Probabilistic Numerics for Ordinary Differential Equations

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Eberhard Karls Universität Tübingen

imprs-is

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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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<u>*Fun with ODE filters*</u>

- 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

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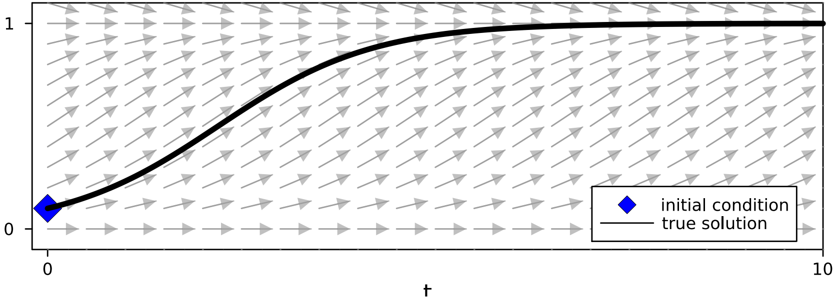
$$\dot{x}(t) = f\left(x(t), t\right)$$

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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- Forward Euler:

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

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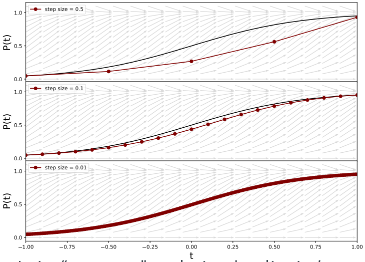
Forward Euler for different step sizes:



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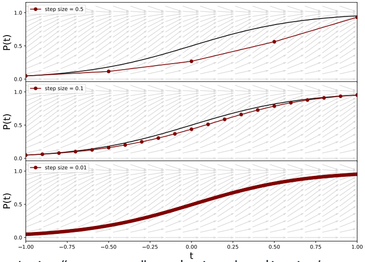

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Numerical ODE solvers **estimate** $x(t)$ *by evaluating f on a discrete set of points.*

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:

$$
\begin{aligned}
\text{Initial distribution:} \quad & x_0 \sim \mathcal{N}\left(x_0; \mu_0, \Sigma_0\right), \\
\text{Prior / dynamics:} \quad & x_{i+1} \mid x_i \sim \mathcal{N}\left(x_{i+1}; f(x_i), Q_i\right), \\
\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}.
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The extended Kalman filter/smoother (EKF/EKS) recursively computes Gaussian approximations:

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\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), \\
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PREDICT

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

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UPDATE

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\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), \\
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Similarly SMOOTH.

Today: ***Probabilistic*** **numerical ODE solutions**

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

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1. Prior:
2. Likelihood:
3. Data:

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Prior: General Gauss–Markov processes

You saw this in lecture 5 (I believe)

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)*:

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

$$\begin{aligned}
\mathrm{d}X^{(i)}(t) &= X^{(i+1)}(t)\,\mathrm{d}t, \qquad i = 0, \dots, q-1, \\
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- **Discrete-time transitions**:

$$\begin{aligned} X(t+h) \mid X(t) &\sim \mathcal{N}\left(X(t+h); A(h)X(t), \sigma^2 Q(h)\right), \\ [A(h)]_{ij} &= \mathbb{I}_{i \leq j} \frac{h^{j-i}}{(j-i)!}, \\ [Q(h)]_{ij} &= \frac{h^{2q+1-i-j}}{(2q+1-i-j)(q-i)!(q-j)!}, \end{aligned}$$

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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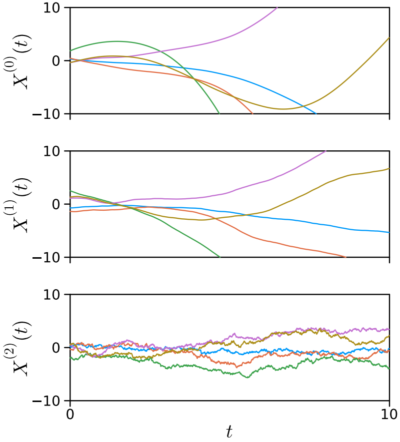

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- **Discrete-time transitions**:

