Practical Probabilistic Numerical Solvers

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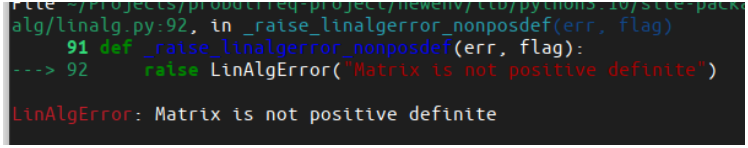
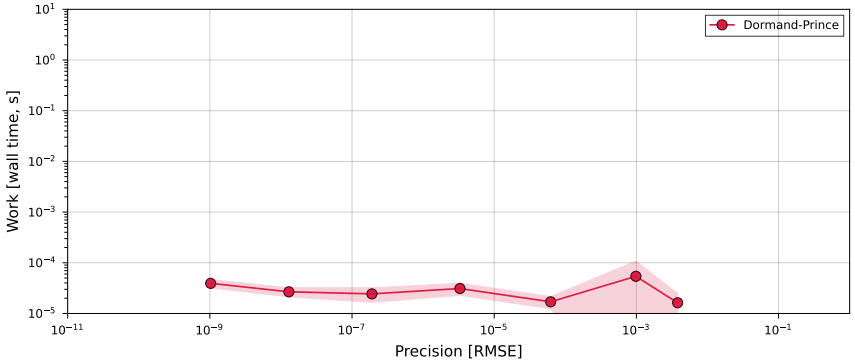
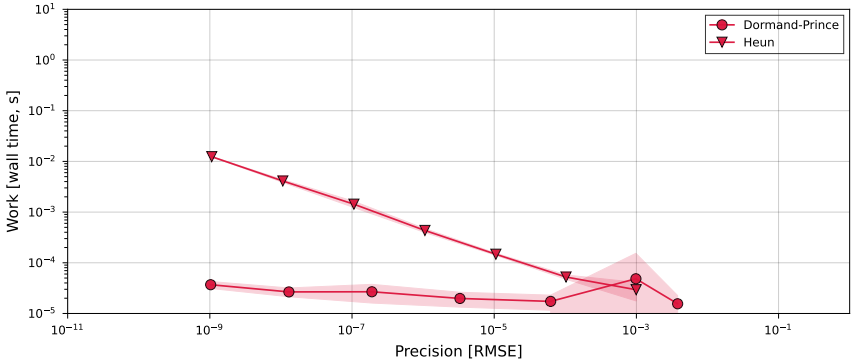
I have bad news.



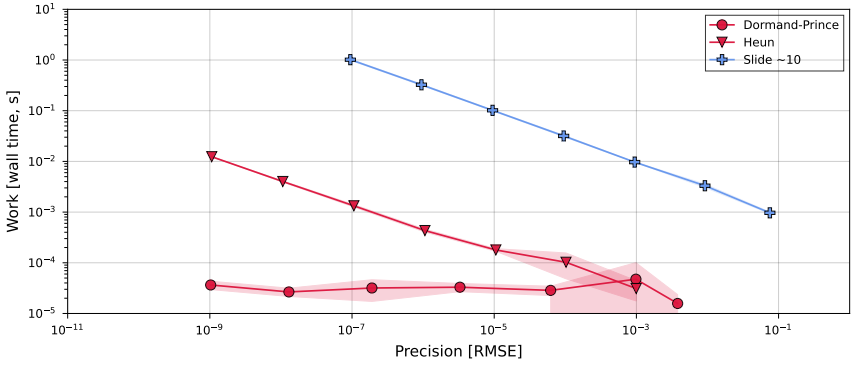
Work vs. precision



Work vs. precision



Work vs. precision



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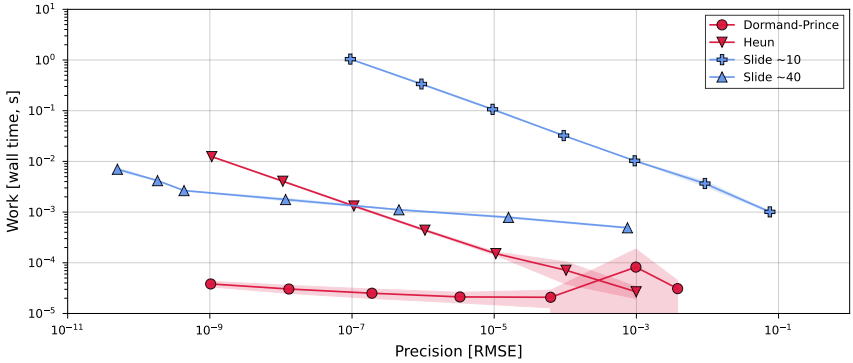

Practical Probabilistic Numerical Solvers (now for real)

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Probabilistic solvers in a nutshell

- ◇ Initial value problem (IVP):

$$\frac{\mathrm{d}}{\mathrm{d}t} y(t) = f(y(t), t), \quad y(0) = y_0$$

- ◇ Hypothesize $Y \sim \mathrm{GP}$. Grid $t_0, ..., t_N$. Approximate y by estimating (variations of)

$$p\left(Y(\cdot) \;\middle|\; \left\{ \dot{Y}(t_n) = f(Y(t_n), t_n) \right\}_{n=0}^{N}, \; Y(t_0) = y_0 \right)$$

(WLOG $t_0 = 0$) *Tronarp et al., Cockayne et al.*

- ◇ We call this *probabilistic IVP solution*
- ◇ Same for BVPs, PDEs, mass-matrices, etc. *Krämer & Hennig, Krämer et al., Bosch et al.*
- ◇ Gauss–Markov prior $p(y) \Rightarrow$ probabilistic solution in $O(N)$ *Schober et al.*

Probabilistic solvers in a nutshell

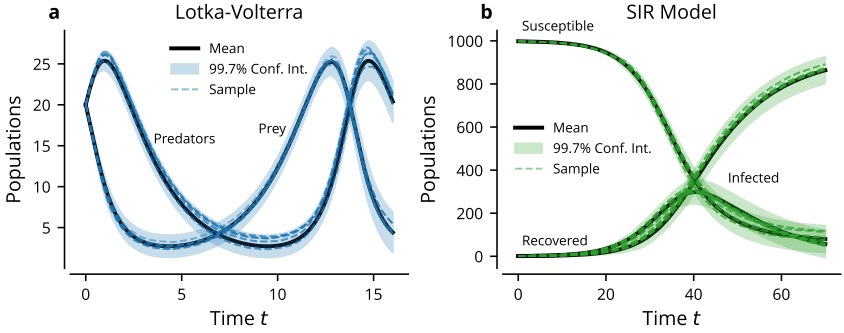


Figure: Krämer & Hennig

$$Y \sim \mathrm{GP}$$

Stochastic differential equation priors

$$\frac{\mathrm{d}^{\nu+1}}{\mathrm{d}t^{\nu+1}} Y(t) - \sum_{k=0}^{\nu} A_k \frac{\mathrm{d}^k}{\mathrm{d}t^k} Y(t) = \sigma w(t) \quad + \text{Gaussian initial condition}$$

