Probabilistic Numerics for Ordinary Differential Equations

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Eberhard Karls Universität Tübingen

imprs-is

erc some of the presented work is supported by the European Research Council.

Background

- Ordinary differential equations and how to solve them

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

- "ODE filters": **How to solve ODEs with extended Kalman filtering and smoothing**

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- "ODE filters": **How to solve ODEs with extended Kalman filtering and smoothing**

Fun with ODE filters

- Generalizing ODE filters to other related problems (higher-order ODEs, DAEs, …)
- ODE filters for parameter inference

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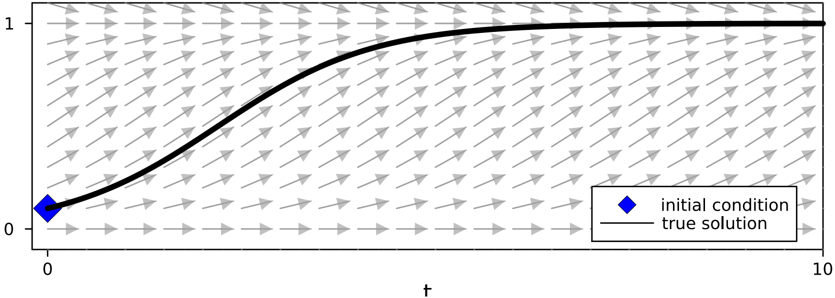
$$\dot{y}(t) = f\left(y(t), t\right)$$

with $t \in [0, T]$, vector field $f : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$, and initial value $y(0) = y_0$. Goal: "Find y".

- **Simple example**: Logistic ODE

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



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- Forward Euler:
  $$\hat{y}(t + h) = \hat{y}(t) + hf(\hat{y}(t), t)$$

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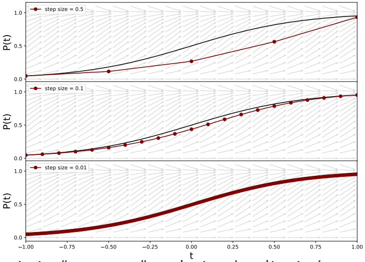
Forward Euler for different step sizes:



$\Rightarrow$ It is "correct" only in the limit $h \to 0$!

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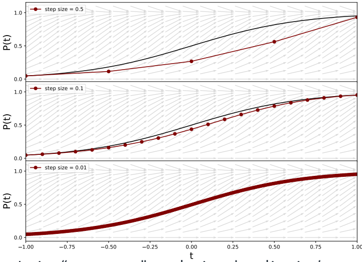

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Numerical ODE solvers **estimate** $y(t)$ *by evaluating f on a discrete set of points.*

Probabilistic numerical ODE solvers

or "How to treat ODEs as a Bayesian state estimation problem"

Probabilistic Numerical ODE Solvers

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

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

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- **Prior:** $y(t) \sim \mathcal{GP}$ a Gauss–Markov process

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- **Prior:** $y(t) \sim \mathcal{GP}$ a Gauss–Markov process with state-space representation $x(t)$:

$$x(0) \sim \mathcal{N}(\mu_0^-, \Sigma_0^-),$$
$$\mathrm{d}x(t) = Fx(t)\mathrm{d}t + \sigma\Gamma\mathrm{d}w(t),$$
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- **Likelihood:** (aka “observation model” or “information operator”)

$$z_0 = E_0 x(0) - y_0 = 0, \qquad \& \qquad z(t_n) = E_1 x(t_n) - f(E_0 x(t_n), t_n) = 0.$$

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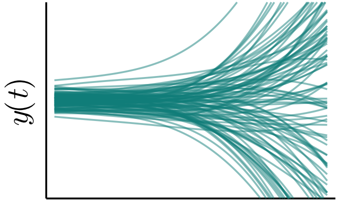
- **Inference:** Extended Kalman filter/smoother (or other Bayesian filtering and smoothing methods).

Prior



Probabilistic Numerical ODE Solvers in pictures

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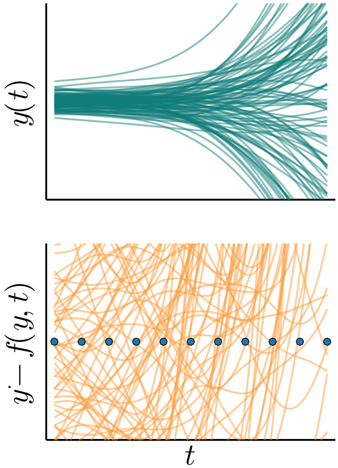

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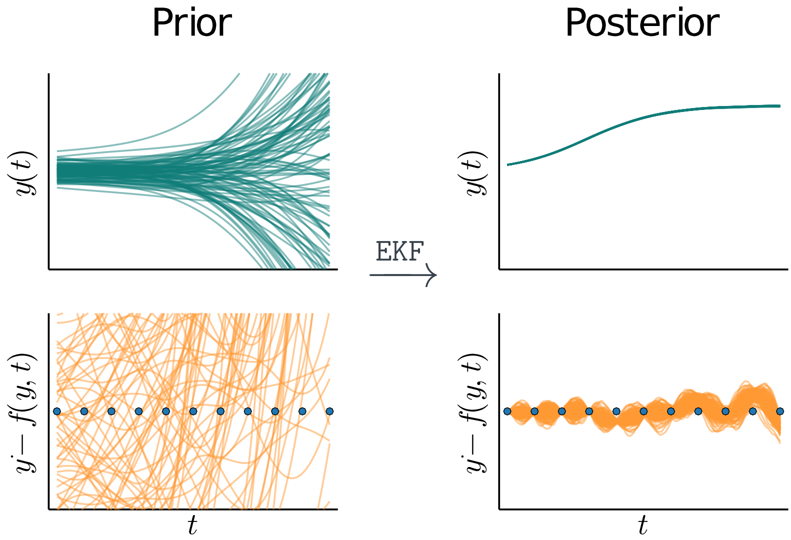
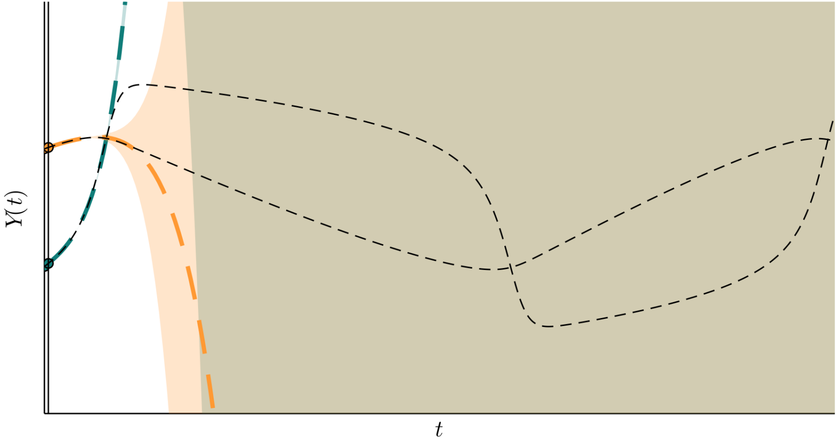


Probabilistic Numerical ODE Solvers in action

Fixed steps — the vanilla way as introduced so far



Probabilistic Numerical ODE Solvers in code

We can solve ODEs with basically just an extended Kalman filter

Algorithm The extended Kalman ODE filter

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

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

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- Properties and features:
  - Polynomial convergence rates [Kersting et al., 2020, Tronarp et al., 2021]

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Probabilistic Numerics: Computation as Machine Learning

Philipp Hennig, Michael A. Osborne, Hans P. Kersting, 2022

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Flexible Information Operators

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Flexible Information Operators

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(it's all just likelihood models)

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, Krämer and Hennig, 2021]

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

$$\dot{y}(t) = f(y(t), t), \quad y(0) = y_0.$$

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:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_1 x(t_i) - f(E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

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, Krämer and Hennig, 2021]

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

$$\ddot{y}(t) = f(\dot{y}(t), y(t), t), \quad y(0) = y_0, \quad \dot{y}(0) = \dot{y}_0.$$

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:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_1 x(t_i) - f(E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

Extending ODE filters to other related differential equation problems

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ODE likelihood:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_2 x(t_i) - f(E_1 x(t_i), E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$
Initial derivative likelihood:	$z_1^{\text{init}} \mid x(0) \sim \delta\left(z_1^{\text{init}}; E_1 x(0)\right),$	$z_1^{\text{init}} \triangleq \dot{y}_0$

Extending ODE filters to other related differential equation problems

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

$$\dot{y}(t) = f(y(t), t), \quad y(0) = y_0. \quad g(y(t), \dot{y}(t)) = 0.$$

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:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_1 x(t_i) - f(E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