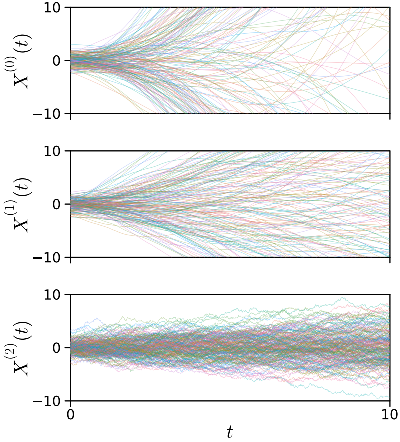
$$X(t+h) \mid X(t) \sim \mathcal{N}\left(X(t+h); A(h)X(t), \sigma^2 Q(h)\right),$$

$$[A(h)]_{ij} = \mathbb{I}_{i \leq j} \frac{h^{j-i}}{(j-i)!},$$

$$[Q(h)]_{ij} = \frac{h^{2q+1-i-j}}{(2q+1-i-j)(q-i)!(q-j)!},$$

for any $i, j = 0, \dots, q$. (one-dimensional case).
(proof: [Kersting et al., 2020])

- **Example**: IWP(2)



Probabilistic numerical ODE solutions

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

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

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

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

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2. Likelihood:
3. Data:

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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

- **Ideal but intractable goal:** Want $x(t)$ to satisfy the ODE
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The likelihood and data relate the prior to the desired posterior: the numerical ODE solution

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

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$$
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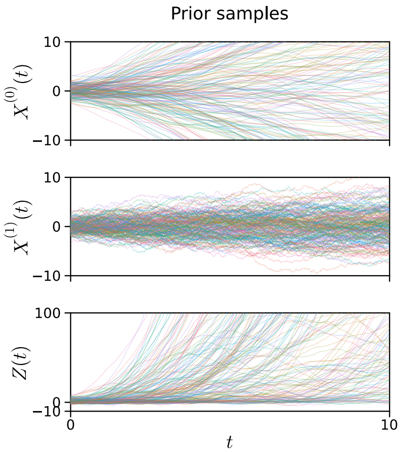
Example: Logistic ODE $\dot{x} = x(1 - x)$



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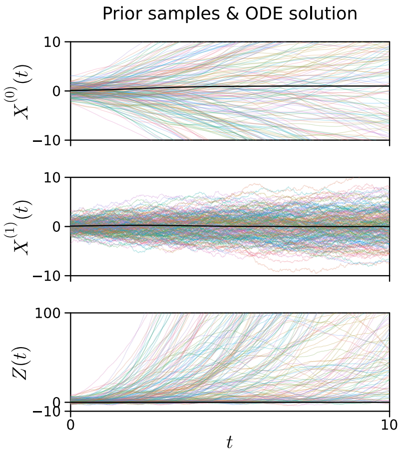

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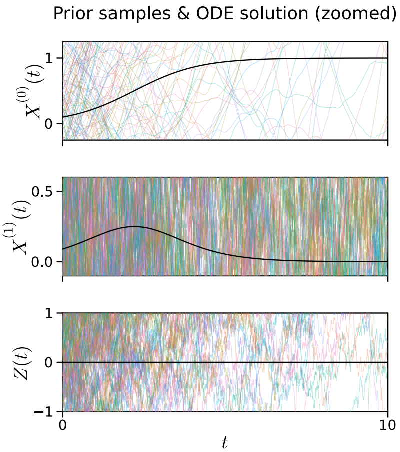

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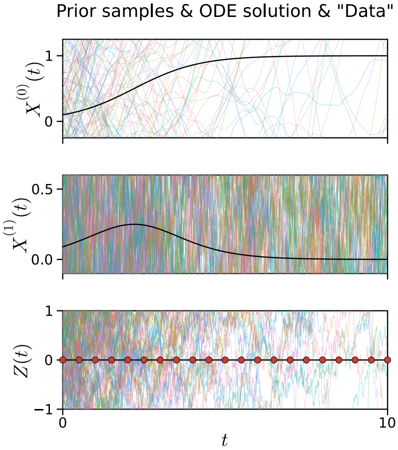

