Backward Filtering Forward Guiding for Markov processes

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VU GENERAL MATH COLLOQUIUM

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Warming up

A finite state Markov chain

- Consider process that starts at time 0 and evolves over times $1, 2, \ldots$.
- At each time, the process takes values in $E := \{①, ②, ③\}$.
- Draw initial state $x_0 \in E$ from probability vector π_0 (row vector):

x	①	②	③
$\mathbb{P}(X = x)$	$\pi_0(1)$	$\pi_0(2)$	$\pi_0(3)$

- Once x_0 is drawn, proceed iteratively: sample $X_i | X_{i-1} = x_{i-1}$.
- Summarise transition probabilities by matrix

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

Distribution of the chain

- Distribution at time 1 is given by

$$\pi_1 = \pi_0 \kappa.$$

- Likewise

$$\pi_i = \pi_{i-1} \kappa.$$

- κ may depend on unknown parameters. Example

$$\kappa = \begin{bmatrix} 1-\theta & \theta & 0 \\ 0.25 & 0.5 & 0.25 \\ 0.4 & 0.3 & 0.3 \end{bmatrix}.$$

- Observe sequence $(x_0, x_1, \ldots, x_n)$, estimate θ.
- Markov property

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

Likelihood based inference

Define the likelihood function by

$$\theta \mapsto L(\theta; x) = \mathbb{P}_\theta(X_0 = x_0, X_1 = x_1, \ldots, X_n = x_n).$$

Maximum likelihood estimator: find θ that maximises $L(\theta; x)$.

Bayesian approach: cast problem in hierarchical way. Assume the data are generated as follows

1. First sample a realisation θ from the random variable Θ taking values in $[0, 1]$;
2. conditional on θ, generate $x_0, x_1, \ldots, x_n$ as before.
3. Bayesian approach: all inference is based on the posterior distribution

$$f_{\Theta|X}(\theta \mid x) = \frac{L(\theta; x) f_\Theta(\theta)}{\int L(\theta; x) f_\Theta(\theta) \, \mathrm{d}\theta} \propto L(\theta; x) f_\Theta(\theta).$$

Example (1/2)

Observe

$$(x_0, x_1, x_2, x_4, x_4, x_5) = (\textcircled{1}, \textcircled{2}, \textcircled{2}, \textcircled{3}, \textcircled{1}, \textcircled{2}).$$

Assume $\pi_0 = (1/3, 1/3, 1/3)$ and recall

$$\kappa = \begin{bmatrix} 1-\theta & \theta & 0 \\ 0.25 & 0.5 & 0.25 \\ 0.4 & 0.3 & 0.3 \end{bmatrix}.$$

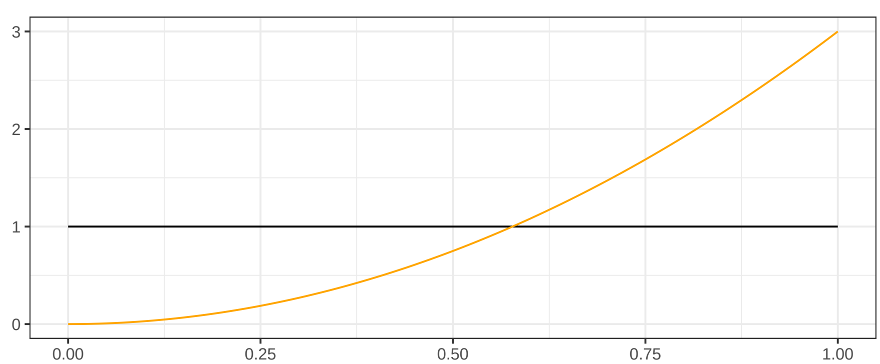
⚠ Estimate for θ?

$$L(\theta; x) = \frac{1}{3} \cdot \theta \cdot 0.5 \cdot 0.25 \cdot 0.4 \cdot \theta \propto \theta^2.$$

Example (2/2)

- MLE $\hat{\theta} = 1$.
- Bayes: assume $\Theta \sim Unif(0, 1)$, then

$$f_{\Theta|X}(\theta \mid x) = 3\theta^2 \mathbf{1}_{[0,1]}(\theta).$$

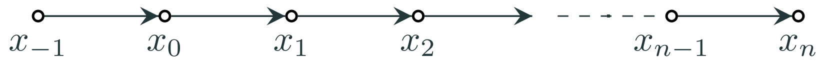


Posterior mean:

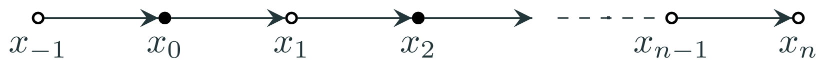
$$\mathbb{E}[\Theta \mid X = x] = \int \theta f_{\Theta|X}(\theta \mid x)\, \mathrm{d}\theta = 3/4.$$

