Backward Filtering Forward Guiding

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Warwick, December 2 (2022)

General problem setting

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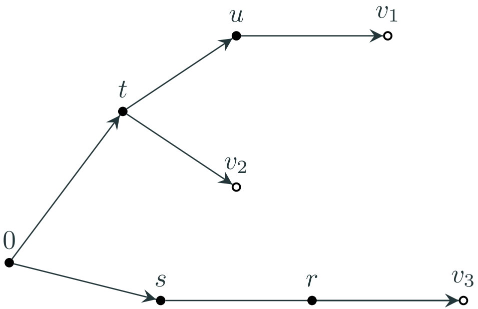
Consider a directed *Markovian* tree:



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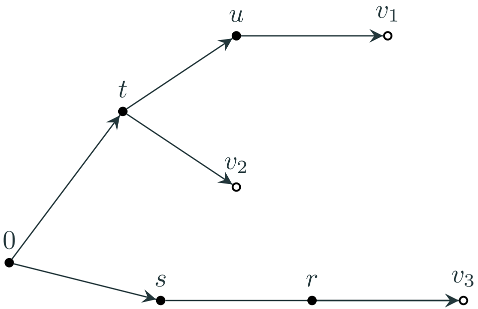

• latent vertices, ∘ leaf/observation-vertices.

To each edge corresponds a Markov kernel $\kappa_{\to t}(x_{\mathrm{pa}(t)}, \mathrm{d}x_t)$.

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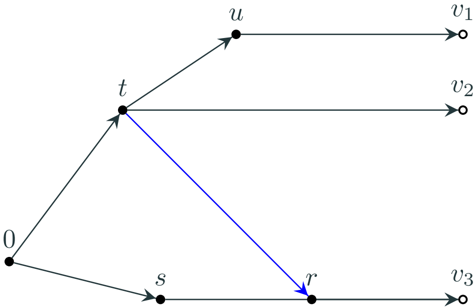
We aim for

1. sampling values at $\bullet$, conditional on values at $\circ$;
2. estimating parameters in kernels;
3. not just on a tree, but on a general Directed Acyclic Graph (DAG).

Example of a DAG



Example 1: interacting particle process

Setup:

- population of n individuals;
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- If $x_i = \mathbf{R}$, it transitions to $\mathbf{S}$ with intensity ν.

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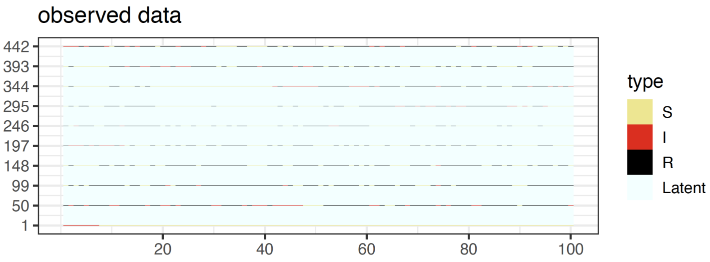
The transition matrix for individual i at time t, given "full state" x:

$$\kappa_i(t,x) = \begin{bmatrix} \psi\left(\lambda N_i(t,x)\right) & 1 - \psi\left(\lambda N_i(t,x)\right) & 0 \\ 0 & \psi(\mu) & 1-\psi(\mu) \\ 1-\psi(\nu) & 0 & \psi(\nu) \end{bmatrix},$$

where $\psi(u) = \exp(-\tau u)$

Example 1: data and challenges



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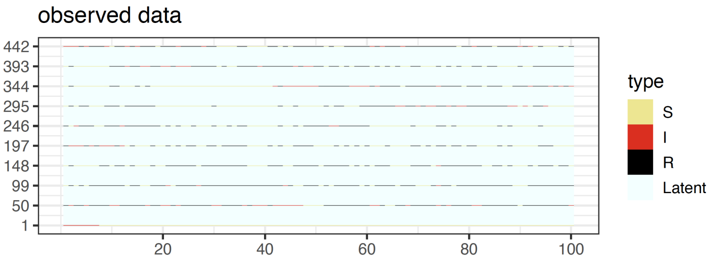

Observe state of each individual at times $t_0 < t_1 < \cdots t_n$.

