Automatic Backward Filtering Forward Guiding
for Markov processes and graphical models

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Abstract

We incorporate discrete and continuous time Markov processes as building blocks into probabilistic graphical models with latent and observed variables. We introduce the automatic Backward Filtering Forward Guiding (BFFG) paradigm (Mider et al. (2021)) for programmable inference on latent states and model parameters. Our starting point is a generative model, a forward description of the probabilistic process dynamics. We backpropagate the information provided by observations through the model to transform the generative (forward) model into a pre-conditional model guided by the data. It approximates the actual conditional model with known likelihood-ratio between the two. The backward filter and the forward change of measure are suitable to be incorporated into a probabilistic programming context because they can be formulated as a set of transformation rules.

The guided generative model can be incorporated in different approaches to efficiently sample latent states and parameters conditional on observations. We show applicability in a variety of settings, including Markov chains with discrete state space, interacting particle systems, state space models, branching diffusions and Gamma processes.

Keywords: Backward information filter, Bayesian network, Branching diffusion process, directed acyclic graph, guided process, Doob’s \( h \)-transform, string diagram.

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1 Introduction

1.1. Problem description. A large number of scientific disciplines makes use of stochastic processes for probabilistic modelling of time evolving phenomena and complex systems under uncertainty. In this setting data assimilation and statistical inference is challenging. More so, if this is to be incorporated as components into larger probabilistic models, to be described using modelling languages, and if it is desired to perform
inference in an at least semi-automated fashion in probabilistic programming. In this paper we provide a way to incorporate Markovian stochastic processes as building blocks into probabilistic graphical models and efficiently perform inference on them.

Probabilistic graphical models capture the structure of a probabilistic model in the form of a graph from which conditional independence properties can easily be extracted. We assume that the dependence structure of random quantities is represented by a directed acyclic graph (DAG) with vertices \( t \in T \) and edges directed from a set of source vertices towards the leaves (commonly used terminology for graphical models is reviewed in appendix B). To each vertex \( t \) of the DAG corresponds a random quantity \( X_t \), constituting a Bayesian network. Often the DAG arises as the dependency structure of a probabilistic program. The conditional distribution of \( X_t \) given all \( X_s \) corresponding to the ancestors \( s \) of \( t \) in the DAG is prescribed and assumed to depend only on the parents, the random quantity \( X_{\text{pa}(t)} \), the set of vertices \( s \) for which there is a directed edge from \( s \) to \( t \). See Figure 1 for a simple example with a single source (root).

Assume we only observe \( X_v \) for each leaf vertex \( v \) of the DAG. Leaves can be attached anywhere in the DAG, also at the sources. Therefore edges ending in leaves can be conceptualised as observation schemes, possibly representing random errors. The smoothing problem consists of finding the exact joint distribution of all \( X_s \), where \( s \in T \) is not a leaf, conditional on the observations. In this paper we give a novel way to sample from the smoothing distribution thereby extending well known algorithms for graphical models. Contrary to other methods, the proposed framework does not require modification of the DAG or dependency structure of the probabilistic program, for example by addition of edges. We are especially interested in models where some \( X_t \) are obtained as the endpoint of the evolution of a Markov process starting from the parent \( X_s \) over a certain time span. The transitions may depend on parameters in the Markov kernel which need to be estimated.

The problem setting encompasses training of stochastic residual neural networks (Wang et al., 2018) and their continuous-time counterparts neural stochastic differential equations (Chen et al., 2018), as well as other settings where the output of a complicated latent process is observed and the latent process is obtained from iteration and composition of models which are tractable (only) locally in time, in space or along single edges in the DAG.

1.2. Approach. We start from a Markovian forward description of the possibly nonlinear, non-reversible process dynamics. In essence, by first filtering backwards an approximate process from the leaves towards the root and then performing a change of measure on the transitions of the generative (forward) model using the filtering information, we derive a generative model \textit{guided} by the data. This model provides a structure preserving approximation to the true model conditional on the observations to sample from. Notably, we also transform transitions which correspond to continuous time Markov processes using an exponential change of measure (Palmowski and Rolski, 2002). This \textit{pre-conditional} model, which combines information from data and the model, can then be incorporated in different approaches to efficiently sample the actual smoothing distri-
bution, for example Hamiltonian Monte Carlo, particle methods or variational inference. The setup allows to obtain a differentiable likelihood through a reparametrisation in a natural way.

As a familiar special case of the procedure we obtain the backwards filtering forward sampling algorithm for linear state space models (in this case the guided approximation is exact and can be directly sampled as latent path given the observations). Also our previously introduced backward filtering forward guiding (BFFG) algorithm for discretely observed stochastic differential equations (Mider et al., 2021) is a special case. More examples, involving Gamma processes, continuous-time Markov chains and Poisson processes are also covered in this paper. Key to this is the insight that the dynamics of a conditioned Markov process or graphical model can be obtained by Doob’s \( h \)-transform and that guided proposals (as defined in Schauer et al. (2017)) result from an approximation to this transform. The idea of using an approximate \( h \)-transform dates back to at least Glynn and Iglehart (1989) in the setting of rare event simulation.

The backward filter and the forward change of measure are suitable to be incorporated into probabilistic programming environments. We use arguments from category theory to derive a principle of compositionality for our method, that is a principle which “describes and quantifies how complex things can be assembled out of simpler parts”, as the eponymous journal Compositionality defines it. Very related properties of Bayesian updates are considered in Smithe (2020). By this it is enough to provide a library of transformation rules and tractable approximations for backward filtering each single transition, the elementary building blocks of a model, and an implementable composition rule to obtain guided processes for larger models. Note that we speak of “guided processes” rather than “guided proposals” (used in earlier works), the motivation being that its applicability is not restricted to a proposal distribution in a Metropolis-Hastings algorithm.

We provide a library of some of such rules and approximations as Julia package Mitosis.jl,\(^1\) following the spirit of the ChainRules.jl package, Revels et al. (2018-2020), providing common differentiation rules to the different automatic differentiation packages in Julia ecosystem.

1.3. Related work. There is a vast literature on filtering and smoothing on graphical models and continuous-time Markov models. Much attention has been paid to state-space models, especially in particle filtering. The proposed framework in this paper is agnostic with respect to the choice of inferential method and fits within the class of message passing algorithms. In Section A we provide a detailed overview of references to related work. The companion paper Van der Meulen (2022) contains a non-technical introduction to this work, targeted at a broader audience.

1.4. Novelty and contribution. Building up on successes with guided processes (Schauer et al., 2017) in the specific, but challenging problem of likelihood-based in-

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\(^1\)https://github.com/mschauer/Mitosis.jl.
ference for diffusion process, this work gives a new, holistic perspective on automatic probabilistic programming in general.

Our approach stands out by being generally applicable to both discrete time as continuous-time processes, discrete and continuous state spaces, agnostic with respect to the choice of inferential method, automatic, being suitable for automatic transformation of probabilistic programs, and compositional, the transformation of a probabilistic program relies on the composition of the transformations of its elementary building blocks in a backward and a forward pass.

1.5. Outline. In Subsection 2.2 we explain the setting and some notation. In Subsection 2.3 we define Doob’s $h$-transform for Markov processes indexed on a tree. In Subsection 2.4 we introduce guided processes for directed trees and, more generally, Bayesian networks. In Subsection 2.5 we explain how continuous time processes, evolving over an edge, can be incorporated. Subsequently, the computational structure of Doob’s $h$-transforms and guided processes is detailed in Section 3 for the specific case of a line graph. Here, we explain how an efficient implementation is obtained by piecing together forward and backward maps. For the more general setting of a directed acyclic graph we explain how the compositional structure can be unpacked in Section 4. In Section 5 we prove compositionality results for the pairing of forward- and backward maps on a directed tree. Examples of guided processes with tractable backward map are given in Section 6. Examples for continuous-time processes are given in Section 7. Various ways in which the obtained results can be used for inference are discussed in Section 8.

Appendix A contains a summary of related work. Some notation for graphical models is reviewed in Appendix B. Appendix C contains some postponed proofs.

2 Doob’s $h$-transform and guided processes

We first recap some elementary definitions on Markov kernels, as these are of key importance in all that follows.
2.1. Markov kernels. Let \( S = (E, \mathcal{B}) \) and \( S' = (E', \mathcal{B}') \) be Borel measurable spaces. A Markov kernel between \( S \) and \( S' \) is denoted by \( \kappa : S \to S' \) (note the special type of arrow), where \( S \) is the “source” and \( S' \) the “target”. That is, \( \kappa : E \times \mathcal{B}' \to [0,1] \), where (i) for fixed \( B \in \mathcal{B}' \) the map \( x \mapsto \kappa(x, B) \) is \( \mathcal{B} \)-measurable and (ii) for fixed \( x \in E \), the map \( B \mapsto \kappa(x, B) \) is a probability measure on \( S' \). On a measurable space \( S \), denote the sets of bounded measures and bounded measurable functions (equipped with the supremum norm) by \( \mathcal{M}(S) \) and \( \mathcal{B}(S) \) respectively. The kernel \( \kappa \) induces a pushforward of the measure \( \mu \) on \( S \) to \( S' \) via

\[
\mu \kappa(\cdot) = \int_E \kappa(x, \cdot) \mu(dx), \quad \mu \in \mathcal{M}(S). \tag{2.1}
\]

The linear continuous operator \( \kappa : \mathcal{B}(S') \to \mathcal{B}(S) \) is defined by

\[
\kappa h(\cdot) = \int_E h(y) \kappa(\cdot, dy), \quad h \in \mathcal{B}(S'). \tag{2.2}
\]

We will refer to this operation as the pullback of \( h \) under the kernel \( \kappa \). Markov kernels \( \kappa_1 : S_0 \to S_1 \) and \( \kappa_2 : S_1 \to S_2 \) can be composed by the Chapman-Kolmogorov equations, here written as juxtaposition

\[
(\kappa_1 \kappa_2)(x_0, \cdot) = \int_{E_1} \kappa_2(x_1, \cdot) \kappa_1(x_0, dx_1), \quad x_0 \in E_0. \tag{2.3}
\]

The unit \( \text{id} \) for this composition is the identity function considered as a Markov kernel, \( \text{id}(x, dy) = \delta_x(dy) \). The product kernel \( \kappa \otimes \kappa' \) on \( S \otimes S' \) is defined on the cylinder sets by \( (\kappa \otimes \kappa')(\{x, x'\}, B \times B') = \kappa(x, B) \kappa'(x', B') \), (where \( x \in E, x' \in E', B \in \mathcal{B}, B' \in \mathcal{B}' \)) and then extended to a kernel on the product measure space.

2.2. Probabilistic graphical models. Let \( \mathcal{G} = (\mathcal{T}, \mathcal{E}) \) be a directed, finite graph without parallel edges and self-loops, with vertices \( \mathcal{T} \) and edges \( \mathcal{E} \), where (\( s, t \)) or \( s \sim t \) denotes a directed edge from \( s \) to \( t \), \( s, t \in \mathcal{T} \). Without first argument, \( s \) denotes the edge or the set of edges directed to \( t \in \mathcal{T} \). We write \( s \leadsto t \) if \( s = t \) or there is a directed path from \( s \) to \( t \). We denote by \( \text{pa}(t), \text{ch}(t), \text{anc}(t) \) the parents, children and ancestors of a vertex \( t \) respectively. The set of leaves (sinks) is denoted by \( \mathcal{V} \). For each vertex \( t \), we denote by \( \mathcal{V}_t = \{ v \in \mathcal{V}, t \leadsto v \} \) the leaves which are descendants of \( t \) (including \( t \), if \( t \) is a leaf). Terms and notations from graph theory used here (see e.g. chapter 10 in Murphy (2012)) are formally defined in Appendix B.

To simplify the presentation we will assume a designated root vertex \( 0 \notin \mathcal{T} \) with deterministic \( X_0 = x_0 \) and formally define \( 0 = \text{pa}(s) \) for sources, that is vertices \( s \in \mathcal{T} \) without parent(s) in \( \mathcal{T} \). In this sense, either \( x_0 \) represents a fixed or \( X_{\text{ch}(0)} \) a random starting configuration with possibly multiple source vertices (sources in \( \mathcal{S} \)).

Finally, define \( \mathcal{S} = \mathcal{T} \setminus \mathcal{V} \) (the set of non-leaf vertices) and \( \text{pa}(\mathcal{V}) \) to be the set of vertices in \( \mathcal{T} \) that are parent of at least one leaf node and set \( \mathcal{S}_0 = \mathcal{S} \cup \{0\} \).

Setting: We consider a probabilistic graphical model on \( \mathcal{G} \), a random process \( (X_t, t \in \mathcal{T}) \) such that \( X_t \) depends on its ancestors \( \text{anc}(t) \) only through its parent(s) \( \text{pa}(t) \) and
where random variables $X_s, X_t$, s $\not\rightarrow$ t, t $\not\rightarrow$ s are independent conditional on all of their parents. We assume that $X_t$ takes values in Borel spaces $S_t = (E_t, \mathcal{B}_t)$ satisfying
\[
\kappa_{\text{pa}(t) \rightarrow t}(x; dy) = P(X_t \in dy \mid X_{\text{pa}(t)} = x)
\]
for given Markov transition kernels $\kappa_{\text{pa}(t) \rightarrow t}$ (where such notation here and in the following should be read as $\int_A \kappa_{\text{pa}(t) \rightarrow t}(x; dy) = P(X_t \in dA \mid X_{\text{pa}(t)} = x)$ for all measurable $A$.)

For $v \in V$ we assume the existence of transition densities $p_{\text{pa}(v) \rightarrow v}$ with respect to a dominating measures $\lambda$
\[
\kappa_{\text{pa}(v) \rightarrow v}(x; dy) = p_{\text{pa}(v) \rightarrow v}(x; y)\lambda(dy), \quad v \in V, \quad x \in E_{\text{pa}(v)} \tag{2.4}
\]

Let $P^*$ denote the law of $X_S$ conditional on $X_V = x_V$. By Bayes theorem
\[
\frac{dP^*}{dP}(X_S) = \frac{\prod_{v \in V \mid V} p_{\text{pa}(v) \rightarrow v}(X_{\text{pa}(v)}; x_v)}{\text{ev}(x_0)}, \tag{2.5}
\]
where $\text{ev}(x_0)$ is known as the evidence. If also the remaining transition kernels have a transition density $p$ with respect to a measure $\lambda$, i.e. $\kappa_{\text{pa}(t) \rightarrow t}(x; dy) = p_{\text{pa}(t) \rightarrow t}(x, y)\lambda(dy)$, the joint density factorises as
\[
p(x_T) = \prod_{t \in \mathcal{T}} p_{\text{pa}(t) \rightarrow t}(x_{\text{pa}(t)}; x_t). \tag{2.6}
\]

### 2.3. Doob’s h-transform on a directed tree.

Doob’s $h$-transform characterises the conditional distribution of a Markov process given information at the end of a time horizon/life time in a succinct, but not always tractable form. It generalises to the setting where $\mathcal{G}$ is a connected tree directed to the leaves, i.e. each vertex has a unique parent, except from the formal root vertex 0. Thus, edges point towards the leaves and “backwards” is to be understood as pointing from leaves to the root.

We are interested in the distribution of $X_S$ conditional on $X_V$, i.e. the smoothing distribution. The values at the leaf vertices can be interpreted as observations without error. Alternatively, $X_{\text{pa}(v)}$ can be thought of as observed quantities with the edges $\text{pa}(v) \rightarrow v$, $v \in V$ representing observation errors. Note that each vertex, including the root 0, may have one or more leaves as its children. A simple example is depicted in Figure 1.