Other observation schemes

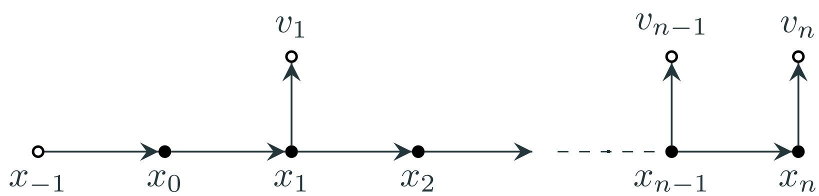
Fully observed:



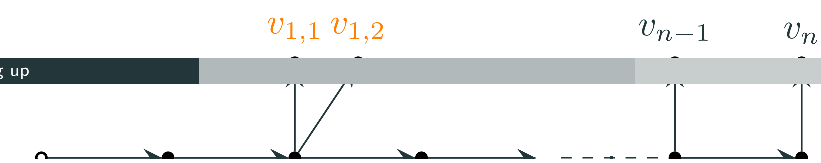
Partially observed: ● =unobserved, ○=observed.



Partially observed:



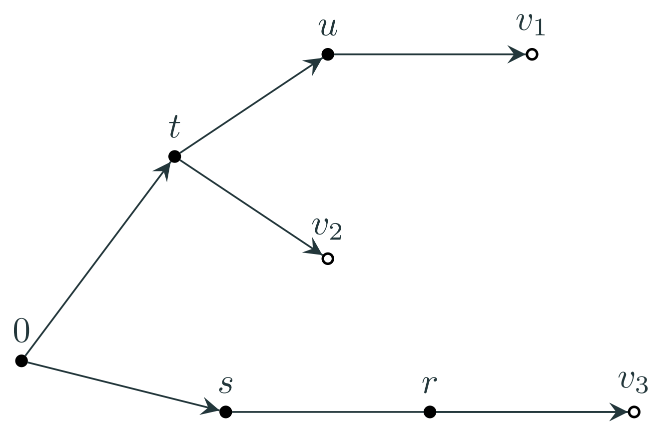
Partially observed:



General problem setting

Problem setting

Consider a directed *Markovian* tree:



• denotes latent vertices, ○ leaf/observation-vertices.

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.

Problem setting

To each edge corresponds a Markov kernel:

$$\kappa_{\to t}(x_{\mathrm{pa}(t)}, \mathrm{d}x_t)$$

(pointing towards vertex t).

We aim for

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

Example 1: interacting particle process

Setup:

- population of n individuals;
- each individual is either **S**usceptible, **I**nfected or **R**ecovered;
- each individual has a known (possibly time varying) set of neighbours .

Dynamics:

- If $x_i = \mathbf{S}$, then it transitions to $\mathbf{I}$ with intensity $\lambda N_i(t, x)$, with $N_i(t, x)$ number of infected neighbours of individual i at time t.
- If $x_i = \mathbf{I}$, then it transitions to $\mathbf{R}$ with intensity μ.
- If $x_i = \mathbf{R}$, it transitions to $\mathbf{S}$ with intensity ν.

Example 1: Dynamics of each particle

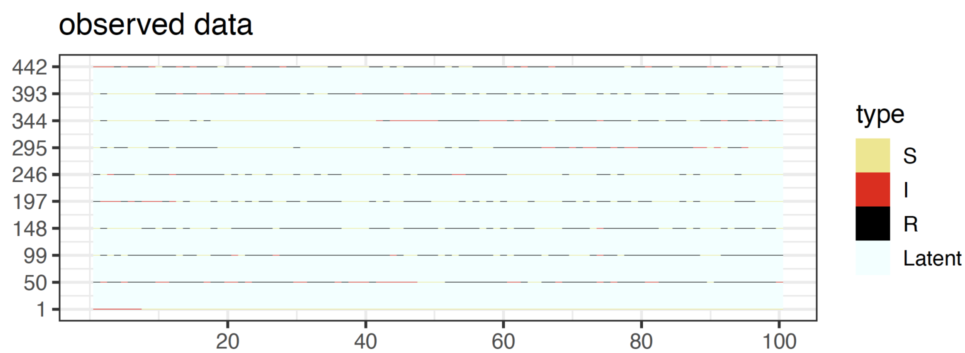
- Time-discretised version of the problem, where time steps are multiples of $\tau > 0$.
- In each time interval of length τ, conditional on the the present state of all individuals, each individual independently remains in its present state or transitions.

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



Goals:

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

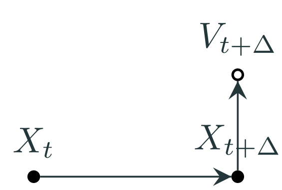
⚠ Dimension of state-space is 3^n.

