Exact Bayesian Inference on Discrete Models via Probability Generating Functions: A Probabilistic Programming Approach

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Abstract

We present an exact Bayesian inference method for discrete statistical models, which can find exact solutions to many discrete inference problems, even with infinite support and continuous priors. To express such models, we introduce a probabilistic programming language that supports discrete and continuous sampling, discrete observations, affine functions, (stochastic) branching, and conditioning on events. Our key tool is *probability generating functions*: they provide a compact closed-form representation of distributions that are definable by programs, thus enabling the exact computation of posterior probabilities, expectation, variance, and higher moments. Our inference method is provably correct, fully automated and uses automatic differentiation (specifically, Taylor polynomials), but does not require computer algebra. Our experiments show that its performance on a range of real-world examples is competitive with approximate Monte Carlo methods, while avoiding approximation errors.

1 Introduction

Bayesian statistics is a highly successful framework for reasoning under uncertainty that has found widespread use in a variety of fields, such as AI / machine learning, medicine and healthcare, finance and risk management, social sciences, climate science, astrophysics, and many other disciplines. At its core is the idea of representing uncertainty as probability, and updating prior beliefs based on observed data via Bayes' law, to arrive at posterior beliefs. A key challenge in Bayesian statistics is computing this posterior distribution: analytical solutions are usually impossible or intractable, which necessitates the use of approximate methods, such as Markov-chain Monte Carlo (MCMC) or variational inference. In this work, we identify a large class of discrete models for which exact inference is in fact possible, in particular time series models of count data (e.g. autoregressive models, hidden Markov models, switchpoint models). We achieve this by leveraging *probability generating* functions (GF_s) as a representation of distributions. The GF of a random variable X is defined to be the function $G(t) := \mathbb{E}[t^X]$. In probability theory, it is a well-known tool to study random variables and their distributions, related to the moment generating and the characteristic functions [12, Chapter 4]. In computer science, GFs have previously been used for the analysis of probabilistic programs [14, 3] and for exact inference on certain classes of graphical models [22, 23]. Here we apply them uniformly in a much more general context via probabilistic programming, enabling exact inference on more expressive Bayesian models.

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We characterize the class of supported models with the help of a probabilistic programming language. *Probabilistic programming* [21] has recently emerged as a powerful tool in Bayesian inference. Probabilistic programming systems (PPSs) allow users to specify complex statistical models as programs in a precise yet intuitive way, and automate the Bayesian inference task. This allows practitioners to focus on modelling, leaving the development of general-purpose inference algorithms to experts. Consequently, probabilistic programming systems such as Stan [2] enjoy increasing popularity among statisticians and data scientists. We describe a programming language, called SGCL (statistical guarded command language), that extends pGCL (probabilistic GCL) [14]. This language is carefully designed to be simple yet expressive, and just restrictive enough to enable exact Bayesian inference on all programs that can be written in it.

Contributions We provide a new framework for exact inference on discrete Bayesian models.

- (a) Our method is applicable to a large class of discrete models with infinite support, in particular time series models of count data, such as autoregressive models for population dynamics, Bayesian switchpoint models, mixture models, and hidden Markov models. To our knowledge, no exact inference method for all but the simplest population models was known before.
- (b) The models are specified in a probabilistic programming language (PPL), which provides flexibility in model definition, thus facilitating model construction. Our PPL supports stochastic branching, continuous and discrete priors, discrete observations, and conditioning on events.
- (c) Every program written in the language is translatable to a generating function that represents the posterior distribution in an automatic and provably correct way. From this generating function, one can extract posterior mean, variance, and higher moments, as well as the posterior probability masses (for a discrete distribution).
- (d) We have built an optimized tool implementation that takes a probabilistic program as input and automatically computes the aforementioned set of descriptive statistics about the posterior distribution.
- (e) We demonstrate that its performance on a range of real-world examples is competitive with approximate Monte Carlo methods, while (as exact inference) achieving 0 approximation errors.

Related Work Computing the exact posterior distribution of probabilistic programs is intractable in general as it requires analytical solutions to integrals [7]. For this reason, existing systems either restrict the programming language to allow only tractable constructs (this is our approach) or cannot guarantee successful inference. In the former category are Dice [13] which only supports finite discrete distributions, and SPPL [18] which supports some infinite-support distributions but requires finite discrete priors. In the latter category are the systems PSI [7] and Hakaru [17], which do not impose syntactic restrictions. Both rely on computer algebra techniques to try to find a closed-form solution for the posterior. Such a form need not exist in general but, even if it does, the running time is unpredictable and unscalable [18], or the systems may still fail to find the solution. None of the case studies featuring in our evaluation (Section 5) can be handled by the aforementioned tools.

Probability generating functions are a useful tool in probability theory to study random variables with infinite support, e.g. in the context of branching processes [5, Chapter 12]. On the Bayesian inference side, Winner and Sheldon [22] find a symbolic representation of the generating function for a Poisson autoregressive model and extract posterior probabilities from it. Subsequently, Winner et al. [23] extend this model to latent variable distributions other than the Poisson distribution, where symbolic manipulation is no longer tractable. Instead they evaluate generating functions and their derivatives using automatic differentiation, which enable exact inference for graphical models. Probabilistic programming is an elegant way of generalizing graphical models, allowing a much richer representation of models [8, 21, 10]. Our contribution here is a new framework for exact inference on Bayesian models via probabilistic programming.

In the context of discrete probabilistic programs without conditioning, Klinkenberg et al. [14] use generating functions to analyze loop invariants and determine termination probabilities. In follow-up work, Chen et al. [3] extend these techniques to check (under certain restrictions) whether a looping program generates a specified distribution. Both papers rely on computer algebra, which only scales to real-world probabilistic programs under special circumstances: as demonstrated by Winner et al. [23], the size of the generating functions usually grows quickly with the data conditioned on.

Limitations Exact posterior inference is PSPACE-hard (so at least NP-hard) already for probabilistic programs involving only finite discrete distributions [13, Section 6]. It follows that our method cannot always be performant and has to restrict the supported class of probabilistic programs. Indeed, our programming language forbids certain constructs, such as nonlinear transformations and observations of continuous variables, in order to preserve a closed-form representation of the generating functions (Section 2). For the same reason, our method cannot compute probability density functions for continuous parameters (but probability masses for discrete parameters and exact moments for all parameters are fine). Regarding performance, the running time of inference is polynomial in the numbers observed in the program and exponential in the number of program variables (Section 4). Despite these limitations, our approach shows that exact inference is possible in the first place, and our evaluation (Section 5) demonstrates support for many real-world models and efficient exact inference in practice.

2 Bayesian Probabilistic Programming

Probabilistic programming languages extend ordinary programming languages with two additional constructs: one for sampling from probability distributions and one for conditioning on observed values. We first discuss a simple program that can be written in our language using a simplified example based on population ecology (cf. [22]).

Suppose you're a biologist trying to estimate the size of an animal population migrating into a new habitat. The immigration of animals is often modeled using a Poisson distribution. You cannot count the animals exhaustively (otherwise we wouldn't need estimation techniques), so we assume that each individual is observed independently with a certain probability; in other words the count is binomially distributed. For simplicity, we assume that the rate of the Poisson and the probability of the binomial distribution are known, say 20 and 0.1. (For more realistic population models, see Section 5.) As a generative model, this would be written as $X \sim \text{Poisson}(20)$; $Y \sim \text{Binomial}(X, 0.1)$.

Suppose you observe Y = 2 animals. The Bayesian inference problem is to compute the *posterior* distribution $\mathbb{P}(X = x \mid Y = 2)$ given by Bayes' rule as $\mathbb{P}(X = x \mid Y = 2) = \frac{\mathbb{P}(X=x) \mathbb{P}(Y=2|X=x)}{\mathbb{P}(Y=2)}$, where $\mathbb{P}(X = x)$ is called the *prior* probability, $\mathbb{P}(Y = 2 \mid X = x)$ the *likelihood* and $\mathbb{P}(Y = 2)$ the *evidence* or *normalization* constant.

Example 2.1. In our probabilistic programming language, this simplified population model would be expressed as:

$$X \sim \text{Poisson}(20); Y \sim \text{Binomial}(X, 0.1); \text{observe } Y = 2;$$

The syntax looks similar to generative model notation except that the observations are expressible as a command. Such programs denote a joint probability distributions of their program variables, which are viewed as random variables. The program statements manipulate this joint distribution. After the first two sampling statements, the distribution has the probability mass function (PMF) $p_1(x,y) = \mathbb{P}[X = x, Y = y] = \text{Poisson}(x; 20) \cdot \text{Binomial}(y; x, 0.1)$. Observing Y = 2 restricts this to the PMF $p_2(x,y) = \mathbb{P}[X = x, Y = y = 2]$, which equals $\mathbb{P}[X = x, Y = 2] = p_1(x, 2)$ if y = 2 and 0 otherwise. Note that this is not a probability, but a *subprobability*, distribution because the total mass is less than 1. So, as a final step, we need to *normalize*, i.e. rescale the subprobability distribution back to a probability distribution. This corresponds to the division by the evidence in Bayes' rule, yielding the PMF $p_3(x,y) = \frac{p_2(x,y)}{\sum_{x,y} p_2(x,y)}$. To obtain the posterior $\mathbb{P}[X = x \mid Y = 2]$, which is a distribution of the single variable X, not the joint of X and Y, we need to marginalize p_3 and find $\sum_y p_3(x,y) = \frac{\sum_y p_2(x,y)}{\sum_{x,y} p_2(x,y)} = \frac{\mathbb{P}[X=x,Y=2]}{\mathbb{P}[Y=2]} = \mathbb{P}[X = x \mid Y = 2]$, as desired.