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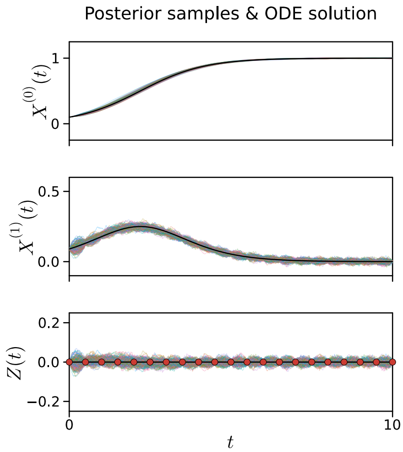

(here: $Z = X^{(1)} - X^{(0)}(1 - X^{(0)})$)
Spoiler: **This is the thing we want!**

***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:

1. Prior: q-times integrated Wiener process prior:
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This describes a state-space model

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This describes a state-space model $\Rightarrow$ 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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Initial distribution:	$X(0) \sim \mathcal{N}\left(X(0); \mu_0, \Sigma_0\right)$
Prior / dynamics model:	$X(t+h) \mid X(t) \sim \mathcal{N}\left(X(t+h); A(h)X(t), Q(h)\right)$
Likelihood / measurement model:	$Z(t_i) \mid X(t_i) \sim \delta\left(Z(t_i); X^{(1)}(t_i) - f(X^{(0)}(t_i), t_i)\right)$
Data:	$z_i \triangleq 0, \qquad i = 1, \dots, N.$

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One thing is still missing:

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

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$$
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\text{Data:} \quad & z_i \triangleq 0, \qquad i = 1, \dots, N.
\end{aligned}
$$

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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    $\mu_k^-, \Sigma_k^- \leftarrow$ KF_PREDICT$(\mu_{k-1}, \Sigma_{k-1}, A(h_k), Q(h_k))$ // Kalman filter prediction

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  end for

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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

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Algorithm Kalman filter prediction

procedure KF_PREDICT(μ, Σ, A, Q)
    $\mu^P \leftarrow A\mu$ // Predict mean
    $\Sigma^P \leftarrow A\Sigma A^\top + Q$ // Predict covariance
    return μ^P, Σ^P
end procedure

Algorithm Extended Kalman filter update

procedure EKF_UPDATE(μ, Σ, h, R, y)
    $\hat{y} \leftarrow h(\mu)$ // evaluate the observation model
    $H \leftarrow J_h(\mu)$ // Jacobian of the observation model
    $S \leftarrow H\Sigma H^\top + R$ // Measurement covariance
    $K \leftarrow \Sigma H^\top S^{-1}$ // Kalman gain
    $\mu^F \leftarrow \mu + K(y - \hat{y})$ // update mean
    $\Sigma^F \leftarrow \Sigma - KSK^\top$ // 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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- **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:

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

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

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$\Rightarrow$ **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

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

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

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

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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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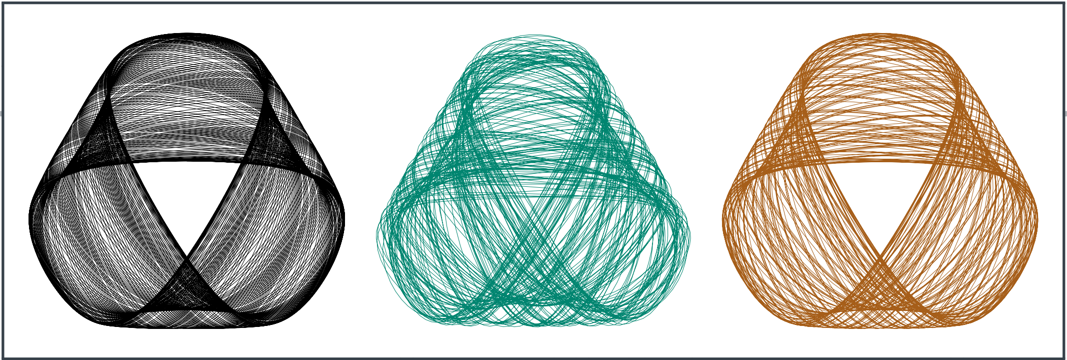