Goals:

- identify most probable latent states (partial observations...);
- estimate rate parameters λ, μ and ν.

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Ju, Heng, Jacob – Sequential Monte Carlo algorithms for agent-based models of disease transmission

Example 2: Wright-Fisher diffusion on a tree

Diffusion approximation to Wright-Fisher model (with mutation) for N diploid individuals.

Consider a directed tree where along each branch

$$\mathrm{d}X_t = (\beta_1(1 - X_t) + \beta_2 X_t)\,\mathrm{d}t + \sqrt{X_t(1 - X_t)}\,\mathrm{d}W_t.$$

At a leaf vertex observe $V \sim \mathit{Bin}(2n, x)$, where x is the state at the parent vertex.

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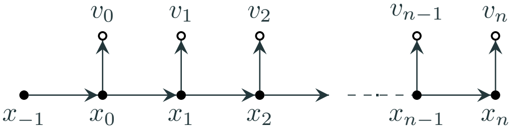
Wish to

- reconstruct X_t along edges;
- estimate parameters (β_1, β_2).

Stoltz et al. – Bayesian inference of species trees using diffusion models

State-space models / hidden Markov models



Well-known filtering, smoothing algorithms dating back to 1960-1970.

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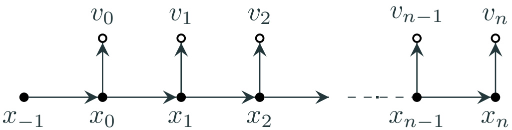

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- Finite state space: Baum-Welch, Viterbi, forward-backward algorithm.
- Linear Gaussian models: Kalman filter, Rauch-Tung-Striebel smoother.
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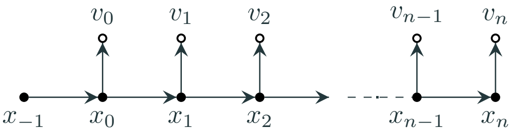

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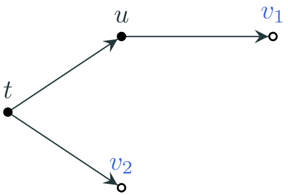
More recently much work on SMC
(twisted particle samplers, controlled SMC).

Conditioning, Doob's h-transform and the Backward Information Filter

Conditioning on a tree

Define

- $\mathcal{V}_t$: all leaf descendants of vertex t.
- $\mathcal{V}_t = \{v_1, v_2\}$.



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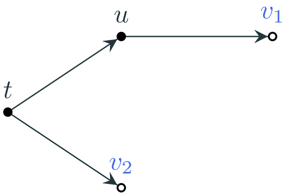

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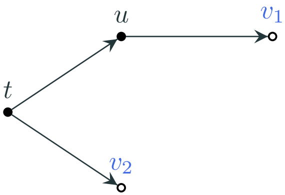

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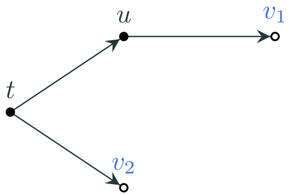

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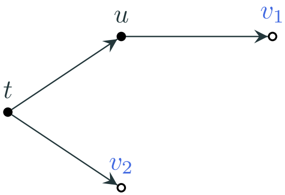

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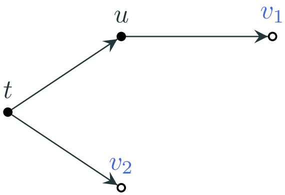

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⚠ Within the subtree, $h_t(x_t)$ is the likelihood of x_t.

Doob's h-transform

- *Doob's h-transform*: Transformation of each κ_s with h_s to $\kappa_s^\star$:

$$\kappa_{\to s}^\star(x,\, \mathrm{d}y) = \frac{\kappa_{\to s}(x,\, \mathrm{d}y) h_s(y)}{\int \kappa_{\to s}(x,\, \mathrm{d}y) h_s(y)}, \quad s \in \mathcal{S}.$$