Next we describe all constructs of our probabilistic programming language SGCL more formally. It is based on the *probabilistic guarded command language* (pGCL) from [14] but augments it with statistical features like conditioning on events and normalization, which is why we call it *Statistical GCL* (SGCL). Each program operates on a fixed set of variables $\mathbf{X} = \{X_1, \ldots, X_n\}$ taking values in $\mathbb{R}_{\geq 0}$. A program consists of a list of statements $P_1; P_2; \ldots; P_m$. The simplest statement is skip, which does nothing and is useful in conditionals (like pass in Python). Variables can be transformed using affine maps, e.g. $X_2 := 2X_1 + 7X_3 + 2$ (note that the coefficients must be nonnegative to preserve nonnegativity of the variables). Programs can branch based on the value of a (discrete) variable (e.g. if $X_k \in \{1,3,7\} \{\ldots\}$ else $\{\ldots\}$), and sample new values for variables from distributions (e.g. $X_k \sim \text{Binomial}(10, 0.5)$ or $X_k \sim \text{Binomial}(X_j, 0.5)$). The supported distributions are Bernoulli, Categorical, Binomial, Uniform (both discrete and continuous), NegBinomial, Geometric, Poisson, Exponential, Gamma. These distributions need to have constant (non-variable) parameters except for

Table 1: GFs for common distributions with constant (left) and random variable parameters (right)

Distribution D	$gf(X \sim D)(x)$	Distribution	$D(Y)$ gf $(X \sim D(Y))(x)$
Binomial(n,p)	$(px+1-p)^n$	Binomial(Y,	p) $gf(Y)(1-p+px)$
Geometric(p)	$\frac{p}{1-(1-p)x}$	NegBinomia	$I(Y,p) \qquad gf(Y)\left(\frac{p}{1-(1-p)x}\right)$
$Poisson(\lambda)$	$e^{\lambda(x-1)}$	$Poisson(\lambda \cdot Y)$	(Y) $\operatorname{gf}(Y)(e^{\lambda(x-1)})$
Exponential(λ)	$\frac{\lambda}{\lambda - \log x}$	Bernoulli(Y)	$1 + (x - 1) \cdot (gf(Y))'(1)$

Binomial(X, p), NegBinomial(X, p), Poisson $(\lambda \cdot X)$, and Bernoulli(X), where X can be a random variable itself. One can observe events involving discrete variables (e.g. observe $X_k \in \{3, 5\}$) and values from (discrete) distributions directly (e.g. observe $3 \sim \text{Binomial}(X_j, 0.5)$). Note that observe $m \sim D$ can be seen as a convenient abbreviation of $Y \sim D$; observe Y = m with a fresh variable Y. After an observation, the variable distribution is usually not a probability distribution anymore, but a subprobability distribution ("the numerator of Bayes' rule").

In summary, the syntax of programs P has the following BNF grammar:

$$P ::= \mathsf{skip} \mid P_1; P_2 \mid X_k := a_1 X_1 + \dots + a_n X_n + c \mid \text{if } X_k \in A \{P_1\} \text{ else } \{P_2\} \\ \mid X_k \sim D \mid X_k \sim D(X_j) \mid \text{observe } X_k \in A \mid \text{observe } m \sim D \mid \text{observe } m \sim D(X_j) \end{cases}$$

where P, P_1 and P_2 are subprograms; $a_1, \ldots, a_n, c \in \mathbb{R}_{\geq 0}$; $m \in \mathbb{N}$; A is a finite subset of the naturals; and D is a supported distribution. A fully formal description of the language constructs can be found in Appendix A.

Restrictions Note that in SGCL, we impose several restrictions on the syntax in order to enable exact inference using generating functions: (a) only affine functions are supported (e.g. no X^2 or $\exp(X)$), (b) only comparisons between variables and constants are supported (e.g. no test for equality X = Y), (c) only observations from discrete distributions on \mathbb{N} and only comparisons of such random variables are supported (e.g. no observe $1.5 \sim \text{Normal}(0, 1)$), (d) a particular choice of distributions and their composites is supported, (e) loops or recursion are not supported.

3 Generating Functions

Consider Example 2.1. Even though the example is an elementary exercise in probability, it is challenging to compute the normalizing constant, because one needs to evaluate an infinite sum: $\mathbb{P}[Y=2] = \sum_{x \in \mathbb{N}} \mathbb{P}[Y=2 \mid X=x] \mathbb{P}[X=x] = \sum_{x \in \mathbb{N}} {x \choose 2} 0.1^2 0.9^{x-2} \cdot \frac{20^x e^{-20}}{x!}$. It turns out to be $2e^{-2}$ (see Example 3.1), but it is unclear how to arrive at this result in an automated way. If X had been a continuous variable, we would even have to evaluate an integral. We will present a technique to compute such posteriors mechanically. It relies on probability generating functions, whose definition includes an infinite sum or integral, but which often admit a closed form, thus enabling the exact computation of posteriors.

Definition Probability generating functions are a well-known tool in probability theory to study random variables and their distributions, especially discrete ones. The probability generating function of a random variable X is defined to be the function $G(x) := \mathbb{E}[x^X]$. For a discrete random variable supported on \mathbb{N} , this can also be written as a power series $G(x) = \sum_{n \in \mathbb{N}} \mathbb{P}[X = n] \cdot x^n$. Since we often deal with subprobability distributions, we omit "probability" from the name and refer to $G(x) := \mathbb{E}_{X \sim \mu}[x^X]$, where μ is a subprobability measure, simply as a *generating function* (GF). For continuous variables, it is often called *factorial moment generating function*, but we stick with the former name in all contexts. We will use the notation $gf(\mu)$ or gf(X) for the GF of μ or X. Note that for discrete random variables supported on \mathbb{N} , the GF is always defined for $x \in [-1, 1]$, and for continuous ones for x = 1, but it need not be defined for other x.

Probability masses and moments Many common distributions admit a closed form for their GF (see Table 1). In such cases, GFs are a compact representation of a distribution, even if it has infinite or continuous support like the Poisson or Exponential distributions, respectively. Crucially, one can extract probability masses and moments of a distribution from its generating function. For discrete random variables X, P[X = n] is the *n*-th coefficient in the power series representation of G, so

Table 2: Generating function semantics of SGCL constructs				
Language construct P	$\llbracket P \rrbracket_{\sf gf}(G)({m x})$			
skip	$G(oldsymbol{x})$			
$P_1; P_2$	$\llbracket P_2 \rrbracket_{gf}(\llbracket P_1 \rrbracket_{gf}(G))(\boldsymbol{x})$			
$X_k := \mathbf{a}^\top \mathbf{X} + c$	$x_k^c \cdot G(\boldsymbol{x}')$ where $x_k' := x_k^{a_k}$ and $x_i' := x_i x_k^{a_i}$ for $i \neq k$			
$if X_k \in A \{P_1\} else \{P_2\}$	$\llbracket P_1 \rrbracket_{gf}(G_{X_k \in A}) + \llbracket P_2 \rrbracket_{gf}(G - G_{X_k \in A})$			
	where $G_{X_k \in A}(\mathbf{x}) = \sum_{i \in A} \frac{\partial_k^i G(\mathbf{x}[k \mapsto 0])}{i!} x_k^i$			
$X_k \sim D$	$G(\mathbf{x}[k\mapsto 1]) \cdot gf(D)(x_k)$			
$X_k \sim D(X_j)$	$G(\mathbf{x}[k \mapsto 1, j \mapsto x_j \cdot gf(D(1))(x_k)])$			
	for $D \in \{ Binomial(-, p), NegBinomial(-, p), Poisson(\lambda \cdot -) \}$			
	$G(\boldsymbol{x}[k\mapsto 1]) + x_j(x_k-1) \cdot \partial_j G(\boldsymbol{x}[k\mapsto 1]) \text{for } D = Bernoulli(-)$			
observe $X_k \in A$	$G_{X_k \in A}(\mathbf{x}) = \sum_{i \in A_{\mathbf{x}}} \frac{\partial_k^i G(\mathbf{x}^{[k \mapsto 0]})}{i!} x_k^i$			
Normalization	$normalize(G) := \frac{G}{G(1_n)}$			

can be computed as the Taylor coefficient at 0: $\frac{1}{n!}G^{(n)}(0)$ (hence the name "probability generating function"). For a discrete or continuous random variable X, its expected value is $\mathbb{E}[X] = G'(1)$, and more generally, its *n*-th factorial moment is $\mathbb{E}[X(X-1)\cdots(X-n+1)] = \mathbb{E}[\frac{d^n}{dx^n}x^X]|_{x=1} = G^{(n)}(1)$ (hence the name "factorial moment generating function"). The ordinary and central moments can easily be computed from the factorial moments. For instance, the variance is $\mathbb{V}[X] = G''(1)+G'(1)-G'(1)^2$. We will exploit these properties of generating functions through automatic differentiation.