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ODE likelihood:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_1 x(t_i) - f(E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
Conservation law likelihood:	$z_i^c(t_i) \mid z(t_i) \sim \delta\left(z_i^c(t_i); g(E_0 x(t), E_1 x(t))\right),$	$z_i^c \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

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Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$
Initial derivative likelihood:		

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

$\ddot{y}(t)$ … $= 0.$

This leads to the **pro**

Initial distr

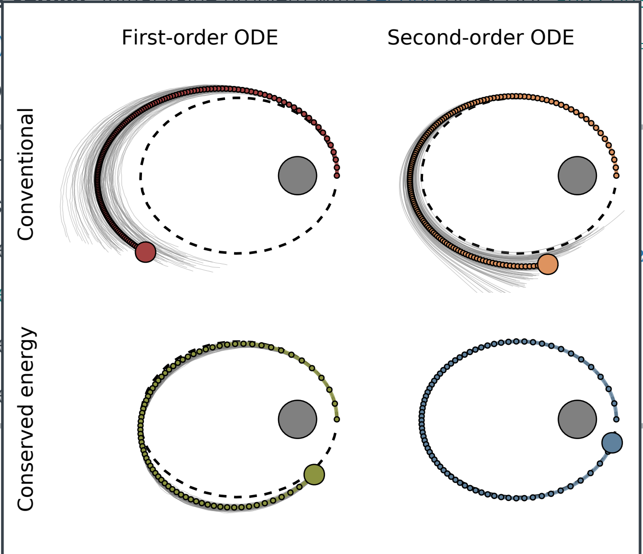
Prior / dynamics

ODE lik … $x(t_i) - f(E_1 x(t_i), E_0 x(t_i), t_i)$

Conservation law lik

Initial value lik

Initial derivative lik



Extending ODE filters to other related differential equation problems

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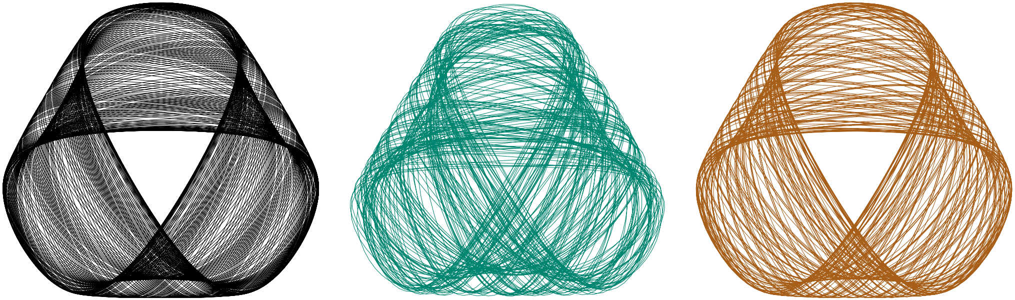

$(t_i), t_i)$

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

$$0 = F\left(\dot{y}(t), y(t), t\right), \quad y(0) = y_0.$$

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:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); E_1 x(t_i) - f(E_0 x(t_i), t_i)\right),$	$z_i \triangleq 0$
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DAE likelihood:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); F\left(E_1 x(t_i), E_0 x(t_i), t_i\right)\right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

Extending ODE filters to other related differential equation problems

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Numerical problems setting: Boundary value problem (BVP) with first-order ODE

$$\dot{y}(t) = f(y(t), t), \quad Ly(0) = y_0, \quad Ry(T) = y_T.$$

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ODE likelihood:	$z(t_i) \mid x(t_i) \sim \delta\left(z(t_i); \right),$	$z_i \triangleq 0$
Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; E_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$

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Initial value likelihood:	$z^{\text{init}} \mid x(0) \sim \delta\left(z^{\text{init}}; LE_0 x(0)\right),$	$z^{\text{init}} \triangleq y_0$
Boundary value likelihood:	$z_1^{\text{R}} \mid x(T) \sim \delta\left(z_1^{\text{R}}; RE_0 x(T)\right),$	$z_1^{\text{init}} \triangleq y_T$

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The measurement model provides a very flexible way to easily encode desired properties.
But it's all just Bayesian state estimation!

Probabilistic Numerics for ODE Parameter Inference

Using the ODE solution as a “physics-enhanced” prior for regression

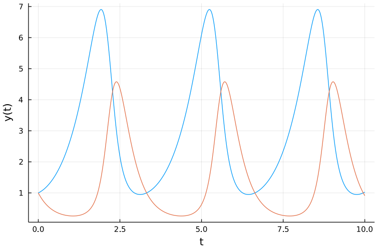
“Forward” and “Inverse” Problems

Going from formula to plot, or from plot to formula

Forward Problem

$$\dot{y}_\theta = f_\theta(y_\theta, t) \qquad y_\theta(t_0) = y_0(\theta).$$

solve $\Longrightarrow$



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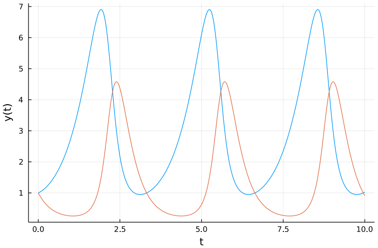
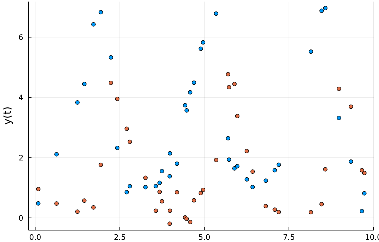


Inverse Problem

$$\hat{\theta} = \arg\max_\theta p\left(\mathcal{D} \mid \theta\right)$$

find $\Longleftarrow$



“Forward” and “Inverse” Problems

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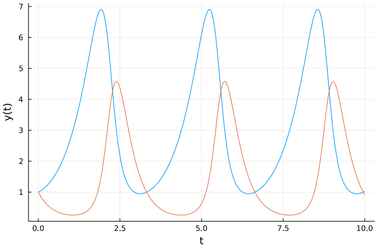

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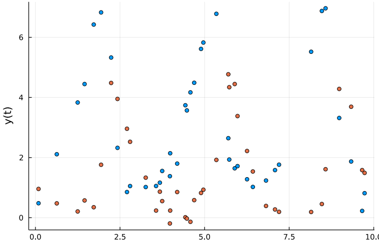

Problem: The *marginal likelihood* $p(\mathcal{D} \mid \theta) = \prod \mathcal{N}\left(u(t); y_\theta(t), R_\theta\right)$ is intractable. (because the true ODE solution is intractable!)

Context: Between classic integration and gradient matching

We're doing both: Integrating first, then GP regression

1. **Classical Numerical Integration**
   - (i) Solve the IVP to compute $\hat{y}_\theta(t)$
   - (ii) Approximate the marginal likelihood as $\widehat{\mathcal{M}}(\theta) = \prod_n \mathcal{N}(u(t_n); \hat{y}_\theta(t_n), R_\theta)$
   - (iii) Optimize to get $\hat{\theta} = \arg\max \widehat{\mathcal{M}}(\theta)$

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2. **Gradient Matching**
   - (i) Fit a curve $\hat{y}(t)$ *to the data* $\{u(t_i)\}$
   - (ii) Estimate θ by minimizing $\dot{\hat{y}}(t) - f_\theta(\hat{y}(t))$

   Exists in both classic (splines) or probabilistic versions (GPs)

Context: Between classic integration and gradient matching

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Context: Between classic integration and gradient matching

We're doing both: Integrating first, then GP regression

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3. **Probabilistic Numerical Integration**
   - $$\widehat{\mathcal{M}}_{PN}(\theta, \kappa) = \int \underbrace{\prod_n \mathcal{N}\left(u(t_n); y(t_n), R_\theta\right)}_{\text{Likelihood}} \cdot \underbrace{\gamma_{PN}\left(y(t_{1:N}) \mid \theta, \kappa\right)}_{\text{PN ODE Solution}} \mathrm{d}y(t_{1:N}) \tag{1}$$

Context: Between classic integration and gradient matching

We're doing both: Integrating first, then GP regression

1. **Classical Numerical Integration**
   - (i) Solve the IVP to compute $\hat{y}_\theta(t)$
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   - (i) *Probabilistically* solve IVP to compute $\gamma_{PN}(y(t) \mid \theta, \kappa)$

Context: Between classic integration and gradient matching

We're doing both: Integrating first, then GP regression

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   - (i) *Probabilistically* solve IVP to compute $\gamma_{\text{PN}}(y(t) \mid \theta, \kappa)$
   - (ii) Perform Kalman filtering on the data, with γ_{PN} as a "physics-enhanced" **prior**