Stochastic differential equation priors

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} Y(t) \\ \frac{\mathrm{d}}{\mathrm{d}t}Y(t) \\ \vdots \\ \frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}Y(t) \end{pmatrix} = \begin{pmatrix} 0 & I & & \\ & \ddots & \ddots & \\ & & 0 & I \\ -A_0 & \dots & \dots & -A_\nu \end{pmatrix} \begin{pmatrix} Y(t) \\ \frac{\mathrm{d}}{\mathrm{d}t}Y(t) \\ \vdots \\ \frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}Y(t) \end{pmatrix} + \sigma \begin{pmatrix} 0 \\ \vdots \\ 0 \\ I \end{pmatrix} w(t)$$

Stochastic differential equation priors

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Y}(t) = \mathbf{A}\mathbf{Y}(t) + \sigma\mathbf{B}w(t)$$

where

$$\mathbf{Y}(t) = \begin{pmatrix} Y(t) \\ \frac{\mathrm{d}}{\mathrm{d}t}Y(t) \\ \vdots \\ \frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}Y(t) \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 0 & I & & \\ & \ddots & \ddots & \\ & & 0 & I \\ -A_0 & \dots & \dots & -A_\nu \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ I \end{pmatrix}$$

Our favourite example: integrated Wiener processes

- ν-times integrated Wiener process

$$\frac{\mathrm{d}^{\nu+1}}{\mathrm{d}t^{\nu+1}} Y(t) = \sigma w(t) \tag{1}$$

  (i.e. $A_0 = A_1 = ... = 0$)
- Corresponds to spline models

see works by Wahba

- It is just fantastic

Integrated Wiener processes

$A_0 = A_1 = ... = 0$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Y}(t) = \mathbf{A}\mathbf{Y}(t) + \sigma\mathbf{B}w(t)$$

where

$$\mathbf{Y}(t) = \begin{pmatrix} Y(t) \\ \frac{\mathrm{d}}{\mathrm{d}t}Y(t) \\ \vdots \\ \frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}Y(t) \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 0 & I & & \\ & \ddots & \ddots & \\ & & 0 & I \\ 0 & \dots & 0 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ I \end{pmatrix}$$

Discretised integrated Wiener process

$$p(\mathbf{Y}(t+\Delta t) \mid \mathbf{Y}(t), \sigma) = \mathsf{N}((\Phi(\Delta t) \otimes I)\mathbf{Y}(t), \Sigma(\Delta t, \sigma) \otimes I),$$

with

e.g. Schober et al., Kersting et al.

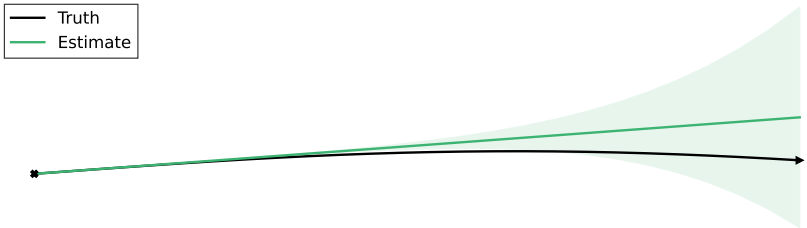
$$\Phi(\Delta t) = 1_{i \leq j} \left(\frac{(\Delta t)^{j-i}}{(j-i)!} \right)_{ij}, \quad \Sigma(\Delta t, \sigma) = \sigma^2 \left(\frac{\Delta t^{2\nu+1-i-j}}{(2\nu+1-i-j)(\nu-i)!(\nu-j)!} \right)_{ij}$$

for example with $\nu = 2$:

$$\Phi(\Delta t) = \begin{pmatrix} 1 & \Delta t & (\Delta t)^2/2 \\ 0 & 1 & \Delta t \\ 0 & 0 & 1 \end{pmatrix}, \quad \Sigma(\Delta t, \sigma) = \sigma^2 \begin{pmatrix} (\Delta t)^5/20 & (\Delta t)^4/8 & (\Delta t)^3/6 \\ (\Delta t)^4/8 & (\Delta t)^3/6 & (\Delta t)^2/2 \\ (\Delta t)^3/6 & (\Delta t)^2/2 & \Delta t \end{pmatrix}$$

Discretised integrated Wiener process

$$\begin{pmatrix} Y(t+\Delta t) \\ \frac{\mathrm{d}}{\mathrm{d}t} Y(t+\Delta t) \\ \frac{\mathrm{d}^2}{\mathrm{d}t^2} Y(t+\Delta t) \end{pmatrix} = \begin{pmatrix} 1 & \Delta t & (\Delta t)^2/2 \\ 0 & 1 & \Delta t \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y(t) \\ \frac{\mathrm{d}}{\mathrm{d}t} Y(t) \\ \frac{\mathrm{d}^2}{\mathrm{d}t^2} Y(t) \end{pmatrix} + \mathsf{N}(0, \Sigma(\Delta t, \sigma))$$



Sequential IVP solution

- Probabilistic IVP solution

$$p\left(Y \;\middle|\; \left\{\dot{Y}(t_n) = f(Y(t_n), t_n)\right\}_{n=0}^{N},\; Y(t_0) = y_0\right)$$

- Implement as

$$p\left(Y, \frac{\mathrm{d}}{\mathrm{d}t}Y, ..., \frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}Y \;\middle|\; \left\{\dot{Y}(t_n) = f(Y(t_n), t_n)\right\}_{n=0}^{N},\; Y(t_0) = y_0, \sigma\right)$$

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- Implement as

$$p\left(\{\mathbf{Y}(t_n)\}_{n=0}^{N} \;\middle|\; \left\{\dot{Y}(t_n) = f(Y(t_n), t_n)\right\}_{n=0}^{N},\; Y(t_0) = y_0, \sigma\right)$$

Sequential IVP solution

- Probabilistic IVP solution

$$p\left(Y \;\middle|\; \left\{\dot{Y}(t_n) = f(Y(t_n), t_n)\right\}_{n=0}^{N},\; Y(t_0) = y_0\right)$$

- Implement as

$$p\left(\{\mathbf{Y}(t_n)\}_{n=0}^{N} \;\middle|\; \left\{\dot{Y}(t_n) - f(Y(t_n), t_n) = 0\right\}_{n=0}^{N},\; Y(t_0) = y_0, \sigma\right)$$

Sequential IVP solution

- Probabilistic IVP solution

$$p\left(Y \;\middle|\; \left\{\dot{Y}(t_n) = f(Y(t_n), t_n)\right\}_{n=0}^{N},\; Y(t_0) = y_0\right)$$

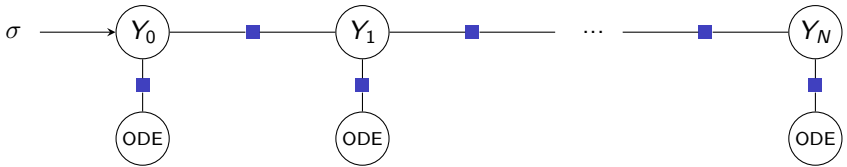
- Implement as

$$p\left(\mathbf{Y}(t_{0:N}) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma\right)$$

