Backward Filtering Forward Guiding for Markov processes

Frank van der Meulen – joint work with Moritz Schauer

VU GENERAL MATH COLLOQUIUM

Vrije Universiteit Amsterdam
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Warming up

A finite state Markov chain

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- Summarise transition probabilities by matrix

$$\kappa = \begin{bmatrix} ① \to ① & ① \to ② & ① \to ③ \\ ② \to ① & ② \to ② & ② \to ③ \\ ③ \to ① & ③ \to ② & ③ \to ③ \end{bmatrix}$$

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- Markov property

$$\begin{aligned} &\mathbb{P}(X_0 = x_0, X_1 = x_1, \ldots, X_n = x_n) \\ &\qquad = \mathbb{P}(X_0 = x_0) \prod_{i=1}^{n} \mathbb{P}(X_i = x_i \mid X_{i-1} = x_{i-1}). \end{aligned}$$

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Example (1/2)

Observe

$$(x_0, x_1, x_2, x_4, x_4, x_5) = (①, ②, ②, ③, ①, ②).$$

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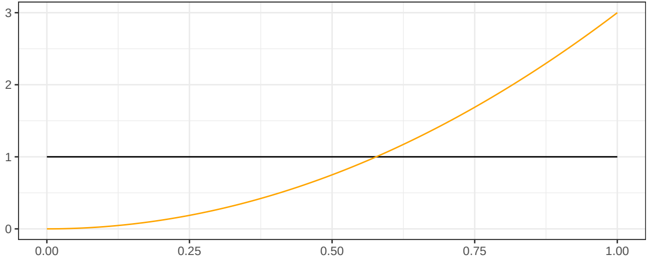

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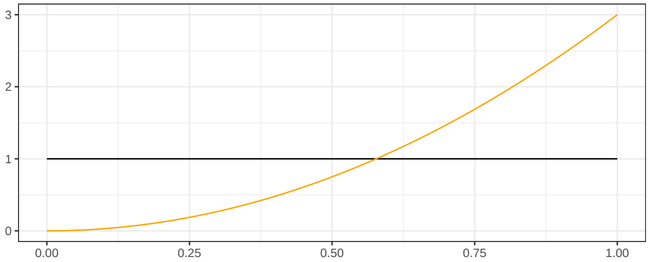
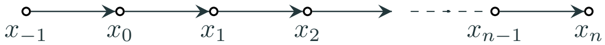


Posterior mean:

$$\mathbb{E}[\Theta \mid X = x] = \int \theta f_{\Theta|X}(\theta \mid x)\,\mathrm{d}\theta = 3/4.$$

Other observation schemes

Fully observed:



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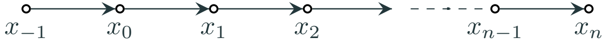

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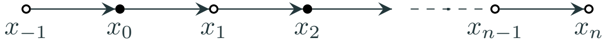

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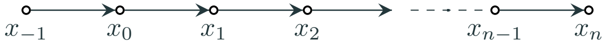

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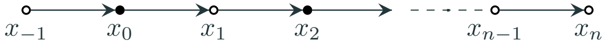

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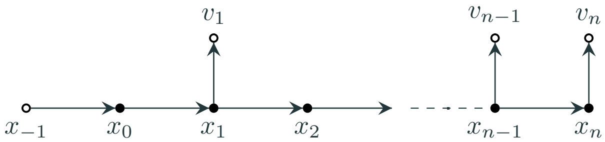

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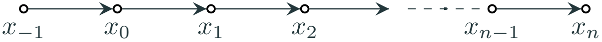

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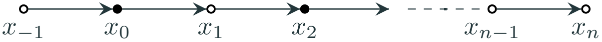

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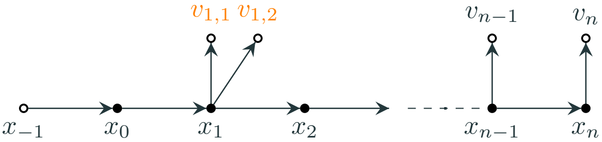
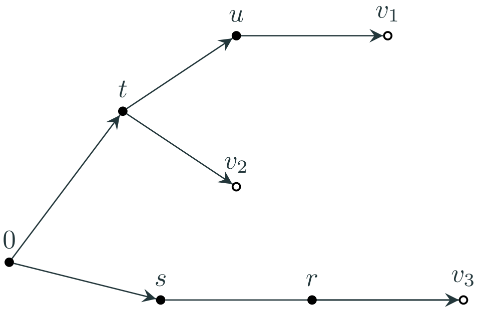