Multivariate case The definition of GFs is extended to multidimensional distributions in a straightforward way: for random variables $X = (X_1, \ldots, X_n)$, their GF is the function $G(x) := \mathbb{E}[x^X]$ where we write $x := (x_1, \ldots, x_n)$ and $x^X := x_1^{X_1} \cdots x_n^{X_n}$. We generally follow the convention of using uppercase letters for random and program variables, and lowercase letters for the corresponding parameters of the generating function. Marginalization can also be expressed in terms of generating functions: to obtain the GF \tilde{G} of the joint distribution of (X_1, \ldots, X_{n-1}) , i.e. to marginalize out X_n , one simply substitutes 1 for x_n in $G: \tilde{G}(x_1, \ldots, x_{n-1}) = G(x_1, \ldots, x_{n-1}, 1)$. This allows us to compute probability masses and moments of a random variable in a joint distribution: we marginalize out all the other variables and then use the previous properties of the derivatives.

3.1 Translating programs to generating functions

The standard way of describing the meaning of probabilistic programs is assigning (sub-)probability distributions to them. An influential example is Kozen's distribution transformer semantics [15], where each program statement transforms the joint distribution of all the variables $X = (X_1, \ldots, X_n)$. Since Kozen's language does not include observations, we present the full semantics in Appendix A. We call this the *standard semantics* of a probabilistic program and write $[\![P]\!]_{std}(\mu)$ for the transformation of μ by the program P. As a last step, the subprobability distribution μ has to be normalized, which we write normalize(μ) := $\frac{\mu}{\int d\mu}$. This reduces the Bayesian inference problem for a given program to computing its semantics, starting from the joint distribution Dirac($\mathbf{0}_n$) in which all n variables are initialized to 0 with probability 1. While mathematically useful, the distribution transformer semantics is hardly amenable to computation as it involves integrals and infinite sums.

Instead, we shall compute the generating function of the posterior distribution represented by the probabilistic program. Then we can extract posterior probability masses and moments using automatic differentiation. Each statement in the programming language transforms the generating function of the distribution of program states, i.e. the joint distribution of the values of the variables $\mathbf{X} = (X_1, \ldots, X_n)$. Initially, we start with the constant function $G = \mathbf{1}$, which corresponds to all variables being initialized with 0 since $\mathbb{E}[x^0] = 1$. The generating function semantics of a program $[P]_{gf}$ describes how to transform G to the generating function $[P]_{gf}(G)$ for the distribution at the end.

This generating function semantics $\llbracket P \rrbracket_{gf}$ is defined in Table 2, where the update notation $x[i \mapsto a]$ denotes $(x_1, \ldots, x_{i-1}, a, x_{i+1}, \ldots, x_n)$ and $\mathbf{1}_n$ means the *n*-tuple $(1, \ldots, 1)$. The first five rules were already described in [3], so we only explain them briefly: skip leaves everything unchanged and P_1 ; P_2 chains two statements by transforming with $\llbracket P_1 \rrbracket_{gf}$ and then $\llbracket P_2 \rrbracket_{gf}$. To explain linear

assignments, consider the case of only two variables: $X_1 := 2X_1 + 3X_2 + 5$. Then

$$\llbracket P \rrbracket_{\mathsf{gf}}(G)(\boldsymbol{x}) = \mathbb{E}[x_1^{2X_1 + 3X_2 + 5} x_2^{X_2}] = x_1^5 \mathbb{E}[(x_1^2)^{X_1} (x_1^3 x_2)^{X_2}] = x_1^5 \cdot G(x_1^2, x_1^3 x_2).$$

For conditionals if $X_k \in A \{P_1\}$ else $\{P_2\}$, we split the generating function G into two parts: one where the condition is satisfied $(G_{X_k \in A})$ and its complement $(G - G_{X_k \in A})$. The former is transformed by the then-branch $\llbracket P_1 \rrbracket_{gf}$, the latter by the else-branch $\llbracket P_2 \rrbracket_{gf}$. The computation of $G_{X_k \in A}$ is best understood by thinking of G as a power series where we keep only the terms where the exponent of x_k is in A. Sampling $X_k \sim D$ from a distribution with constant parameters works by first marginalizing out X_k and then multiplying by the generating function of D with parameter x_k .

The first new construct is sampling $X_k \sim D(X_j)$ from compound distributions (see Appendix B). Observing events $X_k \in A$ uses $G_{X_k \in A}$ like conditionals do, which was explained above. Just like the subprobability distribution that the program represents has to be normalized as a last step, we have to normalize the generating function. The normalizing constant is easily obtained by marginalizing out all variables: $G(1, \ldots, 1)$. So we obtain the generating function representing the normalized posterior distribution by rescaling with the inverse: normalize $(G) := \frac{G}{G(1_n)}$. These intuitions can, in fact, be made rigorous in the form of the following theorem, which is proved in Appendix B.2.

Theorem 3.1. The GF semantics is correct w.r.t. the standard semantics: for any SGCL program P and subprobability distribution μ on $\mathbb{R}^n_{\geq 0}$, we have $\llbracket P \rrbracket_{gf}(gf(\mu)) = gf(\llbracket P \rrbracket_{std}(\mu))$. In particular, it correctly computes the GF of the posterior distribution of P as normalize($\llbracket P \rrbracket_{gf}(1)$). Furthermore, the GFs $\llbracket P \rrbracket_{gf}(1)$ and thus normalize($\llbracket P \rrbracket_{gf}(1)$) are defined on $[0, R)^n$ for some R > 1.

Novelty The semantics builds upon [14, 3]. To our knowledge, the GF semantics of Poisson $(\lambda \cdot X_j)$ and Bernoulli (X_j) is novel, and the former is required to support most models in Section 5. While the GF of observations has been considered in the context of a specific model [22], this has not been done in the general context of a probabilistic programming language before. More generally, previous works involving GFs only considered discrete distributions, whereas we also allow sampling from continuous distributions. This is a major generalization and requires different proof techniques because the power series representation $\sum_{i \in \mathbb{N}} \mathbb{P}[X = i]x^i$, on which the proofs in [22, 14, 3] rely, is not valid for continuous distributions.

Example 3.1 (GF translation). Consider Example 2.1. We can find the posterior distribution mechanically by applying the rules from the GF semantics. We start with the GF $A(x, y) = \mathbb{E}[x^0y^0] = 1$ corresponding to X and Y being initialized to 0. Sampling X changes this to GF $B(x, y) = A(1, y)e^{20(x-1)} = e^{20(x-1)}$. Sampling Y yields $C(x, y) = B(x(0.1y + 0.9), 1) = e^{2x(y+9)-20}$. Observing Y = 2 yields $D(x, y) = \frac{1}{2!}y^2 \frac{\partial^2}{\partial y^2}C(x, 0) = 2x^2y^2e^{18x-20}$. To normalize, we divide by $D(1, 1) = 2e^{-2}$, obtaining $E(x, y) = \frac{D(x, y)}{D(1, 1)} = x^2y^2e^{18(x-1)}$ since A(x, y) = 1.

As described above, we can extract from this GF the posterior probability of, for example, exactly 10 individuals $\mathbb{P}[X = 10] = \frac{1}{10!} \frac{\partial^{10}}{\partial x^{10}} E(0, 1) = 991796451840e^{-18}$ and the expected value of the posterior $\mathbb{E}[X] = \frac{\partial}{\partial x} E(1, 1) = 20$.

4 Implementation & Optimizations

The main difficulty in implementing the GF semantics is the computation of the partial derivatives. A natural approach (as followed by [3]) is to manipulate symbolic representations of the generating functions and to use computer algebra for the derivatives, however this scales badly for the following reason: every observe $X_k = d$ statement in the program is translated to a *d*-th partial derivative. Since probabilistic programs tend to contain many data points, it is common for the total order of derivatives to be in the hundreds. The size of the symbolic representation of a function can (and typically does) grow exponentially in the order of the derivative: the derivative of the product of two functions $f \cdot g$ is $f' \cdot g + f \cdot g'$, a sum of two products, so the representation doubles in size. Hence the running time would be $\Omega(2^d)$ where *d* is the sum of all observed values, which is clearly unacceptable.

Instead, we exploit the fact that we do not need to generate the full representation of a GF, but merely to *evaluate it and its derivatives*. We implement our own *automatic differentiation* framework for this because existing automatic differentiation frameworks are not designed for computing derivatives of order greater than, say, 4 or 5. In fact, it is more efficient to work with Taylor polynomials instead

of higher derivatives directly. Winner et al. [23] already do this for the population model (with only one variable), and we extend this to our more general setting with more than one variable, requiring multivariate Taylor polynomials. In this approach, derivatives are the easy part (they can be read off the Taylor coefficients), but the composition of Taylor polynomials is the bottleneck. Winner et al. [23] use a naive $O(d^3)$ approach, which is fast enough for their single-variable use case.

For n variables, naive composition of Taylor polynomials takes $O(d^{3n})$ time, where d is the sum of all observations in the program, i.e. the total order of differentiation, i.e. the degree of the polynomial. Note that this is polynomial in d, contrary to the symbolic approach, but exponential in the number of variables n. This is not as bad as it seems because in many cases, the number of variables can be kept to one or two, as opposed to the values of data points (such as the models from Section 5). In fact, we exploit the specific composition structure of generating functions to achieve $O(d^3)$ for n = 1 and $O(d^{n+3})$ for $n \ge 2$ in the worst case, while often being faster in practice. Overall, our implementation takes $O(sd^{n+3})$ time in the worst case, where s is the number of statements in the program, d is the sum of all observed values, and n is the number of program variables (see Appendix C.3).