Sequential solution

$$
\begin{aligned}
&p(\mathbf{Y}(t_{0:N}) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma) \\
&\qquad = p(\mathbf{Y}(t_N) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma) \\
&\qquad\qquad \times \prod_{n=0}^{N-1} p((\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), (\mathcal{R}\mathbf{Y})(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)
\end{aligned}
$$

e.g. Tronarp, Bosch, Hennig



Sequential solution

$$
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&\qquad = p(\mathbf{Y}(t_N) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma) \\
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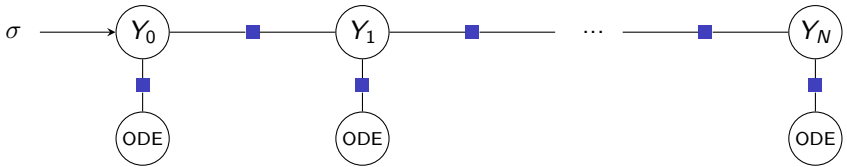
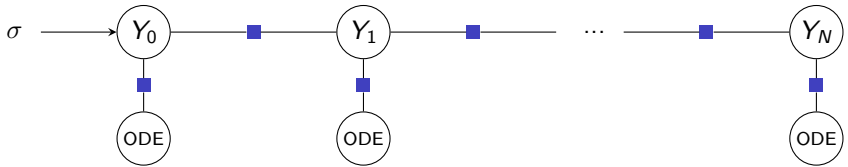


Sequential solution

$$
\begin{aligned}
p(\text{IVP solution}) &= p(\text{Terminal-value solution}) \times \prod_{n=0}^{N-1} p(\text{backward-transitions}) \\
&= [\text{Simulate forward-in-time}] \times [\text{Byproducts of forward simulation}] \\
&= [\text{Always interesting}] \times [\text{Optional}]
\end{aligned}
$$

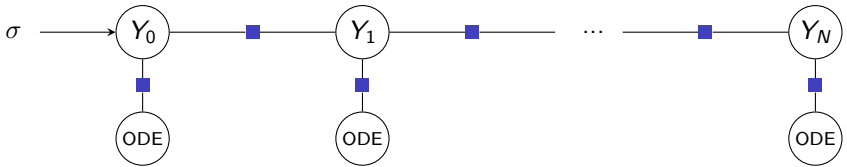
e.g. Tronarp, Bosch, Hennig



Sequential solution

$$
\begin{aligned}
&p(\mathbf{Y}(t_{0:N}) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma) \\
&\qquad = p(\mathbf{Y}(t_N) \mid (\mathcal{R}\mathbf{Y})(t_{0:N}) = 0, Y(t_0) = y_0, \sigma) \\
&\qquad\qquad \times \prod_{n=0}^{N-1} p((\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), (\mathcal{R}\mathbf{Y})(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)
\end{aligned}
$$

e.g. Tronarp, Bosch, Hennig

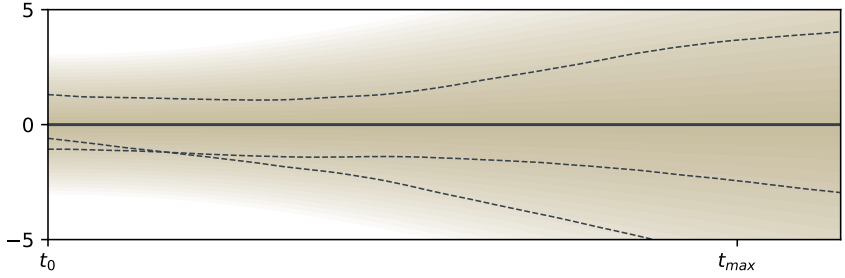


Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

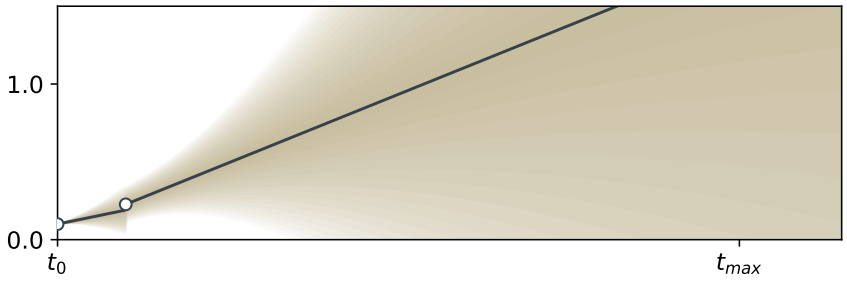
Like Kalman filtering, sum-product algorithm, sequential least-squares, etc.

Algorithm: Sequential IVP solver



https://www.youtube.com/watch?v=vlMibwkanQw

Algorithm: Sequential IVP solver



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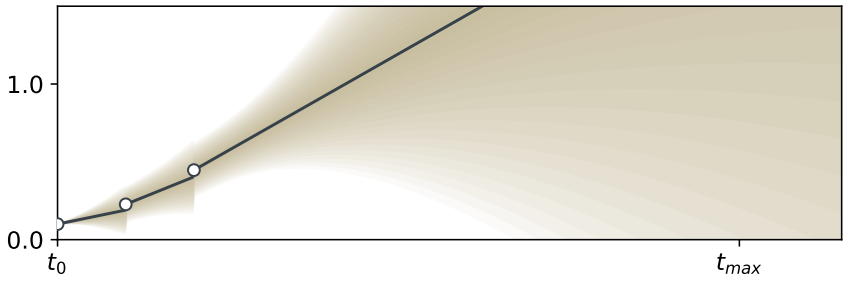

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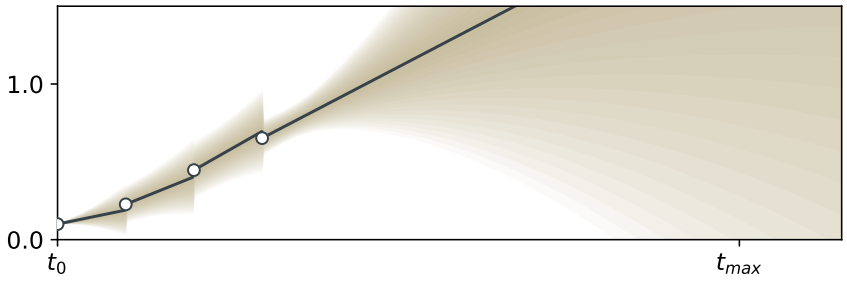

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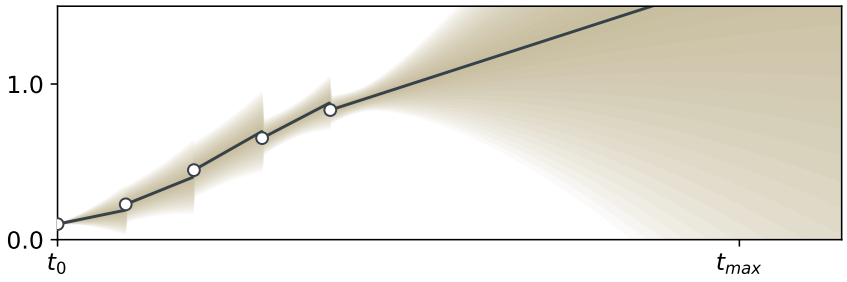