Example 2: stochastic differential equations

- Consider the SDE

$$\mathrm{d}X_s = b_\theta(s, X_s)\,\mathrm{d}s + \sigma_\theta(s, X_s)\,\mathrm{d}W_s.$$

- Graphical model



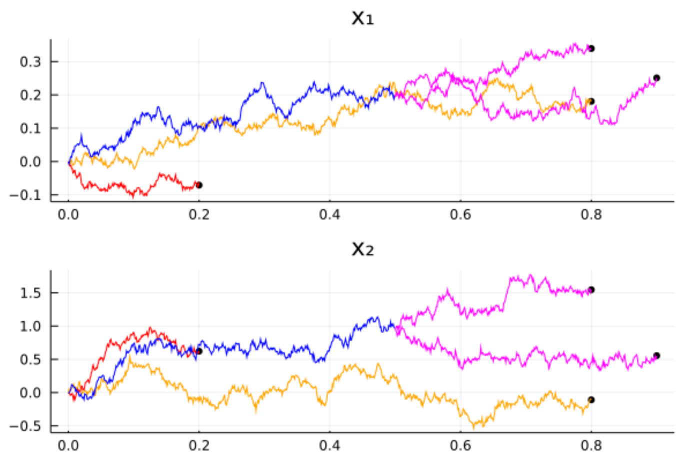
where

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

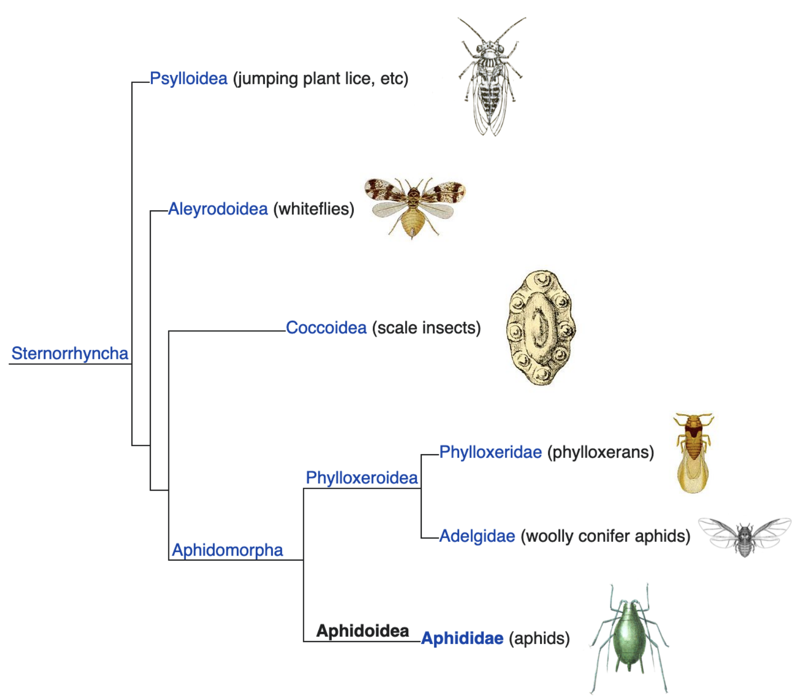
Example 2: branching diffusion

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



Example 3: phylogenetics

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Stochastic Mapping of Morphological Characters

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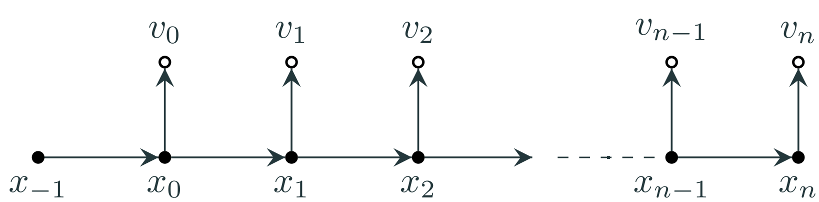
Abstract.— Many questions in evolutionary biology are best addressed by comparing traits in different species. Often such studies involve mapping characters on phylogenetic trees. Mapping characters on trees allows the nature, number, and timing of the transformations to be identified. The parsimony 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.]

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



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

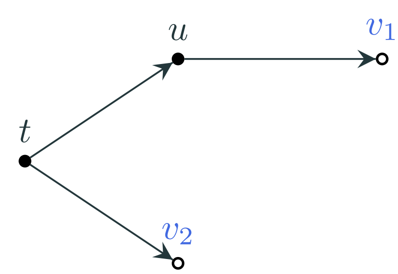
- finite state space: Baum-Welch, Viterbi, forward-backward algorithm.
- linear Gaussian models: Kalman filter, Rauch-Tung-Striebel smoother.
- linear stochastic differential equations: Kalman-Bucy filter & smoother.