General problem setting

Problem setting

Consider a directed *Markovian* tree:



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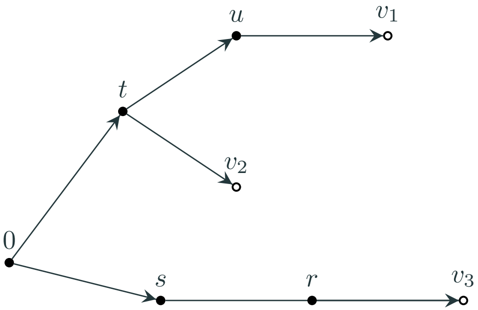

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Along each edge the process evolves according to either one step of a discrete-time Markov chain or a time-span of a continuous-time Markov process.

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To each edge corresponds a Markov kernel:

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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).

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- population of n individuals;
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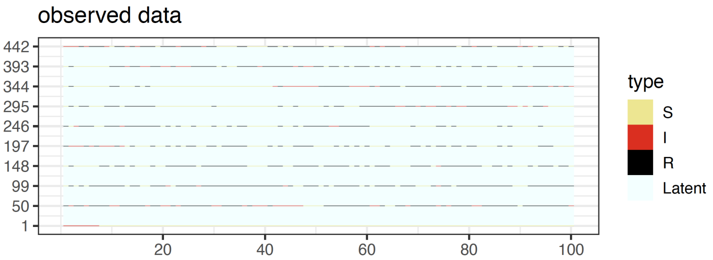
The transition matrix for individual i at time t, given "full state" x:

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

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

Example 1: challenges



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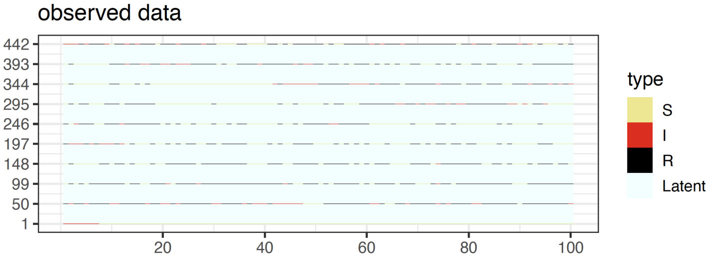

Goals:

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

⚠ Dimension of state-space is 3^n.

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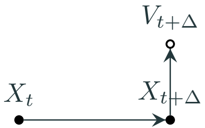
- Graphical model



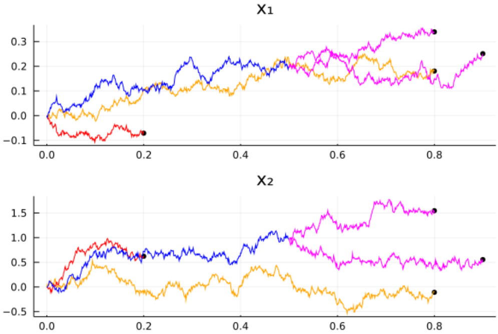
where

$$V_{t+\Delta} \mid X_{t+\Delta} \sim N(X_{t+\Delta}, \Sigma).$$

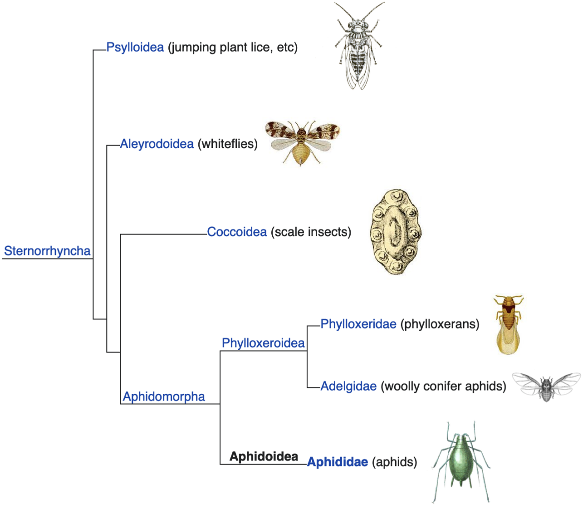
Example 2: branching diffusion

SDE on a tree where on each branch

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



Example 3: phylogenetics



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Syst. Biol. 52(2):131–158, 2003
DOI: 10.1080/10635150390192780