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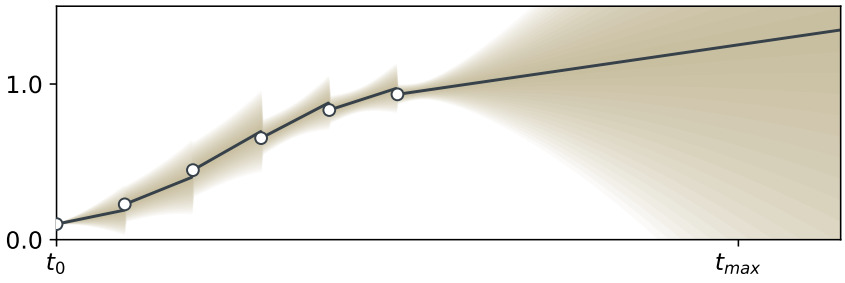

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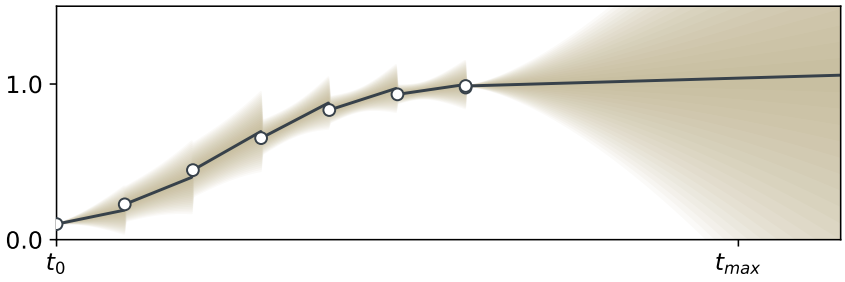

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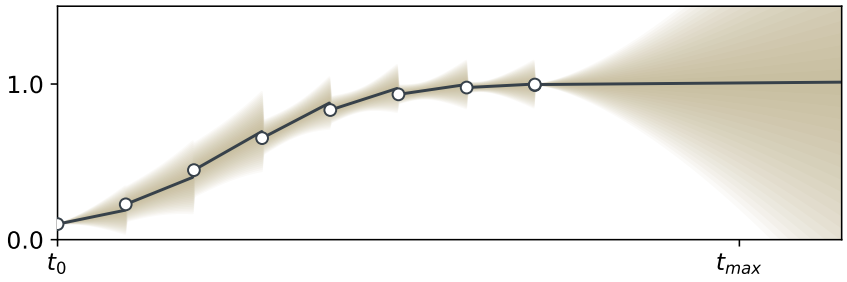

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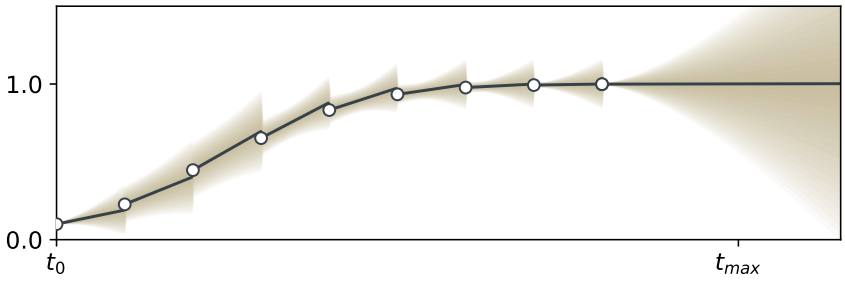

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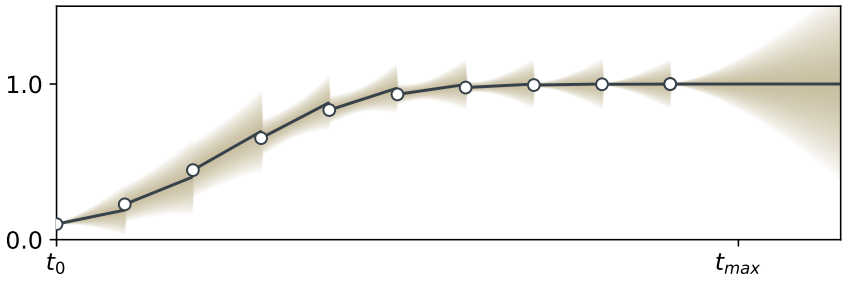

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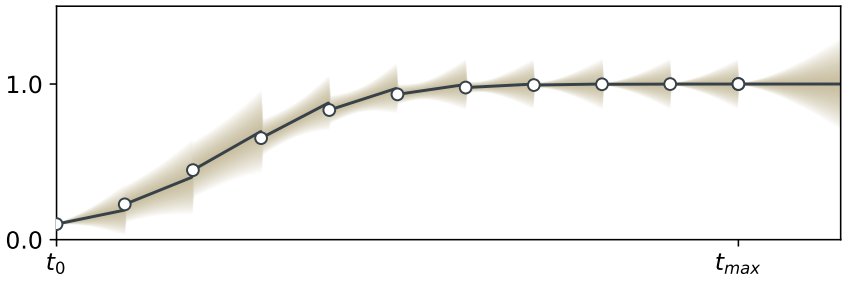

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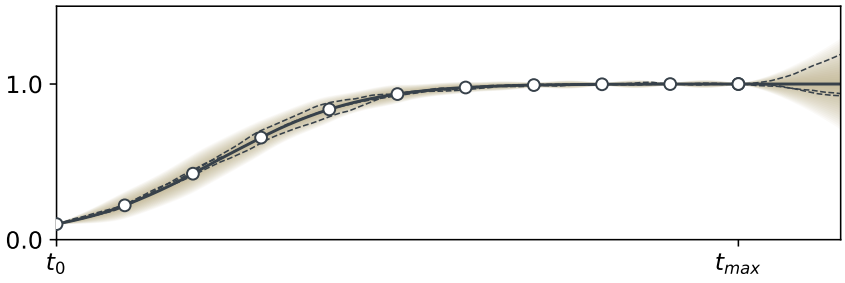

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     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Where's the Kalman filter?

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution
   and (optionally) the backward transitions

Where's the Rauch–Tung–Striebel smoother?

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Where's the extended/unscented filter/smoother?

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Where's Gauss–Newton?

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   3.1 Extrapolate: Compute
   - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$

   3.2 Repeat until convergence:
   - Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

see works by Bell

Where's parameter estimation?

$\frac{\mathrm{d}}{\mathrm{d}t} y(t) = f_\theta(y(t), t)$

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma, \theta)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma, \theta)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $\diamond$ $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma, \theta)$
     - $\diamond$ $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma, \theta)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma, \theta)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

e.g. Kersting, Krämer, et al.; Tronarp, Bosch, Hennig.