Observations from compound distributions In Bayesian inference, observing data points from distributions with random parameters may well be the most common operation. To help with this, we introduce the shorthand observe $d \sim D(X_k)$ for $X_{n+1} \sim D(X_k)$; observe $X_{n+1} = d$, where X_{n+1} is a fresh variable. Probabilistic programs typically contain many observations, so it is worthwhile to optimize this construct and to avoid the extra variable X_{n+1} . In fact, this is essential to achieving good performance for many of the examples in Section 5. Winner and Sheldon [22] do this for the binomial distribution in the context of a specific model. We extend this to our more general setting with continuous variables, and also present optimized semantics for the Poisson and Bernoulli distributions. The proof can be found in Appendix C.2.

Theorem 4.1. *The transformation of GFs by observations can be equivalently expressed without an extra variable as follows:*

$$\begin{split} [\text{observe } d &\sim \text{Binomial}(X_k, p)]_{\text{gf}}(G) &= \frac{1}{d!}(px_k)^d \cdot \partial_k^d G(\boldsymbol{x}[k \mapsto (1-p)x_k]) \\ [\text{[observe } d &\sim \text{Poisson}(\lambda X_k)]_{\text{gf}}(G) &= \frac{1}{d!}D_{k,\lambda}^d(G)(\boldsymbol{x}[k \mapsto e^{-\lambda}x_k]) \\ & \text{where } D_{k,\lambda}(G)(\boldsymbol{x}) &:= \lambda x_k \cdot \partial_k G(\boldsymbol{x}). \\ [\text{[observe } d &\sim \text{Bernoulli}(X_k)]_{\text{gf}}(G) &= \begin{cases} G(\boldsymbol{x}) - x_k \cdot \partial_k G(\boldsymbol{x}) & d = 0 \\ x_k \cdot \partial_k G(\boldsymbol{x}) & d = 1 \end{cases} \end{split}$$

Implementation Our implementation reads a program file and outputs the posterior mean, variance, skewness, and kurtosis for a specified variable of interest. For discrete variables supported on \mathbb{N} , it also computes the posterior probability masses up to a configurable threshold. To have tight control over performance, especially for the multivariate Taylor polynomials, we implemented our method in Rust [16], a safe systems programming language. Our implementation is available in the supplementary material and will be made available on Github after the review process.

Numerical issues To ensure that the results are numerically stable, we also implemented interval arithmetic to bound the rounding errors. Initially, we found that programs with continuous distributions led to catastrophic cancelation errors, due to the logarithmic term in their GFs, whose Taylor expansion is badly behaved. We fixed this problem with a slightly modified representation of the GFs, avoiding the logarithms (details in Appendix C). For all the examples we tested, our implementation is accurate up to at least 6 significant digits (using 64-bit floating point numbers).

5 Empirical Evaluation

It is impossible to compare our approach with other exact inference methods: as mentioned in Related Work (Section 1), none of the existing exact inference systems, such as DICE [13], SPPL [18], Hakaru [17] and PSI [7], support discrete models with priors that have infinite support, which is the kind of models we are targeting. Hence, we compare our approach with approximate (Monte Carlo) inference methods. Specifically, we choose the Anglican [20] probabilistic programming system because it implements many state-of-the-art inference algorithms suitable for discrete models, which is what our benchmark models need. Other potential candidate systems are less suitable according to these criteria: Gen [4] specializes in programmable inference, while Stan [2], Turing [6] and Pyro [1] focus on continuous models and have weaker or no support for discrete models. WebPPL [9] also



Figure 1: Comparison of the population model and its modifications with approximate inference: mean and standard error of the computation time and TVD over 20 repeated runs.

satisfies many criteria. However, although it supports discrete models, its inference algorithms are less sophisticated and extensive than Anglican's (for example, it does not support Sequential Monte Carlo (SMC), particle Gibbs, or interacting particle MCMC). We considered comparing with truncated versions of each model, as [22] did for their specific model. However, truncation is much more difficult to achieve for probabilistic programs and impossible for continuous priors. Since Winner and Sheldon [22] already showed that truncation is inferior to exact inference for the population model, we decided to compare with Monte Carlo methods.

The approximation error of a Monte Carlo inference algorithm depends on its Methodology settings¹ (e.g. the number of particles for SMC) and decreases the longer it is run (more samples). To ensure a fair comparison, we use the following setup: for each inference problem, we run several inference algorithms with various configurations (settings and sampling budgets) and report the approximation error and the elapsed time. To measure the quality of the approximation, we report the total variation distance (TVD) between the exact solution and the approximate posterior distribution. Our method can also compute moments exactly, so we report the approximation errors of the posterior mean μ , standard deviation σ , skewness (third standardized moment) S, and kurtosis K, as well. We want our errors to be invariant with respect to the location and scale of the posterior distribution, because otherwise the error measurements could change dramatically if the posterior distribution is simply shifted far to the right or scaled up or down. For this reason, we report the error of the mean as $\frac{|\hat{\mu}-\mu|}{2}$, where μ is the true posterior mean, $\hat{\mu}$ its approximation, and σ the true posterior standard deviation; the relative error of the standard deviation σ (because σ is invariant under translation but not scaling), and the absolute error of skewness and kurtosis (because they are invariant under both translation and scaling). To reduce noise, we average all these error measures and the computation times over 20 runs and report the standard error as error bars. We run several well-known inference algorithms implemented in Anglican: importance sampling (IS), Lightweight Metropolis-Hastings (LMH), Random Walk Metropolis-Hastings (RMH), SMC, particle Gibbs (PGibbs), and interacting particle MCMC (IPMCMC). For comparability, in all experiments, each algorithm is run with two sampling budgets and, if possible, two different settings (one being the defaults) for a total of four configurations. The sampling budgets were 1000 or 10000, because significantly lower sample sizes gave unusable results and significantly higher sample sizes took much more time than our exact method. We discard the first 20% of the samples, a standard procedure called "burn-in".

Note that this setup is generous to the approximate methods because we only report the average time for runs of each configuration. However, in practice, one does not know the best configuration, so the algorithms need to be run several times with different settings. By contrast, our method requires only one run because the result is exact.

5.1 Benchmarks

Population ecology Our first benchmark comes from [22, 23] and describes the dynamics of e.g. animal populations. A simplified version of it was presented in Example 2.1. Here we model a population N_k at time steps k = 0, ..., m. At each time step, there is a Poisson-distributed number of new arrivals, which are added to the binomially distributed number of survivors from the previous time step. Each individual is observed with a fixed probability δ , so the number of observed individuals is

¹See https://probprog.github.io/anglican/inference/ for a full list of Anglican's options.



(a) Error of the mean (b) Error of the std. dev. (c) Error of the skewness (d) Error of the kurtosis

Figure 3: Comparison of moments for the switchpoint model: approximate inference vs our method.

binomially distributed:

$$New_k \sim \text{Poisson}(\lambda_k);$$
 $Survivors_k \sim \text{Binomial}(N_{k-1}, \delta);$
 $N_k := New_k + Survivors_k;$ observe $y_k \sim \text{Binomial}(N_k, \rho);$

where the model parameters $\lambda_k \in \mathbb{R}, \delta \in [0, 1]$ are taken from [22] and the detection probability ρ is set to 0.2 ([22] considers a range of values, but we pick one because of the page limit). The $y_k \in \mathbb{N}$ is the observed number of individuals in the population at time step k, which is simulated from the same ground truth as [22]. The goal is to infer the final number N_m of individuals in the population. We set the (population size) model parameter (and hence the observed values which influence the running time) to be 4 times larger than the largest in [22] (see details in Appendix D.1). The results (Fig. 1a) show that our method is superior to MCMC methods in both computation time and accuracy (since it is exact).

While this model was already solved exactly in [22], our probabilistic programming approach makes it trivial to modify the model, since the whole inference is automated and one only needs to change a few lines of the program: (a) we can model the possibility of natural disasters affecting the offspring rate of a certain generation with a conditional: $Disaster \sim \text{Bernoulli}(0.1)$; if $Disaster = 1 \{New_k \sim \text{Poisson}(\lambda')\}$ else $\{New_k \sim \text{Poisson}(\lambda)\}$, or (b) instead of a single population, we can model populations of two kinds of individuals that interact, i.e. a *multitype* branching process (see Fig. 1c). None of these modifications can be handled by [22] or [23]. The results of the first modification (Fig. 1b) are very similar. The (more complex) second modification takes longer to solve exactly, but the running time is similar to the approximate inference with 10000 samples, while achieving zero error.

Switchpoint model Our second benchmark is Bayesian switchpoint analysis, which is about detecting a change in the frequency of certain events over time. We use the model from [19] with continuous priors and its 111 real-world data points about the frequency of coal-mining accidents. We compare both the moment errors (Fig. 3) and the TVD errors (Fig. 2a). In both cases, the approximations are either inaccurate or take longer than our exact method.

Mixture model We consider a binary mixture model on the same data set, with equal mixture weights and a geometric prior for the rates: each data point is observed from a mixture of two Poisson distributions with different rates and the task is to infer these rates. Due to their multimodality, mixture models are notoriously hard for approximate inference methods, which is confirmed in Fig. 2b. Even the runs with the lowest error cover only one of the two modes (cf. the sample histogram in Fig. 2c).