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

Conditioning on a tree

Define

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



Key identity (Bayesian notation):

$$
\begin{aligned}
p(x_t \mid x_{\mathrm{pa}(t)}, x_{\mathcal{V}_t}) &\propto p(x_t, x_{\mathcal{V}_t} \mid x_{\mathrm{pa}(t)}) \\
&= p(x_t \mid x_{\mathrm{pa}(t)})\, \underbrace{p(x_{\mathcal{V}_t} \mid x_t, \cancel{x_{\mathrm{pa}(t)}})}_{h_t(x_t)}
\end{aligned}
$$

Rewrite to $\boxed{\kappa^{\star}_{\rightarrow t}(x; \mathrm{d}y) \propto \kappa_{\rightarrow t}(x; \mathrm{d}y) h_t(y)}$.

⚠ If x_t is observed, then $h_t(x_t)$ is the likelihood in the subtree from node t.

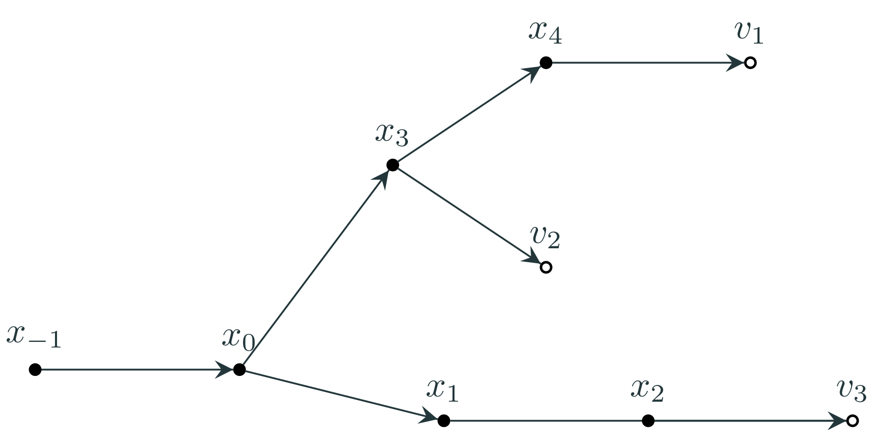
Doob's h-transform

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

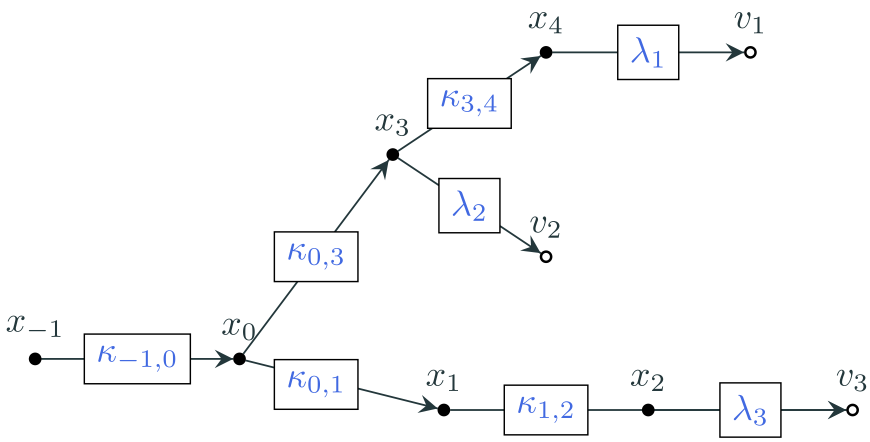
$$\kappa^\star_{\to s}(x, \mathrm{d}y) = \frac{\kappa_{\to s}(x, \mathrm{d}y) h_s(y)}{\int \kappa_{\to s}(x, \mathrm{d}y) h_s(y)}, \quad s \in \mathcal{S}.$$

  A forward pass: Needs $\kappa_{\to s}$ and h_s.
- Recursive computation of h_s in a backward pass: (Backward Information Filter):
  - Compute h_s from the leaves back to the roots.
  - Acyclic belief propagation, sum-product algorithm, Felsenstein algorithm...
  - ⚠ Only in very specific models tractable.
- ⚠ 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



Example: finite state space

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

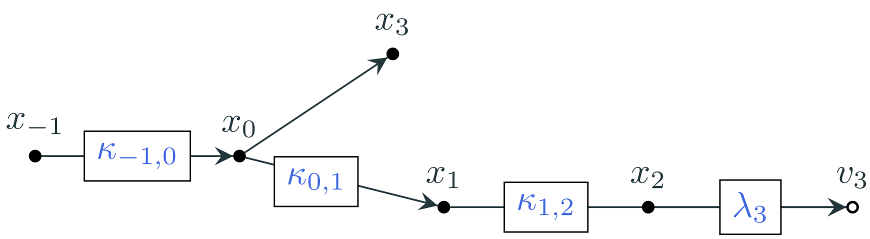
$$\kappa_{-1,0} = [\pi_1,\ \pi_2,\ \pi_3] =: \boldsymbol{\pi}.$$