Can we solve second-order problems?

$\frac{\mathrm{d}^2}{\mathrm{d}t^2} y(t) = f(y(t), t)$

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Bosch et al.

Can we solve 8th-order problems?

$\frac{\mathrm{d}^8}{\mathrm{d}t^8} y(t) = f(y(t), t)$

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Bosch et al.

Can we solve mass-matrix problems?

$\mathsf{M}\frac{\mathrm{d}}{\mathrm{d}t}y(t) = f(y(t), t)$

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Bosch et al.

Where's the boundary value problem solver?

$\frac{\mathrm{d}^2}{\mathrm{d}t^2} y(t) = f(y(t), t),\ y(0) = y_0,\ y(1) = y_1$

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, Y(t_N) = y_1, \sigma)$
2. Linearise: $\mathcal{R}\mathbf{Y}(t_{0:N}) \approx R_0 + \hat{\mathcal{R}}\mathbf{Y}(t_{0:N})$
3. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, Y(t_N) = y_1, \sigma)$
4. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 4.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, Y(t_N) = y_1, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, Y(t_N) = y_1, \sigma)$
   - 4.2 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, Y(t_N) = y_1, \sigma)$
5. Rinse and repeat from 2.
6. Do something fun with the terminal-value solution and (optionally) the backward transitions

Krämer & Hennig

Wait!

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. For all $(t_n, t_{n+1} = t_n + \Delta t_n ???]$:
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Δt_n ???

Step-size adaptation

- ◇ Choose $t_0, ..., t_N$ adaptively.
- ◇ Ensure that all "local errors" are equal to tolerance.
- ◇ If error at $t_n + \Delta t_n$ is too large:
  1. Estimate the error introduced by the previous step *Schober et al., Bosch et al.*
  2. Assume the local error decays as $(\Delta t)^\rho$
  3. Then, choosing ("integral"-controller) *e.g. Hairer & Wanner*

$$t_{n+1}^{\text{new}} = t_n + \Delta t_n^{\text{new}}, \quad \Delta t_n^{\text{new}} \sim \left(\frac{\text{tol}}{\text{error}}\right)^{1/\rho} \Delta t_{n-1}$$

  will (usually) yield a sufficiently small step
- ◇ Use a more sophisticated version ("proportional-integral" controller) *See works by Gustafsson*

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

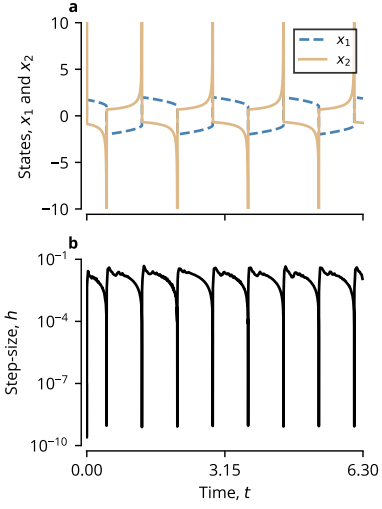
Adaptive steps are mandatory

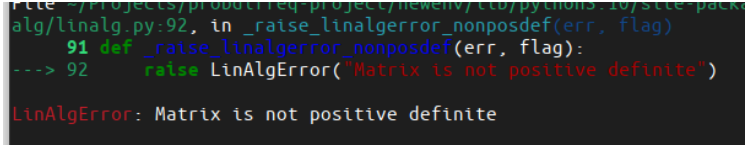
Stiff van-der-Pol system,

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}y(t) = 10^6(1 - y(t)^2)\frac{\mathrm{d}}{\mathrm{d}t}y(t) - y(t)$$

- ◇ Crazy "spikes"
- ◇ Requires non-uniform steps

see Bosch et al.; Figure: Krämer & Hennig





Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
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     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix}\star\\ \star\\ \star\\ \star\end{pmatrix}, \begin{pmatrix}\star & \star & \star & \star\\ \star & \star & \star & \star\\ \star & \star & \star & \star\\ \star & \star & \star & \star\end{pmatrix}\right)$$

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ \star \\ \star \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \star & \star & \star \\ 0 & \star & \star & \star \\ 0 & \star & \star & \star \end{pmatrix}\right)$$

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ f(y_0, t_0) \\ \star \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \star & \star \\ 0 & 0 & \star & \star \end{pmatrix}\right)$$

$(\nu = 3)$

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ f(y_0, t_0) \\ J_y f(y_0, t_0) f(y_0, t_0) + J_t f(y_0, t_0) \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \star \end{pmatrix}\right)$$

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ f(y_0, t_0) \\ J_y f(y_0, t_0) f(y_0, t_0) + J_t f(y_0, t_0) \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \star \end{pmatrix}\right)$$

Taylor approximation of IVP solutions

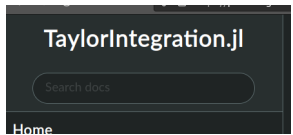
$$
\begin{aligned}
y &= y_0 \\
\frac{\mathrm{d}}{\mathrm{d}t} y &= f \\
\frac{\mathrm{d}^2}{\mathrm{d}t^2} y &= [J_y f](f) + [J_t f](1) \\
\frac{\mathrm{d}^3}{\mathrm{d}t^3} y &= [J_y^2 f](f, f) + [J_y f]([J_y f](f)) + [J_t^2 f](1, 1)
\end{aligned}
$$

$$
[n\text{-th Taylor coefficient of } y] = [(n-1)\text{-th Taylor coefficient of } (f \circ y)]
$$

Taylor arithmetic

$$\mathcal{A} : (f, [n\text{-th order Taylor series of } y]) \longrightarrow [n\text{-th order Taylor series of } f \circ y]$$

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}y(t), ..., \frac{\mathrm{d}^{(n+1)}}{\mathrm{d}t^{(n+1)}}y(t)\right] = \mathcal{A}\left(f, \left[y(t), \frac{\mathrm{d}}{\mathrm{d}t}y(t), ..., \frac{\mathrm{d}^{n}}{\mathrm{d}t^{n}}y(t)\right]\right)$$



e.g. Griewank & Walther

$(\nu = 3)$

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ f(y_0, t_0) \\ J_y f(y_0, t_0) f(y_0, t_0) + J_t f(y_0, t_0) \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \star \end{pmatrix}\right)$$

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y_0 \\ f(y_0, t_0) \\ J_y f(y_0, t_0) f(y_0, t_0) + J_t f(y_0, t_0) \\ \star \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \star \end{pmatrix}\right)$$

($\nu = 3$)

$$p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$$

$$\mathsf{N}\left(\begin{pmatrix} y(t_0) \\ \frac{\mathrm{d}^1}{\mathrm{d}t^1} y(t_0) \\ \frac{\mathrm{d}^2}{\mathrm{d}t^2} y(t_0) \\ \frac{\mathrm{d}^3}{\mathrm{d}t^3} y(t_0) \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\right)$$

Extrapolation

$$p(\mathbf{Y}(t+\Delta t) \mid \mathbf{Y}(t), \sigma) = \mathsf{N}((\Phi(\Delta t) \otimes I)\mathbf{Y}(t), \Sigma(\Delta t, \sigma) \otimes I),$$

with

e.g. Schober et al., Kersting et al.