Hidden Markov model We use a hidden Markov model based on [18, Section 2.2], but involving infinite (geometric) priors. It is a two-state system with known transition probabilities and the rate for the observed data depends on the hidden state. We run this model on 30 simulated data points. For this model as well, our method clearly outperforms approximate methods (Fig. 2d).

For brevity, we only presented the important aspects of these benchmarks, relegating the details and their encoding as probabilistic programs to Appendix D.1. To our knowledge, our approach is the first to find an exact solution to these problems, except the very first problem (without the modifications), which appeared in [22]. In the supplementary material, code and instructions to reproduce the above results are provided, which takes a few hours of CPU time on a laptop computer.

Conclusion

By leveraging generating functions, we have developed and proven correct a framework for exact Bayesian inference on discrete models, even with infinite support and continuous priors. We have demonstrated competitive performance on a range of models specified in an expressive probabilistic programming language, which our tool processes automatically.

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A Details on the Probabilistic Programming Language SGCL

A.1 A minimal grammar

A minimal grammar of SGCL looks like this:

$$P ::= \mathsf{skip} \mid P_1; P_2 \mid X_k := a_1 X_1 + \dots + a_n X_n + c \mid \text{if } X_k \in A \{P_1\} \text{ else } \{P_2\}$$

| fail | $X_k \sim D \mid X_k \sim D(X_j)$

where $a_1, \ldots, a_n, c \in \mathbb{R}_{\geq 0}$, $p \in [0, 1]$ are literals, and A is a finite subset of \mathbb{N} . The X_k for $k = 1, \ldots, n$ are variables that can take on values in $\mathbb{R}_{\geq 0}$. To explain, skip leaves everything unchanged, $P_1; P_2$ runs P_1 and then P_2 , and $X_k := \mathbf{a}^\top \mathbf{X} + c$ performs an affine transformation where $\mathbf{a} \in \mathbb{R}_{\geq 0}^n$ and $c \in \mathbb{R}_{\geq 0}$ (to ensure that the support of X_k is a subset of $\mathbb{R}_{\geq 0}$). The if construct allows branching based on comparisons of a variable X_k with constant natural numbers, with the requirement that X_k be a discrete variable on \mathbb{N} , and $X_k \sim D$ samples X_k from a primitive distribution (with constant parameters)

$$\begin{aligned} \mathcal{D} &= \{\mathsf{Bernoulli}(p), \mathsf{Categorical}(p_0, \dots, p_m), \mathsf{Binomial}(m, p), \mathsf{Uniform}\{l..m\}, \\ & \mathsf{NegBinomial}(m, p), \mathsf{Geometric}(p), \mathsf{Poisson}(\lambda), \\ & \mathsf{Exponential}(\alpha), \mathsf{Gamma}(\alpha, \beta), \mathsf{Uniform}[a, b] \\ & \mid p \in [0, 1], \alpha, \beta \in \mathbb{R}_{>0}, l, m \in \mathbb{N}, a, b \in \mathbb{R}_{>0}, a \leq b \} \end{aligned}$$

whereas $X_k \sim D(X_j)$ samples X_k from a compound distribution (with a parameter that is again a variable)

$$\mathcal{D}(X_j) = \{\mathsf{Binomial}(X_j, p), \mathsf{NegBinomial}(X_j, p), \mathsf{Poisson}(\lambda \cdot X_j), \mathsf{Bernoulli}(X_j) \\ \mid p \in [0, 1], j \in \{1, \dots, n\}, \lambda \in \mathbb{R}_{\geq 0}\}.$$

A.2 Syntactic sugar

For convenience, we add some syntactic sugar, which is expanded as follows:

$$\begin{array}{l} \mathsf{observe}\,c\sim D\rightsquigarrow X'\sim D; \mathsf{observe}\,X'=c\quad (X'\,\mathsf{fresh})\\ \mathsf{observe}\,\phi\rightsquigarrow \mathsf{if}\,\phi\,\{\mathsf{skip}\}\,\mathsf{else}\,\{\mathsf{fail}\}\\ \mathsf{if}\,\neg\phi\,\{P_1\}\,\mathsf{else}\,\{P_2\} \rightsquigarrow \mathsf{if}\,\phi\,\{P_2\}\,\mathsf{else}\,\{P_1\}\\ \mathsf{if}\,\phi_1\wedge\phi_2\,\{P_1\}\,\mathsf{else}\,\{P_2\} \rightsquigarrow \mathsf{if}\,\phi_1\,\{\mathsf{if}\,\phi_2\,\{P_1\}\,\mathsf{else}\,\{P_2\}\}\,\mathsf{else}\,\{P_2\}\\ \mathsf{if}\,\phi_1\vee\phi_2\,\{P_1\}\,\mathsf{else}\,\{P_2\} \rightsquigarrow \mathsf{if}\,\phi_1\,\{P_1\}\,\mathsf{else}\,\{\mathsf{if}\,\phi_2\,\{P_1\}\,\mathsf{else}\,\{P_2\}\}\\ \end{array}$$

A.3 Standard measure semantics

Notation and Conventions Throughout the text, we always assume that \mathbb{N} carries the discrete σ -algebra $\mathcal{P}(\mathbb{N})$ and \mathbb{R} the Borel σ -algebra $\mathcal{B}(\mathbb{R})$. Products of these spaces (e.g. $\mathbb{N} \times \mathbb{R}$) are endowed with the product σ -algebra. In the following, we write \boldsymbol{x} for (x_1, \ldots, x_n) and use the update notation $\boldsymbol{x}[i \mapsto a]$ to denote $(x_1, \ldots, x_{i-1}, a, x_{i+1}, \ldots, x_n)$. Finally, we write $\mathbf{1}_k$ for the k-tuple $(1, \ldots, 1)$ and similarly for $\mathbf{0}_k$. We write $\mathbf{0}$ for the zero measure or the constant zero function. We also use Iverson brackets $[\phi]$ for a logical condition $\phi: [\phi]$ is 1 if ϕ is satisfied and 0 otherwise. For example, the indicator function $\mathbf{1}_S$ of a set S can be defined using Iverson brackets: $\mathbf{1}_S(x) = [x \in S]$. For a measure μ on \mathbb{R}^n , we define $\mu_{X_k \in A}(S) = \mu(\{\boldsymbol{x} \in S \mid x_k \in A\})$.

Standard transformer semantics The standard semantics for such a probabilistic program uses distribution transformers [15]. Since our language includes conditioning, the distribution of program states will not always be a probability distribution, but a subprobability distribution μ on $\mathbb{R}^n_{\geq 0}$ for n variables, i.e. a function $\mu : \mathcal{B}(\mathbb{R}^n_{\geq 0}) \to [0, 1]$ with $\mu(\mathbb{R}^n_{\geq 0}) \leq 1$. The semantics of a program P is thus a measure transformer $[\![P]\!]_{std} : \operatorname{Meas}(\mathbb{R}^k_{\geq 0}) \to \operatorname{Meas}(\mathbb{R}^k_{\geq 0})$. We assume that the initial measure is the probability distribution where every variable X_k is 0 with probability 1, i.e. $X \sim \operatorname{Dirac}(\mathbf{0}_n)$. The semantics is shown in Fig. 4 where X is a vector of length n.

The first 5 rules were essentially given by [15], with slightly different notation and presentation. (Kozen defines some of the measures on rectangles ($S = S_1 \times \cdots \times S_n$) only, which uniquely extends

$$\begin{split} \llbracket \mathsf{skip} \rrbracket_{\mathsf{std}}(\mu) &= \mu \\ \llbracket P_1; P_2 \rrbracket_{\mathsf{std}}(\mu) &= \llbracket P_2 \rrbracket_{\mathsf{std}}(\llbracket P_1 \rrbracket_{\mathsf{std}}(\mu)) \\ \llbracket X_k &:= \mathbf{a}^\top \mathbf{X} + c \rrbracket_{\mathsf{std}}(\mu)(S) = \mu(\{\mathbf{X} \in \mathbb{R}^n \mid \mathbf{X}[k \mapsto \mathbf{a}^\top \mathbf{X} + c] \in S\}) \\ \llbracket \mathsf{if} \ X_k \in A \{P_1\} \ \mathsf{else} \ \{P_2\} \rrbracket_{\mathsf{std}}(\mu) &= \llbracket P_1 \rrbracket_{\mathsf{std}}(\mu_{X_k \in A}) + \llbracket P_2 \rrbracket_{\mathsf{std}}(\mu - \mu_{X_k \in A}) \\ \mathsf{where} \ \mu_{X_k \in A}(S) &= \mu(\{\mathbf{X} \in S \mid X_k \in A\}) \\ \llbracket X_k \sim D \rrbracket_{\mathsf{std}}(\mu)(S) &= \int \int [\mathbf{X}[k \mapsto Y] \in S] \ \mathrm{d}D(Y) \ \mathrm{d}\mu(\mathbf{X}) \\ \llbracket X_k \sim D(X_j) \rrbracket_{\mathsf{std}}(\mu)(S) &= \int \int [\mathbf{X}[k \mapsto Y] \in S] \ \mathrm{d}D(X_j)(Y) \ \mathrm{d}\mu(\mathbf{X}) \\ \llbracket \mathsf{fail} \rrbracket_{\mathsf{std}}(\mu) &= \mathbf{0} \\ \mathsf{normalize}(\mu) &= \frac{\mu}{\int \ \mathrm{d}\mu(\mathbf{X})} \end{split}$$

Figure 4: The standard measure semantics $[-]_{std}$.

to a measure on all sets in the product space σ -algebra. By contrast, we directly define the measure on all sets in the σ -algebra using integrals.)