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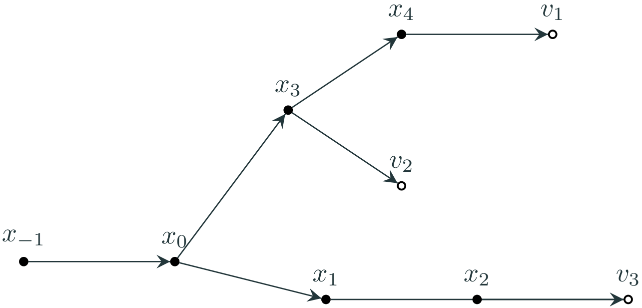
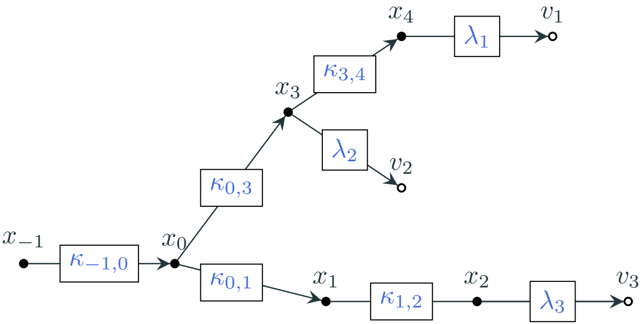
- ⚠ On a DAG conditioning changes the dependency structure. There are no conditional kernels $\kappa^\star_{\to s}$ from $\mathrm{pa}(s)$ to s.

Backward Information Filter



Make kernels explicit



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  Idea: in observations we cannot distinguish ① and ②.
- Finite state space $\Longrightarrow$ Markov kernels can be identified with matrices

$$\lambda_i = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \kappa_{s,t} = \begin{bmatrix} 1-\theta & \theta & 0 \\ 0.25 & 0.5 & 0.25 \\ 0.4 & 0.3 & 0.3 \end{bmatrix},$$

for $i \in \{1, 2, 3\}$, $s \in \{0, 1, 3\}$ and $t \in \mathrm{ch}(s)$.

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  for $i \in \{1, 2, 3\}$, $s \in \{0, 1, 3\}$ and $t \in \mathrm{ch}(s)$.
- Prior on initial state: set $x_{-1} = 0$ and

$$\kappa_{-1,0} = [\pi_1,\ \pi_2,\ \pi_3] =: \boldsymbol{\pi}.$$

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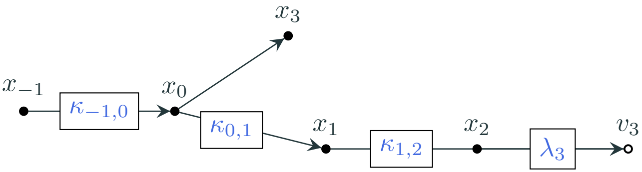
- ⚠ For finite state space this map can be identified with a vector h_t.
- Initialise from observations: for $t = 1, 2, 3$

$$h_t^{\text{obs}} := \begin{bmatrix} 1 \\ 0 \end{bmatrix} \mathbf{1}\{v_t = 1{,}2\} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \mathbf{1}\{v_t = 3\}.$$

Pullback along edges



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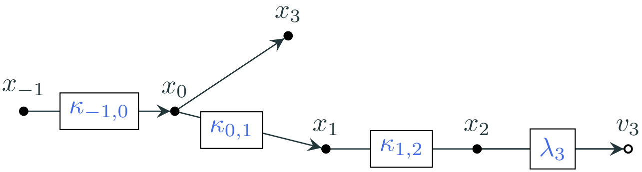

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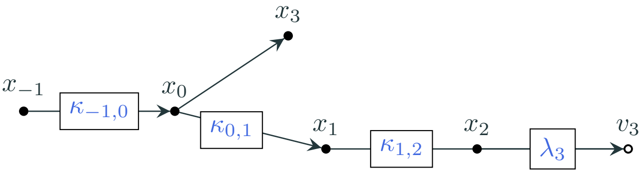

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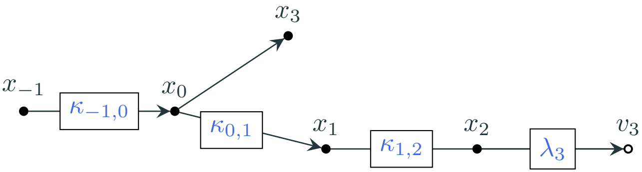