With this notation, the process $X$ that is conditioned on its values on the leaves has transition kernels
\[
P(X_s \in dx_s \mid X_{\text{pa}(s)} = x_{\text{pa}(s)}, X_{V_s} = x_{V_s}) = \kappa^*_s(x_{\text{pa}(s)}; dx_s), \quad s \in S
\]
characterised by
\[
\kappa^*_s(x_{\text{pa}(s)}; dx_s) = \frac{\kappa(x_{\text{pa}(s)}, dx_s)h_s(x_s)}{\int \kappa(x_{\text{pa}(s)}, dx_s)h_s(x_s)}, \tag{2.7}
\]
where the term on $h$ on the right-hand-side is the $h$-transform at vertex $t$, i.e. $h_t(x_t) = p(x_{V_t} \mid x_t)$ in Bayesian notation. Within the subtree with root vertex $t$, this can be
interpreted as the likelihood of $x_t$ with respect to the measure $\lambda$. Alternatively, if we would imply a flat prior on $x_t$, then $h_t(x_t)$ would be proportional to the posterior density of $x_t$ (assuming $x \mapsto h_t(x)$ to be integrable) where $x_t$ is the parameter and $V_t$ the observation. Note that the observations are dropped from the notation as they are fixed throughout (the same convention is used for example in Cappé et al. (2005); Section 3.1.4 in there). In case of hidden Markov models, a rigorous proof that the conditioned latent process is an inhomogeneous Markov chain is given in Section 3.3 of Cappé et al. (2005) and the same argument can adapted to formally justify (2.7).

It is well known how $h_s$ can be computed recursively starting from the leaves back to the root. These recursive relations have reappeared in many papers, see for instance Felsenstein (1981), Briërs et al. (2010), Guarniero et al. (2017) and Heng et al. (2020). This recursive computation is known as the Backward Information Filter (BIF). Firstly, for any leaf vertex $v$ we define

$$h_{\text{pa}(v) \rightarrow v}(x) := p_{\text{pa}(v) \rightarrow v}(x; x_v) \quad v \in V.$$

(2.8)

For other vertices $s$ we define

$$h_{\text{pa}(s) \rightarrow s} := \kappa_{\text{pa}(s) \rightarrow s} h_s, \quad s \in S,$$

(2.9)

where $\kappa_{\text{pa}(s) \rightarrow s} h_s$ is the pullback (as defined in Equation (2.2)) of $h_s$ under the kernel $\kappa_{\text{pa}(s) \rightarrow s}$. By the Markov property we have

$$h_s(x) = \prod_{t \in \text{ch}(s)} h_{s \rightarrow t}(x), \quad s \in S_0.$$

(2.10)

This can be interpreted as fusion, collecting all messages from children at vertex $s$, the messages being $x \mapsto h_{s \rightarrow t}(x)$. Then the dynamics of the conditional process is given in short

$$\kappa_{\text{pa}(s) \rightarrow s}^* f h_s(x; dy) = \kappa_{\text{pa}(s) \rightarrow s}^* h_s(x; dy) \frac{h_s(y)}{h_s(x)}$$

(2.11)

and $h_s(x)$ shows up as normalising constant and one could define it that way. Note that equivalently $\kappa^*$ is characterised by the relation

$$\frac{\kappa_{\text{pa}(s) \rightarrow s}^* f h_s}{\kappa_{\text{pa}(s) \rightarrow s}^* h_s} = \kappa_{\text{pa}(s) \rightarrow s}^* f,$$

(2.12)

for bounded measurable test functions $f \in B(S_s)$. If $h$ is the Doob $h$-transform, then (on a directed tree) the evidence defined in (2.5) satisfies $\text{ev}(x_0) = h_0(x_0)$.

Let $X^*$ be the process $X$ on the vertex set of $\mathcal{G}$, starting in $x_0$ and conditioned on observations at $V$. As $\mathcal{G}$ is a tree, $X^*$ is Markov process on $\mathcal{G}$ at well and evolving according to the transition kernels in (2.11).

2.4. Guided processes. The $h$-transform can only be computed in closed form in few cases: it assumes the graphical model to be a directed tree and even there, in general, it is intractable and so is $\kappa^*$. 

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Suppose it is possible to work with an approximation $g$ of $h$, for example by choosing a Gaussian approximation to $X$, and then computing the $h$-transform for that approximation instead. Then one can use this $g$ to define an approximate $h$-transform, to be used as pre-conditional model which then serves as approximation of the conditional process and can be transformed into the actual conditional process via a change of measure, that is through sampling.

Similar to the $h$-transform we define the guided process $X^\circ$ by transforming each transition along an edge of the DAG by applying a change of measure to the forward kernel by specifying functions $g_{s,t}$ on all edges. Note that on a DAG, contrary to a directed tree, conditioning on the values at leaf-vertices changes the dependency structure (there is a conditional process $X^\star$ defined on the vertex set, but its dependency graph is different from that of $X$, in particular there is no meaningful transition $\kappa_{pa(s) \rightarrow s}$ for all $s$). The guided process, unlike the conditioned process, is constructed to have the same dependency structure as the (unconditional) forward process. Crucially this means a sampler for the guided process has a similar complexity as a sampler for $X$, predisposing guided process for sampling based inference.

**Definition 2.1.** Let the maps $x \mapsto g_{s,t}(x)$ be specified for each edge $(s,t)$ in $T$ and define

$$g_s(x) = \prod_{t \in ch(s)} g_{s,t}(x), \quad s \in S_0. \quad (2.13)$$

We define the guided process $X^\circ$ as the process starting in $X^\circ_0 = x_0$ and from the roots onwards evolving on the DAG $\mathcal{G}$ according to transition kernel

$$\kappa_{pa(s) \rightarrow s}(x_{pa(s)}; dy) = \frac{g_s(y)\kappa_{pa(s) \rightarrow s}(x_{pa(s)}; dy)}{\int g_s(y)\kappa_{pa(s) \rightarrow s}(x_{pa(s)}; dy)}, \quad s \in S.$$

Samples of $X^\circ$ can be transformed into samples of the conditional process. If $\mathbb{P}^\circ$ denotes the law of $X^\circ_S$, then it follows from the definition of $\kappa^\circ$

$$\frac{d\mathbb{P}^\circ}{d\mathbb{P}}(X_S) = \prod_{s \in S} \left( \frac{g_s(X_s)}{\int g_s(y)\kappa_{pa(s) \rightarrow s}(X_{pa(s)}; dy)} \right).$$

Recall the definition of $\mathbb{P}^*$ in (2.5).

**Theorem 2.2.** If $\mathbb{P}^* \ll \mathbb{P}^\circ$, then for $f \in \mathcal{B}(S_S)$

$$\mathbb{E}[f(X_S) \mid X_V = x_V] = \frac{g_0(x_0)}{e_V(x_0)} \mathbb{E}_{\mathbb{P}^\circ} \left[ f(X^\circ_S) \prod_{s \in S} w_{pa(s) \rightarrow s}(X^\circ_{pa(s)}) \prod_{v \in V} h_{pa(v) \rightarrow v}(X^\circ_{pa(v)}) \right],$$

with weights defined by

$$w_{pa(s) \rightarrow s}(x_{pa(s)}) = \frac{\int g_s(y)\kappa_{pa(s) \rightarrow s}(x_{pa(s)}; dy)}{\prod_{u \in pa(s)} g_u \rightarrow s(x_u)} \quad s \in S. \quad (2.14)$$
Proof. By definition of the weights

\[
\frac{d\mathbb{P}^0}{d\mathbb{P}}(X_S) = \prod_{s \in S} \left( w_{\text{pa}(s)s}(X_{\text{pa}(s)}) \right)^{-1} \times \frac{g_s(X_s)}{\prod_{u \in \text{pa}(s)} g_{u \rightarrow s}(X_u)}.
\]

By Equation (2.10), the second term in brackets can be written as

\[
\prod_{s \in S} \prod_{t \in \text{ch}(s)} g_{s \rightarrow t}(X_s) = \prod_{u \in \mathcal{V}} g_{\text{pa}(v) \rightarrow v}(X_{\text{pa}(v)})
\]

which follows by cancellation of terms (note that the numerator is a product over all edges except those originating from the root node, whereas the denominator is a product over all edges except those ending in a leaf node). Hence

\[
\frac{d\mathbb{P}^0}{d\mathbb{P}}(X_S) = \prod_{v \in \mathcal{V}} g_{\text{pa}(v) \rightarrow v}(X_{\text{pa}(v)}) \cdot \left( \prod_{s \in S} w_{\text{pa}(s)s}(X_{\text{pa}(s)}) \right)^{-1}.
\]  \hspace{1cm} (2.15)

The result now follows from

\[
\frac{d\mathbb{P}^*}{d\mathbb{P}^0}(X_S) = \frac{d\mathbb{P}^*}{d\mathbb{P}}(X_S) \cdot \left( \frac{d\mathbb{P}^0}{d\mathbb{P}}(X_S) \right)^{-1}
\]

and substituting (2.5), (2.8) and (2.15). \( \Box \)

The definitions leaves open the choice of \( g_{s \rightarrow t} \). Recall that for Doob’s h-transform, \( h \) is a marginal likelihood. It stands to reason that good choices for \( g_{s \rightarrow t} \) are approximations of the marginal likelihood of the observations \( x_{\text{pa}(t)} \), given \( x_s \) (and integrating out \( x_u, u \in \text{pa}(t) \setminus \{s\} \) using (prior-) information available).

### 2.5. Continuous-time guided processes.

Up to this point, we have assumed edges to represent “discrete time” Markov-transitions. In some applications it is natural to interpret the transition over an edge \((s,t)\) as the result of evolving a continuous-time Markov process over a fixed time interval \([S,T]\). Let \( X \equiv (X_u, u \in [S,T]) \) be a time-homogeneous \( E \)-valued Markov process with full (extended) generator \( \mathcal{L} \) with domain \( \mathcal{D}(\mathcal{L}) \). Let \( \{\mathcal{F}_t\} \) be a right-continuous history filtration and let \( \mathbb{P}_u \) denote the restriction of \( \mathbb{P} \) to \( \mathcal{F}_u \). The process \( X \) has a family of evolution kernels \( \kappa_{u,v} \) with transition densities \( p \). For \( S < u < v < T \),

\[
\mathbb{P}(X_v \in dy \mid X_u = x) = \kappa_{u,v}(x, dy) = p(u, x; t, v) dy
\]

The discrete pullback of a function \( h_T \) (from vertex \( t \), defined on \( \mathcal{B}(E) \)) by \( \kappa = \kappa_{S,T} \) extends on the interval \( u \in (S,T] \) to a continuous \( h \)-transform by setting

\[
h(u, x) = (\kappa_{u,T} h_T)(x) = E[h_T(X_T) \mid X_u = x], \quad u \in (S,T]. \hspace{1cm} (2.16)
\]
For given $h_T$, the $h$-function at vertex $T$, $h$ satisfies the Kolmogorov backward equation

$$\mathcal{A}h(u, x) = 0, \quad u \in (S, T]$$

subject to $h(T, \cdot) = h_T(\cdot)$, \hspace{1cm} (2.17)

where $\mathcal{A} = \frac{\partial}{\partial t} + \mathcal{L}$ is the generator of the space-time process $(u, X_u)$.$^2$ Only for few Markov processes it is possible to solve this equation in closed form leading to a tractable expression for $h$. However, just as in the discrete-time case, we can specify a function $g$ (not necessarily satisfying (2.17)) and define the guided process by a change of measure. This results in a generalisation of the definition of guided proposals for diffusion processes from Schauer et al. (2017).

**Remark 2.3.** The pullback that we defined for the discrete case can also be seen to satisfy (2.17). To see this, consider the space-(discrete)time process $(t, X_t)$. Consider $t \in \{S, T\}$, where $T$ is a child node of $S$ (in a discrete time Markov chain one may think of $S = t$ and $T = t + 1$, with $t$ indexing time). Then we have the following discrete analogue for the operator $\mathcal{A}$:

$$(\mathcal{A} h)(S, x) : = \mathbb{E}[h(T, X_T) - h(S, X_S) \mid X_S = x] = \int h(T, y) \kappa_{S \to T}(x, dy) - h(S, x).$$

Therefore, solving $(\mathcal{A} h)(S, x) = 0$ is equivalent to computing the pullback of $h(T, x)$ through $\kappa_{S \to T}$. Notationally, in the discrete case we have written $h_T(x)$ rather than $h(T, x)$.

We assume the process $(X_t)$ is defined on $[S, T]$ and consider a fixed initial value $x_S$.

**Definition 2.4.** For $u \in (S, T]$ let

$$D^g_u = \frac{g(u, X_u)}{g(S^+, x_{S^+})} \exp \left( - \int_S^u \frac{Ag}{g}(s, X_s) \, ds \right).$$

Assume $g \in \mathcal{D}(\mathcal{A})$ is a positive function such that $D^g_u$ is a $\mathcal{F}_u$-martingale. Define the change of measure

$$d\mathbb{P}_u^\circ = D^g_u \, d\mathbb{P}_u.$$ \hspace{1cm} (2.18)

The process $X$, with $X_S = x_S$, under the law $\mathbb{P}_u^\circ$ is denoted by $X^\circ$ and referred to as the guided process induced by $h$.

As in Palmowski and Rolski (2002), we will call a function such that $D^g_u$ is a $\mathcal{F}$-martingale a good function (sufficient conditions are given in Proposition 3.2 in Palmowski and Rolski (2002)). By formula (1.2) in Palmowski and Rolski (2002) the full generator of $X^\circ$, characterising the dynamics of $X^\circ$ has the form

$$\mathcal{A}^\circ f = \frac{1}{g} (\mathcal{A}(fg) - fAg).$$ \hspace{1cm} (2.19)

$^2$The space-time process $(t, X_t)$ has full generator $\mathcal{A} = \mathcal{L} + \frac{\partial}{\partial t}$ extending the graph $\{(fh, \mathcal{A}(fh)), f \in \mathcal{D}(\mathcal{L}), h \in C[0, T])\}$, see Theorem 7.1 on page 221 in Ethier and Kurtz (1986).
This implies $g\mathcal{L}^\circ f = \mathcal{L}(fg) - f\mathcal{L}g$ which will be used in multiple examples to identify/recognise the dynamics of the guided process. Note that the change of measure in this definition is similar to the change of measure in Definition 2.1.

If $h$ satisfies (2.17), then we define $dP^*_u = D(u) dP_u$ and denote the process under the law of $P^*$ as $X^*$ having full generator $\frac{1}{h}(Ah - fAh)$.

We obtain the following extension of Theorem 2.2.

**Theorem 2.5.** Consider the guided process on a DAG as defined in Definition 2.1. Suppose that $t \in S$ and assume that the transition kernel on the edge $(s,t)$ corresponds to evolving a continuous-time guided process $X^\circ$ on $[S,T]$ with full (extended) generator $\mathcal{L}$. Then the weight (2.14) over the edge equals

$$w_{s\rightarrow t}(X^\circ) = \exp \left( \int_S^T \frac{Ag}{g}(u, X^\circ_u) \, du \right).$$

**Proof.** This follows from the proof of Theorem 2.2, from which it is seen that the factor $g(T,X^\circ_T)/g(S,X^\circ_S)$ cancels with factors originating from parent and child branches.