Stochastic Mapping of Morphological Characters

JOHN P. HUELSENBECK,[1] RASMUS NIELSEN,[2] AND JONATHAN P. BOLLBACK[1]

[1]*Section of Ecology, Behavior and Evolution, Division of Biology, University of California–San Diego, La Jolla, California 92093-0116, USA*
[2]*Department of Biometrics, Cornell University, 439 Warren Hall, Ithaca, New York 14853-7801, USA*

Abstract.— Many questions in evolutionary biology are best addressed by comparing traits in different species. Often such studies involve mapping characters on phylogenetic trees. Mapping characters on trees allows the nature, number, and timing of the transformations to be identified. The parsimony method is the only method available for mapping morphological characters on phylogenies. Although the parsimony method often makes reasonable reconstructions of the history of a character, it has a number of limitations. These limitations include the inability to consider more than a single change along a branch on a tree and the uncoupling of evolutionary time from amount of character change. We extended a method described by Nielsen (2002, Syst. Biol. 51:729–739) to the mapping of morphological characters under continuous-time Markov models and demonstrate here the utility of the method for mapping characters on trees and for identifying character correlation. [Bayesian estimation; character correlation; character mapping; Markov chain Monte Carlo.]

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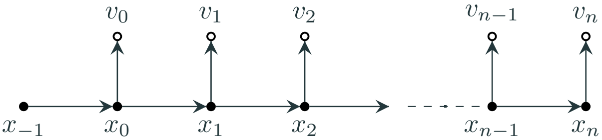
Along each edge, a finite state continuous time Markov process evolves.

Ideally, one would like to randomly sample character histories that consistent with the observations at the tips of a phylogenetic tree.

Related literature

State-space models / hidden Markov models



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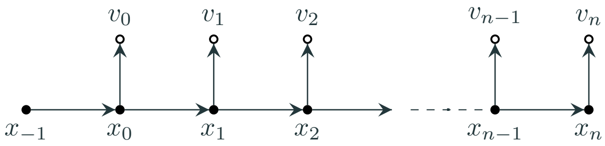

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- finite state space: Baum-Welch, Viterbi, forward-backward algorithm.
- linear Gaussian models: Kalman filter, Rauch-Tung-Striebel smoother.
- linear stochastic differential equations: Kalman-Bucy filter & smoother.

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

Conditioning on a tree

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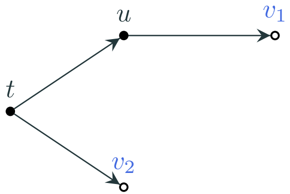

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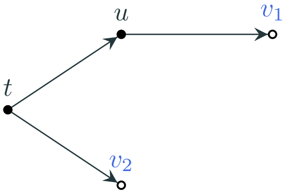

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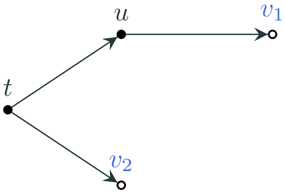

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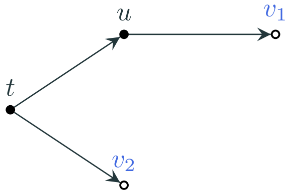

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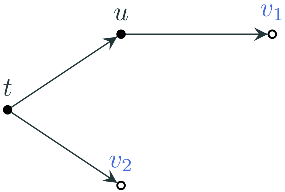

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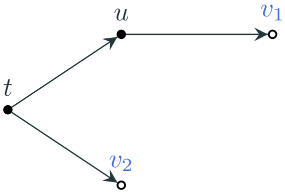