Backward Information Filter (BIF)

- **BIF**: efficient way to compute $x \mapsto h_t(x)$.
- ⚠ For finite state space this map can be identified with a vector h_t.
- Initialise from observations: for $t = 0, \dots, n$

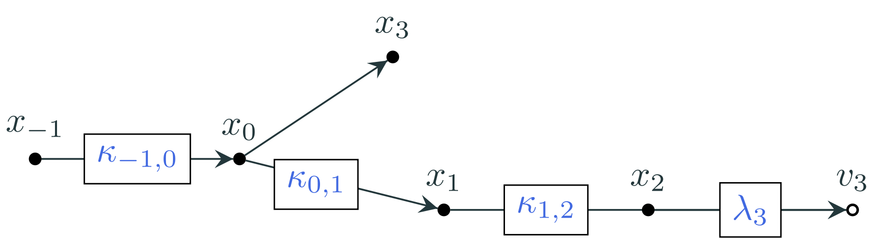
$$h_t^{\text{obs}} := \begin{bmatrix} 1 \\ 0 \end{bmatrix} \mathbf{1}\{v_t = \text{(1,2)}\} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \mathbf{1}\{v_t = \text{③}\}.$$

Pullback along edges:



$$h_2 = \lambda_3 h_3^{\text{obs}} \qquad\qquad h_1 = \kappa_{1,2} h_2.$$

Pullback along edges

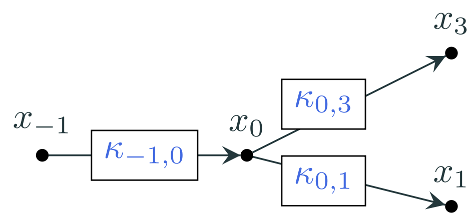


$$h_2 = \lambda_3 h_3^{\text{obs}} \qquad\qquad h_1 = \kappa_{1,2} h_2.$$

Why $h_1 = \kappa_{1,2} h_2$?

$$\begin{aligned} h_1(x_1) = p(v_3 \mid x_1) &= \int p(v_3, x_2 \mid x_1)\, \mathrm{d}x_2 \\ &= \int \underbrace{p(v_3 \mid \cancel{x_1}, x_2)}_{h_2(x_2)} p(x_2 \mid x_1)\, \mathrm{d}x_2. \end{aligned}$$

Backward Information Filter (BIF)



Get

$$h_{0\to3} = \kappa_{0,3} h_3 \quad \text{and} \quad h_{0\to1} = \kappa_{0,1} h_1$$

Fusion: by conditional independence of children we have

$$h_0(x) = h_{0\to1}(x) h_{0\to3}(x).$$

By identifying with vectors

$$h_0 = h_{0\to1} \odot h_{0\to3}.$$

Backward Information Filter (BIF)

- Likelihood: $L(\theta) := h_{-1} = \kappa_{-1,0} h_0$.
- Forward simulate:

$$x_t^\star \mid x_s^\star = i \sim \text{Cat}(\kappa_{s,t}[i,] \odot h_t), \qquad t \in \text{ch}(s).$$

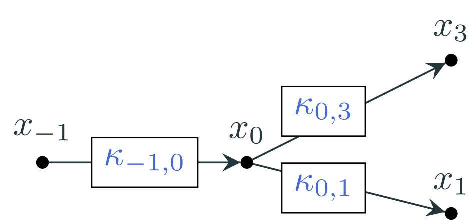
⚠ This is all tractable because

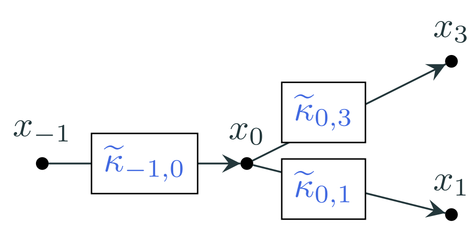
1. the DAG is a directed tree;
2. the state space is finite.

Guided process

Backward Information Filter (BIF)

Key idea: replace $h_{s \to t}$ by $g_{s \to t}$ that makes BIF tractable.





