Extending ODE filters to other related differential equation problems

ODE filters can solve much more than the ODEs that we saw so far! [Bosch et al., 2022]

Numerical problems setting: Initial value problem with first-order ODE

$$\dot{x}(t) = f(x(t), t), \quad x(0) = x_0.$$

This leads to the **probabilistic state estimation problem:**

Initial distribution:	$X(0) \sim \mathcal{N}\left(X(0); \mu_0, \Sigma_0\right)$	
Prior / dynamics model:	$X(t+h) \mid X(t) \sim \mathcal{N}\left(X(t+h); A(h)X(t), Q(h)\right)$	
ODE likelihood:	$Z(t_i) \mid X(t_i) \sim \delta\left(Z(t_i); X^{(1)}(t_i) - f(X^{(0)}(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$Z^{\text{init}} \mid X(0) \sim \delta\left(Z^{\text{init}}; X^{(0)}(0)\right),$	$z^{\text{init}} \triangleq x_0$

Extending ODE filters to other related differential equation problems

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Numerical problems setting: Initial value problem with second-order ODE

$$\ddot{x}(t) = f(\dot{x}(t), x(t), t), \quad x(0) = x_0, \quad \dot{x}(0) = \dot{x}_0.$$

This leads to the **probabilistic state estimation problem:**

Initial distribution:	$X(0) \sim \mathcal{N}(X(0); \mu_0, \Sigma_0)$	
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Initial value likelihood:	$Z^{\text{init}} \mid X(0) \sim \delta\left(Z^{\text{init}}; X^{(0)}(0)\right),$	$z^{\text{init}} \triangleq x_0$
Initial derivative likelihood:	$Z_1^{\text{init}} \mid X(0) \sim \delta\left(Z_1^{\text{init}}; X^{(1)}(0)\right),$	$z_1^{\text{init}} \triangleq \dot{x}_0$

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Numerical problems setting: Initial value problem with *differential-algebraic equation* (DAE) in mass-matrix form

$$M\dot{x}(t) = f(x(t), t), \quad x(0) = x_0.$$

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Numerical problems setting: Initial value problem with first-order ODE and conserved quantities

$$\dot{x}(t) = f(x(t), t), \quad x(0) = x_0, \quad g(x(t), \dot{x}(t)) = 0.$$

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Conservation law likelihood:	$Z_i^c(t_i) \mid X(t_i) \sim \delta\left(Z_i^c(t_i); g(X^{(0)}(t), X^{(1)}(t))\right),$	$z_i^c \triangleq 0$
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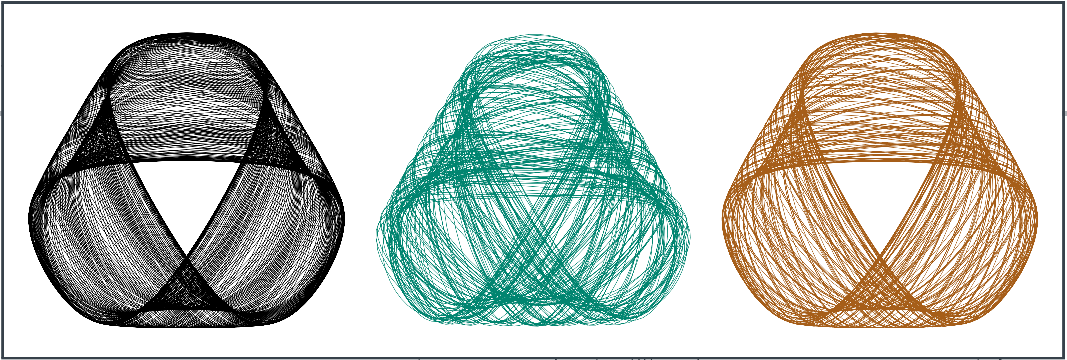

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The measurement model provides a very flexible way to easily encode desired properties!