One way to choose a tractable guided process is to consider a second continuous-time Markov process, with generator $\tilde{\mathcal{L}}$, and take $g$ solving

$$(\tilde{\mathcal{L}} + \frac{\partial}{\partial u})g(u,x) = 0, \text{ subject to } g(T,\cdot) = g_T(\cdot).$$

(2.20)

In this case $Ag = (\mathcal{L} - \tilde{\mathcal{L}})g$, which leads to the following corollary.

**Corollary 2.6.** Assume $h$ and $g$ satisfy (2.17) and (2.20) respectively. Suppose both $h$ and $g$ are good functions. Then

$$\frac{dP^*_T(X^\circ)}{dP^*_T}(X^\circ) = \frac{h_T(X^\circ_T)}{g_T(X^\circ_T)} \frac{g(S,X^\circ_S)}{h(S,X^\circ_S)} \exp \left( \int_S^T \frac{(\mathcal{L} - \tilde{\mathcal{L}})g}{g}(s, X^\circ_s) \, ds \right).$$

(2.21)

**Remark 2.7.** The result is indeed a continuous-time analogue of Theorem 2.2. With (2.17) the continuous analogue of (2.9), $h$ describes the true conditional evolution along the continuous time edge given information encoded in $h_T$. It can be used for sampling a continuous-time Markov process conditioned on exact observations. In this case $g(t,X^\circ_t)$ and $h(t,X^\circ_t)$ approach the same Dirac measure for $t \rightarrow T$. In the setting where $X$ is defined by a stochastic differential equation sufficient conditions such that the first ratio on the-right hand-side of equation (2.21) cancels in the limit $t \rightarrow T$ have been derived in Schauer et al. (2017) and Bierkens et al. (2020). In Corstanje et al. (2021) sufficient conditions are derived for a wider class of Markov processes.

Using a different $h$ on the unconditioned dynamics $\kappa$, rather than directly approximating the dynamics of the conditioned process $\kappa^*$, we aim to approximate the information brought by future observations, and let this approximation guide the process in a natural way. In absence of information from observations, the process evolves just as the unconditional one. This is emphatically the right thing to do to preserve absolute continuity when the graph becomes large.
3 Compositionality: first steps

In this section we give a principle of compositionality for the task of sampling a guided process using the Backwards Filtering Forward Guiding algorithm.

3.1. Sequential composition. To shift to a compositional perspective, it is convenient to frame the graphical structure, that is the evolution of the process along the edges of a DAG, differently as sequential composition of Markov kernels (as defined in (2.3)). We sequentially order the vertices, by partitioning the set $S$ in generations $\Gamma_1, \Gamma_2, \ldots, \Gamma_n$ and $\Gamma_0 = \{0\}$, $\Gamma_{n+1} = V$, such that all parents of vertices $s \in \Gamma_i$ are in $\bigcup_{0 \leq j < i} \Gamma_j$. Write $X_i = X_{\Gamma_i}$ and set

$$\kappa_i(x_{i-1}; dx_i) = P(X_i \in dx_i \mid X_{i-1} = x_{i-1}).$$

We assume $\kappa_{n+1}(x, \cdot)$ has density $p_{n+1}$ with respect to the dominating measure $\lambda$ (consistent with (2.4)). Consequently the distribution of $X_i$ is given by a composition of kernels

$$\delta_{x_0} \kappa_1 \kappa_2 \cdots \kappa_i,$$

obtained by repeatedly pushing forward the initial law (a Dirac measure in $x_0$ as we assumed deterministic $X_0 = x_0$). Parentheses can be omitted by associativity. Note that $\{0, \ldots, n+1\}$ are the vertices of a line graph with a single observation vertex $n+1$, and Doob’s $h$-transform applies on the level of generations. By repeatedly applying the pullback operation, we obtain the backward filter

$$h_n(x) = p_{n+1}(x, x_{n+1})$$
$$h_{i-1} = \kappa_i \kappa_{i+1} \cdots \kappa_n h_n.$$

The $h$-transform maps $(\kappa_i, h_i)$ to $\kappa^*_i$, where for $(\kappa_i, h_i)$, $i \in \{1, \ldots, n\}$,

$$\frac{\kappa^*_i(x, dy)}{\kappa_i(x, dy)} = \frac{h_i(y)}{(\kappa_i h_i)(x)} =: m(x, y)$$

(not for $\kappa^*_{n+1}$, which is just a Dirac measure in the observation). We will interpret $m$ as a message obtained from backward filtering, to be used in forward sampling.

3.2. Forward and backward maps for guided processes. The following definition is motivated by the backward filter in (3.2). In the upcoming definitions we assume kernels $\kappa: S \rightarrow S'$ and $\tilde{\kappa}: S \rightarrow S'$, where $S = (E, \mathcal{B})$ and $S' = (E', \mathcal{B}')$

Definition 3.1. For a Markov kernel $\kappa: S \rightarrow S'$ and function $h \in \mathcal{B}(S')$ define the backward map $\mathcal{B}_\kappa: \mathcal{B}(S') \rightarrow \mathcal{B}(S \times S') \times \mathcal{B}(S)$ by

$$\mathcal{B}_\kappa(h) = (m, \kappa h), \ \text{where} \ m(x, y) = \frac{h(y)}{(\kappa h)(x)}.$$

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This map returns both the pullback \( \kappa h \) and an appropriate message \( m \) for the map \( \mathcal{F}_\kappa \) specified in the following definition.

**Definition 3.2.** For a Markov kernel \( \kappa: S \rightarrow S' \), message \( m \in \mathcal{B}(S \times S') \) (as defined in (3.3)) and measure \( \mu \in \mathcal{M}(S) \) define the forward map \( \mathcal{F}_\kappa : \mathcal{B}(S \times S') \times \mathcal{M}(S) \rightarrow \mathcal{M}(S') \) by

\[
\mathcal{F}_\kappa(m, \mu) = \nu, \quad \nu(dy) = \int m(x, y)\mu(dx)\kappa(x, dy).
\] (3.4)

In case the pullback is intractable or computationally demanding, we propose to replace the kernels \( \kappa \) in the backward map by simpler kernels \( \tilde{\kappa} \). Specification of \( \tilde{\kappa} \) is a way to define \( g_{\text{opt}} \) in Definition 2.1. If \( \mu \) is a probability measure and \( \mathcal{B}_\kappa \) sends the message \( m \), then \( \mathcal{F}_\kappa(m, \mu) \) is again a probability measure. If instead, as for guided processes, \( \mathcal{B}_\kappa \) sends the message \( m \) (rather than \( \mathcal{B}_\kappa \)), then \( \mathcal{F}_\kappa(m, \mu) \) need not be a probability measure, even if \( \mu \) is. This motivates the following definition, which is actually an application and suggestive rewriting of the backward- and forward maps.

For a guided process with backward kernel \( \tilde{\kappa}: S \rightarrow S' \) we have for \( g \in \mathcal{B}(S') \)

\[
\mathcal{B}_{\tilde{\kappa}}(g) = (m, \tilde{\kappa}g), \quad \text{where} \quad m(x, y) = \frac{g(y)}{(\kappa g)(x)}.
\]

If \( \varpi \geq 0 \) and \( \mu \) is a probability measure then

\[
\mathcal{F}_\kappa(m, \varpi \cdot \mu)(dy) = (\varpi \omega_\kappa(m, \mu)) \cdot \nu(dy)
\]

where the weight \( \omega_\kappa(m, \mu) \) and probability measure \( \nu \) are defined by

\[
\omega_\kappa(m, \mu) = \int \int m(x, y)\kappa(x, dy)\mu(dx) = \int \frac{(\kappa g)(x)}{(\kappa g)(x)}\mu(dx)
\]

\[
\nu(dy) = \omega_\kappa^{-1}(m, \mu) \int \frac{g(y)}{(\kappa g)(x)}\mu(dx)\kappa(x, dy).
\] (3.5)

Clearly, \( \mathcal{F}_\kappa \) and \( \mathcal{B}_{\tilde{\kappa}} \) work as a pair which we denote as \( (\mathcal{F}_\kappa | \mathcal{B}_{\tilde{\kappa}}) \) and refer to as optic. We define the map \( F \) that takes kernels \( \kappa, \tilde{\kappa}: S \rightarrow S' \) and returns the optic

\[
F(\kappa, \tilde{\kappa}) = (\mathcal{F}_\kappa | \mathcal{B}_{\tilde{\kappa}}).
\] (3.6)

**3.3. Backward Filtering Forward Guiding.** With these definitions, a first form of compositionality is easily obtained for the forward evolution on the level of generations (cf. Equation (3.1)). Hence, assume the forward evolution \( \delta_{x_0\kappa_1\kappa_2 \cdots \kappa_n} \). Then sampling from the guided process is obtained by iteratively applying the forward and backward maps in the following way:

\[
m_i, g_{i-1} = \mathcal{B}_{\tilde{\kappa}_i}(g_i), \quad i = n, \ldots, 1 \quad \text{and} \quad \omega_i \cdot \delta_{x_i} = \mathcal{F}_{\kappa_i}(m_i, \omega_{i-1} \delta_{x_{i-1}}),
\]

\[
\omega_i \cdot \delta_{x_i} \sim \mathcal{F}_{\kappa_i}(m_i, \omega_{i-1} \delta_{x_{i-1}}), \quad i = 1, \ldots, n,
\] (3.7)

initialised from \( h_n, \omega_0 = 1 \) and \( x_0 = x_0 \). Here, for an unnormalised bounded measure \( \nu \), we write \( \varpi \cdot \delta_x \sim \nu \) if \( x \sim \nu/\int \nu \) and \( \varpi = \int \nu \).
Hence, for each \( i \in \{1, \ldots, n\} \), \( x_i^0 \) is a sample drawn independently from \( \mathcal{F}_{\kappa_i}(m_i, \omega_{i-1} \delta_{x_{i-1}^0})/\omega_i \). Then \( \omega_n \cdot (x_0^0, \ldots, x_n^0) \) is a weighted sample from the conditioned process, i.e.

\[
\mathbb{E}[f(X_0, X_1, \ldots, X_n) \mid X_V = x_V] = \mathbb{E}[\omega_n f(X_0^0, X_1^0, \ldots, X_n^0)].
\] (3.8)

As we backward filter the process using the kernel \( \tilde{\kappa} \), followed by forward propagating a weighted sample by guiding we call this procedure \textit{backward filtering forward guiding}.

We introduce a \textit{message passing diagram} to display the compositional structure of (3.7).

\[
\begin{array}{c}
\omega' \cdot \delta_{(x^0)_V}' \\
\Downarrow \quad m \\
F \\
\Downarrow \quad g' \\
B \\
\Downarrow \quad \omega \cdot \delta_{x^0} \\
g
\end{array}
\] (3.9)

The message flow of the diagram is right to left in the direction of the arrows and illustrates how the output of \( B \) (the message \( m \) and pullback \( g \)) serves as input for \( F \).

Figure 2, which reminds of a physical zipper is a composition of the elementary diagram (3.9), in case the forward evolution is \( \delta_{x_0} \kappa_1 \kappa_2 \cdots \kappa_4 \). The diagram should be read starting from the very right, where the observation from leaf 4 comes in via \( g_3 \). Then the \( h \)-transform is computed back to the root by moving south-west towards \( g_0 \). Subsequently, the conditional marginal is propagated from \( \mu_0 \) onwards by moving in north-west direction. Simulation of the conditioned process follows the same pattern. The diagram reveals the dependency structure and recursive nature of the algorithm for computing the \( h \)-transform.

A corresponding pseudo-program in unrolled form, consisting of a function accepting \( g_3 \) and \( x_0 \) and sampling, has a similar structure:

```plaintext
function transform123(x0, g3)
    message3, g2 = backward(kernel3, g3)
    message2, g1 = backward(kernel2, g2)
    message1, g0 = backward(kernel1, g1)
    omega1, x1 = forwardsample(kernel1, message1, omega0, x0)
    omega2, x2 = forwardsample(kernel2, message2, omega1, x1)
    omega3, x3 = forwardsample(kernel3, message3, omega2, x2)
    return h0, omega3, (x0,x1,x2,x3) # return evidence and weighted sample
end
```

\textbf{Remark 3.3.} The message \( m \) from \( B_{\tilde{\kappa}} \) could equivalently be transmitted as pair \((g, \tilde{\kappa} g)\) and then combined in the recipient \( \mathcal{F}_{\tilde{\kappa}} \), or even just as \( g \), with \( \tilde{\kappa} g \) computed in \( \mathcal{F}_\kappa \). We
choose the quotient form as it is convenient for the exposition and acknowledges that while other choices are sometimes convenient, they are essentially equivalent: the format of the message $m_i$ is something between $F_κ$ and $B_˜κ$. Also note that the forward map is invariant under multiplying $g$ by an arbitrary strictly positive constant $c$, as the constant is cancelled in the message $m$.

4 Unpacking the compositional structure within generations

In the previous section, backward filtering, forward guiding was only introduced on the level of generations. Just applying the $h$-transform at the level of generations is unsatisfactory, as the additional structure that the Markov kernels $κ_i$ inherit from the graphical model is ignored. In this section we show how to deal with this using string diagrams, duplication- and product-kernels.

4.1. String diagrams. Our use of string diagrams originates from applied category theory. See e.g. Chapter 3.1 in Jacobs (2019), Cho and Jacobs (2019) or Selinger (2011). These diagrams give a representation of a probabilistic model on a DAG by explicitly representing Markov kernels which “sit” on the edges of a graphical model. Typically, the joint law of $(X_s, s \in \Gamma_i)$ is not tractable, all one has is a mechanism of creating samples $X_i = X_{\Gamma_i}$ using the forward model. It can be described using products of kernels with the identity kernel id as neutral element for the product and the special duplication Markov kernel $\bowtie$, which we now define.
Figure 3: A simple DAG with three leaves (left) and the corresponding string diagram (right) with 3 observables reaching the upper figure boundary. The root 0 is not drawn. The black bullet symbol denotes the duplication (copy) \( \triangleleft \). The string diagram can be written as \( \kappa_1 \triangleleft \left( \kappa_{2a} \otimes \text{id} \right) \left( \triangleleft \otimes \text{id} \right) \left( \kappa_{3a} \otimes \kappa_{3b} \otimes \kappa_{2b} \right) \).

**Definition 4.1.** Define the (\( k \)-fold) duplication kernel as the Markov kernel

\[
\kappa_k(x, dy) = \delta_x(dy_1) \delta_x(dy_2) \ldots \delta_x(dy_k)
\]

and let \( \triangleleft = \triangleleft_2 \).

The duplication kernel allows two different kernels \( \kappa_1, \kappa_2 \) to apply independently to the same argument, giving the probability kernel \( \left( \kappa_1 \otimes \kappa_2 \right)(x, \cdot) = (\kappa_1 \otimes \kappa_2)(\langle (x, x), \cdot \rangle) \) representing a conditionally independent transition from one parent to two children (as part of a DAG).

Now we are able to express in detail the conditional distribution \( \kappa_i \) of a generation of children \( \Gamma_i \) given their parents (which may belong to different generations \( 0 \leq j < i \)). Each \( \kappa_i \) can be written as product of \( \kappa_{p \rightarrow s} \) (where \( p \in \text{pa}(s) \)), duplication kernels and identity kernels \( \text{id} \) acting on \( X_{i-1} \).