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- *Doob's h-transform*: Transformation of each κ_s with h_s to $\kappa_s^\star$:

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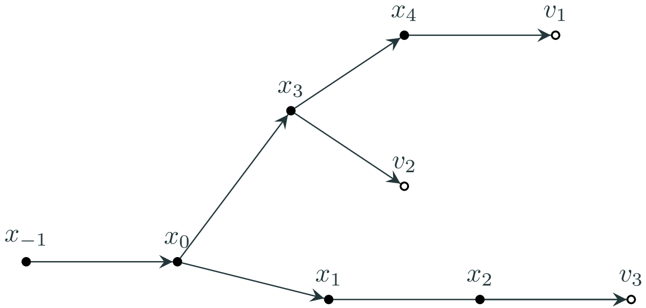
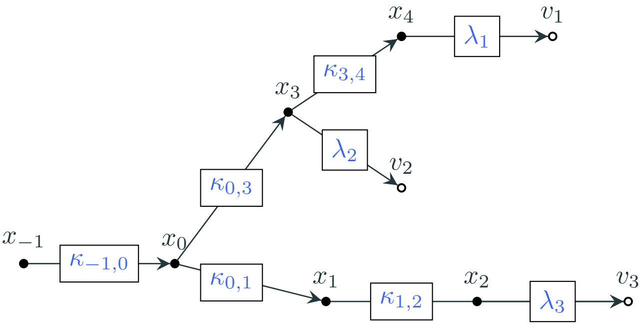


Make kernels explicit



Example: finite state space

- Suppose $x_t \in \{\textcircled{1}, \textcircled{2}, \textcircled{3}\}$ and $v_t \in \{\textcircled{1,2}, \textcircled{3}\}$.

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- Prior on initial state: set $x_{-1} = ⓪$ and

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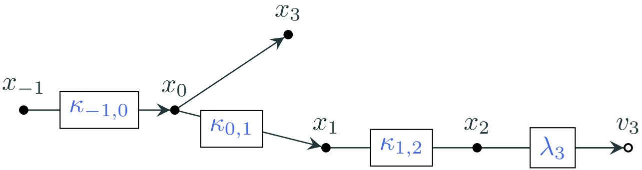

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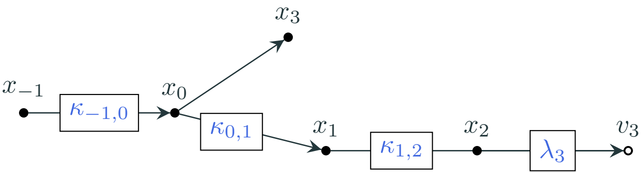

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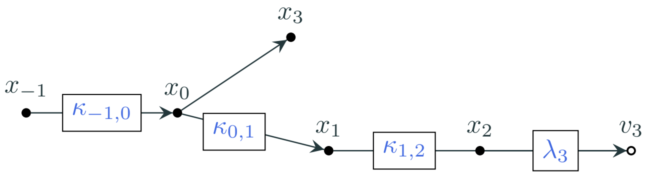

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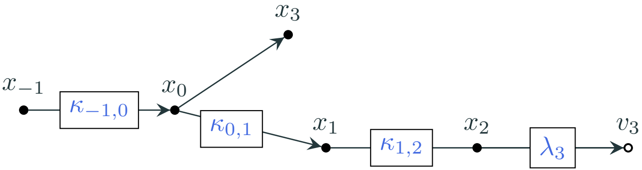

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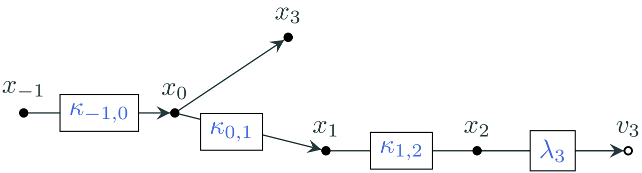

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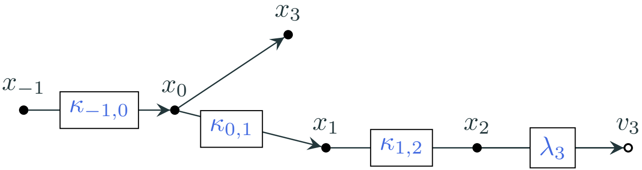