Context: Between classic integration and gradient matching

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   - (ii) Perform Kalman filtering on the data, with γ_{PN} as a "physics-enhanced" **prior**
   - (iii) Optimize the approximate marginal likelihood

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

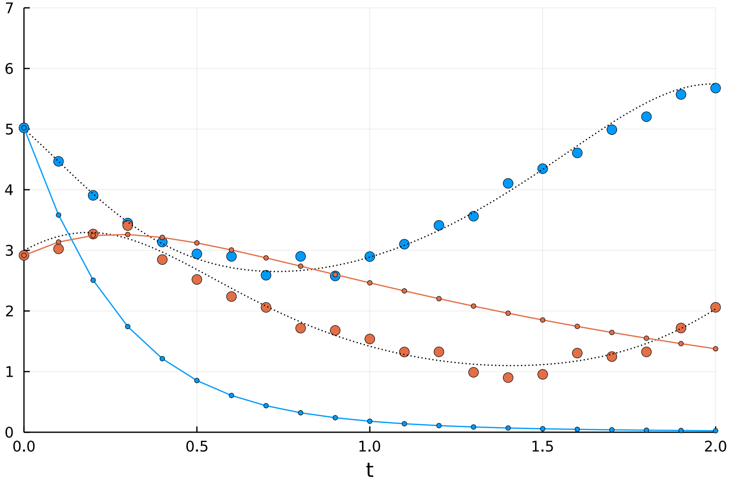

Figure: i=1

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

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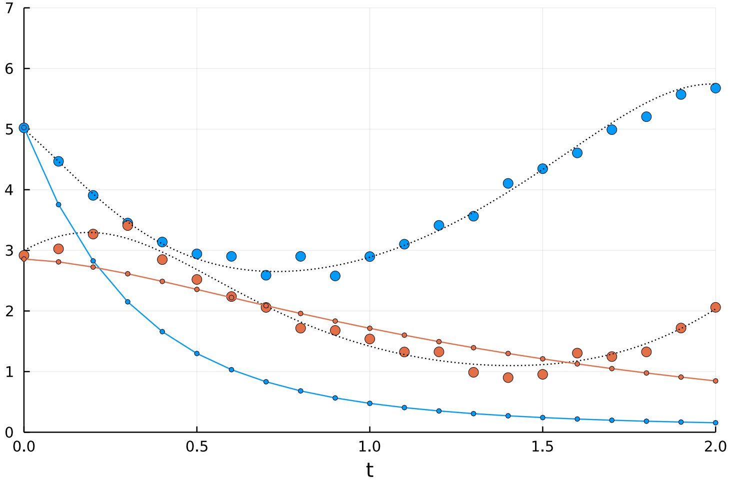


Figure: i=2

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

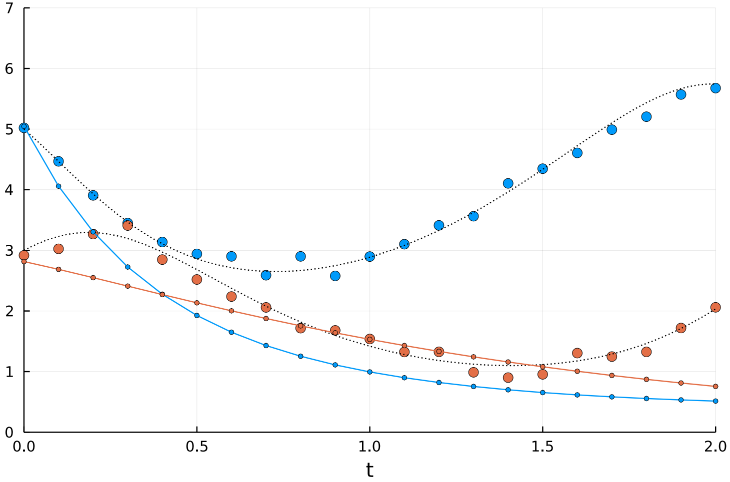


Figure: i=3

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

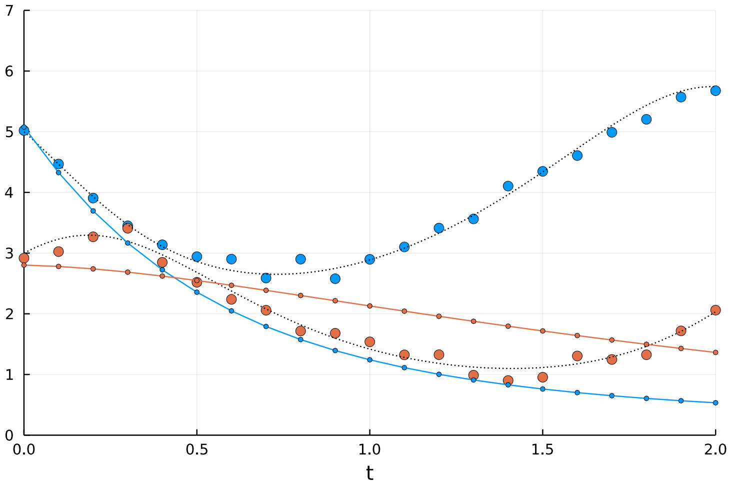


Figure: i=4

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

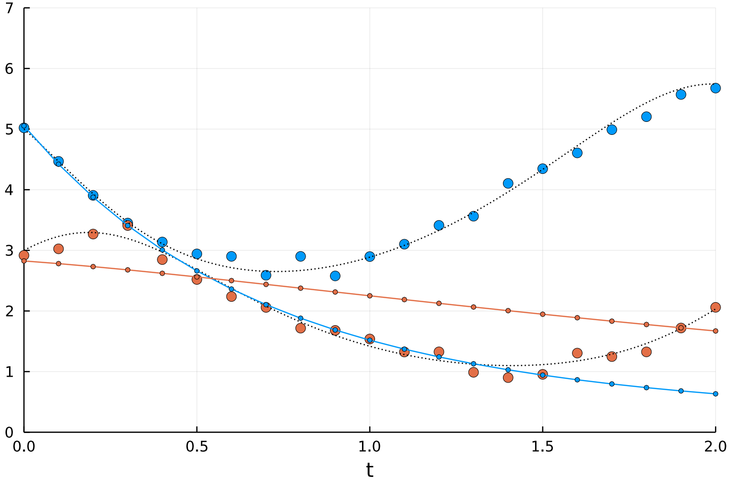


Figure: i=5

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

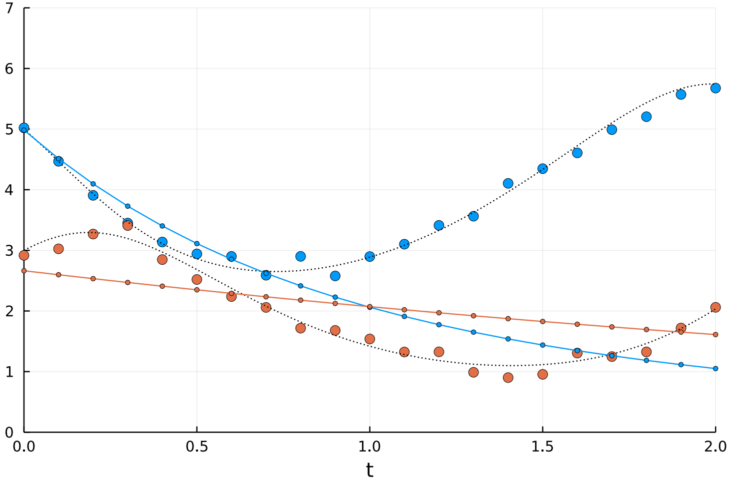
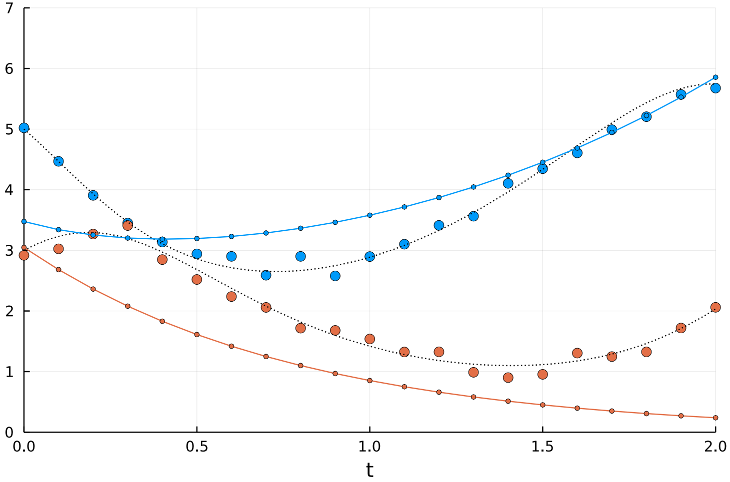