Get

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

Get

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

Get

Guided process

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

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

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

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

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

with weights defined by

$$w_{\mathrm{pa}(s)\to s}(x_{\mathrm{pa}(s)}) = \frac{\int g_s(y)\kappa_{\mathrm{pa}(s)\to s}(x_{\mathrm{pa}(s)}; \mathrm{d}y)}{\prod_{u \in \mathrm{pa}(s)} g_{u \to s}(x_u)} \qquad s \in \mathcal{S}.$$

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.
- 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

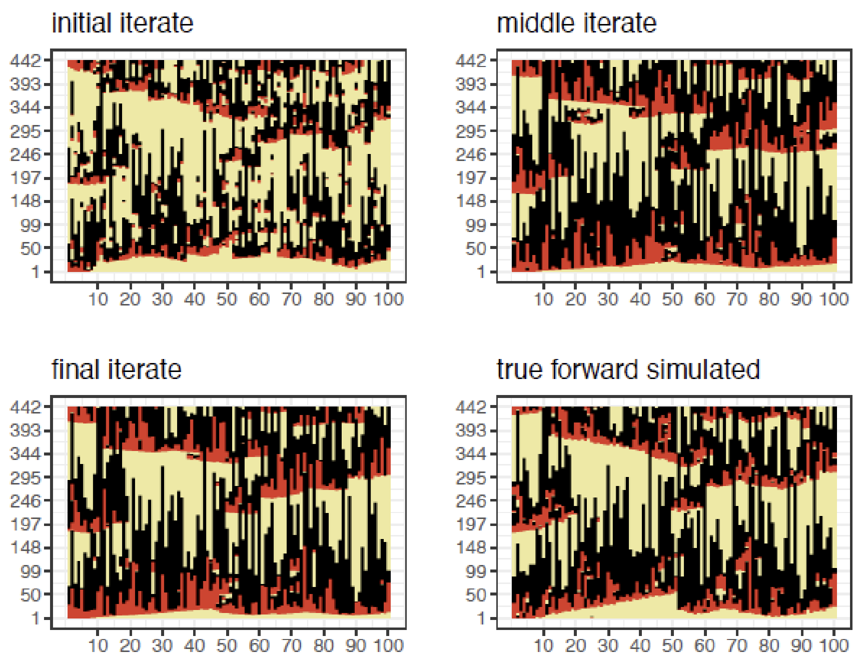
$$N_i(x) = \{\text{number of infected neighbours of individual } i \text{ in state } x\}$$

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

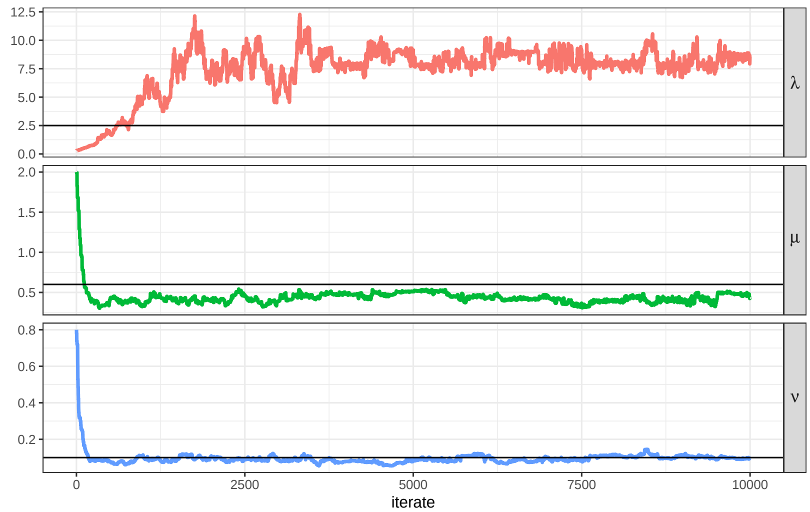
Auxiliary kernel for backward filtering:

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

Application: interacting particle process



Application: interacting particle process



Continuous time transitions

Rethinking the discrete-time case:

- Edge

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

- "Discrete-time" generator

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

- ⚠ 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 $S \leq s < s + h \leq T$

$$
\begin{aligned}
(\mathcal{A}h)(s, x) &= \lim_{h \downarrow 0} h^{-1}\mathbb{E}[h(s + h, X_{s+h}) - h(s, X_s) \mid X_s = x] \\
&= (\mathcal{L}h)(s, x) + \frac{\partial}{\partial s} h(s, x).
\end{aligned}
$$

- Obtain $x \mapsto h(S, x)$ from solving

$$(\mathcal{A}h)(s, x) = 0 \quad \text{subject to} \quad h(T, \cdot).$$

- h induces a change of measure from X to the process $X^\star$ with inf. generator

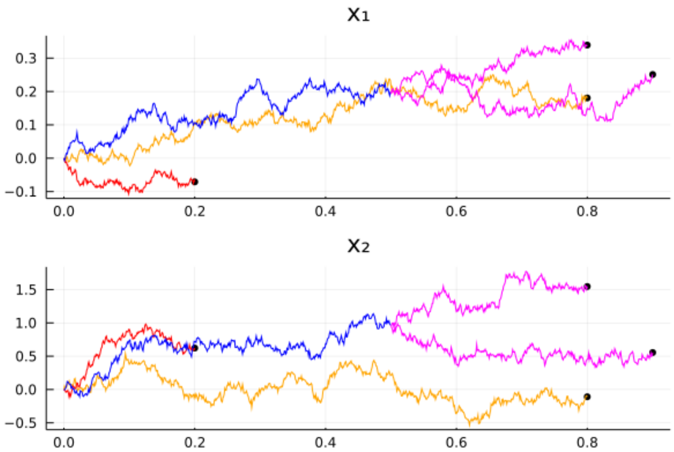
$$h\mathcal{L}^\star f = \mathcal{L}(fh) - f\mathcal{L}h.$$