DEMO TIME: Solving a second-order ODE

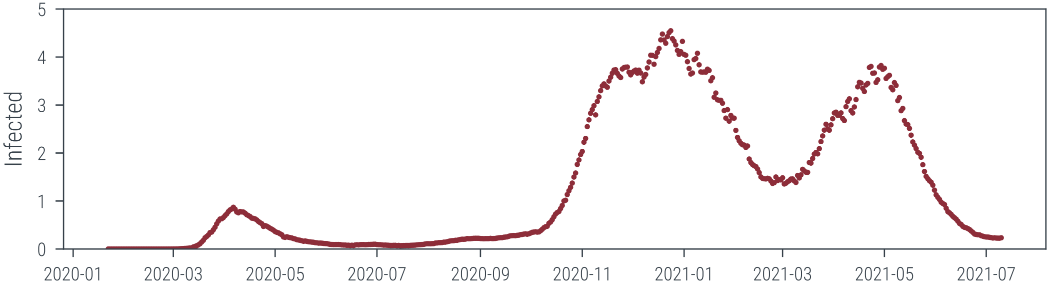
`demo.jl`

Next: **Combine ODEs and GP regression via *latent force inference***

Latent force inference: GP regression on both ODEs and data

An example we know all too well: COVID-19

Paper: [Schmidt et al., 2021]



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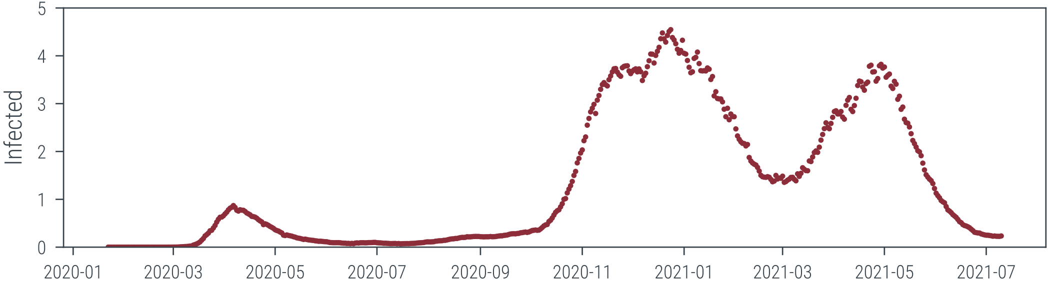

ODE dynamics:

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

Latent force inference: GP regression on both ODEs and data

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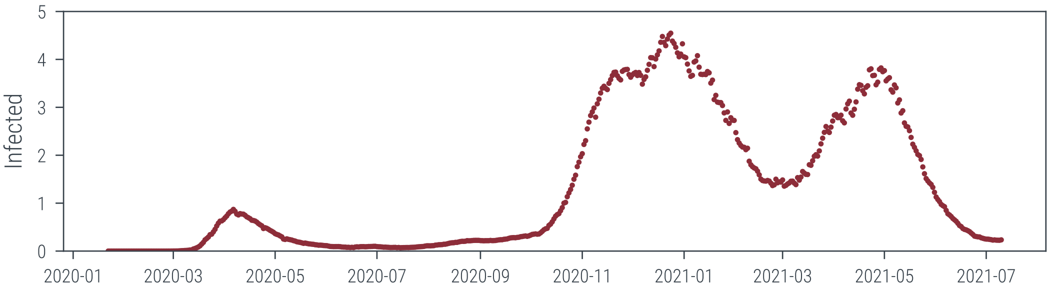
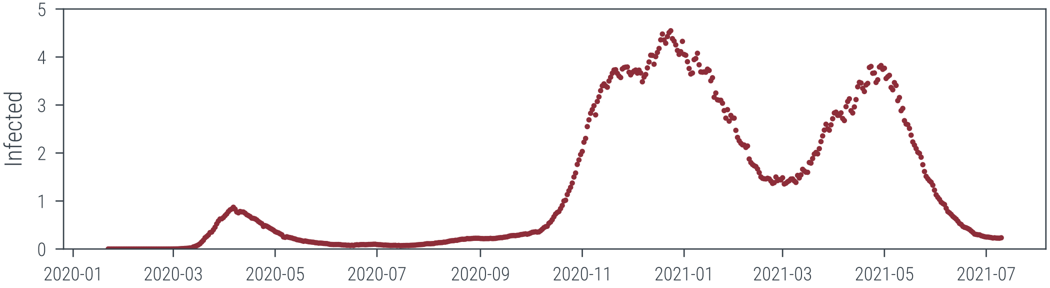


ODE dynamics with time-varying contact rate:

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



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Latent force model: Gauss–Markov prior

$$\beta(t+h) \mid \beta(t) \sim \mathcal{N}\left(A_\beta(h)\beta(t), Q_\beta(h)\right)$$