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ODE likelihood:	$Z(t_i) \mid X(t_i) \sim \delta\left(Z(t_i); X^{(1)}(t_i) - f(X^{(0)}(t_i), t_i)\right),$	$z_i \triangleq 0$
Conservation law likelihood:	$Z^c_i(t_i) \mid X(t_i) \sim \delta\left(Z^c_i(t_i); g(X^{(0)}(t), X^{(1)}(t))\right),$	$z^c_i \triangleq 0$
Initial value likelihood:	$Z^{\text{init}} \mid X(0) \sim \delta\left(Z^{\text{init}}; X^{(0)}(0)\right),$	$z^{\text{init}} \triangleq x_0$

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

DEMO TIME: Solving a second-order ODE

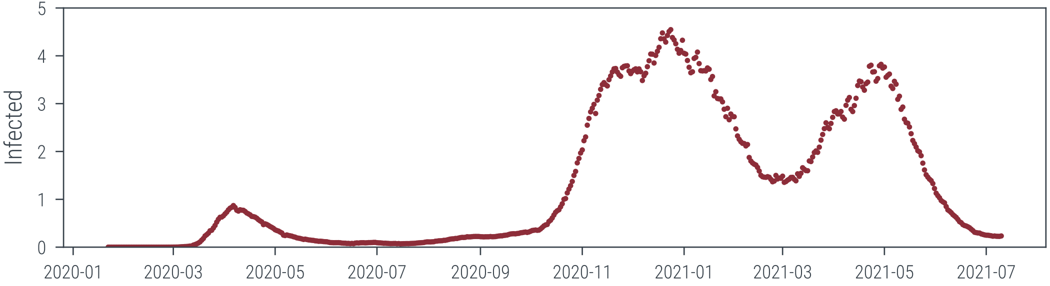
`demo.jl`

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]



Latent force inference: GP regression on both ODEs and data

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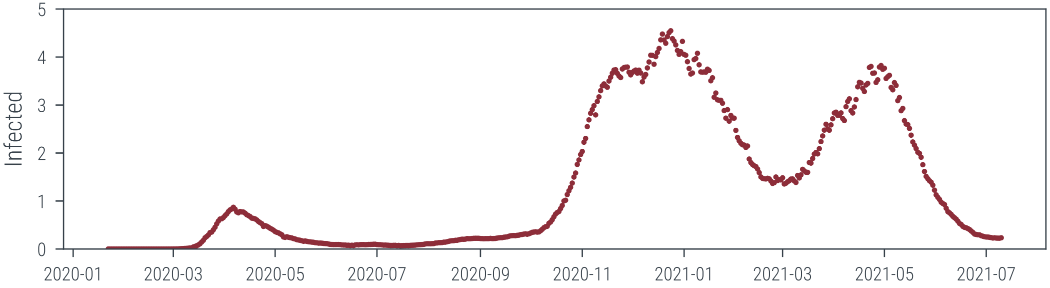

ODE dynamics:

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

Latent force inference: GP regression on both ODEs and data

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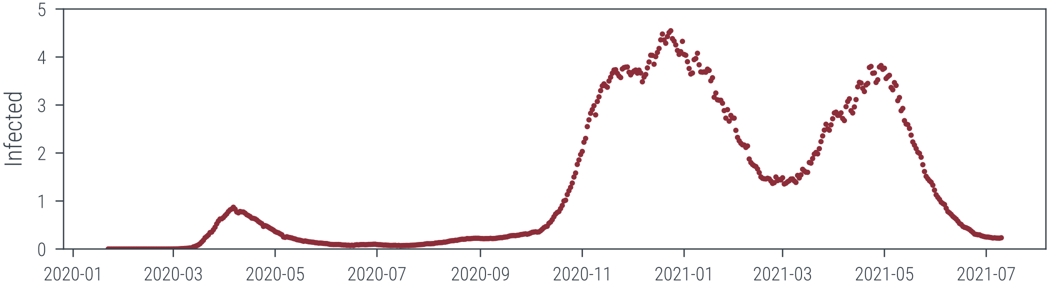

ODE dynamics with time-varying contact rate:

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

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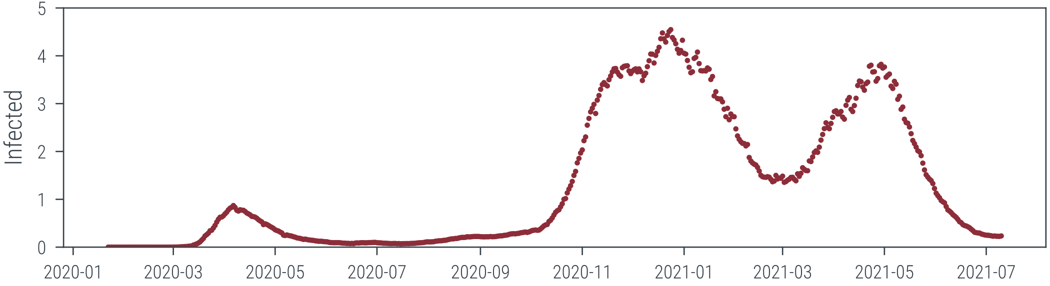

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Latent force model: Gauss–Markov prior

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

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

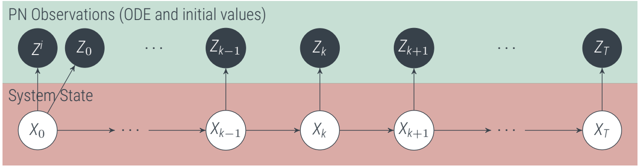
Once again we can just build a custom state-space model for the problem setup of interest

Paper: [Schmidt et al., 2021]

Initial value problem:

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

ODE filter setup:



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]

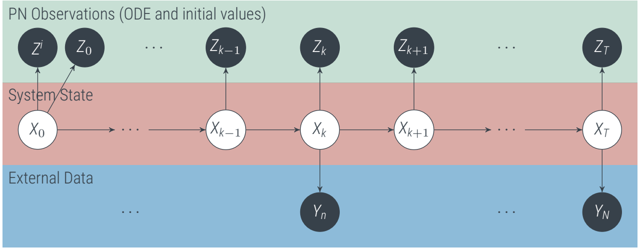
Initial value problem:

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

External observations / data:

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

ODE filter setup:



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:

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

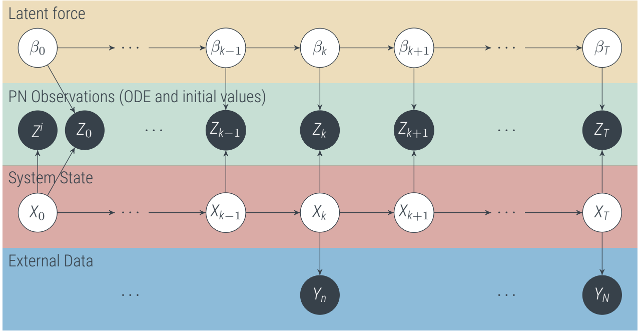
External observations / data:

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

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:



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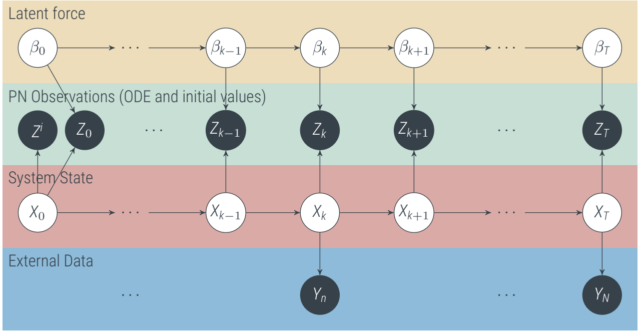


Again: **This is just state-space model**

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:

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

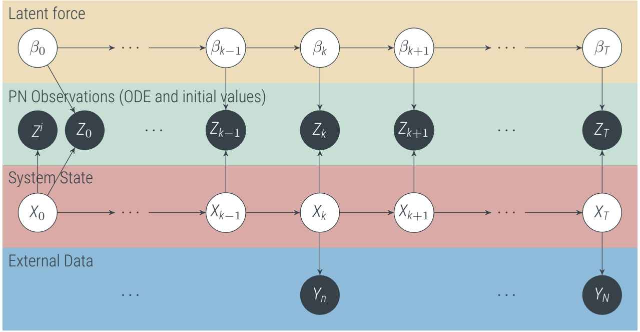
External observations / data:

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

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* $\tilde{X} = [X, \beta]$:

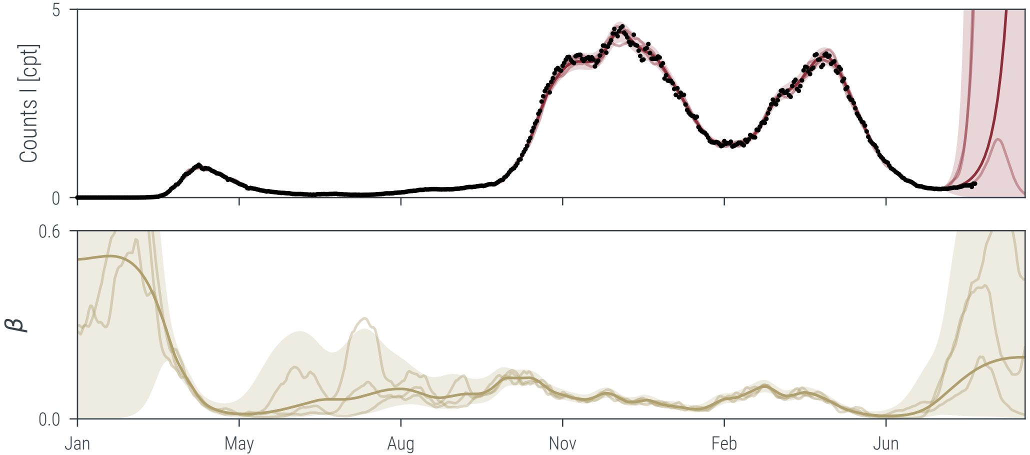
Initial distribution:	$\tilde{X}(0) \sim \mathcal{N}\left(\tilde{\mu}_0, \tilde{\Sigma}_0\right)$	
Prior / dynamics model:	$\tilde{X}(t+h) \mid \tilde{X}(t) \sim \mathcal{N}\left(\tilde{A}(h)\tilde{X}(t), \tilde{Q}(h)\right)$	
ODE likelihood:	$Z(t_i) \mid \tilde{X}(t_i) \sim \delta\left(E_1\tilde{X}(t_i) - f(E_0\tilde{X}(t_i), E_\beta\tilde{X}(t_i), t_i)\right),$	$z_i \triangleq 0$
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

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

Other facts and further reading

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]

Come to the Probabilistic Numerics Spring School!

Register at `https://probnumschool.org/`

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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

Please give Feedback:

Software packages

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

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

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

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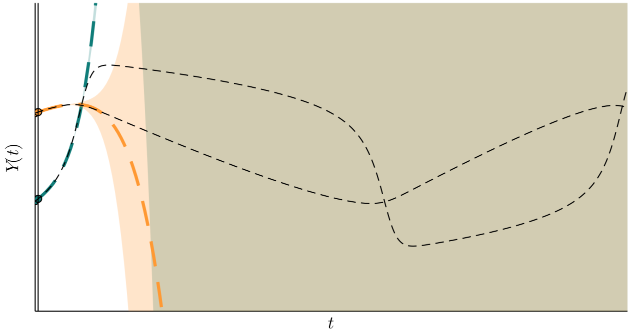
BACKUP

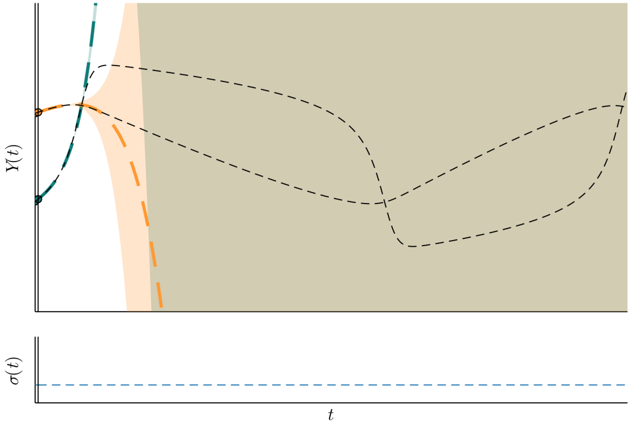
Local calibration and step-size adaptation