$$\Phi(\Delta t) = \begin{pmatrix} 1 & \Delta t & (\Delta t)^2/2 \\ 0 & 1 & \Delta t \\ 0 & 0 & 1 \end{pmatrix},$$

$$\Sigma(\Delta t, \sigma) = \begin{pmatrix} (\Delta t)^4/20 & (\Delta t)^3/8 & (\Delta t)^2/6 \\ (\Delta t)^3/8 & (\Delta t)^2/6 & \Delta t/2 \\ (\Delta t)^2/6 & \Delta t/2 & 1 \end{pmatrix} \cdot \sigma \cdot \Delta t$$

Extrapolation

$$p(\mathbf{Y}(t+\Delta t) \mid \mathbf{Y}(t), \sigma) = \mathsf{N}((\Phi(\Delta t) \otimes I)\mathbf{Y}(t), \Sigma(\Delta t, \sigma) \otimes I),$$

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Extrapolation

$$C(t + \Delta t) \approx 0 + \Sigma(\Delta t, \sigma)$$

with

$$\Phi(\Delta t) = \begin{pmatrix} 1 & \Delta t & (\Delta t)^2/2 \\ 0 & 1 & \Delta t \\ 0 & 0 & 1 \end{pmatrix},$$

$$\Sigma(\Delta t, \sigma) = \begin{pmatrix} (\Delta t)^4/20 & (\Delta t)^3/8 & (\Delta t)^2/6 \\ (\Delta t)^3/8 & (\Delta t)^2/6 & \Delta t/2 \\ (\Delta t)^2/6 & \Delta t/2 & 1 \end{pmatrix} \cdot \sigma \cdot \Delta t$$

Extrapolation

$$C(t + \Delta t) = \Phi(\Delta t) C(t) \Phi(\Delta t)^\top + \Sigma(\Delta t, \sigma)$$

with

$$\Phi(\Delta t) = \begin{pmatrix} 1 & \Delta t & (\Delta t)^2/2 \\ 0 & 1 & \Delta t \\ 0 & 0 & 1 \end{pmatrix},$$

$$\Sigma(\Delta t, \sigma) = \begin{pmatrix} (\Delta t)^4/20 & (\Delta t)^3/8 & (\Delta t)^2/6 \\ (\Delta t)^3/8 & (\Delta t)^2/6 & \Delta t/2 \\ (\Delta t)^2/6 & \Delta t/2 & 1 \end{pmatrix} \cdot \sigma \cdot \Delta t$$

Extrapolation

$$C(t+\Delta t) = T(\Delta t)\left[\Phi_0 T(\Delta t)^{-1} C(t) T(\Delta t)^{-\top} \Phi_0^\top + \Sigma_0\right] T(\Delta t)^\top$$

with

$$T(\Delta t) = \sqrt{\Delta t}\begin{pmatrix} \frac{(\Delta t)^2}{2} & 0 & 0 \\ 0 & \Delta t & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \Phi_0 = \begin{pmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T(\Delta t)^{-1} = \frac{1}{\sqrt{\Delta t}}\begin{pmatrix} 2/(\Delta t)^2 & 0 & 0 \\ 0 & \frac{1}{\Delta t} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \Sigma_0 = \begin{pmatrix} 1/5 & 1/4 & 1/3 \\ 1/4 & 1/3 & 1/2 \\ 1/3 & 1/2 & 1 \end{pmatrix}$$

Krämer & Hennig

see also: Nordsieck methods, balanced representations

Linearisation

- Taylor-linearise

$$f(y,t) \approx f(y_0,t) + J_y f(y_0,t_0)(y-y_0)$$

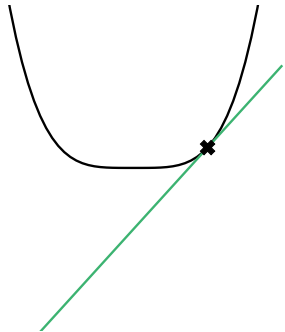
- Statistical linear regression

$$f(y,t) \approx Hy + b, \quad b \sim \mathrm{N}(\lambda, \Lambda)$$

- Approximate *Bosch et al.*

$$\mathcal{R}_1\mathbf{Y}(t) \approx \dot{Y}(t) - HY - b$$
$$\mathcal{R}_2\mathbf{Y}(t) \approx \ddot{Y}(t) - H_1 Y - H_2 \dot{Y} - b$$
$$\mathcal{R}_M\mathbf{Y}(t) \approx M\dot{Y}(t) - HY - b$$

- Plug into solver *Tronarp et al.*
- Iterate? *e.g. Tronarp et al., Krämer & Hennig*



Zeroth-order Linearisation

- ◇ Taylor-linearise *Schober et al., Kersting et al.*

$$f(y, t) \approx f(y_0, t)$$

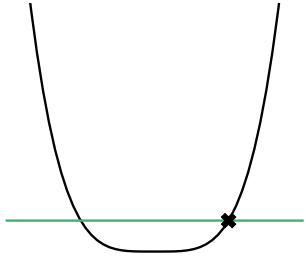
- ◇ Statistical linear regression *Kersting & Hennig*

$$f(y, t) \approx b, \quad b \sim \mathrm{N}(\lambda, \Lambda)$$

- ◇ Approximate *Bosch et al.*

$$\mathcal{R}_1 \mathbf{Y}(t) \approx \dot{Y}(t) - b$$
$$\mathcal{R}_2 \mathbf{Y}(t) \approx \ddot{Y}(t) - b$$
$$\mathcal{R}_M \mathbf{Y}(t) \approx M\dot{Y}(t) - b$$

- ◇ Plug into solver *e.g. Schober et al.*
- ◇ Iterate? *Arvanitidis et al.*



Why does linearisation matter?

- ◇ Jacobians → stability *c.f. Rosenbrock methods*
- ◇ First-order: A-stable *Tronarp et al.*
- ◇ First-order: for stiff problems
- ◇ Zeroth-order: lightning fast *Krämer et al.*

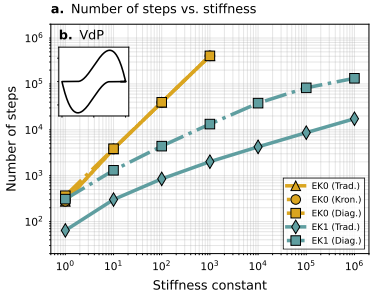
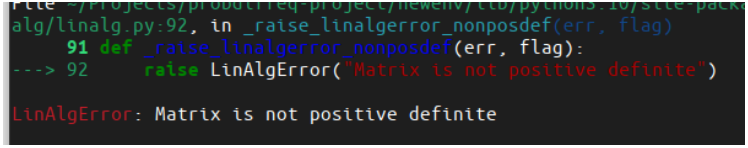