Data:

$$y_i \mid x(t_i) \sim \mathcal{N}\left(Hx(t_i), \sigma^2 I\right)$$

Latent force inference: GP regression on both ODEs and data

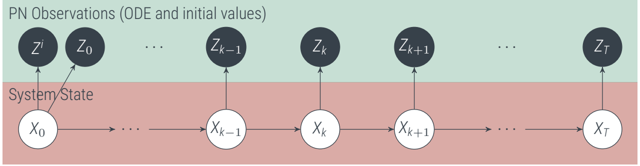
Once again we can just build a custom state-space model for the problem setup of interest

Paper: [Schmidt et al., 2021]

Initial value problem:

$$\dot{x}(t) = f(x(t), t), \quad x(0) = x_0.$$

ODE filter setup:



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External observations / data:

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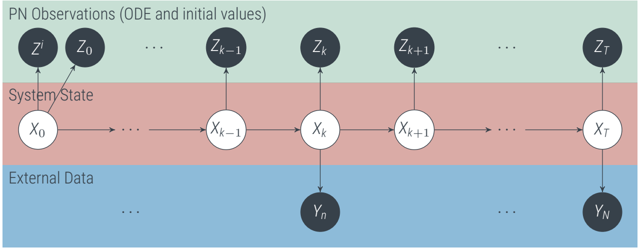

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EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Paper: [Schmidt et al., 2021]

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$$\dot{x}(t) = f(x(t), \beta(t), t), \quad x(0) = x_0.$$

External observations / data:

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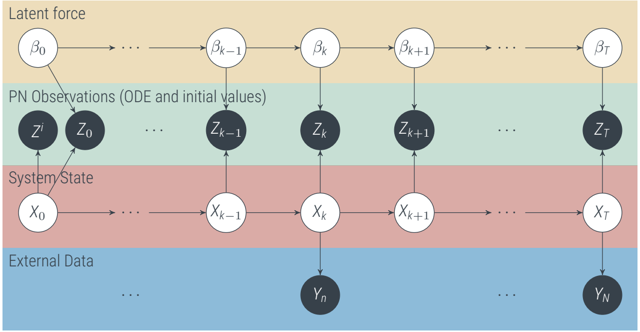
Latent Gauss–Markov process:

$$\beta(t+h) \mid \beta(t) \sim \mathcal{N}\left(A_\beta(h)\beta(t), \sigma_\beta^2 Q_\beta(h)\right).$$

ODE filter setup:



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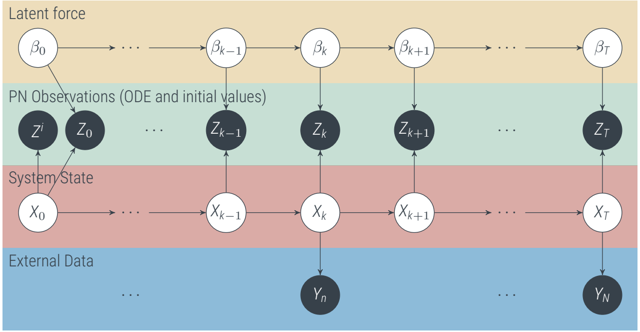

Again: **This is just state-space model**

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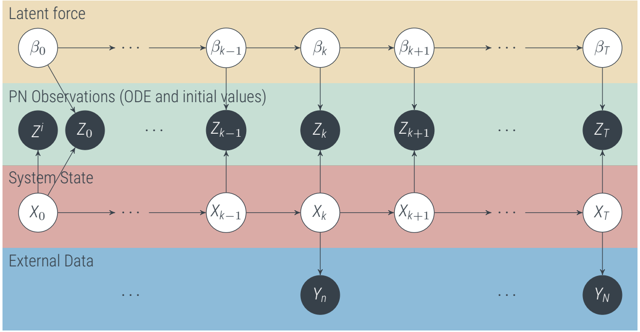
$$y_i = Hx(t_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2).$$

Latent Gauss–Markov process:

$$\beta(t+h) \mid \beta(t) \sim \mathcal{N}\left(A_\beta(h)\beta(t), \sigma_\beta^2 Q_\beta(h)\right).$$

ODE filter setup:



Again: **This is just state-space model $\Rightarrow$ inference with EKF/EKS!**

Formally we obtain the **probabilistic state estimation problem:**

State initial distribution:	$X(0) \sim \mathcal{N}(\mu_0, \Sigma_0)$	
State dynamics:	$X(t+h) \mid X(t) \sim \mathcal{N}(A(h)X(t), Q(h))$	
Latent force initial distribution:	$\beta(0) \sim \mathcal{N}\left(\mu_0^\beta, \Sigma_0^\beta\right)$	
Latent force dynamics:	$\beta(t+h) \mid \beta(t) \sim \mathcal{N}(A_\beta(h)\beta(t), Q_\beta(h))$	
ODE likelihood:	$Z(t_i) \mid X(t_i), \beta(t_i) \sim \delta\left(X^{(1)}(t_i) - f(X^{(0)}(t_i), \beta(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$Z^{\text{init}} \mid X(0) \sim \delta\left(X^{(0)}(0)\right),$	$z^{\text{init}} \triangleq x_0$
Data likelihood:	$Y_i \mid X(t_i) \sim \mathcal{N}\left(HX^{(0)}(t_i), \sigma^2 I\right),$	$y_i \in \mathcal{D}_y$

Formally we obtain the probabilistic state estimation problem, *simplified by stacking* $\tilde{X} = [X, \beta]$:

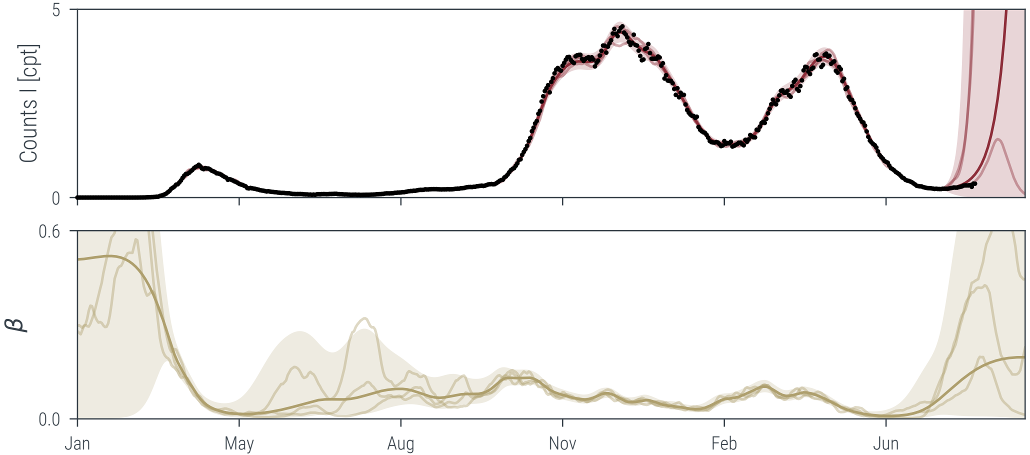
Initial distribution:	$\tilde{X}(0) \sim \mathcal{N}\left(\tilde{\mu}_0, \tilde{\Sigma}_0\right)$	
Prior / dynamics model:	$\tilde{X}(t+h) \mid \tilde{X}(t) \sim \mathcal{N}\left(\tilde{A}(h)\tilde{X}(t), \tilde{Q}(h)\right)$	
ODE likelihood:	$Z(t_i) \mid \tilde{X}(t_i) \sim \delta\left(E_1\tilde{X}(t_i) - f(E_0\tilde{X}(t_i), E_\beta\tilde{X}(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$Z^{\text{init}} \mid \tilde{X}(0) \sim \delta\left(E_0\tilde{X}(0)\right),$	$z^{\text{init}} \triangleq x_0$
Data likelihood:	$Y_i \mid \tilde{X}(t_i) \sim \mathcal{N}\left(HE_0\tilde{X}(t_i), \sigma^2 I\right),$	$y_i \in \mathcal{D}_y$

with $E_0\tilde{X} := X^{(0)}$, $E_1\tilde{X} := X^{(1)}$, $E_\beta\tilde{X} := \beta$.