⚠ 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.
- g induces a change of measure from X to X° with inf. generator
$$g\mathcal{L}^\circ f = \mathcal{L}(fg) - f\mathcal{L}g$$
Identify guided process from $\mathcal{L}^\circ$.
- Correct for "wrong" h by weight
$$\exp\left(\int_{t_i}^{t_{i+1}} \frac{(\mathcal{L}-\widetilde{\mathcal{L}})g}{g}(u, X^\circ_u)\,\mathrm{d}u\right).$$

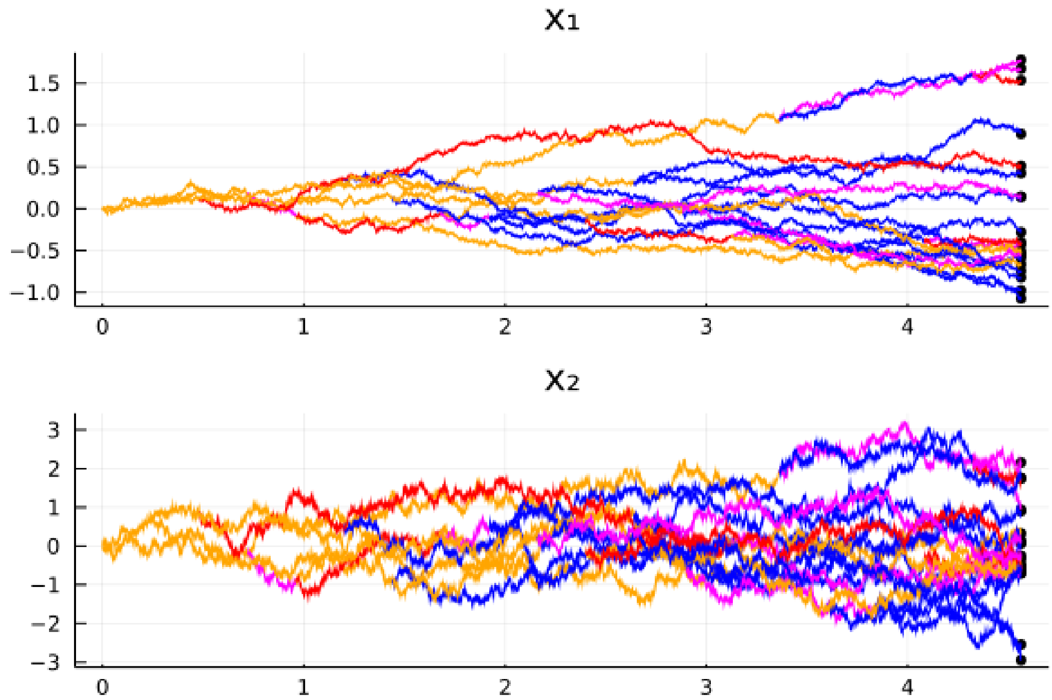
Example 2: branching diffusion

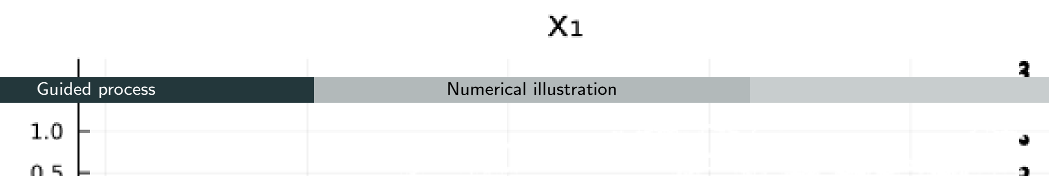


SDE on a tree where on each branch

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

Numerical illustration: SDE on a tree





Numerical illustration: SDE on a tree

On each branch

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

- Backward filter a linear process (essentially $\widetilde{\kappa}$)
- Write X° as pushforward of (x_0, ξ, Z), with $\xi = (\theta_1, \theta_2, \sigma_1, \sigma_2)$
- MCMC on (ξ, Z)