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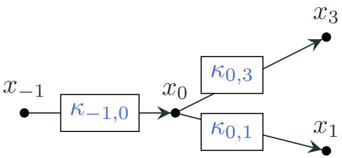

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$$h_{0\to 3} = \kappa_{0,3} h_3 \quad \text{and} \quad h_{0\to 1} = \kappa_{0,1} h_1$$

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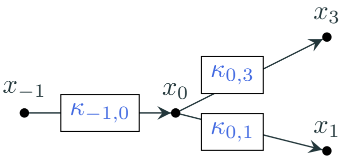

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Fusion: by conditional independence of children we have

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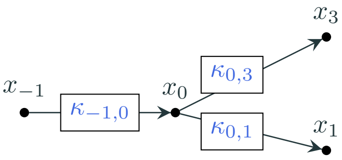

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By identifying with vectors

$$h_0 = h_{0\to 1} \odot h_{0\to 3}.$$

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⚠ This is all tractable because

1. the DAG is a directed tree;
2. the state space is finite.

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Natural to convert DAG to string diagram...

Guided process

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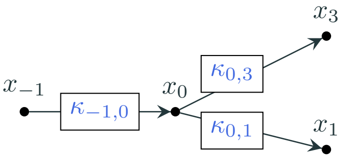

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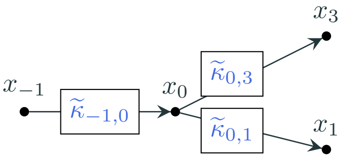

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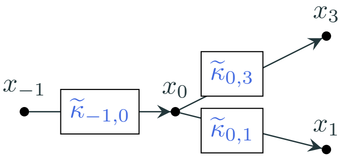

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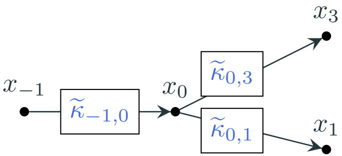

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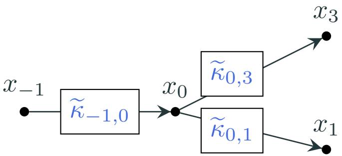

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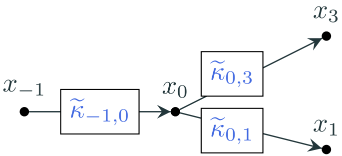

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Fusion: by conditional independence of children we have

$$g_0(x) = g_{0 \to 1}(x) g_{0 \to 3}(x).$$

By identifying with vectors

$$g_0 = g_{0 \to 1} \odot g_{0 \to 3}.$$

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Let the maps $x \mapsto g_{s \to t}(x)$ be specified for each edge (s, t) and define

$$g_s(x) = \prod_{t \in \mathrm{ch}(s)} g_{s \to t}(x), \qquad s \in \mathcal{S}_0. \tag{1}$$

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Practical way to choose $g_{s \to t}$: replace kernel $\kappa_{s \to t}$ by approximation $\widetilde{\kappa}_{s \to t}$.

Define the guided process X° as the process starting in $X_0^\circ = x_0$ and from the roots onwards evolving *on* the DAG $\mathcal{G}$ according to transition kernel

$$\kappa^\circ_{\mathrm{pa}(s) \to s}(x_{\mathrm{pa}(s)}; \mathrm{d}y) = \frac{g_s(y) \kappa_{\mathrm{pa}(s) \to s}(x_{\mathrm{pa}(s)}; \mathrm{d}y)}{\int g_s(y) \kappa_{\mathrm{pa}(s) \to s}(x_{\mathrm{pa}(s)}; \mathrm{d}y)}, \qquad s \in \mathcal{S}.$$

Use of guided process

Let $\mathcal{S}$ denote the set of non-leaf vertices.