We quickly explain the rules. The skip command does nothing, so the distribution μ of the program is unchanged. Chaining commands P_1 ; P_2 has the effect of composing the corresponding transformations of μ . Affine transformations of program variables yield a measure that is given by the original measure of the preimage of the event S under the affine map. For conditionals if $X_k \in A \{P_1\}$ else $\{P_2\}$, we consider only outcomes satisfying $X_k \in A$ in the first branch and the complement in the second branch and then sum both possibilities. Sampling from distributions $X_k \sim D$ is a bit more complicated. Note that $\mu(S) = \int [\mathbf{X} \in S] d\mu(\mathbf{X})$. To obtain the measure after sampling $X_k \sim D$, we care about the new state $\mathbf{X}[k \mapsto Y]$ being in S, where Y has distribution D. This is exactly expressed by the double integral. The rule for compound distributions $X_k \sim D$, except the dependency on X_j needs to be respected.

The two new rules (not derivable from Kozen's work) are for fail and the implicit normalization normalize(μ) as a final step at the end of a program. The rule for fail departs from Kozen's semantics in the sense that it yields a subprobability distribution (i.e. the total mass can be less than 1). Intuitively, fail "cuts off" or assigns the probability 0 to certain branches in the program. This is called *hard conditioning* in the PPL literature. For example, if $X_1 = 5$ {skip} else {fail} has the effect of conditioning on the event that $X_1 = 5$ because all other scenarios are assigned probability 0.

The normalization construct corresponds to the division by the evidence in Bayes' rule and scales the subprobability distribution of a subprogram P back to a probability distribution. The semantics is $\frac{\mu}{\int d\mu(\mathbf{X})}$, so the distribution μ is scaled by the inverse of the total probability mass of μ , thus normalizing it.

B Details on Generating Functions

An exhaustive list of the supported distributions and their generating functions can be found in Tables 3a and 3b.

B.1 Generating function semantics

The full generating function semantics can be found in Fig. 5. The first five rules in Fig. 5 were presented in [14, 3]. The GF for sampling from $\text{Binomial}(X_j, p)$ was first given in [22]. Chen et al. [3] also implicitly describe the GF semantics of sampling from $\text{Binomial}(X_j, p)$ and $\text{NegBinomial}(X_j, p)$ by expressing it as summing X_j iid samples from Bernoulli(p) and Geometric(p), respectively.

Distribution D	$gf(X \sim D)(x)$	_	
Dirac(a)	x^a	_	
Bernoulli(p)	px + 1 - p		
$Categorical(p_0,\ldots,p_n)$	$\sum_{i=0}^{n} p_i x^i$	(b) GFs for commo	n compound distributions
Binomial(n,p)	$(px + 1 - p)^n$	\mathbf{D}' (1) $\mathbf{D}(\mathbf{V})$	(X - D(X))(x)
$Uniform\{ab\}$	$\frac{x^a - x^{b+1}}{(b-a+1)(1-x)}$	Distribution $D(Y)$	$gf(X \sim D(Y))(x)$
	$(n)^r$	- Binomial (Y, p)	gf(Y)(1-p+px)
NegBinomial (r, p)	$\left(\frac{p}{1-(1-p)x}\right)$	NegBinomial(Y, p)	$\operatorname{gf}(Y)\left(\frac{p}{1-(1-r)r}\right)$
Geometric(p)	$\frac{p}{1-(1-p)x}$	$Poisson(\lambda \cdot Y)$	$\operatorname{sf}(Y)(e^{\lambda(x-1)})$
$Poisson(\lambda)$	$e^{\lambda(x-1)}$	Bernoulli (Y)	$1 + (x - 1) \cdot (gf(Y))'(1)$
$Exponential(\lambda)$	$\frac{\lambda}{\lambda - \log x}$		
$Gamma(\alpha,\beta)$	$\left(\frac{\beta}{\beta - \log x}\right)^{\alpha}$		
Uniform[a,b]	$\begin{cases} \frac{x^b - x^a}{(b-a)\log x} & x \neq 1 \\ 1 & 1 \end{cases}$		
	$1 \qquad x=1$		

(a) GFs for common distributions

$$\begin{split} \llbracket \mathsf{skip} \rrbracket_{\mathsf{gf}}(G) &= G \\ \llbracket P_1; P_2 \rrbracket_{\mathsf{gf}}(G) &= \llbracket P_2 \rrbracket_{\mathsf{gf}}(\llbracket P_1 \rrbracket_{\mathsf{gf}}(G)) \\ \llbracket X_k &:= \mathbf{a}^\top \mathbf{X} + c \rrbracket_{\mathsf{gf}}(G)(\mathbf{x}) = x_k^c \cdot G(\mathbf{x}') \\ & \text{where } x_k' := x_k^{a_k} \text{ and } x_i' := x_i x_k^{a_i} \text{ for } i \neq k \\ \llbracket \text{if } X_k \in A \{P_1\} \text{ else } \{P_2\} \rrbracket_{\mathsf{gf}}(G) &= \llbracket P_1 \rrbracket_{\mathsf{gf}}(G_{X_k \in A}) + \llbracket P_2 \rrbracket_{\mathsf{gf}}(G - G_{X_k \in A}) \\ & \text{where } G_{X_k \in A}(\mathbf{x}) = \sum_{i \in A} \frac{\partial_k^i G(\mathbf{x}[k \mapsto 0])}{i!} x_k^i \quad \text{and } A \subset \mathbb{N} \text{ finite} \\ & \text{if } X_k \text{ has support in } \mathbb{N} \\ \llbracket X_k \sim D \rrbracket_{\mathsf{gf}}(G)(\mathbf{x}) &= G(\mathbf{x}[k \mapsto 1]) \mathsf{gf}(D)(x_k) \\ \llbracket X_k \sim D(X_j) \rrbracket_{\mathsf{gf}}(G)(\mathbf{x}) &= G(\mathbf{x}[k \mapsto 1, j \mapsto x_j \cdot \mathsf{gf}(D(1))(x_k)]) \\ & \text{ for } D \in \{\mathsf{Binomial}(-, p), \mathsf{NegBinomial}(-, p), \mathsf{Poisson}(\lambda \cdot -)\} \\ \llbracket X_k \sim \mathsf{Bernoulli}(X_j) \rrbracket_{\mathsf{gf}}(G)(\mathbf{x}) &= G(\mathbf{x}[k \mapsto 1]) + x_j(x_k - 1) \cdot \partial_j G(\mathbf{x}[k \mapsto 1]) \\ & \text{ if } X_j \text{ has support in } [0, 1] \\ & \llbracket \mathsf{fail} \rrbracket_{\mathsf{gf}}(G) &= \mathbf{0} \\ & \mathsf{normalize}(G) &= \frac{G}{G(\mathbf{1}_n)} \end{split}$$

Figure 5: The generating function (GF) semantics $[\![-]\!]_{gf}.$

Let us discuss each rule in detail. The skip command leaves the distribution and hence the generating function unchanged. Chaining commands P_1 ; P_2 is again achieved by composing the individual transformers for each command. To obtain some intuition for the affine transformation case $X_k := \mathbf{a}^\top \mathbf{X} + c$, suppose we only have 2 variables: $X_1 := 2X_1 + 3X_2 + 5$. The idea is that the transformed generating function is given by $[X_1 := 2X_1 + 3X_2 + 5]_{gf}(G)(\mathbf{x}) = \mathbb{E}[x_1^{2X_1+3X_2+5}x_2^{X_2}] = x_1^5 \mathbb{E}[(x_1^2)^{X_1}(x_1^3x_2)^{X_2}] = x_1^5 \cdot G(x_1^2, x_1^3x_2)$.

The semantics of if $X_k \in A \{P_1\} \operatorname{else} \{P_2\}$ uses $G_{X_k \in A}$. If G is the generating function for a measure μ then $G_{X_k \in A}$ is the generating function for the measure $\mu_{X_k \in A}(S) := \mu(\{x \in S \mid x_k \in A\})$. To get intuition for this, remember that for discrete variables X_1, X_2 , we have $G(x_1, x_2) = \sum_{X_1, X_2} \mu(\{(X_1, X_2)\}) \cdot x_1^{X_1} x_2^{X_2}$. If we want to obtain the generating function for $X_1 = 5$, we want to keep only terms where x_1 has exponent 5. In other words, we need the Taylor coefficient $\frac{\partial_1^5 G(0, x_2)}{5!}$. This should give some intuition for $G_{X_k \in A}$. The semantics of if $X_k \in A \{P_1\}$ else $\{P_2\}$ transforms $G_{X_k \in A}$ in the then-branch and the complement $G - G_{X_k \in A}$ in the else branch, summing the two possibilities.