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

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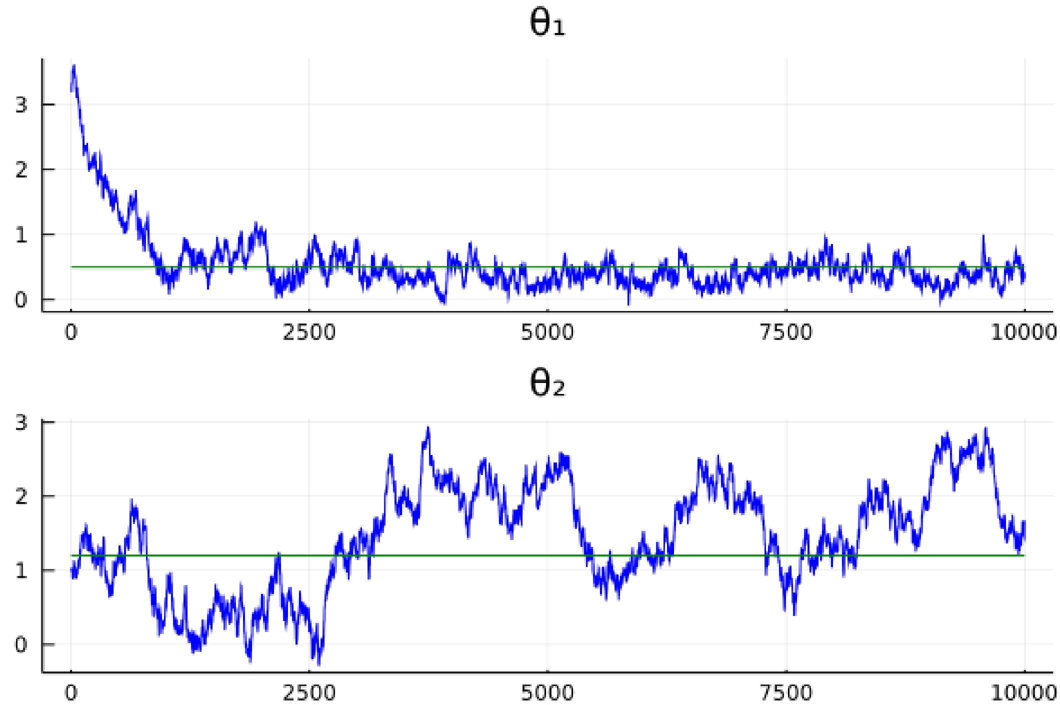

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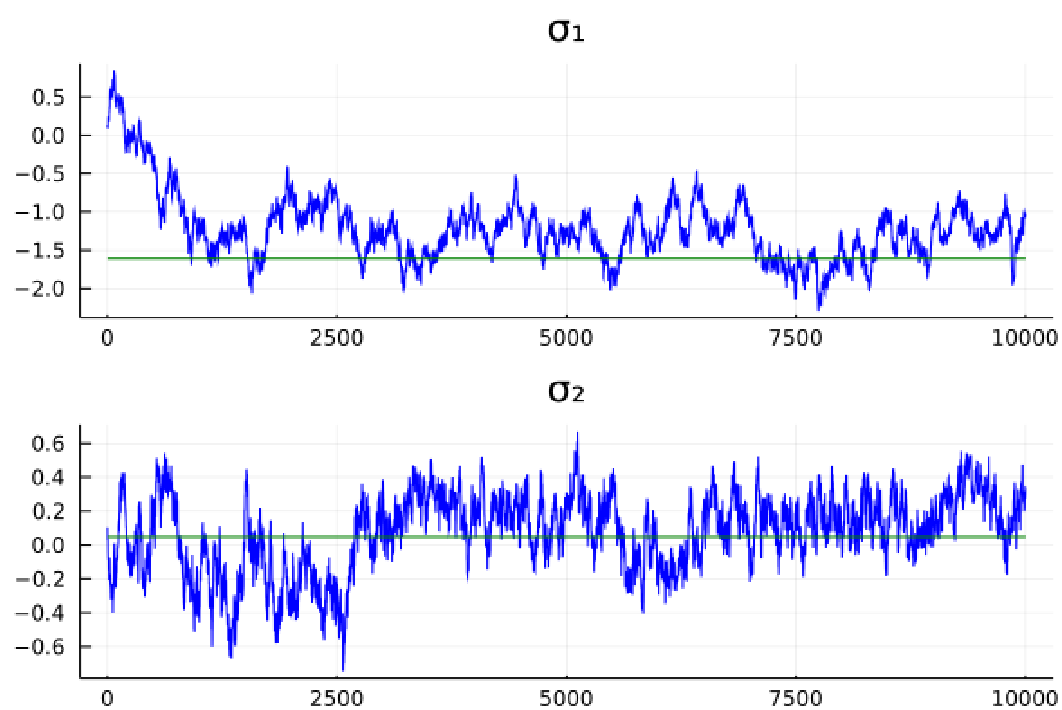

Wrap-up / conclusions

Wrap-up

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.
- Illustrations for interacting particle process and branching diffusion.
- Not covered: compositionality results (some category theory, see preprint).

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

References

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

  Bayesian inference for partially observed diffusions.
- 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.