Figure 3 illustrates the interplay between \( \triangleleft \) and \( \otimes \). The string diagram on the right corresponds to the composition

\[
\kappa_1 \triangleleft \left( \kappa_{2a} \otimes \kappa_{2b} \right) \left( \triangleleft \otimes \text{id} \right) \left( \kappa_{3a} \otimes \kappa_{3b} \otimes \text{id} \right).
\]

The black bullet symbol in Figure 3 denotes the duplication (copy) \( \triangleleft \). As \( \kappa \text{id} = \kappa \) and \( \kappa \otimes \text{id} = \text{id} \otimes \kappa \), the composition in (4.2) is not unique and an equivalent decomposition is given by

\[
\kappa_1 \triangleleft \left( \kappa_{2a} \otimes \text{id} \right) \left( \triangleleft \otimes \text{id} \right) \left( \kappa_{3a} \otimes \kappa_{3b} \otimes \kappa_{2b} \right).
\]

As we require that the kernels at the leaves have a \( \lambda \)-density in equation (3.2) it is this decomposition that we intend to use.

**Example 4.2.** For a state-space model both the “familiar” graphical model, as also the corresponding string-diagram are depicted in Figure 4.
Figure 4: Top: DAG for state-space model. Bottom: the corresponding string diagram, rotated 90° to the right. Here, $\kappa_i$ denote the morphism from node $i-1$ to $i$ and $\kappa'_i$ is the morphism of node $i$ to the observations $x_i$.

4.2. Forward and backward maps for the duplication and product kernels.

As the duplication kernel is a Markov kernel, forward and backwards maps are well defined.

Proposition 4.3. For the $k$-fold duplication kernel $\llangle_k$ defined in (4.1) we have

$$B_{\llangle_k}(h) = (m, \llangle_k h), \quad m(x, y) = \frac{h(y_1, \ldots, y_k)}{(\llangle_k h)(x)},$$

where $(\llangle_k h)(x) = h(x, \ldots, x)$ ($k$ times). and

$$F_{\llangle_k}(m, \mu) = f_{\llangle_k} (\mu),$$

with $f_{\llangle_k}(\mu)$ the image measure of $\mu$ under the diagonal map $f_{\llangle_k} : x \mapsto (x, \ldots, x)$ ($k$ elements). If $\mu$ is a probability measure, then so is $\nu$.

The proof follows directly from the definition of the forward- and backward maps.

Note in particular that sampling $F_{\llangle_k}(m, \mu)$ means drawing $z$ from $\mu/\int d\mu$ and setting $y_1 = \cdots = y_k = z$ with weight equal to $(\int \mu dx)^{1/k}$ (other choices are possible as long as the product of the weights is the same). The backward- and forward maps can be applied to product kernels $\kappa_1 \otimes \kappa_2$ upon direction application of their definitions (Definition 3.1 and Definition 3.2 respectively). The following results shows that in case $h$ has special structure, this structure is preserved in the backward map for both the duplication and product kernel.

Corollary 4.4. For $h \in \mathcal{B}(S), h' \in \mathcal{B}(S')$, if we define the pointwise product as

$$(h \odot h')(x, y) = h(x) \cdot h'(y), \quad x \in E, y \in E'$$

then $\llangle_k(h_1 \odot \cdots \odot h_k) = \prod_{i=1}^k h_i$ and $(\kappa \otimes \kappa')(h \odot h') = (\kappa h) \odot (\kappa' h').$
In this way we recover the $h$-transform presented in Section 2.3, in particular Equation (2.10) (the fusion operation). For this, note that $h_n$ in (3.2), corresponding to initialisation of $h$ from the leaves, has product form, with components as in (2.8).

As a tree consists of composing products of “ordinary” kernels and duplication kernels we have all ingredients for backwards filtering and forward guiding on a tree. We show this using the following representative example:

**Example 4.5** (Backward-forward diagram on a directed tree). Consider the directed tree and string diagram in Figure 5. Assume we backward filter with kernels $\tilde{\kappa}_i$. Abbreviate $B_i$ for $B_{\tilde{\kappa}_i}$ and $F_i$ for $F_{\kappa_i}$. Corresponding to the string-diagram we have the following dependency diagram which shows the compositional structure of forward and backward maps for this example:
This diagram should be read starting from the very right, where observations from the leaves 5a, 5b come in via \((g_{4a}, g_{4b})\). Then the \(h\)-transform is computed back to the root by moving south-west towards \(g_0\). Subsequently, the conditional marginal is propagated from \(\delta_{x_0}\) onwards by moving in north-west direction. Simulation of the conditioned process follows the same pattern, but then we would also include the weights explicitly in the diagram.

**Remark 4.6.** In applying the scheme (3.1) intermediate values \(X_i\) are lost. To keep them one can make a duplicate and keep one of these by formally applying the identity kernel \(\text{id}\) to it in each subsequent composition.\(^3\) By doing so, no longer all leaves are being observed. To deal with this consider the case where only a subset of the leaves are observed. It suffices to consider \(\kappa_{n+1}\) of product form, \(\kappa_{n+1} = \kappa_{(n+1)a} \otimes \kappa_{(n+1)b}\) and assume only \(X_{(n+1)a} = x_{(n+1)a}\) to be observed. In that case it suffices to define

\[
g_n(x) = p_{(n+1)a}(x, x_{(n+1)a}).
\]

**Remark 4.7.** So far we have assumed conditionally independent observations. Suppose this is not the case, for example when \(X_{n+1} = (Y, Y')\) with \(\kappa_{n+1}: S_n \to T \otimes T'\) and only \(Y' = y'\) was observed. Then with \(\bar{\kappa}: S_n \to T, \bar{\kappa}': S_n \to T',\) and distribution of \((\bar{Y}_x, \bar{Y}'_x)\) given by \(\bar{\kappa}(x, \cdot) \otimes \bar{\kappa}'(x, \cdot)\)

\[
\mathbb{E}[f(X_{n+1}) \mid X_n = x, Y' = y'] = \frac{\mathbb{E}[f(\bar{Y}_x, y')\Phi(x, \bar{Y}_x, y')}}{\mathbb{E}\Phi(x, \bar{Y}_x, y')},
\]

where

\[
\Phi(x, y, y') = \frac{d\kappa(x, \cdot)}{d\tilde{\kappa}(x, \cdot)}(y, y').
\]

Thus, (3.2) can be replaced by \(g_n(x) = \mathbb{E}\Phi(x, \bar{Y}_x, y')\).

### 4.3. Extension from a directed tree to a DAG.

In this section we extend our approach from a directed tree to a true DAG. Whereas on the former each vertex has a unique parent vertex, on a DAG a vertex can have multiple parent vertices. Correspondingly, in the diagram a box with several input edges denotes a Markov kernel whose domain is a tensor product.

Note that if \(\kappa = \kappa_1 \kappa_2\), then \(\kappa^* = \kappa_1^* \kappa_2^*\). Moreover, if \(\kappa_2 = \kappa_2 a \otimes \kappa_2 b\) has product form, we also get

\[
(\kappa_1 \kappa_2)^* = (\kappa_1 (\kappa_2 a \otimes \kappa_2 b))^* = \kappa_1^* (\kappa_2 a^* \otimes \kappa_2 b^*).
\]

This corresponds to our earlier observation, that the \(h\)-transform can be computed in the tree one vertex and its children at a time. It illustrates that the transform as we have considered it until now is structure preserving on a directed tree. This property is lost in case of a general DAG.

To illustrate the issue, we consider Doob’s \(h\)-transform for the DAG in Figure 6. The rightmost picture shows the situation corresponding to a collider in graphical models.\(^2\) A string diagram is called **accessible** if all its internal connections are also accessible externally (Jacobs (2019), Section 3.3).
Upon defining \( \pi \), recall that for \( \lambda \), as a consequence to this proposition (with \( X \)), typically won’t have product form, the states become entwined (Jacobs, 2019). Here \( \kappa_1 = \kappa_{1a} \otimes \kappa_{1b} \) has product form, but \( \kappa_2 \) does not. The transformed kernel \( \kappa_1^* \) typically won’t have product form, the states become entwined (Jacobs, 2019).

Consider a kernel with multiple parents, say \( \kappa_{\text{pa}(s)-s}(x, dy) \). Its input \( x = \{x_u, u \in \text{pa}(s)\} \) is a concatenation of values of the process at the parent vertices. For an approximation \( \tilde{\kappa}_{\text{pa}(s)-s}(x, dy) \) of \( \kappa_{\text{pa}(s)-s}(x, dy) \), we have pullback

\[
g(x_{\text{pa}(s)}) := (\tilde{\kappa}_{\text{pa}(s)-s}g)(x_{\text{pa}(s)}). \tag{4.6}
\]

To backpropagate this function, we want to have a function in product form \( \prod_{u \in \text{pa}(s)} g_u(x_u) \) to each parent individually. To this end, write \( x_{\text{pa}(s)} = (x_1, \ldots, x_d) \) and suppose the density of \( x_{\text{pa}(s)} \) is given by \( \pi(x_1, \ldots, x_d) \). Then the joint distribution of \( X_{\text{pa}(s)} \) and its leaf descendants is proportional to \( \pi(x_1, \ldots, x_d)g(x_1, \ldots, x_d) \). Let \( \pi_i \) denote the marginal distribution of \( X_i \). Denote \( x_{-i} \) the vector \( x \) without its \( i \)-th component. Recall that for \( \lambda \)-probability densities \( p \) and \( q \), the KL-divergence of \( p \) to \( q \) is given by \( \text{KL}(p, q) = \int p \log p/q \, d\lambda \).

**Proposition 4.8.** The minimiser of \( \text{KL}(\pi g, \prod_{i=1}^{d} \pi_i g_i) \) over \( g_1, \ldots, g_d \), subject to \( \int g_i(x_i)\pi_i(x_i) \, d\lambda(x_i) = c_i \) (1 \( \leq i \leq d \)) is given by

\[
g_i(x_i) = c_i^{-1} \mathbb{E}_{\pi}[g(X_1, \ldots, X_d \mid X_i = x_i)].
\]

As a consequence to this proposition (with \( c_j = 1 \) for all \( j \)) we define \( g_u \) by

\[
g_u(x_u) = \int g(x_{\text{pa}(s)})\pi(x_{-u} \mid x_u) \, dx_{-u}, \quad u \in \text{pa}(s). \tag{4.7}
\]

Upon defining

\[
\tilde{\kappa}_{u\cdot s}(x_u, dy) := \int \tilde{\kappa}_{\text{pa}(s)-s}(x_{\text{pa}(s)}, dy)\pi(x_{-u} \mid x_u) \, dx_{-u}, \tag{4.8}
\]
it follows that we can equivalently define \( g_u \) in terms of these kernels by

\[
g_u(x_u) = \int \tilde{\kappa}_{pa(s)}(x_{pa(s)}, dy) g(y) dy \pi(x_{-u} | x_u) dx_{-u}
= \int \kappa_{-u}(x_u, dy) g(y) dy = (\kappa_{-u} g)(x_u)
\]

(use Fubini’s theorem). Here, the prediction kernels \( \tilde{\kappa}_{u}(x_u, \cdot) \), \( u \in pa(s) \) serve as a priori predictor of \( X_s \) if only \( x_u \) is known. (From this perspective, \( \kappa_{pa(s)}(x, \cdot) \) is the prior predictive distribution of \( X_s \) if \( x = \{ x_u, u \in pa(s) \} \) is known.)

**Definition 4.9.** Assume \( |pa(s)| \geq 2 \). To the kernel \( \kappa_{pa(s)} \) we define the pullback-kernel \( \bar{\kappa}_{pa(s)} \) induced by \( \pi(x_{pa(s)}) \) by its action on functions \( g \in \mathcal{B}(S_s) \)

\[
(\bar{\kappa}_{pa(s)} g)(x) = \prod_{u \in pa(s)} (\tilde{\kappa}_u g)(x_u).
\]

Here, the Markov kernels \( \tilde{\kappa}_u, u \in pa(s) \) are defined in Equation (4.8).

The operator \( \bar{\kappa}_{pa(s)} \) is not a Markov kernel operator and therefore we denote it with a bar rather than a tilde. From it we obtain a backward map \( B_{\bar{\kappa}_{pa(s)}} \) (Definition 3.1)

\[
B_{\bar{\kappa}_{pa(s)}}(g) = (m, \bar{\kappa}_{pa(s)} g), \quad m(x, y) = \frac{g(y)}{\prod_{u \in pa(s)} (\tilde{\kappa}_u g)(x_u)}
\]

to be used with the forward map for \( \kappa_{pa(s)} \): \( S_{pa(s)} \to S, S = (E, \mathcal{B}) \). From the form of the message \( m \) it follows immediately that the forward map picks up the “correct” weight according to (2.14). Summarising, for a kernel \( \kappa(x, dy) \) with \( x = (x_u, u \in pa(s)) \) pullback of \( h \) consists of

- an initial “ordinary” pullback as in Equation (4.6);
- computing \( (\bar{\kappa}_{pa(s)} g)(x_{pa(s)}) = \prod_{u \in pa(s)} g_u(x_u) \) with \( g_u \) as defined in Equation (4.7).

Intuitively, whereas the forward evolution would sample \( y \) based on its “complete” input \( x \), the backward kernel uses a collection of kernels, one for each parent \( u \in pa(s) \). Each of these kernels samples \( y \) based on only \( x_u \).

**Remark 4.10.** Up to this section our framework has been string diagrams of Markov kernels. Note that we make a change of perspective where we focus on the action of kernels on functions \( g \), where the action need not be induced by a Markov kernel.

## 5 Compositionality results for backward filtering forward guiding

Introducing a categorical perspective is motivated by the admission that we have already used the concepts introduced shortly in all but name in the previous section and by the
following testament: “We should approach the problem of statistical modelling and computation in a modular, composable, functional way, guided by underpinning principles from category theory.” Wilkinson (2017). While we defer a discussion of guided processes from a categorical point of view to a companion paper, we do give a number of compositionality results here.

5.1. Composition of kernels. Recall from (3.6) the definition \( F(\kappa, \tilde{\kappa}) = (F_{\kappa} | B_{\tilde{\kappa}}) \). If \( \kappa: S \to S' \) and \( \tilde{\kappa}: S \to S' \), then \( F(\kappa, \tilde{\kappa}) \) acts upon a pair consisting of a bounded function and measure as follows: \( F(\kappa, \tilde{\kappa}): \mathcal{B}(S') \times \mathcal{M}(S) \to \mathcal{B}(S) \times \mathcal{M}(S') \) with

\[
F(\kappa, \tilde{\kappa})(g', \mu) = (\tilde{\kappa}g', F_\kappa(m, \mu)),
\]

where the message \( m \) is defined by \( B_{\tilde{\kappa}}(g') = (m, \tilde{\kappa}g') \). Note that if \( \kappa = \tilde{\kappa} = \text{id} \), then \( \kappa g = g, m(x, y) = g(y)/g(x) \) and \( F_\kappa(m, \mu) = \mu \). Therefore, \( (F_{\text{id}} | B_{\text{id}})(g, \mu) = (g, \mu) \).

Hence there exists an identity optic \( I \), given by \( I = (F_{\text{id}} | B_{\text{id}}) \).

If Markov kernels can be composed, then their induced optics can be composed as well according to the following definition.