Theorem. Assume kernels towards leaf-nodes admit densities $h_{\mathrm{pa}(v)\to v}$. Then

$$h_0(x_0) = g_0(x_0)\mathbb{E}\left[\prod_{s\in\mathcal{S}} w_{\mathrm{pa}(s)\to s}(X^\circ_{\mathrm{pa}(s)}) \prod_{v\in\mathcal{V}} \frac{h_{\mathrm{pa}(v)\to v}(X^\circ_{\mathrm{pa}(v)})}{g_{\mathrm{pa}(v)\to v}(X^\circ_{\mathrm{pa}(v)})}\right]$$

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Computationally, this implies a bidirectional scheme:

1. Backward pass for Filtering;
2. Forward pass for Guiding.

Wrap-up

- If the state space is finite, BIF provides the likelihood.
- Key to tractability is that h can always be represented as a vector.
- ⚠ In general BIF is intractable.

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- If the state space is finite, BIF provides the likelihood.
- Key to tractability is that h can always be represented as a vector.
- ⚠ In general BIF is intractable.
- Resolve by backward filtering with simpler kernels and forward simulating the corresponding guided process.
- This results in weighted samples from the conditioned process.

Application: interacting particle process

Forward transitions:

$$\kappa_i(t,x) = \begin{bmatrix} \psi\left(\lambda N_i(t,x)\right) & 1-\psi\left(\lambda N_i(t,x)\right) & 0 \\ 0 & \psi(\mu) & 1-\psi(\mu) \\ 1-\psi(\nu) & 0 & \psi(\nu) \end{bmatrix},$$

where

$$N_i(x) = \{\text{number of infected neighbours of individual } i \text{ in state } x\}$$

and $\psi(u) = \exp(-\tau u)$.

Auxiliary kernel for backward filtering:

$$\widetilde{\kappa}_i = \begin{bmatrix} \psi(\widetilde{\lambda}_i(t)) & 1-\psi(\widetilde{\lambda}_i(t)) & 0 \\ 0 & \psi(\mu) & 1-\psi(\mu) \\ 1-\psi(\nu) & 0 & \psi(\nu) \end{bmatrix}.$$

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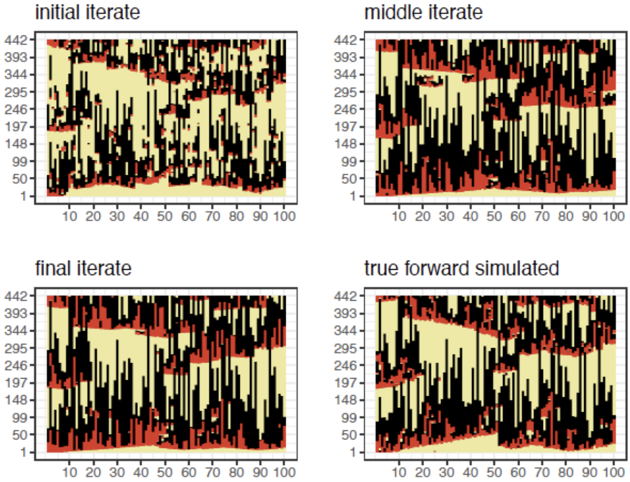

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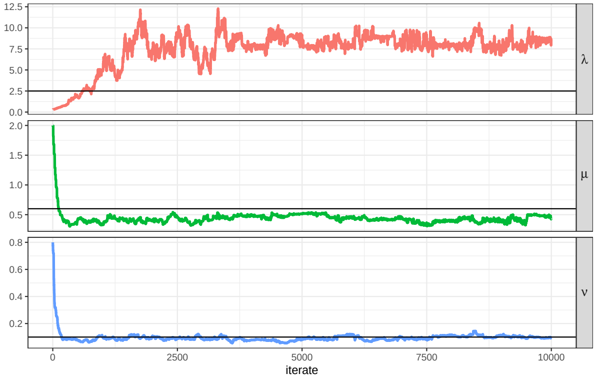

Continuous time transitions

Rethinking the discrete-time case:

- Edge

$$x_S \longrightarrow x_T$$

Suppose $x \mapsto h(T, x)$ is given; wish to find $x \mapsto h(S, x)$.

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$$(\mathcal{A}h)(S, x) : \quad = \quad \mathbb{E}[h(T, X_T) - h(S, X_S) \mid X_S = x]$$

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- ⚠ Obtain $x \mapsto h(S, x)$ by solving $(\mathcal{A}h)(S, x) = 0$.

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⚠ Solving Kolmogorov backward equation is usually intractable.