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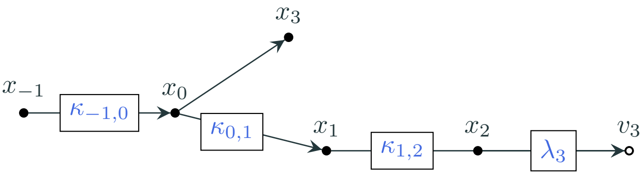

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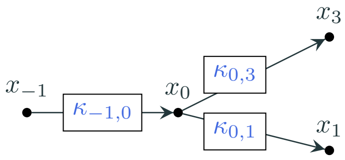

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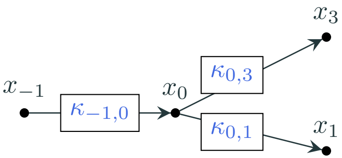

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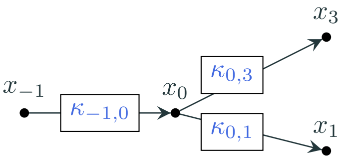

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⚠ This is all tractable because

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

Guided process

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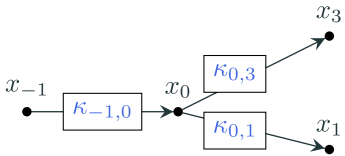

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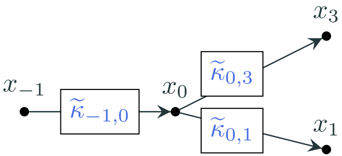

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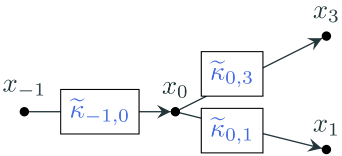

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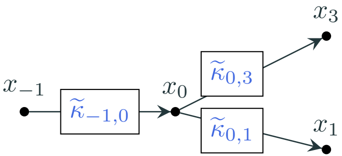

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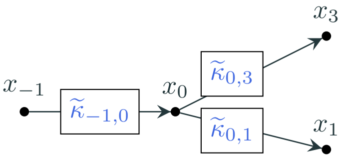

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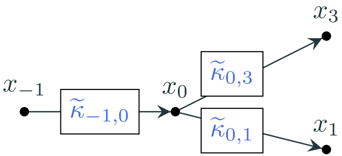

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Let the maps $x \mapsto g_{s \to t}(x)$ be specified for each edge (s, t) and define

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Definition
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 $p_{\mathrm{pa}(v)\rightarrow v}$. Then

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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.
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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

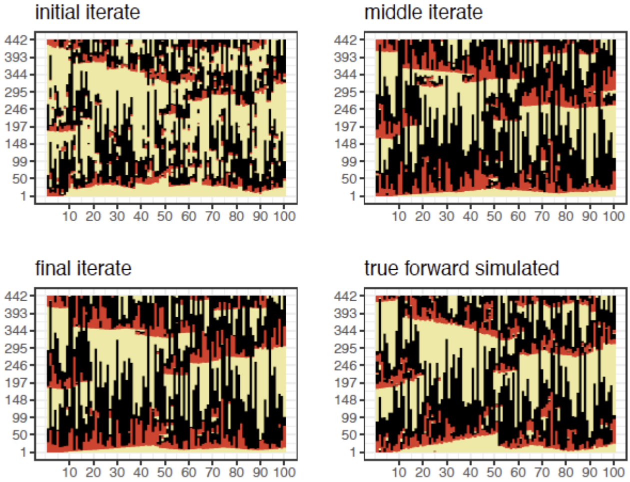
$$N_i(x) = \{\text{number of infected neighbours of individual } i \text{ in state } x\}$$

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

Auxiliary kernel for backward filtering:

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

Application: interacting particle process



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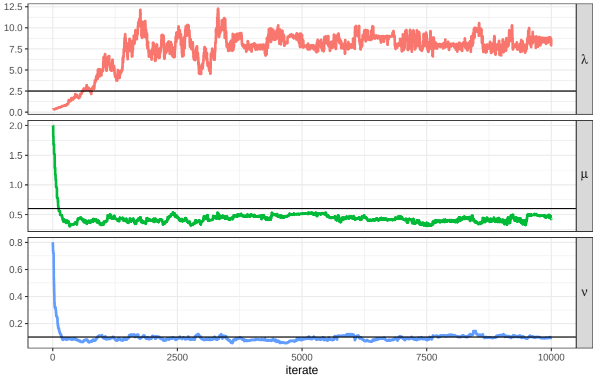

Continuous time transitions

Rethinking the discrete-time case:

- Edge

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

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\begin{aligned}
(\mathcal{A}h)(S, x) : \quad &= \quad \mathbb{E}[h(T, X_T) - h(S, X_S) \mid X_S = x] \\
&= \quad \int h(T, y)\kappa_{S \to T}(x,\, \mathrm{d}y) - h(S, x).
\end{aligned}
$$

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

Continuous time transitions

Define the infinitesimal generator of the space-time process (t, X_t): for $S \leq s < s + h \leq T$

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\begin{aligned}
(\mathcal{A}h)(s,x) &= \lim_{h \downarrow 0} h^{-1} \mathbb{E}[h(s+h, X_{s+h}) - h(s, X_s) \mid X_s = x] \\
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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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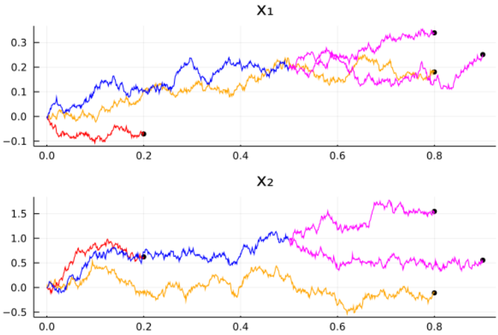
  Identify guided process from $\mathcal{L}^\circ$.
- Correct for "wrong" h by weight

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

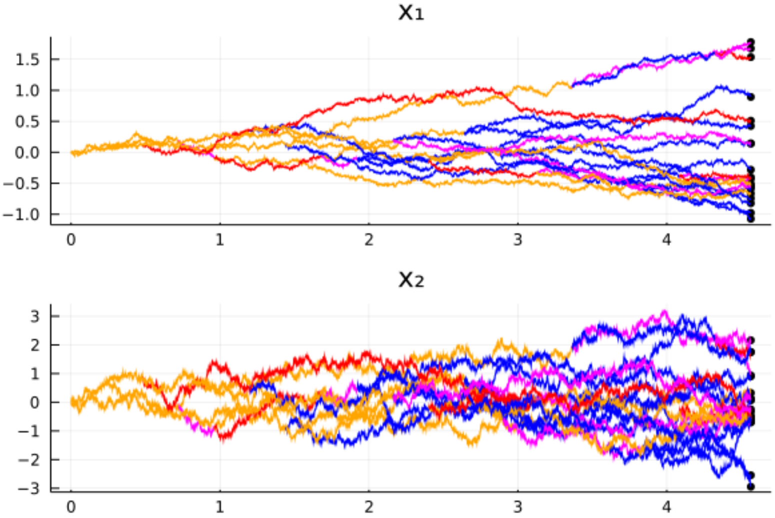
Example 2: branching diffusion



SDE on a tree where on each branch

$$dX_t = \tanh.\left(\begin{bmatrix} -\theta_1 & \theta_1 \\ \theta_2 & -\theta_2 \end{bmatrix} X_t\right) dt + \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} dW_t.$$