Definition 5.1. For \( i \in \{1, 2\} \) assume Markov kernels \( \kappa_i: S_{i-1} \to S_i \) and \( \tilde{\kappa}_i: S_{i-1} \to S_i \). Suppose \( \mu \in \mathcal{M}(S_0) \). We denote the composition of the optics \( F(\kappa_1, \tilde{\kappa}_1) \) with \( F(\kappa_2, \tilde{\kappa}_2) \) by \( F(\kappa_1, \tilde{\kappa}_1)F(\kappa_2, \tilde{\kappa}_2) \). We define \( F(\kappa_1, \tilde{\kappa}_1)F(\kappa_2, \tilde{\kappa}_2): \mathcal{B}(S_2) \times \mathcal{M}(S_0) \to \mathcal{B}(S_0) \times \mathcal{M}(S_2) \) by

\[
(F(\kappa_1, \tilde{\kappa}_1)F(\kappa_2, \tilde{\kappa}_2))(g, \mu) = (g_{12}, \mu_{12}),
\]

where \( (m_2, g_2) = B_{\tilde{\kappa}_2}(g), (m_1, g_{12}) = B_{\tilde{\kappa}_1}(g_2) \) and \( \mu_{12} = F_{\kappa_2}(m_2, F_{\kappa_1}(m_1, \mu)) \).

While this definition may look somewhat complicated, the following figure facilitates understanding the composition rule:

\[
F(\kappa_{12}, \tilde{\kappa}_{12}) = F(\kappa_1, \tilde{\kappa}_1)F(\kappa_2, \tilde{\kappa}_2)
\]

\[
\text{The setting of the following theorem is as in the above definition, with } \kappa_{12} = \kappa_1 \kappa_2 \text{ and } \tilde{\kappa}_{12} = \tilde{\kappa}_1 \tilde{\kappa}_2.
\]

Theorem 5.2. The optic of the composition of kernels is the same as the composition of their induced optics:

\[
F(\kappa_{12}, \tilde{\kappa}_{12}) = F(\kappa_1, \tilde{\kappa}_1)F(\kappa_2, \tilde{\kappa}_2)
\]

Proof. Assume \( \kappa_{12} = \kappa_1 \kappa_2 \) and \( \tilde{\kappa}_{12} = \tilde{\kappa}_1 \tilde{\kappa}_2 \). We show that the right-hand-side of (5.1) equals \( (F_{\kappa_{12}} | B_{\tilde{\kappa}_{12}})(g, \mu) \) which is, by definition,

\[
(F_{\kappa_{12}} | B_{\tilde{\kappa}_{12}})(g, \mu) = (\tilde{\kappa}_{12}g, \nu)
\]
with \( \nu(dy) = \int m_{12}(x, y) \mu(dx) \kappa_{12}(x, dy) \) and \( m_{12}(x, y) = g(y)/(\kappa_{12}g)(x) \). Clearly, \( \tilde{\kappa}_{12}g = \tilde{\kappa}_{1}\tilde{\kappa}_{2}g \). Hence, it remains to show that \( \mu_{12} = \nu \). We have

\[
\mu_{12}(dy) = \iint m_{1}(z, x)m_{2}(x, y) \mu(dz) \kappa_{1}(z, dx) \kappa_{2}(x, dy).
\]

This can be simplified, since

\[
m_{1}(z, x)m_{2}(x, y) = \frac{g_{2}(x)}{(\tilde{\kappa}_{1}g_{2})(z)} \frac{g(y)}{(\tilde{\kappa}_{1}\tilde{\kappa}_{2})(y)} = \frac{g(y)}{(\tilde{\kappa}_{12}g)(z)} = m_{12}(z, y),
\]

using \( g_{2}(x) = (\tilde{\kappa}_{2}g)(x) \). The second equality follows from cancellation of the numerator of the first term and denominator of the second term. Hence

\[
\mu_{12}(dy) = \iint m_{12}(z, y) \mu(dz) \kappa_{1}(z, dx) \kappa_{2}(x, dy) = \int m_{12}(z, y) \mu(dx) \kappa_{12}(z, dy) = \nu(dy).
\]

In particular, this theorem shows compositionality of Doob’s \( h \)-transform in the special case where \( \tilde{\kappa} \) is taken equal to \( \kappa \).

### 5.2. Product of kernels

Next, we define the parallel product of optics. Recall the definition of the \( \circ \)-product from Corollary 4.3.

**Definition 5.3.** Assume Markov kernels \( \kappa : S_{1} \rightarrow T_{1} \) and \( \tilde{\kappa} : S_{1} \rightarrow T_{1} \). Denote the parallel product of the optics \( F(\kappa_{1}, \tilde{\kappa}) \) with \( F(\kappa_{2}, \tilde{\kappa}_{2}) \) by \( F(\kappa_{1}, \tilde{\kappa}) \circ F(\kappa_{2}, \tilde{\kappa}_{2}) \). Let

\[
\mathcal{D}(T_{1}, T_{2}, S_{1}, S_{2}) = \{(h, \mu) \in \mathcal{B}(T_{1} \times T_{2}) \times \mathcal{M}(S_{1} \times S_{2}) : h = h_{1} \circ h_{2}, \mu = \mu_{1} \circ \mu_{2}\}.
\]

Define \( F(\kappa_{1}, \tilde{\kappa}_{1}) \circ F(\kappa_{2}, \tilde{\kappa}_{2}) : \mathcal{D}(T_{1}, T_{2}, S_{1}, S_{2}) \rightarrow \mathcal{D}(S_{1}, S_{2}, T_{1}, T_{2}) \) by

\[
(F(\kappa_{1}, \tilde{\kappa}_{1}) \circ F(\kappa_{2}, \tilde{\kappa}_{2}))(g_{1} \circ g_{2}, \mu_{1} \circ \mu_{2}) = (g_{1}^{′} \circ g_{2}^{′}, \mathcal{F}_{\kappa_{1}}(m_{1}, \mu_{1}) \circ \mathcal{F}_{\kappa_{2}}(m_{2}, \mu_{2})),
\]

where \( (m_{i}, g_{i}^{′}) = \mathcal{B}_{\kappa_{i}}(g_{i}) \) \( (i = 1, 2) \).

The following figure facilitates understanding the composition rule:

Theorem 5.4. On \( \mathcal{D}(T_{1}, T_{2}, S_{1}, S_{2}) \)

\[
F(\kappa_{1}, \tilde{\kappa}_{1}) \circ F(\kappa_{2}, \tilde{\kappa}_{2}) = F(\kappa_{1} \circ \kappa_{2}, \tilde{\kappa}_{1} \circ \tilde{\kappa}_{2}).
\]

(5.5)
Proof. Define 
\((\bar{g}, \bar{\nu}) = (\mathcal{F}_{\hat{\kappa}_1 \otimes \hat{\kappa}_2} | \mathcal{B}_{\hat{\kappa}_1 \otimes \hat{\kappa}_2})(g_1 \circ g_2, \mu_1 \otimes \mu_2)\).

From Definition 5.3 it follows that we need to show that this equals the right-hand-side of (5.4). First note that 
\(\bar{g} = (\hat{\kappa}_1 \otimes \hat{\kappa}_2)(g_1 \circ g_2) = (\hat{\kappa}_1 g_1) \otimes (\hat{\kappa}_2 g_2) = g'_1 \circ g'_2.\)

Now, with 
\(m(x,y) = (g_1 \circ g_2)(y) / (\hat{\kappa}_1 \otimes \hat{\kappa}_2)(g_1 \circ g_2)(x)\)
we have 
\(\bar{\nu}(dy) = \int m(x,y)(\kappa_1 \otimes \kappa_2)(x, dy)(\mu_1 \otimes \mu_2)(dx)\)
\(= \prod_{i=1}^2 \int \frac{g_i(y_i)}{(\hat{\kappa}_i g_i)(x_i)} \kappa_i(x_i, dy_i) \mu_i(dx_i) = \mathcal{F}_{\kappa_1}(m_1, \mu_1) \otimes \mathcal{F}_{\kappa_2}(m_2, \mu_2),\)
where \((m_i, g'_i) = B_{\kappa_i}(g_i) \ (i = 1, 2).\) 

Contrary to the result on sequential composition of optics (Theorem 5.2), this theorem is restricted to product measures. Hence, to forward sample in a compositional way, Theorem 5.4 suggests that we first need to marginalise the measure that is pushed forward by \(\mathcal{F}.\)

Definition 5.5. The marginalisation operator \(M\) acting on measures \(\mu \in \mathcal{M}(S \otimes S')\) is defined by by (using postfix notation for \(M\))
\[(\mu M)(B \times B') = \int \mu(B, dx') \otimes \int \mu(dx, B') \sqrt{\int d\mu} \sqrt{\int d\mu'}, \quad B \in \mathfrak{B}, B' \in \mathfrak{B}'.\]

Rather than pushing forward a measure using the map \(\mathcal{F},\) one can also push forward a weighted sample, which does not suffer from such restrictions. From a statistical perspective, this is the more interesting setting. To define sampling in a compositional way, we recall the following result.

Lemma 5.6 (Kallenberg (2002), p. 56). For a Markov kernel \(\kappa\) between a measure space \((E, \mathfrak{B})\) and a Borel space \((E', \mathfrak{B}')\), there is a measurable function \(\sigma_\kappa: E \times [0,1] \to E'\) and a random variable \(Z \sim U[0,1]\) such that the random variable \(\sigma_\kappa(x, Z)\) has law \(\kappa(x, \cdot)\) for each \(x \in E.\) The random variable \(Z\) is called an innovation variable.

Then, compositionality results for sampling can be obtained by explicitly “carrying along” the innovation variable \(Z.\) A detailed exposition of this approach in the language of category theory is part of ongoing research and considered slightly out of scope for this paper. On a directed tree this yields a fully compositional algorithm, where we are free to either first compose Markov kernels and then use BFFG or to compose optics. Such structure is however lost on a directed acyclic graph which is not a tree. This can be seen from Definition 4.9, where the pullback is defined as an operator, which not necessarily needs to be the pullback of a Markov kernel.
5.3. **Automatic BFFG.** We now have all constituents for a universal procedure of backward filtering and forward guiding (by sampling), which doesn’t put constraints on the program architecture, because it is applicable to any composition of (product-) kernels and it preserves the program architecture. The transformed program is a two-pass algorithm where the forward pass has the same architecture as the program: it has the same Markovian structure, the same function calls, the same diagrammatical form. Also the backward pass has the same architecture, though traversed backwards.

Forwards, a kernel $\kappa$ is replaced by $F_\kappa$, while backwards it is replaced by $B_{\tilde{\kappa}}$. Jointly, they form the optic $F(\kappa, \tilde{\kappa}) = \langle F_\kappa | B_{\tilde{\kappa}} \rangle$. As an example, automatic BFFG entails that the forward evolution

$$\delta x_0 \kappa_1 \otimes (\kappa_2 \otimes \kappa_3) \kappa_4$$

is turned into

$$\delta x_0 F(\kappa_1, \tilde{\kappa}_1) F(\psi_1, \psi) F(\kappa_2 \otimes \kappa_3, \tilde{\kappa}_2 \otimes \tilde{\kappa}_3)$$

by applying $F$ to all terms except for the final kernel pointing to an observation leaf. Kernel $\kappa_4$ emits information in the form of $g_3$, defined by

$$g_3: x \mapsto \frac{d\kappa_4(x, dy)}{\lambda(dy)} \bigg|_{y=x_{\text{obs}}}$$

By applying the program transformation (5.7) to $(g_3, \delta x_0)$ a weighted sample of the smoothing distribution can be obtained, as in (3.8). Equation (5.7) is a translation of Markov kernels in (5.6) to optics.

In this way, for $X$ on any DAG (translated to the corresponding string diagram of kernel compositions) an approximation $X^*$ of the conditional $X$ is obtained that can be sampled from. Note that $X^*$, unlike $X^*$, preserves the Markovian structure of $X$ and does not introduce new edges in the dependency graph (as it was the case in Figure 6). This is of importance: for a probabilistic program which is able to sample $X$, it is easier to adapt it to sample from $X^*$ with weights, than to adapt it to sample from $X^*$ directly (which has a different dependence structure). The former is possible as automatic program transform.

6 Examples of discrete-time guided processes

In this section we provide various examples to illustrate our approach.

The examples make use of the idea that the composition of backward steps is computationally cheap if it preserves a parametrised form of $g$. Hence, suppose $g$ can be parametrised by $g = U(\zeta)$ for a parameter $\zeta$ and a parametrisation $U$. Backward filtering is tractable when

- $\tilde{\kappa}g = U(\zeta')$ for some $\zeta'$;
- $\kappa_{\psi}(g_1 \otimes \cdots \otimes g_k) = U(\zeta')$ for some $\zeta'$ (this corresponds to the fusion step).
In some models the (otherwise intractable) fusion step can be bypassed by only applying the backward map on a line graph, see Section 6.3 for examples. In case \(g\) is proportional to the density of an exponential family member distribution, then the fusion step is tractable.

In applying the forward map for sampling less tractability is required, as for example the pseudo-marginal Metropolis-Hastings algorithm can be used to unbiasedly estimate \((\kappa g)(x)\). Details are given ahead in Section 8.3.

6.1. **Gaussian filtering and smoothing.** Consider the stochastic process on \(G\) with transitions defined by

\[
X_t \mid X_s = x \sim N(\mu_t(x), Q_t(x)), \quad t \in \text{ch}(s). \tag{6.1}
\]

Unfortunately, for this class of models (parametrised by \((\mu_t, Q_t)\)), only in very special cases Doob’s \(h\)-transform is tractable. For that reason, we look for a tractable \(h\)-transform to define a guided process \(X^\circ\). This is obtained in the specific case where

\[
\tilde{X}_t \mid \tilde{X}_s = x \sim N(\Phi_t x + \beta_t, Q_t), \quad t \in \text{ch}(s).
\]

Below we show that backward filtering, sampling from the forward map and computing the weights are all fully tractable.

In the following, we write \(\varphi(x; \mu, \Sigma)\) for the density of the \(N(\mu, \Sigma)\)-distribution, evaluated at \(x\). Similarly, we write \(\varphi^{\text{can}}(x; F, H)\) for the density of canonical Normal distribution with potential \(F = \Sigma^{-1} \mu\) and precision matrix \(H = \Sigma^{-1}\), evaluated at \(x\).

The \(g\) functions can be parametrised by the triple \((c, F, H)\):

\[
g(y) = \exp \left( c - \frac{1}{2} y' H y + y' F \right)
= \varpi(c, F, H) \varphi^{\text{can}}(y; F, H) = \varpi(c, F, H) \varphi(y; H^{-1} F, H^{-1}), \tag{6.2}
\]

where

\[
\log \varpi(c, F, H) = c - \log \varphi^{\text{can}}(0, F, H).
\]

We write \(g(x) = U(c, F, H)(x)\) for \(g\) and parameters as in (6.2).

**Theorem 6.1.** Let \(\kappa(x, dy) = \varphi(y; \mu(x), Q(x)) dy\) and \(\tilde{\kappa}(x, dy) = \varphi(y; \Phi x + \beta, Q) dy\). Assume that \(g = U(c, F, H)\) with invertible \(H\).