Latent force inference: Results

Posteriors over infections and contact rates *in a single forward-backward pass*

Paper: [Schmidt et al., 2021]



Outlook

Other facts and further reading

Probabilistic Numerics: Computation as Machine Learning
Philipp Hennig, Michael A. Osborne, Hans P. Kersting, 2022

Other facts and further reading

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Probabilistic Numerics: Computation as Machine Learning
Philipp Hennig, Michael A. Osborne, Hans P. Kersting, 2022

References for topics not covered today:

- ODE filter theory and details:
  - Convergence rates: [Kersting et al., 2020, Tronarp et al., 2021]
  - Other filtering algorithms (e.g. IEKS and particle filter): [Tronarp et al., 2019, Tronarp et al., 2021]
  - Step-size adaptation and more calibration: [Bosch et al., 2021]
  - Scaling ODE filters to high dimensions: [Krämer et al., 2022]
- More related differential equation problems:
  - Boundary value problems (BVPs): [Krämer and Hennig, 2021]
  - Partial differential equations (PDEs): [Krämer et al., 2022]
- Inverse problems
  - Parameter inference in ODEs with ODE filters: [Tronarp et al., 2022]
  - Efficient latent force inference: [Schmidt et al., 2021]

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Summary

- *ODE solving is state estimation*
  $\Rightarrow$ treat initial value problems as state estimation problems
- *"ODE filters"*: **How to solve ODEs with Bayesian filtering and smoothing**
- *Bells and whistles*: Uncertainty calibration & Square-root filtering
- *Flexible information operators* to solve more than just standard ODEs
- *Latent force inference:* Joint GP regression on both ODEs and data

Software packages

`https://github.com/nathanaelbosch/ProbNumDiffEq.jl`
`]add ProbNumDiffEq`

`https://github.com/probabilistic-numerics/probnum`
`pip install probnum`

`https://github.com/pnkraemer/probdiffeq`
`pip install probdiffeq`

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BACKUP

Background: **Bayesian State Estimation with Extended Kalman filtering and smoothing**

Background: Extended Kalman filtering and smoothing

Bayesian filters and smoothers estimate an unknown *state* (often continuous) from observations

Non-linear Gaussian state-estimation problem:

Initial distribution:	$x_0 \sim \mathcal{N}\left(x_0; \mu_0, \Sigma_0\right),$
Prior / dynamics:	$x_{i+1} \mid x_i \sim \mathcal{N}\left(x_{i+1}; f(x_i), Q_i\right),$
Likelihood / measurement:	$y_i \mid x_i \sim \mathcal{N}\left(y_i; m(x_i), R_i\right),$
Data:	$\mathcal{D} = \{y_i\}_{i=1}^N.$

Background: Extended Kalman filtering and smoothing

Bayesian filters and smoothers estimate an unknown *state* (often continuous) from observations

Non-linear Gaussian state-estimation problem:

$$
\begin{aligned}
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\text{Likelihood / measurement:} \quad & y_i \mid x_i \sim \mathcal{N}\left(y_i; m(x_i), R_i\right), \\
\text{Data:} \quad & \mathcal{D} = \{y_i\}_{i=1}^N.
\end{aligned}
$$

The extended Kalman filter/smoother (EKF/EKS) recursively computes Gaussian approximations:

$$
\begin{aligned}
\text{Predict:} \quad & p(x_i \mid y_{1:i-1}) \approx \mathcal{N}(x_i; \mu_i^P, \Sigma_i^P), \\
\text{Filter:} \quad & p(x_i \mid y_{1:i}) \approx \mathcal{N}(x_i; \mu_i, \Sigma_i), \\
\text{Smooth:} \quad & p(x_i \mid y_{1:N}) \approx \mathcal{N}(x_i; \mu_i^S, \Sigma_i^S), \\
\text{Likelihood:} \quad & p(y_i \mid y_{1:i-1}) \approx \mathcal{N}(y_i; \hat{y}_i, S_i).
\end{aligned}
$$

Background: Extended Kalman filtering and smoothing

Bayesian filters and smoothers estimate an unknown *state* (often continuous) from observations

Non-linear Gaussian state-estimation problem:

Initial distribution: $x_0 \sim \mathcal{N}\left(x_0; \mu_0, \Sigma_0\right),$

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Filter: $p(x_i \mid y_{1:i}) \approx \mathcal{N}(x_i; \mu_i, \Sigma_i),$

Smooth: $p(x_i \mid y_{1:N}) \approx \mathcal{N}(x_i; \mu_i^S, \Sigma_i^S),$

Likelihood: $p(y_i \mid y_{1:i-1}) \approx \mathcal{N}(y_i; \hat{y}_i, S_i).$

PREDICT

$$\mu_{i+1}^P = f(\mu_i),$$
$$\Sigma_{i+1}^P = J_f(\mu_i)\Sigma_i J_f(\mu_i)^\top + Q_i.$$

Background: Extended Kalman filtering and smoothing

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Likelihood: $p(y_i \mid y_{1:i-1}) \approx \mathcal{N}(y_i; \hat{y}_i, S_i)$.