Defining the guided process via its inf.generator

- Backward filter with $\widetilde{\mathcal{L}}$ instead of $\mathcal{L}$, such that solving $(\widetilde{\mathcal{L}}g)(s,x) + \frac{\partial}{\partial s} g(s,x) = 0$ becomes tractable.

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- Correct for "wrong" h by weight

$$\exp\left(\int_{t_i}^{t_{i+1}} \frac{(\mathcal{L} - \widetilde{\mathcal{L}})g}{g}(u, X_u^\circ)\, \mathrm{d}u\right).$$

- Care is needed in choice of $\widetilde{\mathcal{L}}$: matching conditions.

How to solve the Kolmogorov Backward Equation?

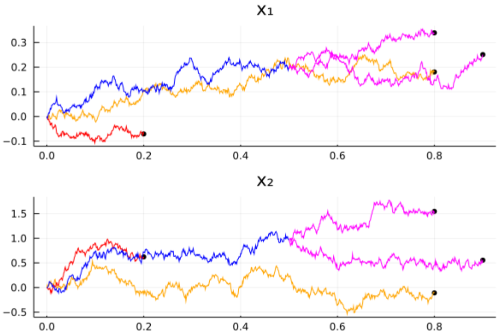
For $s \in (S, T]$,

$$(\widetilde{\mathcal{L}}g)(s,x) + \frac{\partial}{\partial s} g(s,x) = 0, \qquad g(T,\cdot) = g_T(\cdot).$$

Examples/strategies:

1. If $\widetilde{\mathcal{L}}$ is the infinitesimal generator of a linear diffusion process, then $\log g(t,x) = c(t) + F(t)'x + x'H(t)x$ with ODE-system for $(H(t), F(t), c(t))$.
2. Ansatz $g(t,x) = \sum_j c(t)\psi_j(t)$. Derive ODE for $c(t)$.

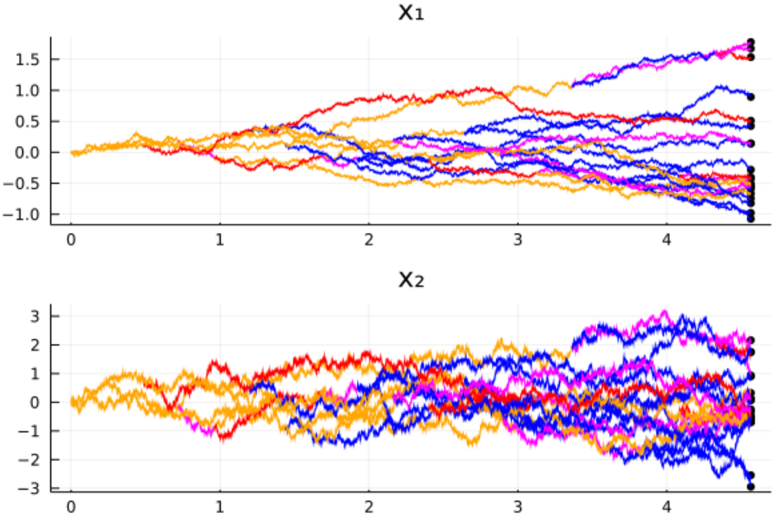
Example: branching diffusion



SDE on a tree where on each branch

$$\mathrm{d}X_t = \tanh . \left(\begin{bmatrix} -\theta_1 & \theta_1 \\ \theta_2 & -\theta_2 \end{bmatrix} X_t \right) \mathrm{d}t + \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \mathrm{d}W_t .$$