(i) Pullback for \(\kappa\): With \(C(x) = Q(x) + H^{-1}\) invertible,

\[
(\kappa g)(x) = \varpi(c, F, H) \varphi(H^{-1} F; \mu(x), C(x)).
\]

(ii) Backward Information Filter initialisation from leaves: if \(y \sim N(\Phi x + \beta, Q)\) is observed at a leaf, then

\[
g(x) = U(\bar{c}, \bar{F}, \bar{H})(x) \quad \text{where} \quad \begin{cases} 
\bar{H} = \Phi' Q^{-1} \Phi \\
\bar{F} = \Phi' Q^{-1} (y - \beta) \\
\bar{c} = \log \varphi(\beta; y, Q).
\end{cases}
\]
(iii) Pullback for $\tilde{\kappa}$: With $C = Q + H^{-1}$ invertible,

$$\tilde{\kappa} g = U(\bar{c}, \bar{F}, \bar{H})$$

where

$$\begin{cases}
\bar{H} = \Phi' C^{-1} \Phi \\
\bar{F} = \Phi' C^{-1} (H^{-1} F - \beta) \\
\bar{c} = c - \log \varphi^{\text{can}}(0, F, H) + \log \varphi(\beta; H^{-1} F, C)
\end{cases}$$

and

$$B_{\tilde{\kappa}} = (m, \tilde{\kappa} g), \quad m(x, y) = \frac{U(c, F, H)(y)}{U(\bar{c}, \bar{F}, \bar{H})(x)}.$$ 

If $\Phi$ is invertible, then alternatively

$$\log \varpi(\bar{c}, \bar{F}, \bar{H}) = \log \varpi(c, F, H) - \log |\Phi|.$$ 

(iv) Forward map:

$$F_{\kappa}(m, \mu) = \nu, \quad \nu(dy) = \int w(x) \varphi^{\text{can}}(y; F + Q(x)^{-1} \mu(x), H + Q(x)^{-1}) \mu(dx) dy,$$

where the weight at $x$ is given by

$$w(x) \equiv \frac{(\kappa g)(x)}{(\tilde{\kappa} g)(x)} = \frac{(\kappa g)(x)}{U(\bar{c}, F, H)(x)} = \frac{\varphi(H^{-1} F; \mu(x), Q(x) + H^{-1})}{\varphi^{\text{can}}(0, F, H) U(\bar{c} - c, F, H)(x)}.$$ 

In particular, if $\mu = \varpi \delta_x$, the forward map gives the importance weight and conditional distribution for the next random draw,

$$\varpi w(x) \cdot N^{\text{can}}(F + Q(x)^{-1} \mu(x), H + Q(x)^{-1}).$$ 

(v) Fusion: if $g_i = U(c_i, F_i, h_i), i = 1, \ldots, k$, then

$$g \equiv g_1 \odot \cdots \odot g_k = U\left(\sum_{i=1}^k c_i, \sum_{i=1}^k F_i, \sum_{i=1}^k H_i\right).$$ 

In particular, $F_{\odot_k}(\cdot, \varpi \delta_x)$, where $\varpi$ is a weight, makes $k$ weighted copies $\varpi^{1/k} \delta_x$.

(vi) Backward splitting of $g$ to two parents nodes: suppose $g(y) = \varpi(c, F, H) \varphi(y; \mu, P)$, with $\mu = H^{-1} F$ and $P = H^{-1}$ and assume a flat prior on the parent vertices. Consider the partitioning

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \end{bmatrix}, \quad \mu = \begin{bmatrix} \mu^{(1)} \\ \mu^{(2)} \end{bmatrix}, \quad P = \begin{bmatrix} P^{(11)} & P^{(12)} \\ P^{(21)} & P^{(22)} \end{bmatrix}.$$ 

Then

$$(\tilde{\kappa} g)(y^{(1)}, y^{(2)}) = \sqrt{\varpi(c, F, H)} \varphi(y^{(1)}; \mu^{(1)}, P^{(11)}) \odot \sqrt{\varpi(c, F, H)} \varphi(y^{(2)}; \mu^{(2)}, P^{(22)}).$$
Proof. The proof is elementary. For completeness, the proof is given in appendix C. For the pullback, similar results have appeared in the literature, for example Chapter 7 in Chopin and Papaspiliopoulos (2020), Wilkinson and Yeung (2002) and Chapter 5 in Cappé et al. (2005).

Taking an inverse of $H$ respective $C$ can be avoided using $(Q + H^{-1})^{-1} = (QH + I)^{-1}, (Q + H^{-1})^{-1} = H - H(Q^{-1})^{-1}. While backward filtering for a linear Gaussian process on a tree is well known (see e.g. Chou et al. (1994), section 3), results presented in the literature often don’t state update formulas for the constant $\varpi$ (or equivalently $c$). If the mere goal is smoothing with known dynamics, this suffices. However, we will also be interested in estimating parameters in $\mu$ and or $Q$ then the constant cannot be ignored.

In case the dynamics of $X$ itself are linear, it simply follows that the weights equal 1. Moreover, if additionally the process lives on a “line graph with attached observation leaves”, where each non-leaf vertex has one child in $\mathcal{S}$ and at most one child in $\mathcal{V}$, our procedure is essentially equivalent to Forward Filtering Backward Sampling (FFBS, Carter and Kohn (1994)), the difference being that our procedure applies in time-reversed order. On a general directed tree however the ordering cannot be changed and the filtering steps must be done backwards, as we propose, just like in message passing algorithms in general.

6.2. Discrete state-space Markov chains and particle systems.

6.2. Branching particle on a tree. Assume a “particle” takes values in a finite state space $E = \{1, \ldots, R\}$ according to the $R \times R$ transition matrix $K$. At each vertex, the particle is allowed to copy itself and branch.

The algorithmic elements can easily be identified. The forward kernel $\kappa(x, dy)$ can be identified with the matrix $K$. Furthermore, the map $x \mapsto g(x)$ can be identified with the column vector $h = [g_1, \ldots, g_R]'$, where $g_i = g(i)$. Hence $g$ is parametrised by $g$ and we write $g = U(g)$.

The following theorem is easily proved. It gives the necessary ingredients for applied the backward and forward map.

Theorem 6.2. Let $\kappa(x, dy)$ and $d \tilde{\kappa}(x, dy)$ be represented by the stochastic matrices $K$ and $\tilde{K}$ respectively. Assume that $h = U(g)$.

(i) Pullback for $\kappa$: $\kappa g = U(Kg)$.

(ii) Pullback for $\tilde{\kappa}$: $\tilde{\kappa} g = U(\tilde{K}g)$ and

$$B_{\tilde{\kappa}} = (m, \tilde{\kappa}g), \quad m(x, y) = \frac{U(Kg)(y)}{U(\tilde{K}g)(x)}.$$ 

Denote by $M$ the matrix with elements $m(x, y), \ x, y \in E.$
(iii) Fusion: if \( g_i = U(g_i), \ i = 1, \ldots, k, \) then
\[
\langle k \rangle(g_1 \odot \cdots \odot g_k) = U\left( \bigodot_{i=1}^{k} g_i \right),
\]
where \( \odot \) denotes the Hadamard (entrywise) product.

(iv) Forward map: Let \( \mu \) be a (row) probability vector. If \( F_{\kappa}(m, \mu) = \nu, \) then for \( k \in E \)
\[
\nu(\{k\}) = \mu(M \odot K)e_k,
\]
with \( e_k \) the \( k \)-th standard basis-vector in \( \mathbb{R}^R. \)

(v) The weight at \( x \in E \) is given by
\[
w(x) = \frac{\langle \kappa g \rangle(x)}{\langle \bar{\kappa} g \rangle(x)} = \frac{\langle K g \rangle_x}{\langle \bar{K} g \rangle_x}
\]
where we denote the \( j \)-th element of the vector \( a \) by \( \langle a \rangle_j \).

(vi) Initialisation at the leaves: at a leaf vertex with observation \( k \in E, \) set \( g = e_k. \)

(vii) Backward splitting of \( g \) to two parents nodes: suppose \( E = \{(x, y): x = 1, \ldots, R_1, y = 1, \ldots, R_2\}. \) Then \( g \) has the form
\[
g = [g_{11} \cdots g_{1R_2} g_{21} \cdots g_{2R_2} \cdots \cdots g_{R_11} \cdots g_{R_1R_2}]'.
\]
Let
\[
g^{(1)}_i = \sum_{j=1}^{R_2} g_{ij} \in B(\{1, \ldots, R_1\}), \quad g^{(2)}_i = \sum_{j=1}^{R_1} g_{ji} \in B(\{1, \ldots, R_2\})
\]
and \( c = \sum_{i,j} h_{ij}, \) then under a flat prior on the parent vertices \( \bar{\kappa} g = g^{(1)}/\sqrt{c} \odot g^{(2)}/\sqrt{c}. \)

While we can simply take \( \bar{\kappa} = \kappa \) on a tree, yielding unit weights, in case \( R \) is very large, it can nevertheless be advantageous to use a different (simpler) map \( \bar{\kappa}. \) To see, this, note that we only need to compute one element of the matrix vector product \( Kg, \) but need to compute the full vector \( \bar{K}g \) in the backward map. Hence, choosing \( \bar{K} \) sparse can give computational advantages.

6.2. Interacting particles – cellular automata – agent based models. Now consider a discrete time interacting particle process, say with \( n \) particles, where each particle takes values in \( \{1, \ldots, R\}. \) Hence, a particle configuration \( x \) at a particular time-instant takes values in \( E = \{1, \ldots, R\}^n. \)

A simple example consists of particles with state \( E = \{1 \equiv S, 2 \equiv I, 3 \equiv R\} \) that represent the health status of individuals that are either Susceptible, Infected or Recovered. Then the probability to transition from state \( S \) to \( I \) may depend on the number of nearby
particles (individuals) that are infected, hence the particles are “interacting”. A similar example is obtained from time-discretisation of the contact process (cf. Liggett (2005)). A visualisation of the DAG is given in Figure 7: time moves from left to right, vertical connects represent state changes of particles and the diagonal connections represent local interactions. Note that each particle has multiple parents defined by a local neighbourhood and that a model like this is sometimes referred to as a cellular automaton.

Let $x \in E$. Without additional assumptions, the forward transition kernel can be represented by a $R^n \times R^n$ transition matrix. With a large number of particles such a model is not tractable computationally. To turn this into a more tractable form, we make the simplifying assumption that conditional on $x$ each particle transitions independently. This implies that the forward evolution kernel $\kappa(x, dy)$ can be represented by $(K_1(x), \ldots, K_n(x))$, where $K_i(x)$ is the $R \times R$ transition matrix for the $i$-th particle. Note that the particles interact because the transition kernel for the $i$-th particle may depend on the state of all particles.

Due to interactions, it will computationally be very expensive to use $\kappa$ for the backward map. Instead, in the backward map we propose to ignore/neglect all interactions between particles. This means that effectively we use a backward map where all particles move independently, and the evolution of the $i$-th particle depends only on $x_i$ (not $x$, as in the forward kernel). Put differently, in the backward map, we simplify the graphical model to $n$ line graphs, one for each particle. See Figure 7.

This choice implies that $\tilde{\kappa}$ can be represented by $(\tilde{K}_1, \ldots, \tilde{K}_n)$ and the map $x \mapsto g(x) = \prod_{i=1}^n g_i(x)$ can be represented by $(g_1, \ldots, g_n)$, where $g_i = [g_{i1}, \ldots, g_{iR}]'$. We write $g = U(g_1, \ldots, g_n)$.

**Theorem 6.3.** Assume $\kappa$ and $\tilde{\kappa}$ are represented by $R \times R$ stochastic matrices $K_1, \ldots, K_n$ and $\tilde{K}_1, \ldots, \tilde{K}_n$ respectively. Assume that $g = U(g_1, \ldots, g_n)$.

(i) Pullback for $\kappa$: $U(\kappa g)(x) = (K_1(x)g_1, \ldots, K_n(x)g_n)$

(ii) Pullback for $\tilde{\kappa}$: $U(\tilde{\kappa} g) = (\tilde{K}_1 g_1, \ldots, \tilde{K}_n g_n)$

(iii) Parametrisation of messages: For each $i \in \{1, \ldots, n\}$ let $M_i$ be the matrix with elements

$$M_i(x,y) = \frac{U(K_i g)(y)}{U(K_i g)(x)}.$$ 

Set $m = (M_1, \ldots, M_n)$.

(iv) Forward map: Let $\mu_1, \ldots, \mu_n$ be a $n$ (row) probability vectors with $\mu_i$ representing the distribution of the $i$-th particle. If $\mu = \otimes_{i=1}^n \mu_i$ and $\mathcal{F}_\kappa(m, \mu) = \nu$, then $\nu = \otimes_{i=1}^n \nu_i$ where for $k \in E$

$$\nu_i(\{k\}) = \mu(M_i \circ K_i(x))e_k,$$

with $e_k$ the $k$-th standard basis-vector in $\mathbb{R}^R$. 

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Figure 7: DAG for the interacting particle process of section 6.2. Particles move from left to right and the grey grid depicts the dependence structure. Here, parents of a vertex are defined by a local neighbourhood (in this case all particles at distance at most 1). For example particle 1 at time 1 (indexed by 1(1)) has parents 1(0) and 2(0). For backward filtering, the dynamics are reduced

(v) The weight at $x$ is given by

$$w(x) = \frac{(\kappa g)(x)}{(\bar{\kappa} g)(x)} = \prod_{i=1}^{n} \frac{\langle K_i(x) g_i \rangle_{x_i}}{\langle \bar{K}_i g_i \rangle_{x_i}}.$$  

(vi) Initialisation at the leaf: for observation $x_{M+1} \in E$ set $g_i = e^{\langle x_{N+1} \rangle_i}$ for $i \in \{1, \ldots, n\}$.

6.3. Backward diagonalisation. The example of the previous section shows a generic way to deal with interacting particles with a pattern as shown in Figure 7. Here, conditional on the state of all particles at a particular “time”, all particles transition independently, though with transition probabilities that may depend on the state of all particles. The backward filtering is however done on $n$ separate line graphs, thereby fully bypassing the need of a tractable fusion step. We call this backward diagonalisation.

In case of a finite-state space, the fusion step can be done, but the computational cost is exponentially increasing with the number of time-steps. The next section provides an example where the fusion step is not tractable at all, but backward diagonalisation ensures it is not needed.

6.4. Independent Gamma increments. In this example, we consider a process with Gamma distributed increments. We consider a line graph (where $|\text{ch}(s)| = 1$ for $s \in S_0$) with a single observational leaf $v$, attached to the end of the single path in $S_0$. We write $Z \sim \text{Gamma}(\alpha, \beta)$ if $Z$ has density $\psi(x; \alpha, \beta) = \beta^\alpha \Gamma(\alpha)^{-1} x^{\alpha-1} e^{-\beta x} 1_{(0, \infty)}(x)$. 

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Choose mappings $\alpha_t, \beta_t: (0, \infty) \to [1/C, C]$ for some $C > 0$. We define a Markov process with Gamma increments on $\mathcal{G}$ by

$$X_t - X_s | X_s = x \sim \text{Gamma}(\alpha_t, \beta_t(x)), \quad \text{if } s = \text{pa}(t), \quad X_0 = x_0.$$ 

This implies

$$\kappa_{\alpha_t}(x; y) = \psi(y - x; \alpha_t, \beta_t(x)).$$

Note that $X$ can be thought of as a time discretised version of the SDE $dX_t = \beta^{-1}(X_t) dL_t$ driven by a Gamma process $(L_t)$ with scale parameter 1, observed at final time $T$. See Belomestny et al. (2019) for a continuous time perspective on this problem. A statistical application will typically involve multiple observations and henceforth multiple line graphs. Simulation on each line graph corresponds to conditional (bridge) simulation for the process $X$.

As the $h$-transform is not tractable, we introduce the process $\tilde{X}$ which is defined as the Markov process with Gamma increments on $\mathcal{G}$ induced by $(\alpha_t, \beta)$, with $\beta$ a user specified nonnegative constant. This process is tractable and is used to define the $h$-transform.