Figure: i=10

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly



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Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

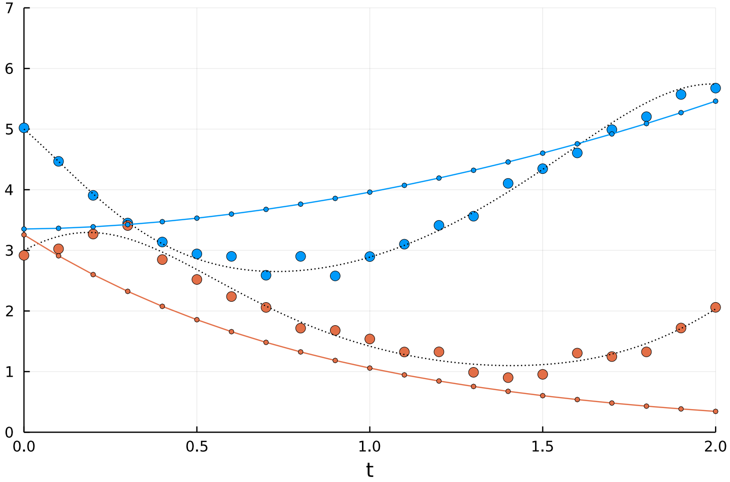

Figure: i=20

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

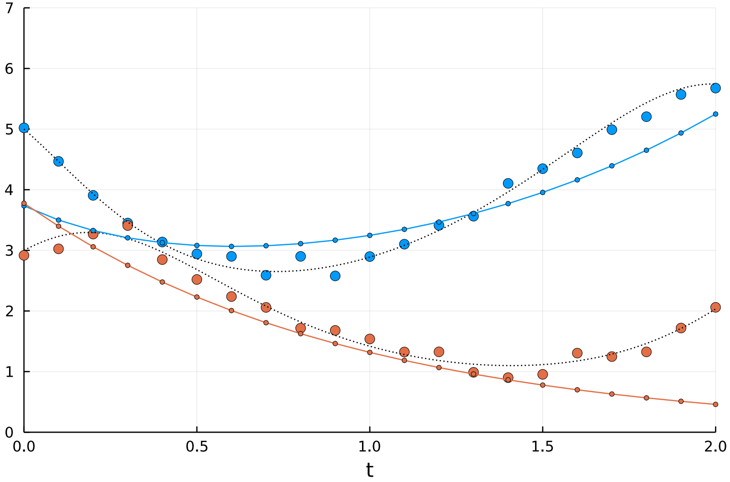

Figure: i=25

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

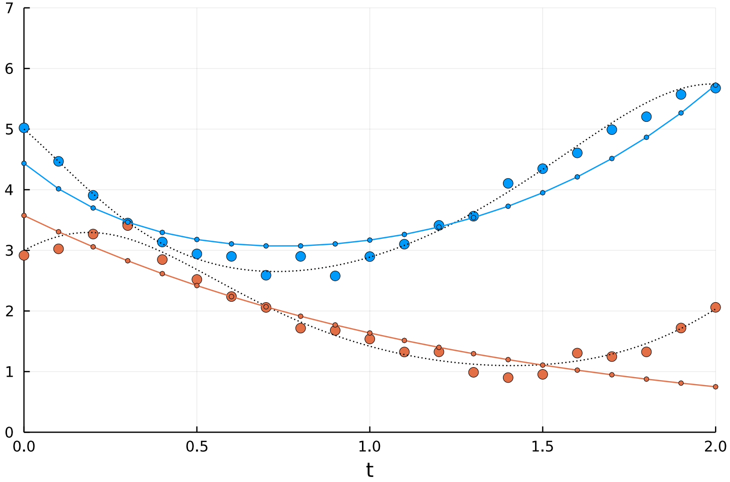

Figure: i=30

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

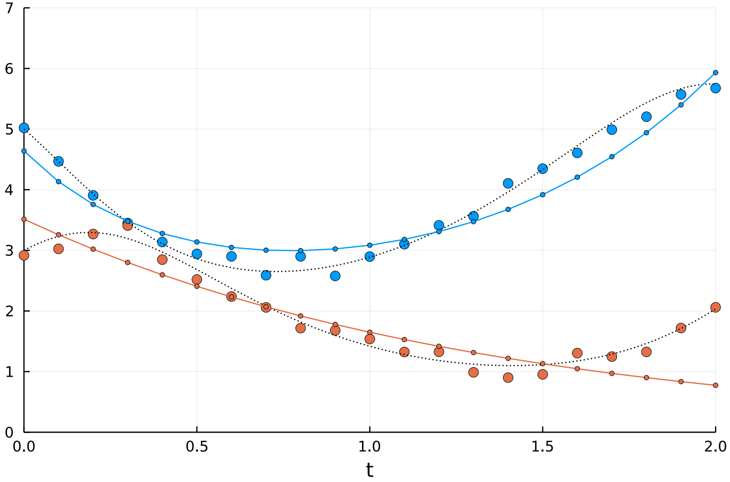

Figure: i=35

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

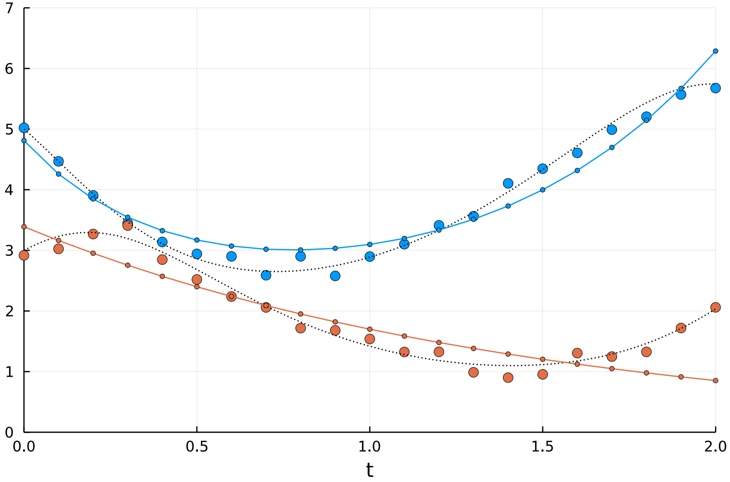

Figure: i=40

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

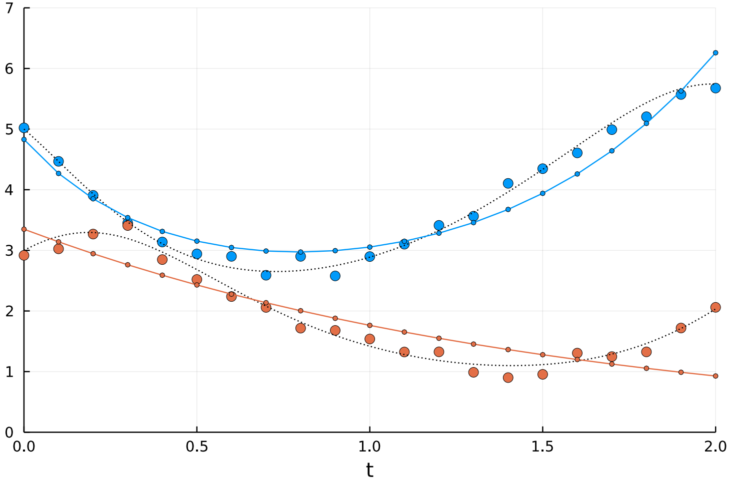

Figure: i=45

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

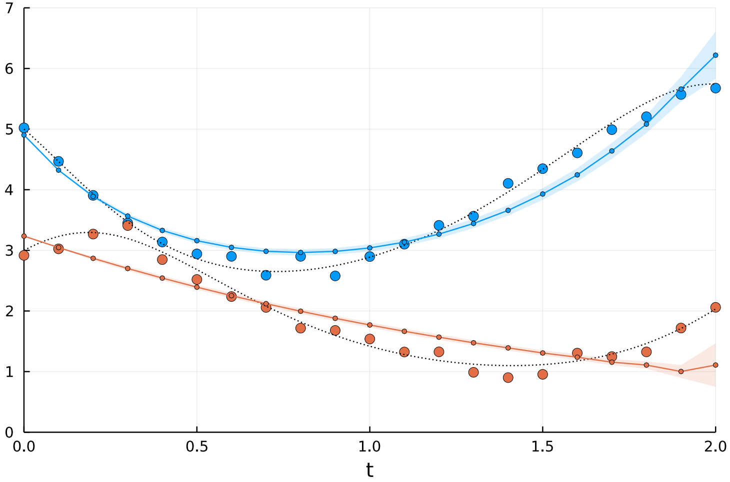