PREDICT

$$\mu_{i+1}^P = f(\mu_i),$$
$$\Sigma_{i+1}^P = J_f(\mu_i)\Sigma_i J_f(\mu_i)^\top + Q_i.$$

UPDATE

$$\hat{z}_i = m(\mu_i^P),$$
$$S_i = J_m(\mu_i^P)\Sigma_i^P J_m(\mu_i^P)^\top + R_i,$$
$$K_i = \Sigma_i^P J_m(\mu_i^P)^\top S_i^{-1},$$
$$\mu_i = \mu_i^P + K_i (z_i - \hat{z}_i),$$
$$\Sigma_i = \Sigma_i^P - K_i S_i K_i^\top.$$

Background: Extended Kalman filtering and smoothing

Bayesian filters and smoothers estimate an unknown *state* (often continuous) from observations

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Non-linear Gaussian state-estimation problem:

$$
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\text{Likelihood / measurement:} \quad & y_i \mid x_i \sim \mathcal{N}\left(y_i; m(x_i), R_i\right), \\
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\end{aligned}
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\text{Likelihood:} \quad & p(y_i \mid y_{1:i-1}) \approx \mathcal{N}(y_i; \hat{y}_i, S_i).
\end{aligned}
$$

PREDICT

$$
\begin{aligned}
\mu_{i+1}^P &= f(\mu_i), \\
\Sigma_{i+1}^P &= J_f(\mu_i)\Sigma_i J_f(\mu_i)^\top + Q_i.
\end{aligned}
$$

UPDATE

$$
\begin{aligned}
\hat{z}_i &= m(\mu_i^P), \\
S_i &= J_m(\mu_i^P)\Sigma_i^P J_m(\mu_i^P)^\top + R_i, \\
K_i &= \Sigma_i^P J_m(\mu_i^P)^\top S_i^{-1}, \\
\mu_i &= \mu_i^P + K_i\left(z_i - \hat{z}_i\right), \\
\Sigma_i &= \Sigma_i^P - K_i S_i K_i^\top.
\end{aligned}
$$

Similarly SMOOTH.

On linearization strategies and their influence on A-Stability

We can actually approximate the Jacobian in the EKF and still get sensible results / algorithms!

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[Tronarp et al., 2019]

- Measurement model: $m(X(t), t) = X^{(1)}(t) - f(X^{(0)}(t), t)$
- A standard extended Kalman filter computes the Jacobian of the measurement mode:
  $J_m(\xi) = E_1 - J_f(E_0\xi, t)E_0$
  $\Rightarrow$ This algorithm is often called `EK1`.
- Turns out the following also works: $J_f \approx 0$ and then $J_m(\xi) \approx E_1$
  $\Rightarrow$ The resulting algorithm is often called `EK0`.

A comparison of `EK1` and `EK0`:

	Jacobian	type	A-stable	uncertainties	speed
`EK1`	$H = E_1 - J_f(E_0\mu^p)E_0$	semi-implicit	yes	more expressive	slower ($O(Nd^3q^3)$)
`EK0`	$H = E_1$	explicit	no	simpler	faster ($O(Ndq^3)$)

Prior: The q-times integrated Wiener process

A very convenient prior with closed-form transition densities

- **q-times integrated Wiener process prior**: $X(t) \sim \mathrm{IWP}(q)$

$$
\begin{aligned}
\mathrm{d}X^{(i)}(t) &= X^{(i+1)}(t)\,\mathrm{d}t, \qquad i = 0, \dots, q-1, \\
\mathrm{d}X^{(q)}(t) &= \sigma\,\mathrm{d}W(t), \\
X(0) &\sim \mathcal{N}(\mu_0, \Sigma_0).
\end{aligned}
$$

- Corresponds to Taylor-polynomial + perturbation:

$$
X^{(0)}(t) = \sum_{m=0}^{q} X^{(m)}(0)\frac{t^m}{m!} + \sigma \int_0^t \frac{t-\tau}{q!}\,\mathrm{d}W(\tau)
$$