Figure: Krämer, Bosch, Schmidt, Hennig

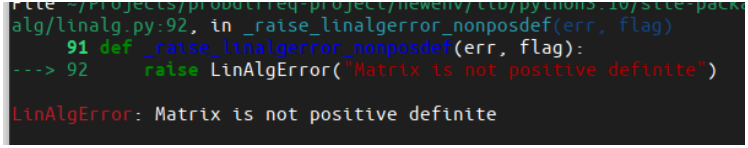


Square-root arithmetic

- ◇ Sometimes, covariance + covariance $\neq$ covariance
- ◇ Factorise $C = \sqrt{C}\sqrt{C}^\top$ (e.g. Cholesky)
- ◇ Then, QR-decomposition $QR = (\sqrt{C_1}^\top, \sqrt{C_2}^\top)$ yields *e.g. Grewal & Andrews*

$$R^\top R = (\sqrt{C_1}, \sqrt{C_2})(\sqrt{C_1}, \sqrt{C_2})^\top = C_1 + C_2$$

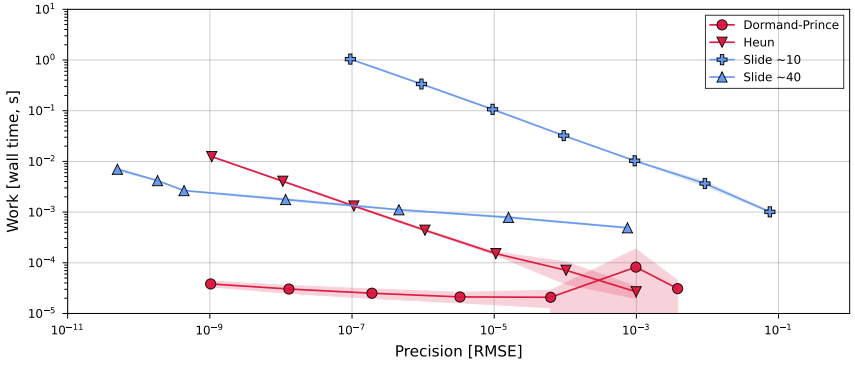
- ◇ Extrapolate covariances in "square-root arithmetic"
- ◇ Conditional covariances: same idea, different QR decomp. ($\rightarrow$ Wednesday)



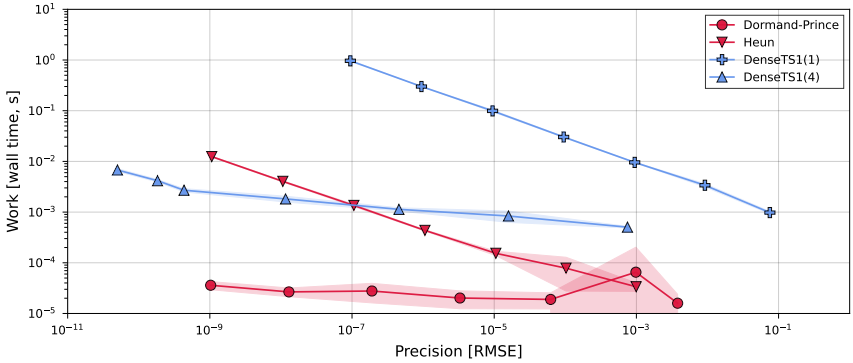
Algorithm: Sequential IVP solver

1. Initialise boundary conditions: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, \sigma)$
2. Initialise first grid point: $p(\mathbf{Y}(t_0) \mid Y(t_0) = y_0, (\mathcal{R}\mathbf{Y})(t_0) = 0, \sigma)$
3. While $t_n + \Delta t_n \leq 1$ (= terminal time):
   - 3.1 Extrapolate: Compute
     - $p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
     - $p(\mathbf{Y}(t_n) \mid \mathbf{Y}(t_{n+1}), \mathcal{R}\mathbf{Y}(t_{0:n}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.2 Linearise: $\mathcal{R}\mathbf{Y}(t_{n+1}) \approx H\mathbf{Y}(t_{n+1}) + b$
   - 3.3 Correct: $\approx p(\mathbf{Y}(t_{n+1}) \mid \mathcal{R}\mathbf{Y}(t_{0:n+1}) = 0, Y(t_0) = y_0, \sigma)$
   - 3.4 Estimate error
   - 3.5 Accept or reject step
   - 3.6 Propose "optimal" Δt_{n+1} and repeat
4. Do something fun with the terminal-value solution and (optionally) the backward transitions

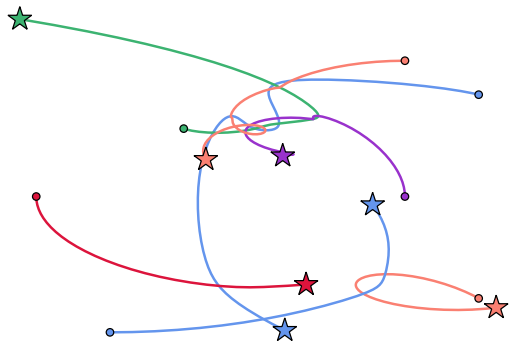
Where are we now?



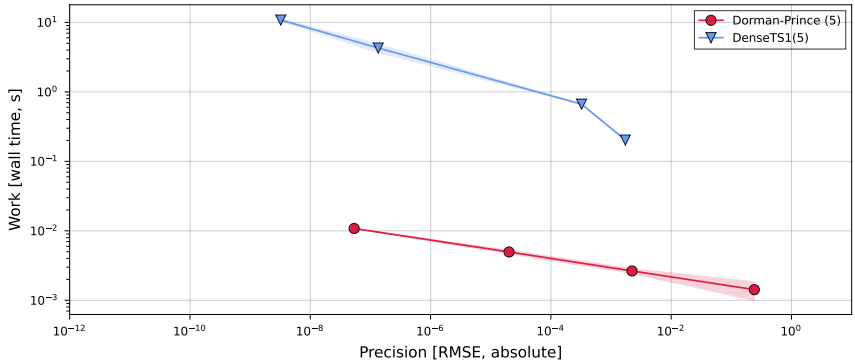
Where are we now?



A medium-dimensional problem



A medium-dimensional problem



$$O([\text{no. time-steps}][\text{no. derivatives}]^3[\text{ODE dimension}]^{\mathbf{3}})$$

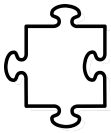


Image source: Pixabay (via Google Images)

Trading correlation for efficiency

Proposition I

If $\Sigma(\Delta t, \sigma)$ is block-diagonal, and if linearisation preserves block-diagonality, all posterior covariances are block-diagonal.

Proposition II

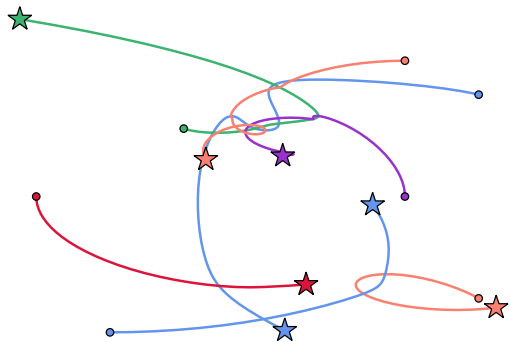
If $\Sigma(\Delta t, \sigma)$ has Kronecker structure, and if linearisation preserves Kronecker structure, all posterior covariances have Kronecker structure.