For sampling, say $X_1 \sim D$, we first marginalize out the old X_1 by substituting 1 for x_1 in G: $\mathbb{E}[x_2^{X_2}] = \mathbb{E}[1^{X_1}x_2^{X_2}] = G(1, x_2)$. Then we multiply with the GF of the new distribution D. The rules for compound distributions $D(X_j)$ are more involved, so we offer the following intuition.

For the compound distributions D(n) = Binomial(n, p), NegBinomial(n, p), Poisson $(\lambda \cdot n)$, we make essential use of their property that $gf(D(n))(x) = (gf(D(1))(x))^n$. So if $G(x) := \mathbb{E}[x^X]$ is the GF of X and $Y \sim D(X)$, then $\mathbb{E}_{X,Y}[x^X y^Y] = \mathbb{E}_X[x^X \mathbb{E}_{Y \sim D(X)}[y^Y]] = \mathbb{E}_X[x^X gf(D(X))(y)] = \mathbb{E}_X[x^X(gf(D(1))(y))^X] = \mathbb{E}[(x \cdot gf(D(1))(y))^X] = G(x \cdot gf(D(1))(y))$. This is not a fully formal argument, but it should give some intuition for the rule.

For D(p) = Bernoulli(p), the intuition is that if $G(x) := \mathbb{E}[x^X]$ is the GF of X and if $Y \sim \text{Bernoulli}(X)$, then $H(x,y) = \mathbb{E}[x^X y^Y] = \mathbb{E}[x^X((1-X)y^0 + Xy^1)] = \mathbb{E}[x^X - (y-1)Xx^X] = G(x) - (y-1)xG'(x)$.

The GF semantics of fail is the zero function because its distribution is zero everywhere. For normalization note that substituting $\mathbf{1}_n$ in the generating function computes the marginal probabilities, similarly to the substitution of 1 in the semantics of sampling. It scales the GF of the subprogram P by the inverse of the normalizing constant obtained by that substitution.

We hope these explanations give some intuition for the GF semantics, but of course, proof is required.

B.2 Correctness proof

Theorem B.1 (Correctness). The GF semantics is correct w.r.t. the standard semantics $[-]]_{std}$: for any SGCL program P and subprobability distribution μ on $\mathbb{R}^n_{\geq 0}$, we have $[\![P]\!]_{gf}(gf(\mu)) = gf([\![P]\!]_{std}(\mu))$. In particular, it correctly computes the GF of the posterior distribution of P as normalize $([\![P]\!]_{gf}(gf(\mu)))$.

Furthermore, if $gf(\mu)$ is defined on $[0, R)^n$ for some R > 1 then $\llbracket P \rrbracket_{gf}(gf(\mu))$ is defined on $[0, R')^n$ for some R' > 1. In particular, the GFs $\llbracket P \rrbracket_{gf}(1)$ and thus normalize($\llbracket P \rrbracket_{gf}(1)$) are defined on $[0, R)^n$ for some R > 1.

Proof. As usual for such statements, we prove this by induction on the structure of the program. The program P can take one of the following forms:

Skip. For the trivial program, we have $\llbracket P \rrbracket_{gf}(G) = G$ and $\llbracket P \rrbracket_{std}(\mu) = \mu$, so the claim is trivial.

Chaining. If P is P_1 ; P_2 , we know by the inductive hypothesis that $\llbracket P_1 \rrbracket_{gf}(gf(\mu)) = gf(\llbracket P_1 \rrbracket_{std}(\mu))$ and similarly for P_2 . Taking this together, we find by the definitions of the semantics:

$$[\![P_1; P_2]\!]_{gf}(gf(\mu)) = [\![P_2]\!]_{gf}([\![P_1]\!]_{gf}(gf(\mu))) = [\![P_2]\!]_{gf}(gf([\![P_1]\!]_{std}(\mu)))$$

$$= \mathsf{gf}(\llbracket P_2 \rrbracket_{\mathsf{std}}(\llbracket P_1 \rrbracket_{\mathsf{std}}(\mu))) = \mathsf{gf}(\llbracket P_1; P_2 \rrbracket_{\mathsf{std}}(\mu)).$$

The claim about the domain of $\llbracket P \rrbracket_{gf}(G)$ follows directly from the inductive hypotheses.

Affine assignments. If P is $X_k := \mathbf{a}^\top \mathbf{X} + c$, we have $\llbracket P \rrbracket_{\mathsf{std}}(\mu)(S) = \mu(\{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}[k \mapsto \mathbf{a}^\top \mathbf{x} + c] \in S\})$ and thus

$$\mathsf{gf}(\llbracket P \rrbracket_{\mathsf{std}}(\mu))(\boldsymbol{x}) = \int \boldsymbol{x}^{\boldsymbol{X}} \, \mathrm{d}(\llbracket P \rrbracket_{\mathsf{std}}(\mu))(\boldsymbol{X})$$

$$= \int x_1^{X_1} \cdots x_{k-1}^{X_{k-1}} x_k^{a_1 X_1 + \dots + a_n X_n + c} x_{k+1}^{X_{k+1}} \cdots x_n^{X_n} d\mu(X_1, \dots, X_n)$$

$$= x_k^c \cdot \int (x_1 x_k^{a_1})^{X_1} \cdots (x_{k-1} x_k^{a_{k-1}})^{X_{k-1}} (x_k^{a_k})^{X_k} \cdot (x_{k+1} x_k^{a_{k+1}})^{X_{k+1}} \cdots (x_n x_k^{a_n})^{X_n} d\mu(\mathbf{X})$$

$$= x_k^c \cdot \mathsf{gf}(\mu) (x_1 x_k^{a_1}, \dots, x_{k-1} x_k^{a_{k-1}}, x_k^{a_k}, x_{k+1} x_k^{a_{k+1}}, \dots, x_n x_k^{a_n})$$

$$= \|P\|_{\mathsf{ff}}(\mathsf{gf}(\mu))(\mathbf{x})$$

The second claim holds if we choose $R' = \min(\sqrt{R}, \min_{i=1}^{n} \sqrt[2a_i]{R})$ because then $x_i x_k^{a_i} < \sqrt{R} (\sqrt[2a_i]{R})^{a_i} \leq R$ for $i \neq k$ and $x_k^{a_k} < (\sqrt[2a_k]{R})^{a_k} \leq \sqrt{R} \leq R$.

Conditionals. If *P* is if $X_k \in A \{P_1\}$ else $\{P_2\}$, the GF semantics defines $(gf(\mu))_{X_k \in A}$, which is the same as $gf(\mu_{X_k \in A})$ by Lemma B.2. Using this fact and the induction hypothesis, we find

$$\begin{aligned} \mathsf{gf}(\llbracket P \rrbracket_{\mathsf{std}}(\mu)) &= \mathsf{gf}(\llbracket P_1 \rrbracket_{\mathsf{std}}(\mu_{X_k \in A})) + \mathsf{gf}(\llbracket P_2 \rrbracket_{\mathsf{std}}(\mu - \mu_{X_k \in A})) \\ &= \llbracket P_1 \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu_{X_k \in A})) + \llbracket P_2 \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu) - \mathsf{gf}(\mu_{X_k \in A})) \\ &= \llbracket P_1 \rrbracket_{\mathsf{gf}}((\mathsf{gf}(\mu))_{X_k \in A}) + \llbracket P_2 \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu) - (\mathsf{gf}(\mu))_{X_k \in A}) \\ &= \llbracket P \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu)) \end{aligned}$$

Also by Lemma B.2, we know that $(gf(\mu))_{X_k \in A}$ is defined on $[0, R)^n$, so the same holds for $[\![P]\!]_{gf}(gf(\mu))$.

Sampling. If *P* is $X_k \sim D$, we find:

$$gf(\llbracket P \rrbracket_{std}(\mu))(\boldsymbol{x}) = \int \boldsymbol{x}^{\boldsymbol{X}} d(\llbracket P \rrbracket_{std}(\mu))(\boldsymbol{X})$$
$$= \int \int \boldsymbol{x}^{\boldsymbol{X}[k \mapsto Y]} dD(Y) d\mu(\boldsymbol{X})$$
$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} \int x_k^Y dD(Y) d\mu(\boldsymbol{X})$$
$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} d\mu(\boldsymbol{X}) \cdot \int x_k^Y dD(Y)$$
$$= gf(\mu)(\boldsymbol{x}[k \mapsto 1])gf(D)(x_k)$$
$$= \llbracket P \rrbracket_{ef}(gf(\mu))(\boldsymbol{x})$$

Regarding the definedness of $\llbracket P \rrbracket_{gf}(gf(\mu))$, note that gf(D) is defined on \mathbb{R} for any finite distribution and for the Poisson distribution (cf. Table 3a). For $D \in \{\text{Geometric}(p), \text{NegBinomial}(n, p)\}$, the GF gf(D) is defined on $[0, \frac{1}{1-p})$, so we can pick $R' := \min(R, \frac{1}{1-p}) > 1$. The GF of Exponential (λ) is defined for $\log x < \lambda$, i.e. $x < \exp(\lambda)$, so we can pick $R' := \min(R, e^{\lambda}) > 1$. The GF of $\text{Gamma}(\alpha, \beta)$ is defined for $\log x < \beta$, i.e. $x < \exp(\beta)$, so we can pick $R' := \min(R, e^{\beta}) > 1$. The GF of Uniform[a, b] is defined on \mathbb{R} , so is not a problem.