Figure: i=50

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

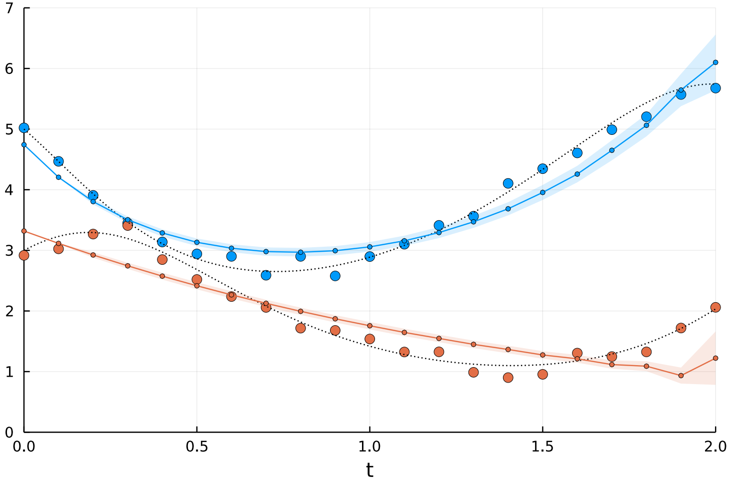

Figure: i=55

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

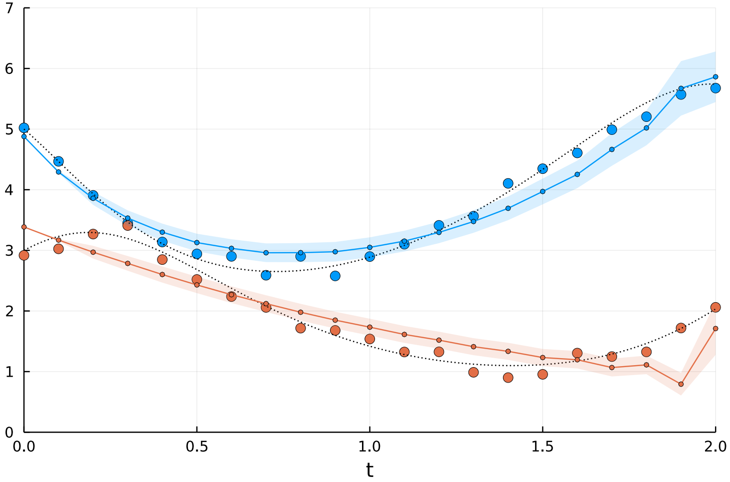

Figure: i=60

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

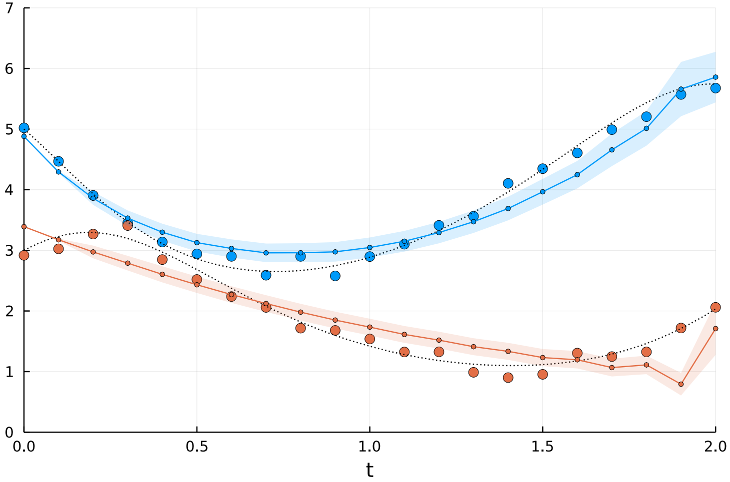

Figure: i=61

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

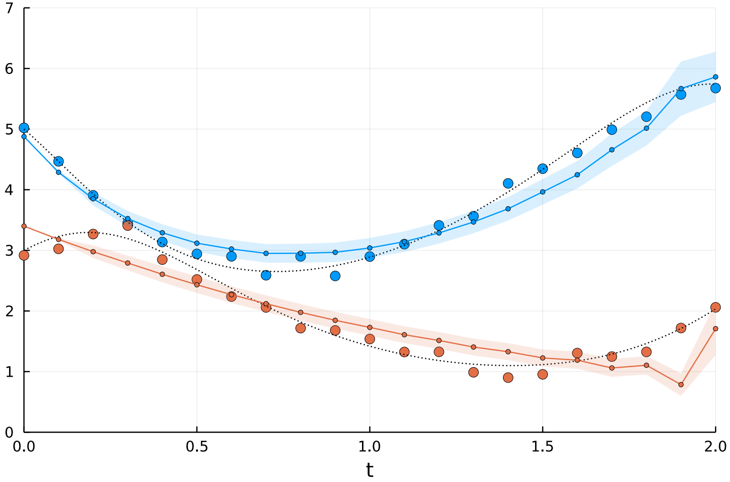

Figure: i=62

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

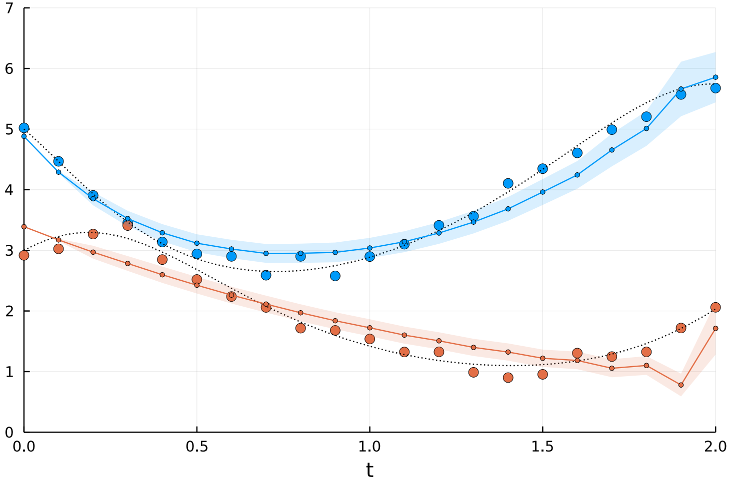

Figure: i=63

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

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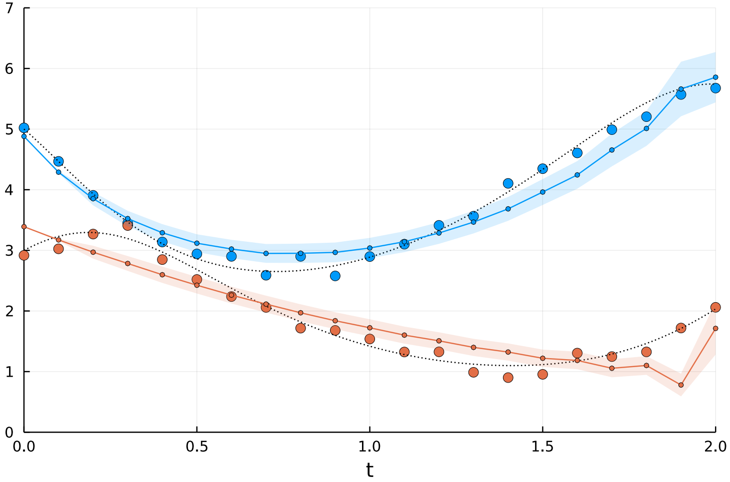

Figure: i=63

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

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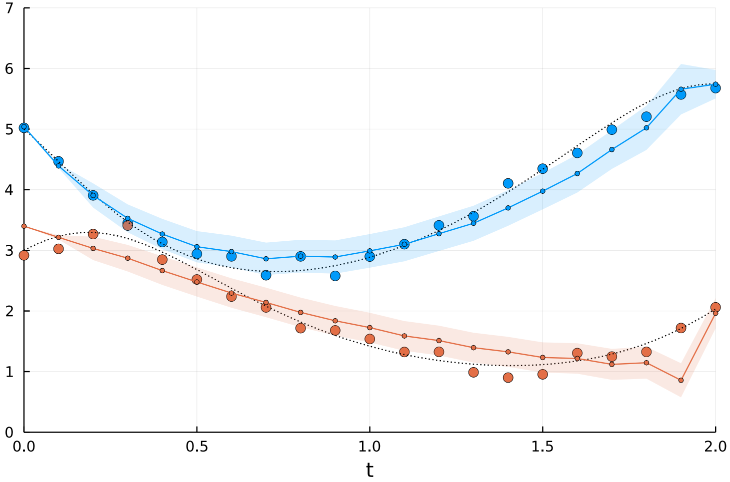