Numerical illustration: SDE on a tree



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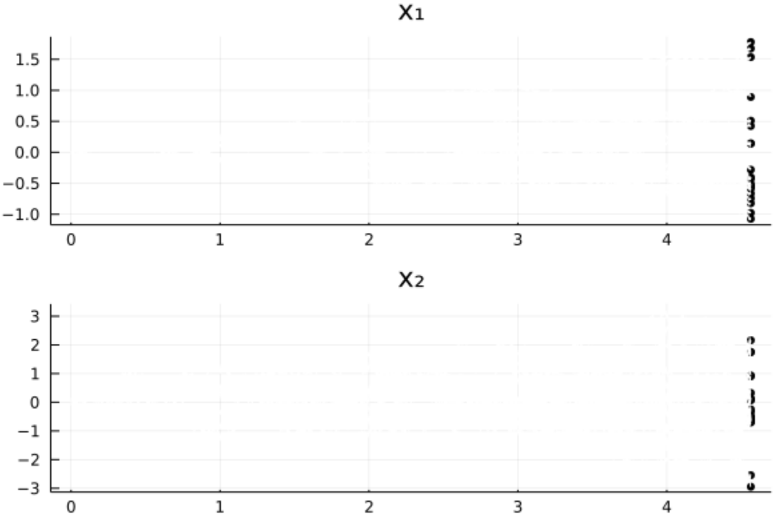

Numerical illustration: SDE on a tree

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

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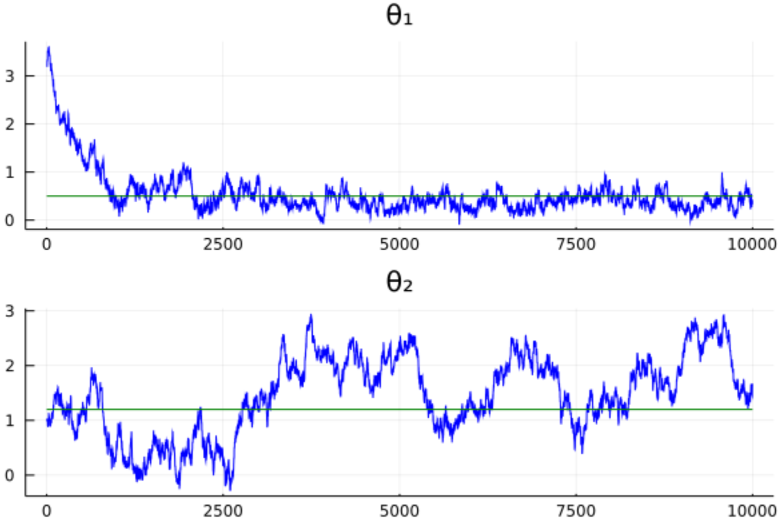

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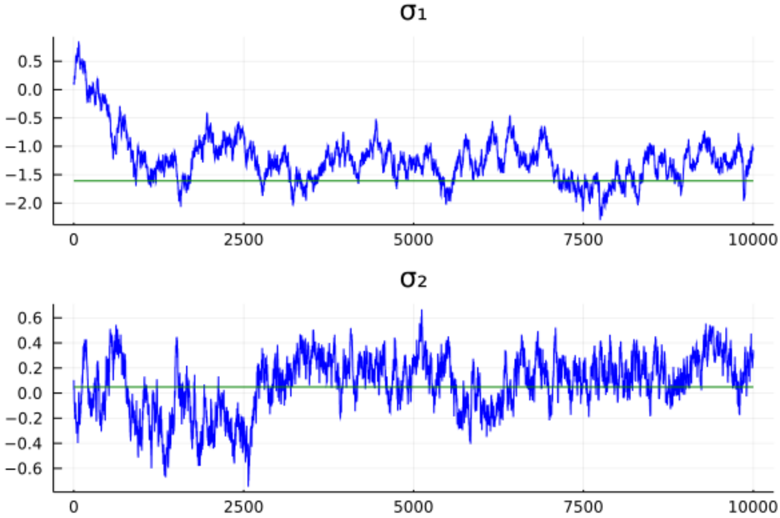

Wrap-up / conclusions

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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.

- Defining guided processes on graphical models
  (for "non-tree"-case: see preprint).
- Both discrete-time and continuous-time transitions incorporated.

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

References

- Continuous-discrete smoothing of diffusions
  Mider, Schauer, VdM, Electronic Journal of Statistics

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- Automatic Backward Filtering Forward Guiding for Markov processes and graphical models, VdM and Schauer, preprint on arXiv.

  A generalisation to Markov processes on graphical models including ideas on compositionality from category theory.

- Introduction to Automatic Backward Filtering Forward Guiding, VdM, preprint on arXiv.

  Gentle introduction to the more advanced paper.

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

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