As before, we state our results using the kernels $\kappa$ and $\tilde{\kappa}$. Define for $A, \beta > 0$

$$g(y) = \psi(x_v - y; A, \beta) \quad (6.3)$$

and write $h = U(A, \beta)$.

Define the exponentially-tilted Beta-distribution with parameters $\gamma_1, \gamma_2 > 0$ and $\lambda \in \mathbb{R}$ as the distribution with density

$$q_{\gamma_1, \gamma_2, \lambda}(z) \propto z^{\gamma_1-1} (1-z)^{\gamma_2-1} e^{-\lambda z} 1_{(0,1)}(z). \quad (6.4)$$

We denote this distribution by $\text{ExpBeta}(\gamma_1, \gamma_2, \lambda)$. Sampling from this distribution can be accomplished for example using rejection sampling, with importance sampling distribution $\text{Beta}(\alpha, A, \xi(x))$.

**Theorem 6.4.** Let $\kappa(x, dy) = \psi(y - x; \alpha, \beta(x)) dy$ and $\tilde{\kappa}(x, dy) = \psi(y - x; \alpha, \beta) dy$. Assume that $g = U(A, \beta)$.

(i) Pullback for $\kappa$: 

$$ (\kappa g)(x) = U(A + \alpha, \beta)(x) \left( \frac{\beta(x)}{\beta} \right)^\alpha e^{-\xi(x)Z}, $$

where $Z \sim \text{Beta}(\alpha, A)$ and $\xi(x) = (\beta(x) - \beta)(x_v - x)$.

(ii) Pullback for $\tilde{\kappa}$: 

$$ (\tilde{\kappa} g)(x) = U(A + \alpha, \beta)(x).$$

(iii) Forward map: if $\mu = \delta_x$, then a draw $y$ from $\mathcal{F}_\kappa(m, \mu)$ can be generated by first drawing $z \sim \text{ExpBeta}(\alpha, A, \xi(x))$ and then setting $y = x + z(x_v - x)$.

(iv) The weight at $x$ is given by

$$ w(x) = \frac{(\kappa g)(x)}{(\tilde{\kappa} g)(x)} = \left( \frac{\beta(x)}{\beta} \right)^\alpha e^{-\xi(x)Z} $$

where $Z \sim \text{Beta}(\alpha, A)$.
Proof. See Appendix C.

Note that the expression for the weight immediately suggests a method to estimate $w(x)$ unbiasedly. The setting is restricted to a line graph, as fusion of $g_1$ and $g_2$ of the form (6.3) does not lead to a fused function of the same form.

The model can be extended to $n$ Markov processes with Gamma increments, which evolve conditionally independent, where it is assumed that the forward evolution consists of composing kernels

$$
\kappa(x, dy) = \prod_{i=1}^{n} \psi(y_i - x_i; \alpha, \beta(x)) dy.
$$

The backward kernel $\tilde{\kappa}$ is then taken to be the same, with $\beta(x)$ replaced with $\tilde{\beta}$. This is an instance of backward diagonalisation.

Remark 6.5. The setting of this section can be generalised: suppose for $s = pa(t)$ that

$$
X_t - X_s \mid X_s = x \sim \mathcal{D}(\theta_t(x)),
$$

with $\mathcal{D}(\theta)$ a distribution with parameter $\theta$ supported on $(0, \infty)$, say with density $\psi(\cdot; \theta)$.

Tracing back the proof, the derivation of $\kappa h$ shows that if $\kappa(x, dy) = \psi(y - x; \theta) dy$, then backward filtering is tractable if

$$
(k g)(x) = \int \psi(x_v - y; \theta) \psi(y - x; \theta(x)) dy = \int \psi(x_v - x - z; \theta) \psi(z; \theta(x)) dz
$$

can be written as $c \psi(x_v - x; \tilde{\theta}(x))$ for some $\tilde{\theta}(x)$. Hence, the results can be extended to the case where increments are closed under convolution. The Gamma distribution has this property, but so does the Inverse Gaussian IG$(\mu, 2\mu^2)$-distribution for example.

7 Examples of continuous-time guided processes

7.1. Stochastic differential equations. Suppose the Markov process $X$ is defined as a solution to the stochastic differential equation (SDE)

$$
dX_t = b(t, X_t) dt + \sigma(t, X_t) dW_t.
$$

Here $\sigma$ is possibly non-constant, as is often the case for physically meaningful local noise structure, for example for those obtained through the stochastically constrained variational principle, Cf. Holm (2015).

Assume we take $g$ derived from the simpler SDE $d\tilde{X}_t = \tilde{b}(t, \tilde{X}_t) dt + \tilde{\sigma}(t, \tilde{X}_t) dW_t$. In case the drift is linear and diffusivity only time-dependent, then $g$ is proportional to a Gaussian density and can be represented as $g(t, x) = \exp (c(t) + F(t)'x - \frac{1}{2}x'H(t)x)$, for scalar-valued $c$, vector-valued $F$ and matrix-valued $H$ (just as in (6.2)). In this case the term in the exponent of the weight in Theorem 2.5 satisfies

$$
\frac{(\mathcal{L} - \tilde{\mathcal{L}})g}{g} = \sum_i (b_i - \tilde{b}_i) \frac{\partial g}{g} + \frac{1}{2} \sum_{i,j} (a_{ij} - \tilde{a}_{ij}) \frac{\partial^2 g}{g},
$$

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where we have omitted arguments \((s, x)\) from the functions and \(\partial_i\) denotes the partial derivative with respect to \(x_i\). If we set \(r_i = (\partial_i g)/g\), then \((\partial_{ij} g)/g = \partial_j r_i + r_i r_j\) and therefore \[
\frac{(\mathcal{L} - \tilde{\mathcal{L}})g}{g} = \sum_i \left( b_i - \tilde{b}_i \right) r_i + \frac{1}{2} \sum_{i,j} \left( a_{ij} - \tilde{a}_{ij} \right) \left( \partial_j r_i + r_i r_j \right). \]

This expression coincides with the expression for the likelihood given in Proposition 1 of Schauer et al. (2017), but the proof given here is much shorter.

In case the process \(\tilde{X}\) defines a linear SDE, then solving the Kolmogorov backwards equation on \([0, T]\) reduces to solving a system of ordinary differential equations. Theorem 2.5 in Mider et al. (2021) gives these ODEs in their “information filter” form. The output of these equations is fully compatible with the form of \(g\) in Subsection 6.1. In particular, fusion is tractable and our approach enables to simulate guided processes for conditioned branching diffusions.

The corresponding rules for Mitosis.jl are provided by MitosisStochasticDiffEq.jl using solvers from Julia’s SciML (sciml.ai) ecosystem for Scientific Machine Learning (Rackauckas and Nie, 2017).

7.2. First hitting time of a diffusion. Doob’s \(h\)-transforms are not restricted to conditioning on the value of a process at a fixed time. Rather, they can generally be applied for different types of conditioning such as for example conditioning on the first hitting time of a set. Accordingly, guided processes can be used for general conditionings.

As a concrete example, suppose that over an edge a one-dimensional diffusion process instead of evolving for a fix time, evolves until it first hits level \(v\), \(v\) being considered fixed and the hitting time is observed. Suppose the dynamics of the diffusion are governed by the SDE \(dX_t = b(X_t) dt + dW_t\). Let \(\tau_v\) denote the first hitting time of \(v\). Now assume existence of the density \(p\) such that \(\mathbb{P}_{s,x}(\tau_v \in dT) = p(s, x; T) dT\). In general \(p\) is intractable, though if \(b \equiv 0\) then
\[
g(t, x) := p(t, x; T) = \frac{|v - x|}{2\pi(T - t)^3} e^{-\frac{(v-x)^2}{2(T-t)}} \]
which can be used to define the guided process. It is easily verified that \(h\) is space-time harmonic, for \(x \neq v\)
\[
\frac{\partial}{\partial t} g(t, x) + \frac{1}{2} \frac{\partial^2}{\partial x^2} g(t, x) = 0.
\]
Furthermore \(\nabla \log g(t, x) = (v - x)/(T - t) + 1/(x - v)\), which implies
\[
\mathcal{L}^g f(x) = \left( b(x) + \frac{v - x}{T - t} + \frac{1}{x - v} \right) f'(x) + \frac{1}{2} f''(x).
\]

Note that in case \(b \equiv 0\), this is the generator of a (shifted and scaled) Bessel bridge.

In the larger picture of continuous processes embedded into graphical models, the observation of such a hitting time may correspond to an “observation operation” (a leaf in the DAG) with transition density \(p(s, x; T)\).
7.3. Continuous time Markov chains on a countable set. Let \( X \) denote a continuous time Markov process taking values in the countable set \( E \). Let \( \mathcal{Q} = (q(x,y), x,y \in E) \) be a \( Q \)-matrix, i.e. its elements \( q(x,y) \) satisfy \( q(x,y) \geq 0 \) for all \( x \neq y \) and \( \sum_y q(x,y) = 0 \). Define \( c(x) = -q(x,x) \). If \( \sup_x c(x) < \infty \), then \( \mathcal{Q} \) uniquely defines a continuous time Markov chain with values in \( E \). Its transition probabilities \( p_t(x,y) \) are continuously differentiable in \( t \) for all \( x \) and \( y \) and satisfy Kolmogorov’s backward equations:

\[
\frac{d}{dt} p_t(x,y) = \sum_z q(x,z)p_t(z,y)
\]

(cf. Liggett (2010), Chapter 2, in particular Corollary 2.34). The infinitesimal generator acts upon functions \( f : E \rightarrow \mathbb{R} \) by

\[
\mathcal{L}f(x) = \sum_{y \in E} q(x,y) (f(y) - f(x)) = \sum_{y \in E} q(x,y)f(y), \quad t \in [0, \infty), \ x \in E. \quad (7.1)
\]

In the specific setting where \( E \) is finite with states labeled by \( 1, 2, \ldots, R \), \( \mathcal{Q} \) is an \( R \times R \)-matrix. Then, by evaluating \( \mathcal{L}f(x) \) for each \( x \in E \) we can identify \( \mathcal{L}f \) by \( Qf \), where \( f \) is the column vector with \( i \)-th element \( f_i = f(i) \).

Suppose an \( h \) transform \( h : [0, \infty) \times E \rightarrow \mathbb{R} \) is specified. It induces a guided process \( X^\circ \) for which the generator of the space-time process can be derived using Equation (2.19) and the preceding display. Some simple calculations reveal that for \( f : [0, \infty) \times E \rightarrow \mathbb{R} \)

\[
h(t,x)(\mathcal{A}^\circ f)(t,x) = \sum_{y \in E} q(x,y) (f(t,y) - f(t,x)) h(t,y) + h(t,x) \frac{\partial f}{\partial t}(t,x)
\]

This implies that the generator of \( X^\circ \) acts upon functions \( f : [0, \infty) \times E \rightarrow \mathbb{R} \) as

\[
(\mathcal{L}^\circ f)(x) = \sum_{y \in E} q(x,y)(f(y) - f(x)) \frac{h(t,y)}{h(t,x)}. \quad (7.2)
\]

Therefore, comparing with (7.1), we see that \( X^\circ \) is a time-inhomogenous Markov process \( X^\circ \) with time dependent generator matrix \( \mathcal{Q}^\circ_t = (q^\circ_t(x,y), x,y \in E) \), where

\[
q^\circ_t(x,y) = q(x,y) \frac{h(t,y)}{h(t,x)} \quad \text{if} \quad y \neq x
\]

and \( q^\circ_t(x,x) = 1 - \sum_{y \neq x} q^\circ_t(x,y) \).

Now assume that \( \tilde{X} \) is a continuous time Markov process on \( E \) with tractable \( h \)-function \( g \) such that \( \tilde{A}g = 0 \), where \( \tilde{A} \) is the generator of the space-time process \( (t, \tilde{X}_t) \). If \( \mathcal{Q} = (\tilde{q}(x,y), x,y \in E) \) denotes the \( Q \)-matrix of \( \tilde{X} \), then the integrand in the exponential of the weight in Theorem 2.5 equals

\[
\int_0^T (\mathcal{L} - \tilde{L})g(t,X^\circ_t) dt = \int_0^T \sum_{y \in E} (q(X^\circ_t,y) - \tilde{q}(X^\circ_t,y))g(t,y) dt.
\]

For finite-state Markov chains transition densities can be computed via \( (p_t(x,y), x,y \in E) = e^{t\mathcal{Q}} \) and this would immediately give \( h \), implying no need for constructing a guided
process via an approximation to Doob’s $h$-transform. While strictly speaking this is true, in case $|E|$ is large, numerically approximating the matrix exponential can be computationally demanding. In that case, by simplifying the dynamics of the Markov process, one may choose an approximating continuous time Markov process $\tilde{X}$ (on $E$) where $\tilde{Q}$ is block diagonal, as this simplifies evaluation of matrix exponentials.

8 Sampling and statistical inference using guided processes

In this section we discuss a variety of ways in which Theorem 2.2 can be used. Let $P^o$ denote the law of $X^o_S$ and let $P^*$ denote the law of $X^o_S | X_V$. Then Theorem 2.2 states

$$\frac{dP^*}{dP^o}(X^o_S) = \frac{g_0(x_0)}{\text{ev}(x_0)^\Psi(X^o_S)} \Psi(X^o_S),$$

where

$$\Psi(X^o_S) = \prod_{s \in S} w_{pa(s) \rightarrow s}(X^o_{pa(s)}) \prod_{v \in V} \frac{h_{pa(v) \rightarrow v}(X^o_{pa(v)})}{g_{pa(v) \rightarrow v}(X^o_{pa(v)})}.$$ 

Taking $f \equiv 1$ in its statement we obtain

$$\text{ev}(x_0) = g_0(x_0)E\Psi(X^o_S). \quad (8.1)$$

Our standing assumption is that we can define $g_s$ for all edges such that $g_s$ can be computed efficiently for all $s \in S_0$. Depending on the the dynamics of $X$ and $g$, it may then be possible to easily forward sample $X^o$ from root vertices towards leaf vertices (for example, in Gaussian nonlinear smoothing this is the case, cf. section 6.1). Then, again depending on $X$ and $g$ the weights $w_s$ may be tractable or not.

Note that $x_0$ may encode any unknown parameters such as the starting point of a stochastic process or a parameter $\theta$ reflecting uncertainty about the forward dynamics. Then formally, there is an edge from $x_0$ to every other vertex in the graph. In the backward filtering step we are free to drop such edges. In that case, the evidence depends on $\theta$. While the backward filter does not return an approximation to the distribution of $\theta$ conditional on the leaf observations, the evidence can still be computed via (8.1) and used to infer the parameter.