Figure: i=64

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

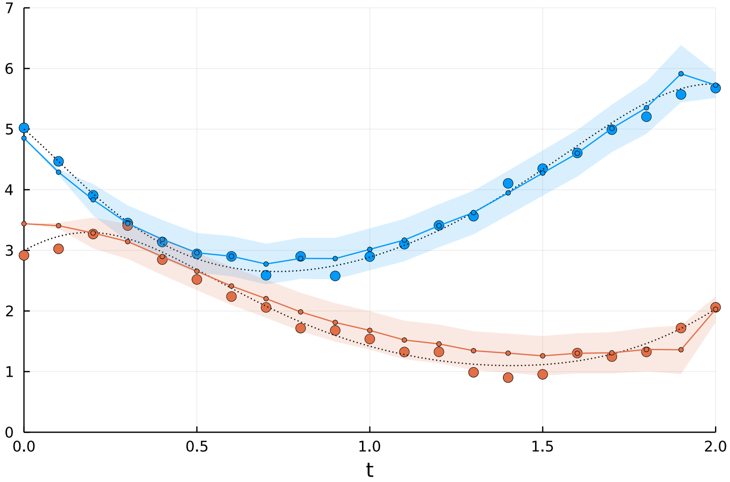


Figure: i=65

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

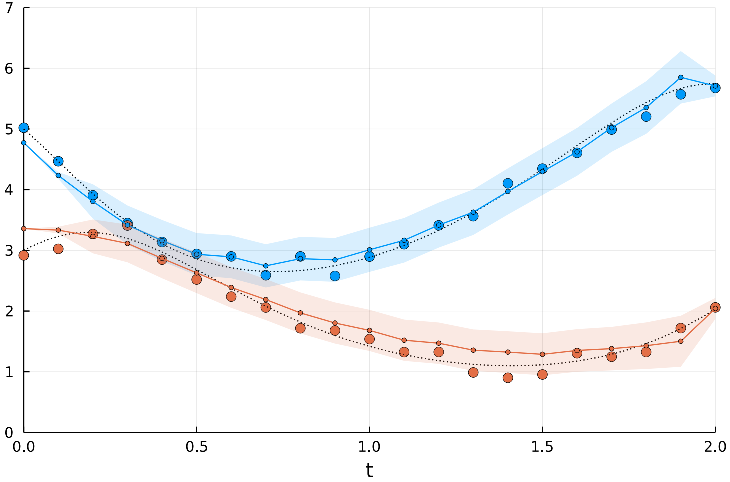


Figure: i=66

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

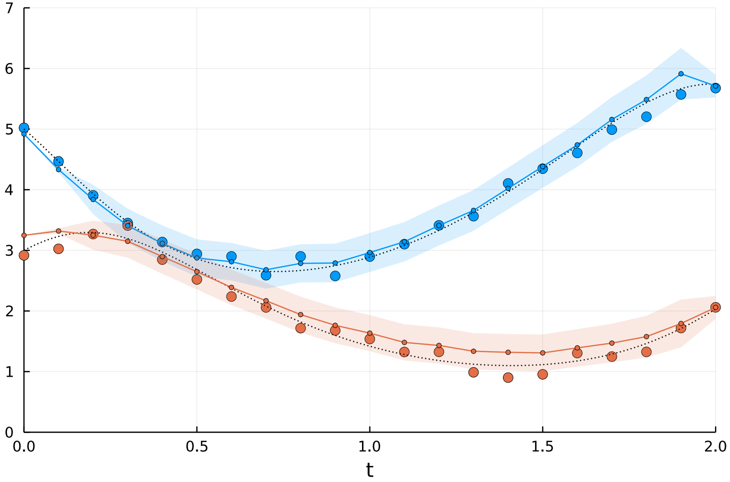


Figure: i=67

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

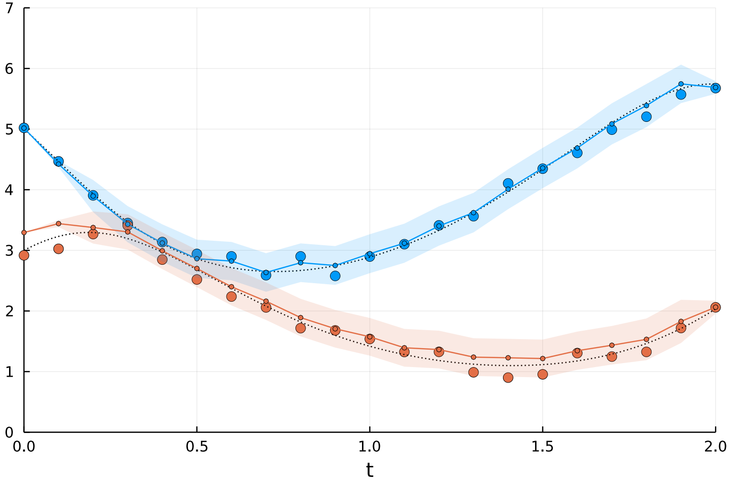


Figure: i=68

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

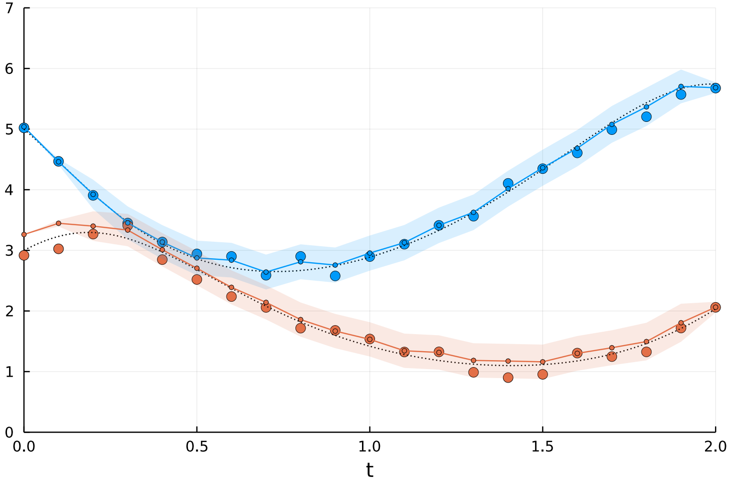


Figure: i=69

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

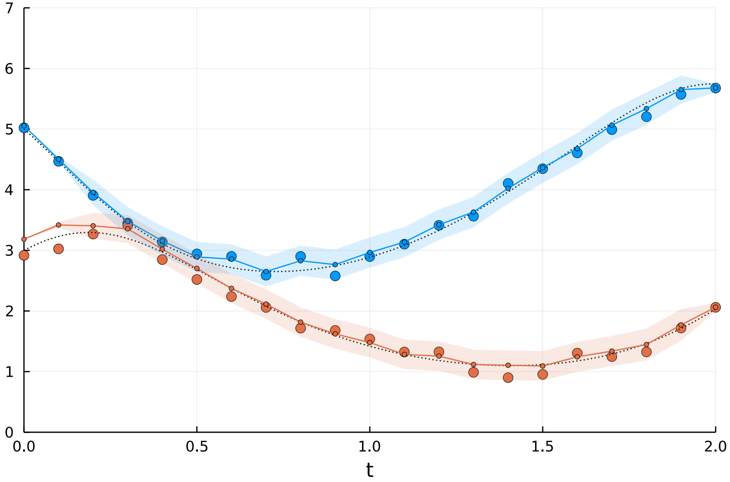


Figure: i=70

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

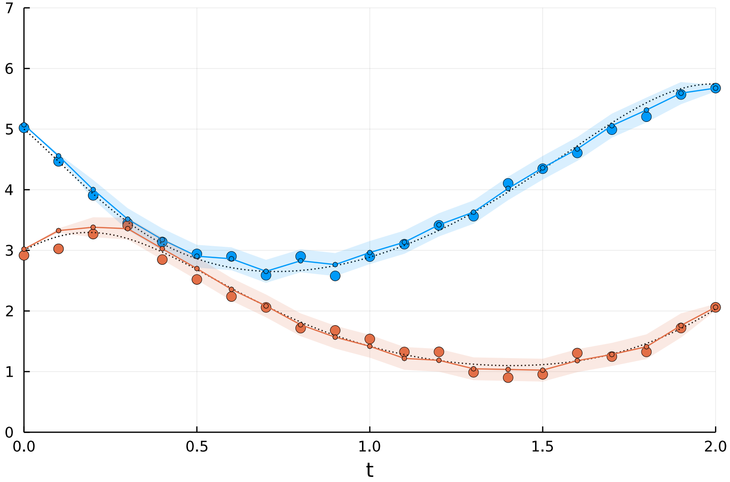


Figure: i=71

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

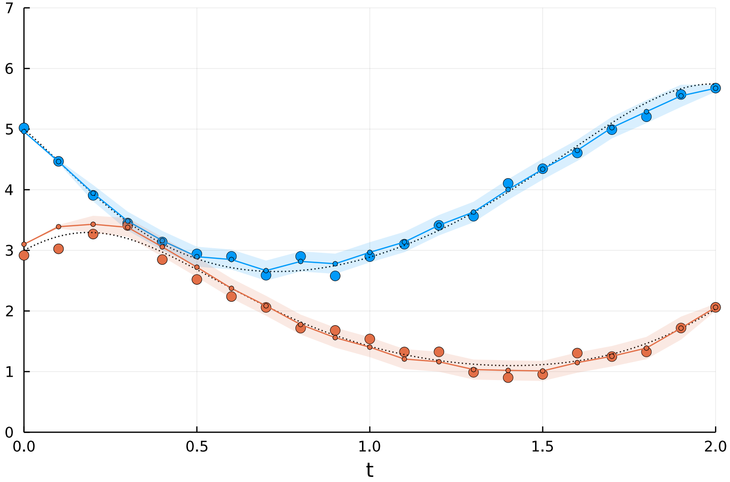


Figure: i=72