Fixed steps — the vanilla way as introduced in the lecture



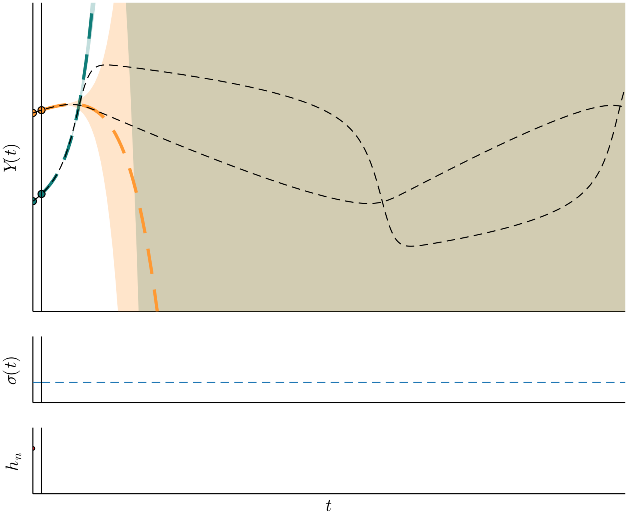
Local calibration and step-size adaptation

Local calibration by estimating a time-varying diffusion model $\sigma(t)$



Local calibration and step-size adaptation

Adaptive step-size selection via local error estimation from the measurement residuals



- 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 ($O(Ndq^3)$)

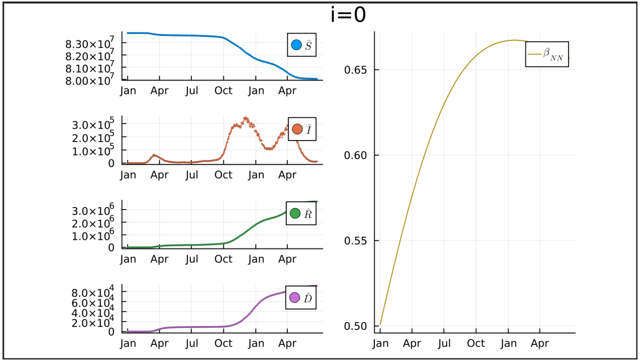
Parameter Inference *on real COVID data* – with neural networks

If we can use a GP we probably can use a NN? In principle, yes – but I did not get it to work well

ODE dynamics with time-varying contact rate $\beta(t)$:

$$\dot{S} = -\beta(t)SE, \qquad \dot{I} = \beta(t)SE - \gamma I - \eta I, \qquad \dot{R} = \gamma I, \qquad \dot{D} = \eta I.$$

Data are the real COVID counts from Germany.
Idea: Just model $\beta(t)$ with a neural network β_θ^{NN}, and do parameter inference on θ.
Result:



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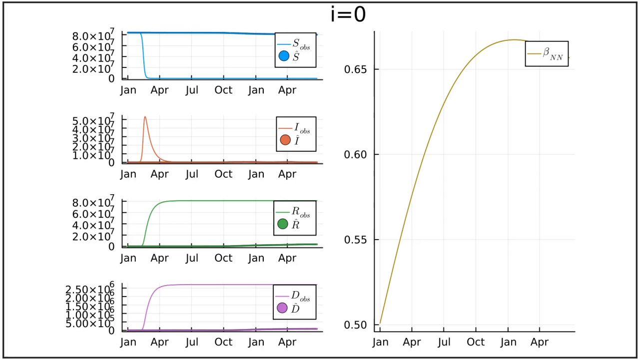

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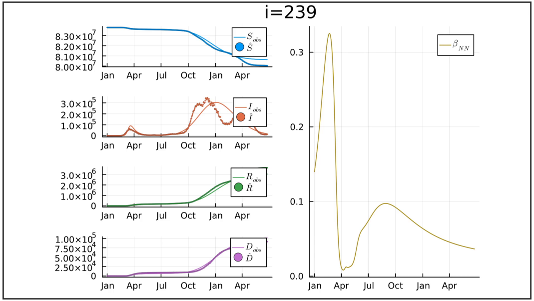
Data are the real COVID counts from Germany.
Idea: Just model $\beta(t)$ with a neural network $\beta_\theta^{\mathrm{NN}}$, and do parameter inference on θ.
Result:



Disclaimer: I only had limited time and it might very well be possible to do this much better!

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:

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