There are links with a variety of popular methods from computational statistics:

8.1. Importance sampling. Suppose interest lies in $I := \mathbb{E}\varphi(X^*)$. We simulate independent copies $\{X^{o,i}, i = 1, \ldots B\}$ under $P^o$. Next, define the importance sampling estimator

$$\hat{I} := \frac{1}{B} \sum_{i=1}^B w_{i}\varphi(X^{o,i}), \quad w_i = \frac{\Psi(X^{o,i})}{\sum_{i=1}^B \Psi(X^{o,i})}.$$ 

Note that $w_i$ does not depend on $\text{ev}(x_0)$ and the estimator requires that the weights can be computed efficiently (if this is not the case, this can however be addressed by Pseudo-Marginal Metropolis-Hastings, see below).
8.2. **Variational inference.** If \( g \) is indexed by a parameter \( \eta \in D \), then it induces a family of laws \( P = \{ P^{\circ(\eta)}, \eta \in D \} \) which can be used as a variational class in variational inference. That is, we find an element in \( P \) that approximates \( P^{\star} \) by the information projection (an early reference in the context of guided processes is Schauer et al. (2017)). More precisely, we aim to find \( \arg\min_{\eta \in D} \text{KL}(P^{\circ(\eta)}, P^{\star}) \), \( \text{KL} \) denoting Kullback-Leibler divergence. The minimisation can be done using stochastic gradient descent, which requires estimating \( \nabla_{\eta} \text{KL}(P^{\circ(\eta)}, P^{\star}) \). Typically, the proposal process can be reparametrised as

\[
X^{\circ(\eta)} = G(\eta, Z) \tag{8.2}
\]

for a deterministic map and a parameter-free innovation process \( Z \) (for example white noise), say with law \( Q \). This enables variational inference with the “reparametrisation trick” (Kingma and Welling, 2014). More precisely, define \( Q^{\star} \) by

\[
\frac{dQ^{\star}}{dQ}(Z) = \frac{dP^{\star}}{dP^{\circ}(G(\eta, Z))}.
\]

By the transformation formula, samples \( Z \sim Q^{\star} \) give \( G(\eta, Z) \sim P^{\star} \). Since

\[
\nabla_{\eta} \log \frac{dP^{\star}}{dP^{\circ}(G(\eta, Z))} = \nabla_{\eta} \log \frac{dQ^{\star}}{dQ}(G(\eta, Z)) = \mathbb{E}_{Q} \nabla_{\eta} \log \frac{dP^{\star}}{dP^{\circ}(G(\eta, Z))}
\]

an estimator for this gradient can be obtained by sampling from \( Q \) (we implicitly assume expectation and differentiation can be interchanged).

Note that the construction of \( X^{\circ(\eta)} \) in (8.2) is a normalising flow, see for instance Rezende and Mohamed (2015) and Kobyzev et al. (2020). Alternatively, it can be seen as a non-centred parametrisation (Papaspiliopoulos et al., 2003) or randomness pushback (Fritz, 2020).

8.3. **Markov chain Monte Carlo methods.** Suppose we can reparametrise \( X^{\circ} = g(Z) \) where \( Z \) is standard normal. Then a Metropolis-Hastings algorithm for sampling from \( P^{\star} \) can be constructed by sampling \( W \sim N(0, I) \) (independently from \( Z \)), choosing \( \alpha \in [0, 1) \) and proposing

\[
Z_{\text{new}} = \alpha Z + \sqrt{1 - \alpha^2} W.
\]

Next, \( Z_{\text{new}} \) is accepted with probability

\[
1 \wedge \frac{\Psi(G(Z_{\text{new}}))}{\Psi(G(Z))}
\]

and upon acceptance \( X^{\circ} \) is updated to \( G(Z_{\text{new}}) \). The update step for \( Z_{\text{new}} \) is often referred to as a preconditioned Crank-Nicolson (pCN) step.

In evaluating \( \Psi(X^{\circ}_{S}) \), the product of weights, \( \prod_{s \in S} w_{s}(X^{\circ}_{pa(s)}) \) may be intractable. The Pseudo-Marginal Metropolis-Hastings (PMMH) algorithm (Andrieu and Roberts, 2009) is based on the observation that if \( \Psi(X^{\circ}_{S}) \) is replaced with an unbiased estimator, the
Metropolis-Hastings algorithm still targets the exact target distribution. Here, this algorithm can be used upon realising that $\Psi(X^s_\circ) \text{ can be unbiasedly estimated by }$

\[
\prod_{s \in S} g_s(X_s) \prod_{u \in \text{pa}(s)} g_{u \circ s}(X_u^0) \prod_{v \in \mathcal{V}} h_{\text{pa}(v \circ s)}(X_{\text{pa}(v)}^0).
\]

where $X_s \sim \mathcal{L}(X_s \mid X_{\text{pa}(s)} = X_{\text{pa}(s)}^0)$.

### 8.4. Hamiltonian Monte Carlo

This is also helpful for derivative-based samplers such as Hamiltonian Monte Carlo. Consider the situation where $X^0 = G(Z)$, for $Z \sim Q = N(0,I)$.

The Hamiltonian to be used in a Hamiltonian Monte Carlo sampler targeting $Z^*$ is

\[
H(z, p) = -\log \frac{dQ^*}{dQ} \frac{dQ}{d\lambda}(z) + \frac{1}{2} ||p||,
\]

where $p$ is the momentum vector and $\lambda$ denotes the Lebesgue measure. Thus with

\[
\psi_s(z) = -\frac{\partial}{\partial z_s} \log \frac{dQ^*}{dQ} \frac{dQ}{d\lambda}(z) = -\sum_{t \in S} \frac{\partial}{\partial z_s} \log w_{s,t}(G(z_{\text{pa}(t)}) - z_s).
\]

the coordinate functions of the gradient of the negative score (the potential energy) and with $\lambda$ the Lebesgue measure, the Hamiltonian dynamics are given by

\[
\frac{\partial p_s}{\partial t} = -\frac{\partial H(z, p)}{\partial z_s} = -\psi_s(z), \quad \frac{\partial z_s}{\partial t} = \frac{\partial H(z, p)}{\partial p_s} = p_s.
\]

Thus a Hamiltonian Monte Carlo method to sample $Z^*$ can be used and samples of the target $X^*$ can then obtained via transformation $G(Z^*)$.

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A Summary of related work

In case of a line graph with edges to observation leaves at each vertex (a hidden Markov model) there are two well known cases for computing the smoothing distribution: (i) if $X$ is discrete the forward-backward algorithm (Murphy (2012), section 17.4.3), (ii) for linear Gaussian systems the Kalman Smoother, also known as Rauch-Tung-Striebel smoother (Murphy (2012), section 18.3.2) for the marginal distributions or its sampling version, where samples from the smoothing distribution are obtained by the forward filtering, backward sampling algorithm, Carter and Kohn (1994). Pearl (1988) gave an extension of the forward-backward algorithm from chains to trees by

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an algorithm known as “belief propagation” or “sum-product message passing”, either on trees or poly-trees. This algorithm consists of two message passing phases. In the “collect evidence” phase, messages are sent from leaves to the root; the “distribute evidence” phase ensures updating of marginal probabilities or sampling joint probabilities from the root towards the leaves. The algorithm can be applied to junction trees as well, and furthermore, the approximative loopy belief propagation applies belief propagation to sub-trees of the graph. A review is given in Jordan (2004).

Chou et al. (1994) extended the classical Kalman smoothing algorithm for linear Gaussian systems to dyadic trees by using a fine-to-coarse filtering sweep followed by a course-to-fine smoothing sweep. This setting arises as a special case of our framework. Extensions of filtering on Triplet Markov Trees and pairwise Markov trees are dealt with in Bardel and Desbouvries (2012) and Desbouvries et al. (2006) respectively.

Particle filters have been employed in related settings, see Doucet and Lee (2018) for an overview, but the resampling operations of particle filters result in the simulated likelihood function being non-differentiable in the parameters, which unlike our approach is an obstacle to gradient based inference. Briers et al. (2010) consider particle methods for state-space models using (an approximation to) the backward-information filter. Twisted particle samplers (Guarniero et al. (2017)) and controlled Sequential Monte Carlo (SMC) (Heng et al. (2020)) essentially use particle methods to find an optimal control policy to approximate the backward-information filter. The approximate backward filtering step in this paper uses a similar idea, formulated in a broader context than particle filtering and discrete-time models.

To easily compare to Heng et al. (2020) (shortly referred to as [H] here), we assist in bridging notation used in that paper and ours. The optimal Backward Information Filter (Cf. Section 2.3), which we denote by \( h_t \) at node \( t \), is denoted \( \psi^* \) in [H]. Approximations to \( h_t \) are specified in our setup by providing \( g_{s,t} \) over all edges (leading to \( \{g_s, s \in S\} \) by fusion). An a state-space model, those approximations are denoted by \( \psi \) in [H]. The set of \( \psi \) functions over all non-leaf vertices is then called a policy. For a state-space model it is shown how \( g_{pa(v),v} \) can be chosen such that the smoothing distribution is exact (this can also easily be deduced from Theorem 2.2). While not the focus of this paper, the idea of policy refinement outlined in [H] is also applicable to our setup.

For variational inference, Ambrogioni et al. (2021) propose an approach which, similar to ours, preserves the Markovian structure of the target by learning local approximations to the conditional dynamics.

\section{Graph theory}

Let \( G = (T, E) \) be a directed, finite graph without parallel edges and self-loops, with vertices \( T \) and edges \( E \), where \( e = (s,t), s, t \in T \) denotes a directed edge from \( s \) to \( t \).

- The parent set of a vertex is the set of all vertices that feed into it: \( \text{pa}(s) = \{ t : e(t, s) \in E \} \).
- The children set of a vertex is the set of all vertices that feed out of it: \( \text{ch}(s) = \{ t : e(s, t) \in E \} \).
- Define \( s \leadsto t \) recursively by \( s = t \) or \( s \leadsto a \) with \( (s,a) \in E \) for some \( a \). That is, \( s = t \) or there is a directed path from \( s \) to \( t \).
- Ancestors of a vertex are its parent, grand-parents, etc.: \( \text{anc}(t) = \{ s \neq t : s \leadsto t \} \). Thus, for fixed \( t \), \( \{ s : s \leadsto t \} = \text{anc}(t) \cup \{ t \} \).
- A leaf (or sink) is a vertex with no children. The set of leaves is denoted by \( \mathcal{V} \).
• For each vertex \( t \), we denote by \( \mathcal{V}_t = \{ v \in \mathcal{V}, t \sim v \} \) the leaves which are descendants of \( t \) (including \( t \), if \( t \) is a leaf).

• A source is a vertex with no parents.

C Proofs

Proof of Proposition 4.8. We aim to find \( g_i \) minimising \(- \sum_{i=1}^{d} \int \pi(x)g(x) \log g_i(x_i) \, dx.\) Writing \( \log g_i = \tilde{g}_i \) and introducing Lagrange multiplier we consider

\[
\mathcal{L}(\tilde{g}_1, \ldots, \tilde{g}_d, \lambda_1, \ldots, \lambda_d) = -\sum_{i=1}^{d} \pi(x)g(x)\tilde{g}_i(x_i) \, dx + \sum_{i=1}^{d} \lambda_i \left( \int e^{\tilde{g}_i(x_i)} \pi_i(x_i) - c_i \right).
\]

Now consider \( \mathcal{L} \) with its \( j \)-th argument taken to be \( \tilde{g}_j(x_j) + \epsilon \delta(x_j) \), subtract \( \mathcal{L} \) and collect terms of \( \mathcal{O}(\epsilon) \) to get

\[
-\int \pi(x)g(x) \delta(x_j) \, dx + \lambda_j \int g_j(x_j) \pi_j(x_j) \delta(x_j) \, dx_j.
\]

Equating this to zero gives

\[
\int \delta(x_j) \left( \lambda_j g_j(x_j) \pi_j(x_j) - \int \pi(x)g(x) \, dx_{-j} \right) \, dx_j = 0
\]

which implies

\[
\lambda_j g_j(x_j) \pi_j(x_j) = \int \pi(x)g(x) \, dx_{-j}.
\]

Integrating over \( x_j \) gives \( \lambda_j c_j = 1 \) from which the result easily follows. \( \square \)

Proof of Theorem 6.1. First note that

\[
(\kappa g)(x) = \int g(y)\kappa(x, dy) = \int \varpi(c,F,H)\varphi(y;\Gamma^{-1}F,\Gamma^{-1})\varphi(y;\mu(x),Q(x)) \, dy = \varpi(c,F,H)\varphi(\Gamma^{-1}F;\mu(x),Q(x) + \Gamma^{-1}).
\]

By using the expression for the weight follows.

To find the parametrisation of \( \kappa h \), let \( C = Q + \Gamma^{-1} \). We have

\[
(\kappa g)(x) = \varpi(c,F,H)\varphi(\Gamma^{-1}F;\Phi x + \beta, Q + \Gamma^{-1})
\]

\[
= \varpi(c,F,H)(2\pi)^{-d/2}|C|^{-1/2} \times \exp \left( -\frac{1}{2}x^{T}\Phi^{-1}x + (\Gamma^{-1}F - \beta)^{T}C^{-1}\Phi x - \frac{1}{2}(\Gamma^{-1}F - \beta)^{T}C^{-1}(\Gamma^{-1}F - \beta) \right)
\]

\[
= U(c - \log \varphi(0,F,H) + \log \varphi(\beta;\Gamma^{-1}F,C), \Phi C^{-1}(\Gamma^{-1}F - \beta), \Phi C^{-1}\Phi)(x).
\]

By equating this to \( U(\kappa, \tilde{F}, \tilde{H}) \) the parametrisation can be inferred directly. If \( \Phi \) is invertible, then

\[
\tilde{F}' \tilde{H} \tilde{F} = (\Gamma^{-1}F - \beta)^{T}C^{-1}(\Gamma^{-1}F - \beta).
\]

A bit of algebra then gives the stated result.

The derivation of the parametrisation of the fusion step is trivial.
To derive the forward map, we write \( \propto \) to denote proportionality with respect to \( y \)
\[
\frac{g(y)\kappa(x, dy)}{dy} \propto \exp \left( -\frac{1}{2} y' H y + y' F \right) \exp \left( -\frac{1}{2} (y - \mu(x))^' Q(x)^{-1} (y - \mu(x)) \right)
\]
\[
\propto \exp \left( -\frac{1}{2} y'(H + Q(x)^{-1})y + y'(F + Q(x)^{-1})\mu(x) \right)
\]
\[
\propto \phi^{\text{can}}(y; F + Q(x)^{-1}\mu(x), H + Q(x)^{-1})
\]
which suffices to be shown.

\( \Box \)

**Proof of Theorem 6.4.** For deriving the pullback of \( \kappa \), we compute
\[
(kg)(x) = \int_x^\infty \psi(x_v - y; A, \beta)\psi(y - x; \alpha, \beta(x)) \, dy
\]
\[
= \frac{\beta^A \beta(x)^\alpha}{\Gamma(A) \Gamma(\alpha)} e^{-\beta x_v + \beta(x)x} \int_x^\infty (x_v - y)^{A-1} (y - x)^{\alpha-1} e^{-(\beta - \beta(x))y} \, dy
\]
\[
= \frac{\beta^A \beta(x)^\alpha}{\Gamma(A) \Gamma(\alpha)} e^{-\beta(x_v - x)} (x_v - x)^{A+\alpha-1} \int_0^1 z^{\alpha-1} (1 - z)^{A-1} e^{-z \xi(x)} \, dz
\]
\[
= g_{A+\alpha, \beta}(x) \frac{1}{B(\alpha, \beta)} \int_0^1 z^{\alpha-1} (1 - z)^{A-1} e^{-z \xi(x)} \, dz
\]
where we made the substitution \( y = x + z(x_v - x) \) at the third equality and \( B(\alpha, \beta) \)-denotes the Beta-function, evaluated at \( (\alpha, \beta) \).

From this expression the pullback for \( \tilde{\kappa} \) follows directly, since \( \xi(x) = \xi \) implies \( \xi(x) = 0 \). This also directly gives the expression for the weight.

If \( \mu = \delta_x \), then drawing from the forward measure entails drawing from a density which is proportional to \( g(y)\kappa(x, dy) \) (proportionality with respect to \( y \)). The claim now follows upon inspecting the derivation of \( (kg)(x) \) and keeping all terms under the integral proportional to \( z \).

\( \Box \)