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

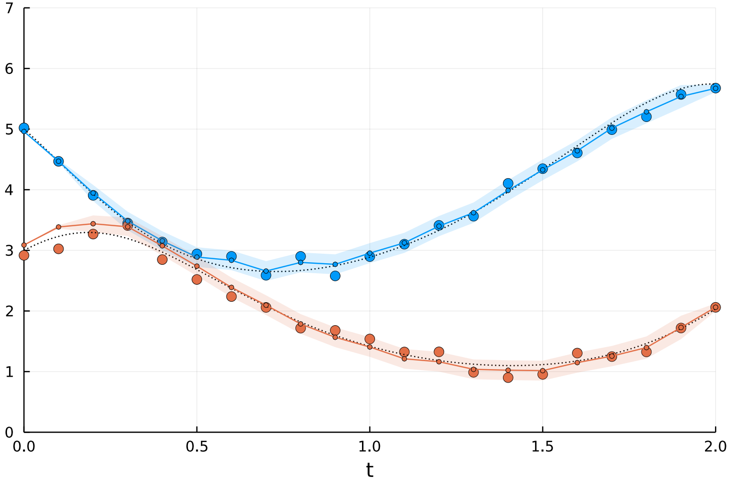


Figure: i=73

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

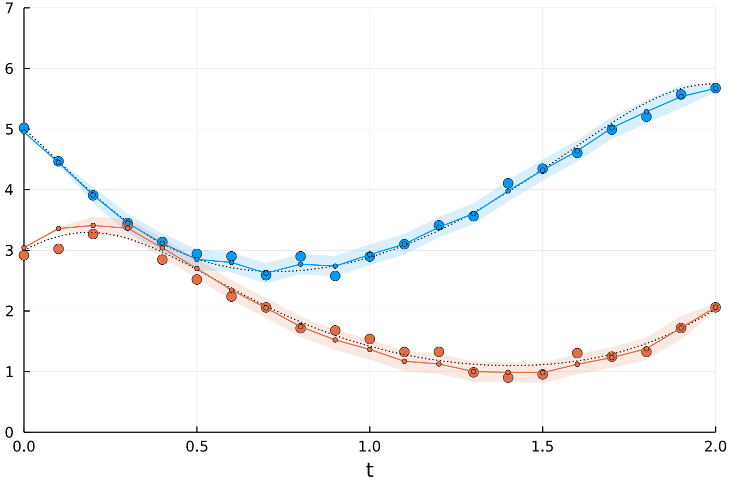


Figure: i=74

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

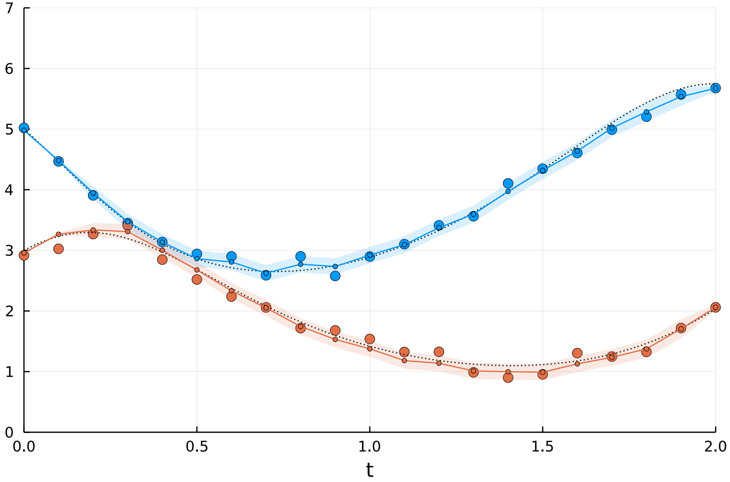


Figure: i=75

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

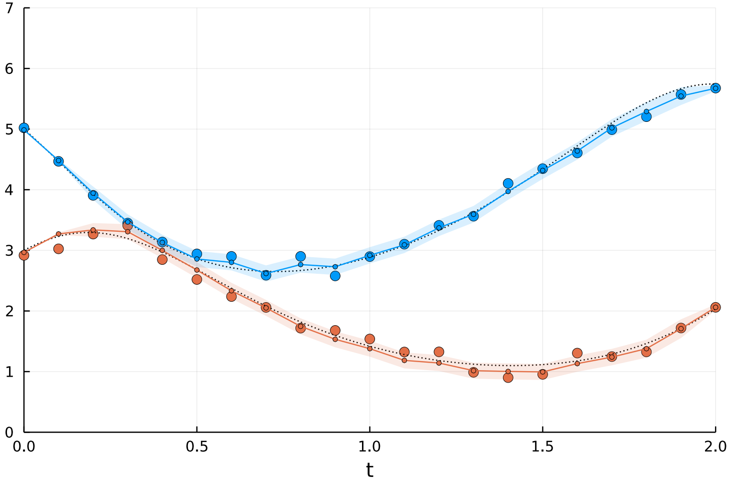


Figure: i=76

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

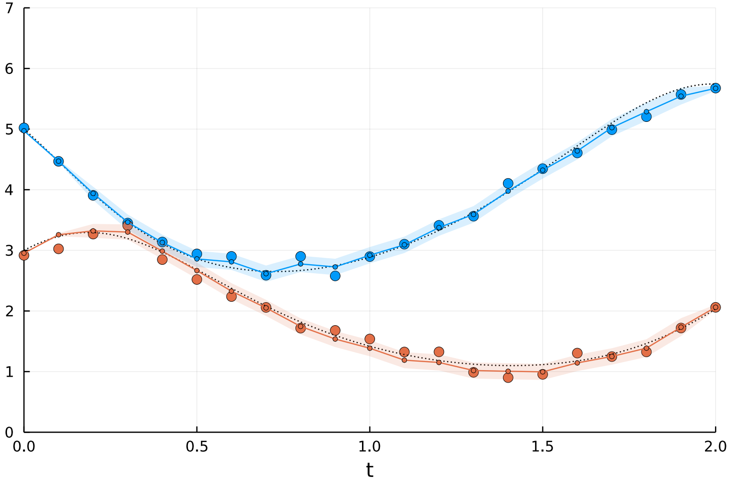


Figure: i=77

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

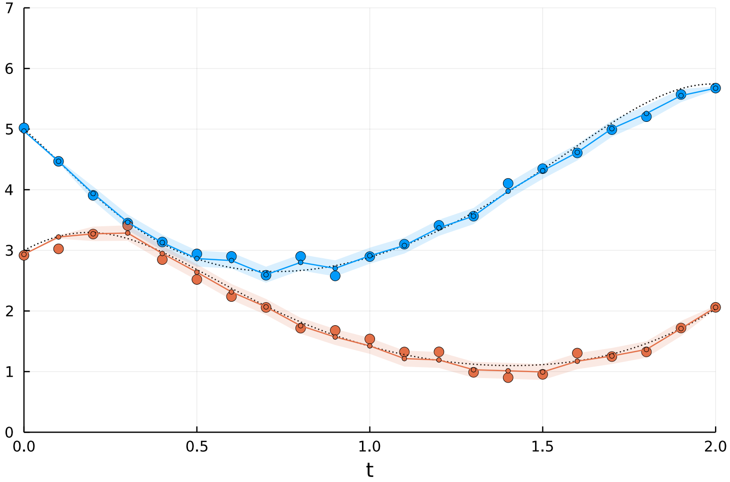


Figure: i=78

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

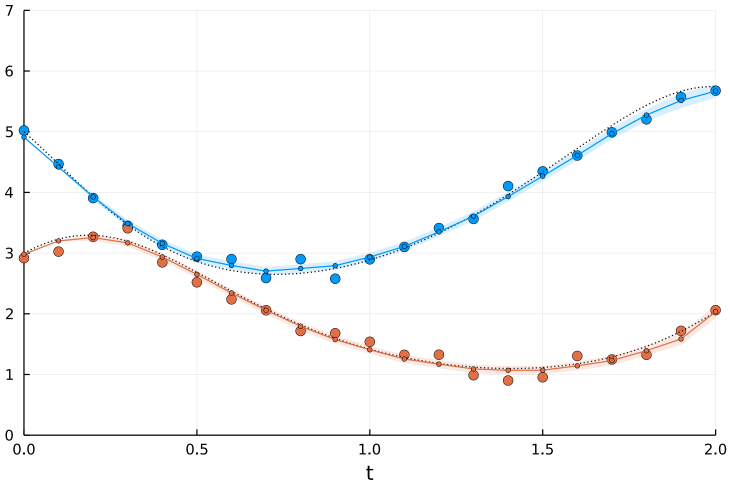


Figure: i=79

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

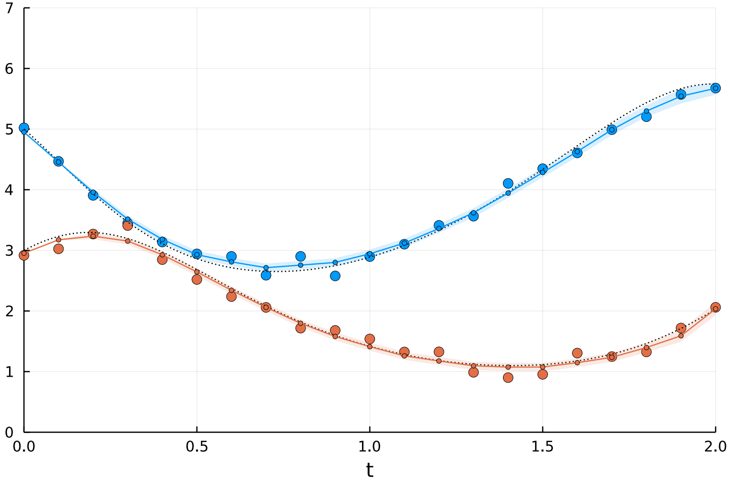


Figure: i=80

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