Corollary

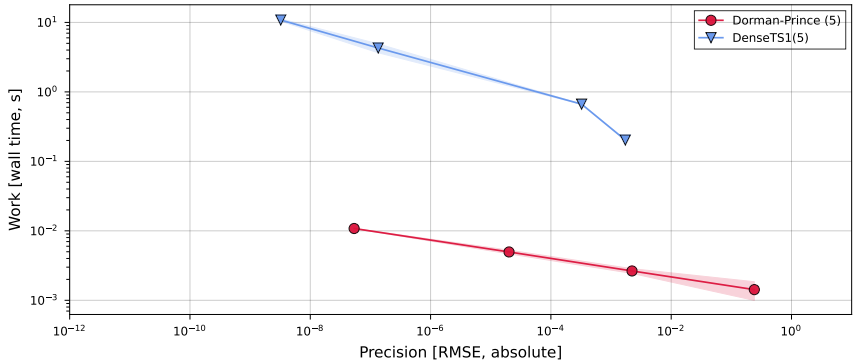
Kronecker-models can be implemented in $O(N(\nu^3 + d\nu^2))$, and block-diagonal models in $O(Nd\nu^3)$.

Krämer, Bosch, Schmidt, Hennig

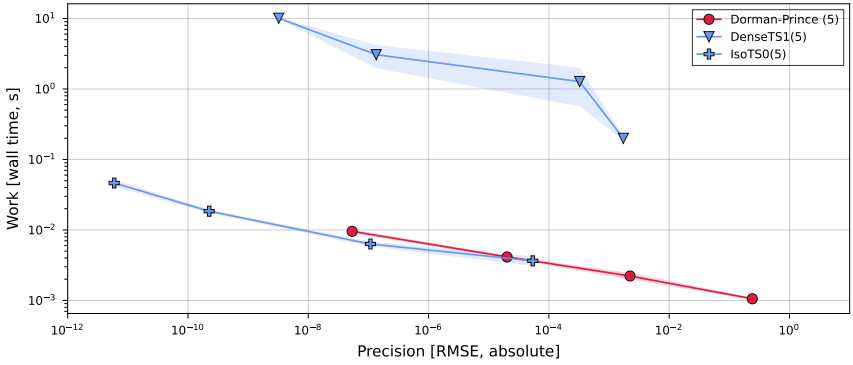
A medium-dimensional problem



A medium-dimensional problem



A medium-dimensional problem



And now the good stuff.

Parameter estimation: Neural ODEs

$$\frac{\mathrm{d}}{\mathrm{d}t}y(t) = \mathrm{NN}_\theta(y(t)), \quad \theta = ???$$

Observations: $\forall n: \; q_n = y(t_n) + \epsilon, \quad \epsilon \sim N(0, \rho^2)$

Parameter estimation

Posterior distribution:

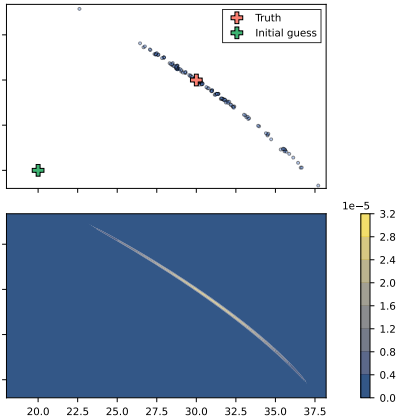
$$\mu(Y \mid \theta) := p(Y \mid \{\dot{Y}(t_n) = f_\theta(Y(t_n), t_n)\}_{n=0}^{N}, Y(t_0) = y_0, \sigma, \theta)$$

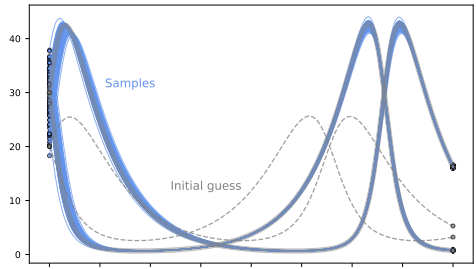
Average likelihood of observations over all IVP solutions:

$$M(\theta) = p(\{q_n\}_n \mid \theta) \approx \int p(q_n \mid Y(t_n))\mu(Y \mid \theta) dY$$

e.g. Kersting et al., Tronarp et al., Cockayne et al.

Probabilistic solvers & MCMC





High resolution images:

https://pnkraemer.github.io/probdiffeq/

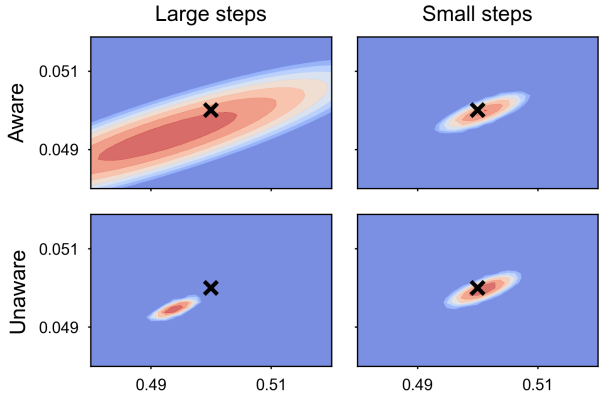


Figure: Kersting, et al.

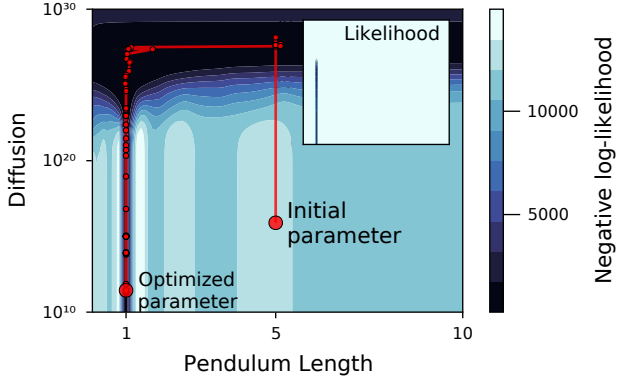


Figure: Tronarp, Bosch, Hennig

Conclusion:

- ◇ Integrated Wiener process priors: estimate IVP solution sequentially
- ◇ Discretise in time. But do it adaptively.
- ◇ Take Taylor series seriously, but not for linearisation.
- ◇ Use only probabilistic solvers for parameter estimation

Future quests:

- ◇ Deep dive into partial differential equations *e.g. Cockayne et al., Krämer et al.*
- ◇ Latent force estimation *Schmidt et al., see work by Särkkä*
- ◇ Other statistical perspectives on numerical differential equation solvers

  see works by Garegnani, Chkrebtii, Wang, Teymur, Pentland, Sullivan, Owhadi, Girolami, Oates, Pförtner, and others

The software landscape


```
pip install probnum
```

```
pip install probdiffeq
```


```
]add ProbNumDiffEq
]add Fenrir
```

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