Numerical illustration: SDE on a tree



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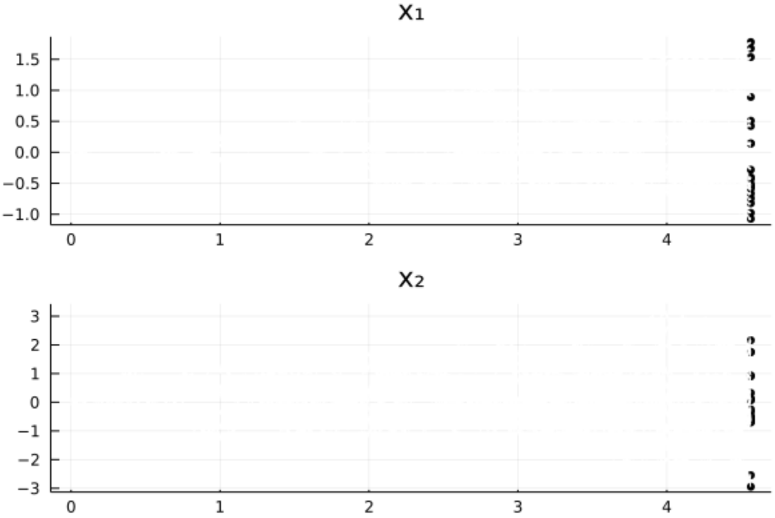

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Implementation in `MitosisStochasticDiffEq.jl` by Frank Schäfer (MIT).

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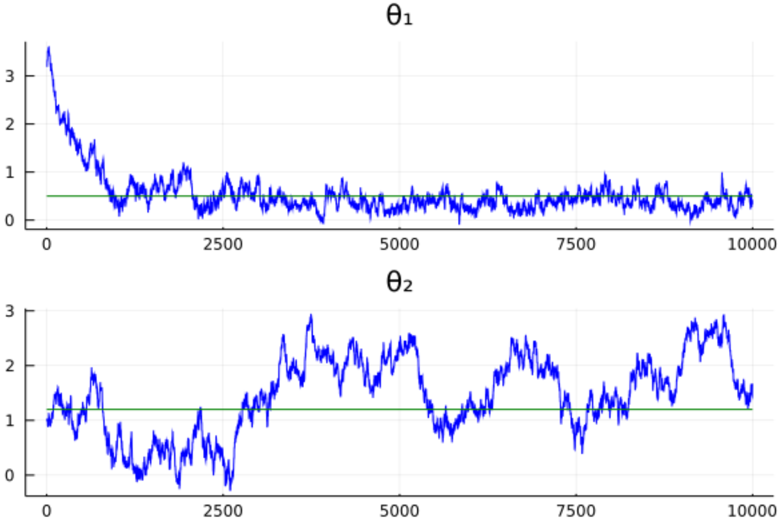

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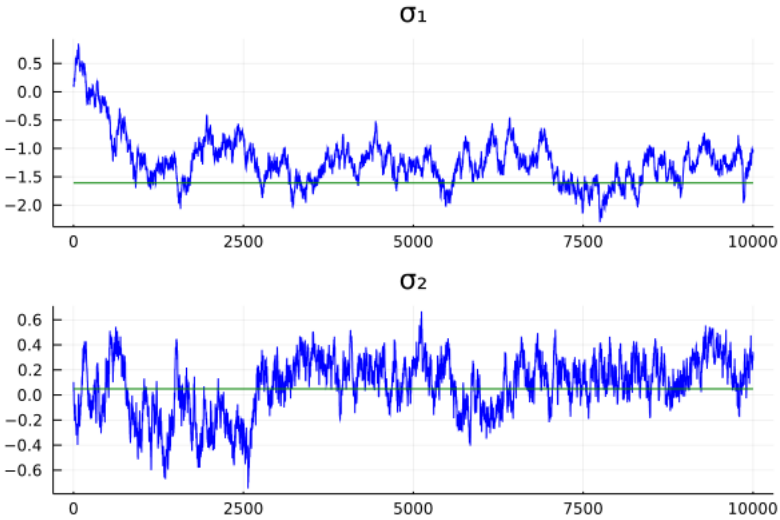

Wrap-up / conclusions

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Backward Filtering Forward Guiding: framework for doing likelihood based inference in directed acyclic graphs, where transitions over edges may correspond to the evolution of a stochastic process for a certain time span.

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- Both discrete-time and continuous-time transitions incorporated.

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Ongoing: SPDEs, SDEs on manifolds, chemical reaction networks.

Open postdoc position at VU Amsterdam.

References

- Continuous-discrete smoothing of diffusions
  MIDER, SCHAUER, VDM, Electronic Journal of Statistics

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- Inference in Hidden Markov Models, Cappé, Moulines and Rydén

  Good source on filtering, smoothing, parameter estimation in HMM.