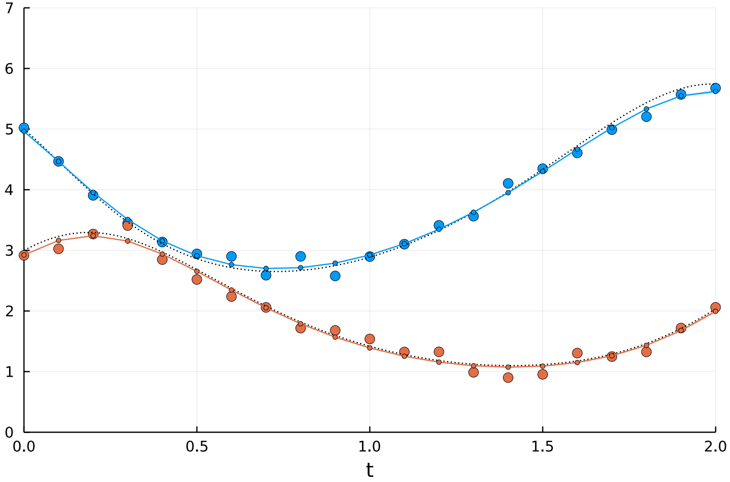


Figure: i=90

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

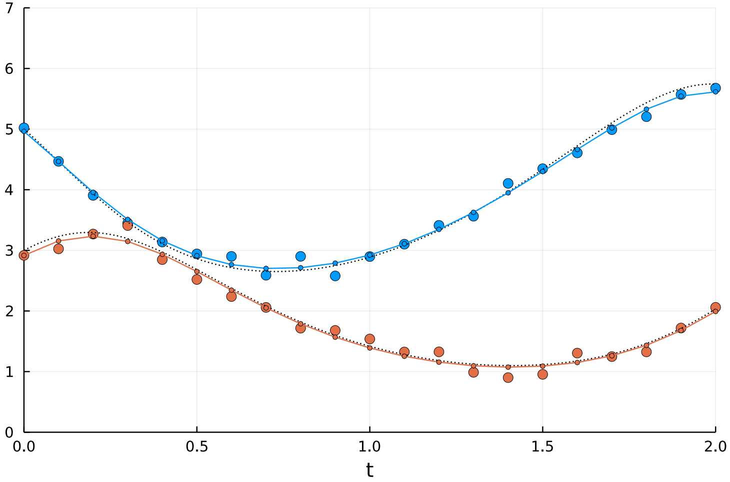


Figure: i=100

Example: Probabilistic Numerical Integration

Optimizing ODE parameters and prior hyperparameters jointly

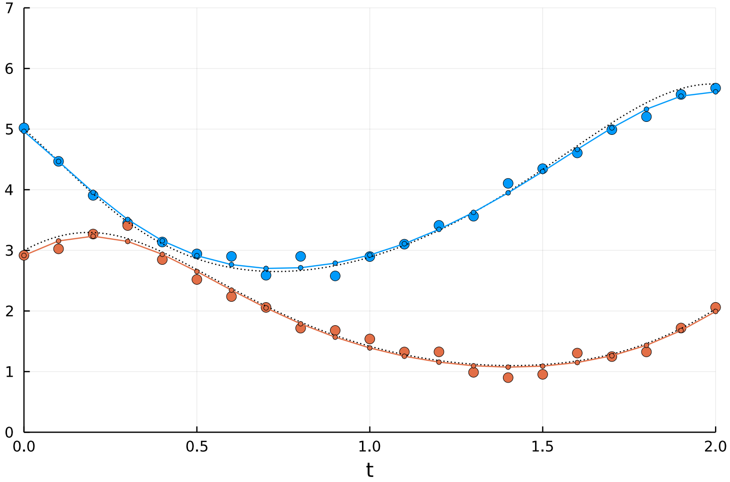
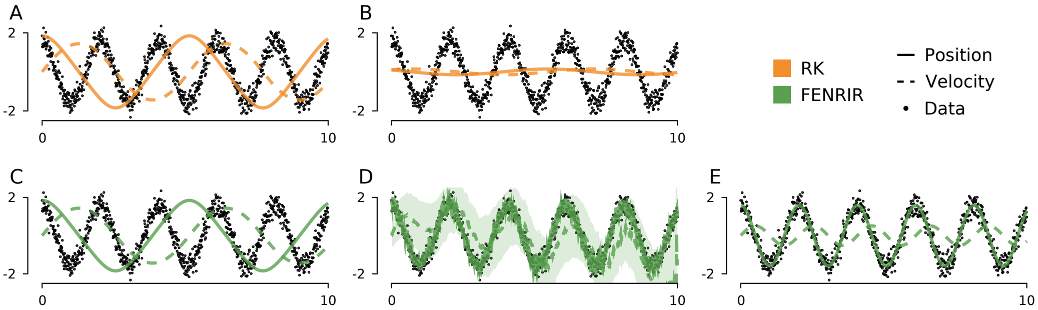


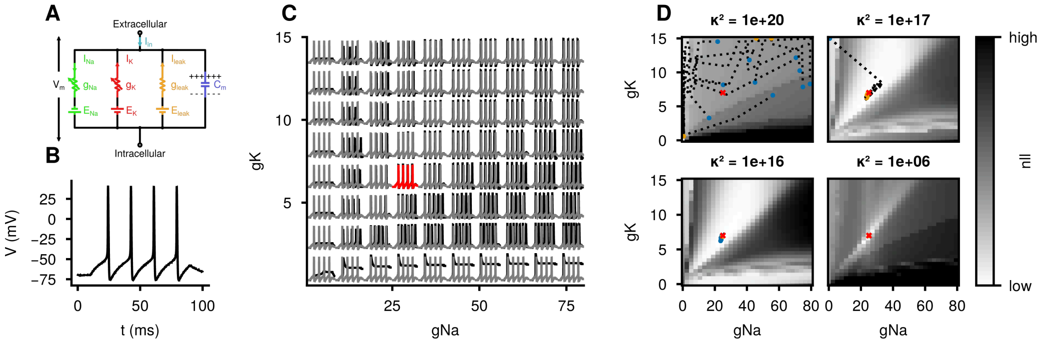
Figure: i=100 DONE

Inference in a partially observed oscillatory system

The probabilistic solver can escape the local optimum



Gradient-based parameter inference in a Hodgkin–Huxley neuron



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**
- *Flexible information operators* to solve more than just standard ODEs
- *Parameter inference:* Being uncertain about the ODE solution allows you to update on 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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