If P is $X_k \sim D(X_j)$, we use the fact that $gf(D(n))(\mathbf{x}) = (gf(D(1))(\mathbf{x}))^n$ for $D(n) \in \{\text{Binomial}(n, p), \text{NegBinomial}(n, p), \text{Poisson}(\lambda \cdot n)\}$, which can easily be checked by looking at their generating functions (cf. Table 3b).

$$gf(\llbracket P \rrbracket_{std}(\mu))(\boldsymbol{x}) = \int \boldsymbol{x}^{\boldsymbol{X}} d(\llbracket P \rrbracket_{std}(\mu))(\boldsymbol{X})$$

$$= \int \int \boldsymbol{x}^{\boldsymbol{X}[k \mapsto Y]} dD(X_j)(Y) d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} \int x_k^Y dD(X_j)(Y) d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} gf(D(X_j))(x_k) d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} (gf(D(1))(x_k))^{X_j} d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1, j \mapsto x_j \cdot gf(D(1))(x_k)])^{\boldsymbol{X}} d\mu(\boldsymbol{X})$$

$$= \mathsf{gf}(\mu)(\boldsymbol{x}[k \mapsto 1, j \mapsto x_j \cdot \mathsf{gf}(D(1))(x_k)])$$

= $\llbracket P \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu))(\boldsymbol{x})$

Regarding the domain of $\llbracket P \rrbracket_{\mathsf{gf}}(\mathsf{gf}(\mu))$, we have to ensure that $x_j \cdot \mathsf{gf}(D(1))(x_k) < R$. For the Binomial(1) distribution, we choose $R' = \sqrt{R}$ such that $x_j(1 - p + px_k) < \sqrt{R}(1 - p + p\sqrt{R}) < R$. For the NegBinomial(1) distribution, we choose $R' = \min(\sqrt{R}, \frac{\sqrt{R}-p}{\sqrt{R}(1-p)}) = \min(\sqrt{R}, 1 + \frac{p(\sqrt{R}-1)}{\sqrt{R}-p\sqrt{R}})$ because then

$$\frac{p}{1 - (1 - p)x_j} < \frac{p}{1 - (1 - p)R'} = \frac{p}{1 - \frac{\sqrt{R} - p}{\sqrt{R}}} = \frac{p\sqrt{R}}{p} = \sqrt{R}$$

and thus $x_j \frac{p}{1-(1-p)x_k} < R$. For the Poisson (λ) distribution, we choose $R' = \min(\sqrt{R}, 1 + \frac{\log(R)}{2\lambda})$ because then $x_j \cdot \exp(\lambda(x_k - 1)) \le \sqrt{R} \exp(\lambda \frac{\log(R)}{2\lambda}) = R$. For the Bernoulli distribution $D(X_j) = \text{Bernoulli}(X_j)$, we reason as follows:

$$gf(\llbracket P \rrbracket_{\mathsf{std}}(\mu))(\boldsymbol{x}) = \dots = \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} gf(D(X_j))(x_k) d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} (1 + X_j(x_k - 1)) d\mu(\boldsymbol{X})$$

$$= \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} d\mu(\boldsymbol{X}) + (x_k - 1) \cdot \int X_j(\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} d\mu(\boldsymbol{X})$$

$$= gf(\mu)(\boldsymbol{x}[k \mapsto 1]) + (x_k - 1) \cdot \int x_j \cdot \partial_j(\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} d\mu(\boldsymbol{X})$$

$$= gf(\mu)(\boldsymbol{x}[k \mapsto 1]) + x_j(x_k - 1) \cdot \partial_j \int (\boldsymbol{x}[k \mapsto 1])^{\boldsymbol{X}} d\mu(\boldsymbol{X})$$

$$= gf(\mu)(\boldsymbol{x}[k \mapsto 1]) + x_j(x_k - 1) \cdot \partial_j gf(\mu)(\boldsymbol{x}[k \mapsto 1])$$

$$= \llbracket P \rrbracket_{\mathsf{sf}}(\mathsf{gf}(\mu))(\boldsymbol{x})$$

Note that the interchange of integral and differentiation is allowed by Corollary B.4. It is also clear that $\llbracket P \rrbracket_{gf}(gf(\mu))(x)$ is defined on $[0, R)^n$ by Corollary B.4.

Fail. If P is fail, then $[\![P]\!]_{std}(\mu)$ is the zero measure and $[\![P]\!]_{gf}(gf(\mu))$ is the zero function, so the claim holds trivially. This GF is clearly defined everywhere.

Normalization. For normalization, we make use of the linearity of gf(-).

$$\begin{split} \mathsf{gf}(\mathsf{normalize}(\mu)) &= \mathsf{gf}\left(\frac{\mu}{\int \mathrm{d}\mu(\boldsymbol{X})}\right) \\ &= \frac{\mathsf{gf}(\mu)}{\int \mathrm{d}\mu(\boldsymbol{X})} \\ &= \frac{\mathsf{gf}(\mu)}{\int 1^{X_1} \cdots 1^{X_n} \mathrm{d}\mu(\boldsymbol{X})} \\ &= \frac{\mathsf{gf}(\mu)}{\mathsf{gf}(\mu)(\mathbf{1}_n)} \\ &= \mathsf{normalize}(\mathsf{gf}(\mu)) \end{split}$$

Furthermore, if $gf(\mu)$ is defined on $[0, R)^n$, then so is normalize $(gf(\mu))$.

This finishes the induction and proves the claim.

Lemma B.2. Let $A \subset \mathbb{N}$ be a finite set. Let μ be a measure on \mathbb{R}^n such that its k-th component is supported on \mathbb{N} , i.e. $\mu(S) = \mu(\{X \in S \mid X_k \in \mathbb{N}\})$ for all measurable $S \subseteq \mathbb{R}_{\geq 0}$. Define $\mu_{X_k \in A}(S) := \mu(\{X \in S \mid X_k \in A\})$. Let $G := \mathsf{gf}(\mu)$. Then

$$\mathsf{gf}(\mu_{X_k \in A})(\boldsymbol{x}) = G_{X_k \in A}(\boldsymbol{x}) := \sum_{i \in A} \frac{\partial_k^i G(\boldsymbol{x}[k \mapsto 0])}{i!} \cdot x_k^i$$

where the derivative is interpreted as the right-hand derivative (since G need not be defined for $x_k < 0$). Furthermore, if G is defined on $[0, R)^n$ then so is $G_{X_k \in A}$.

Proof. Since $\mu_{X_k \in A} = \sum_{i \in A} \mu_{X_k=i}$ where we write $\mu_{X_k=i} := \mu_{X_k \in \{i\}}$, we have:

$$\begin{aligned} \mathsf{gf}(\mu_{X_k=i})(\boldsymbol{x}) &= \int \boldsymbol{x}^{\boldsymbol{X}} \, \mathrm{d}\mu_{X_k=i}(\boldsymbol{X}) \\ &= \int x_1^{X_1} \cdots x_{k-1}^{X_{k-1}} \cdot x_k^{X_k} \cdot x_{k+1}^{X_{k+1}} \cdots x_n^{X_n} \cdot [X_k=i] \, \mathrm{d}\mu(\boldsymbol{X}) \\ &= x_k^i \int x_1^{X_1} \cdots x_{k-1}^{X_{k-1}} \cdot x_{k+1}^{X_{k+1}} \cdots x_n^{X_n} \cdot \left(\frac{1}{i!} \left. \frac{\partial^i x_k^{X_k}}{\partial x_k^i} \right|_{x_k=0} \right) \, \mathrm{d}\mu(\boldsymbol{X}) \end{aligned}$$

The reason for the last step is that for the function $f(x) = x^{l}$, we have

$$f^{(i)}(x) = \begin{cases} 0 & \text{if } l < i \\ \prod_{j=l-i+1}^{l} j \cdot x^{l-i} & \text{if } l \ge i \end{cases}$$

Since 0^{l-i} is 0 for l > i and 1 for l = i, we find that $f^{(i)}(0) = i![i = l]$. This is the fact we used above. We continue:

$$\cdots = x_k^i \int \frac{1}{i!} \left(x_1^{X_1} \cdots x_{k-1}^{X_{k-1}} \cdot \frac{\partial^i x_k^{X_k}}{\partial x_k^i} \cdot x_{k+1}^{X_{k+1}} \cdots x_n^{X_n} \right) \Big|_{x_k=0} \, \mathrm{d}\mu(\mathbf{X})$$

$$= \int \frac{\partial^i}{\partial x_k^i} \mathbf{x}^{\mathbf{X}} \, \mathrm{d}\mu(\mathbf{X}) \Big|_{x_k=0} \cdot \frac{x_k^i}{i!}$$

$$= \frac{\partial^i}{\partial x_k^i} \int \mathbf{x}^{\mathbf{X}} \, \mathrm{d}\mu(\mathbf{X}) \Big|_{x_k=0} \cdot \frac{x_k^i}{i!}$$

$$= \partial_k^i G(\mathbf{x}[k \mapsto 0]) \cdot \frac{x_k^i}{i!}$$

as desired. Note that the integral and differentiation operators can be interchanged by Corollary B.4.

Lemma B.3. Let $w \in \mathbb{N}^n$, p be a polynomial in n variables, and μ a measure on $\mathbb{R}^n_{\geq 0}$. Suppose the integral $\int p(\mathbf{X}) \mathbf{x}^{\mathbf{X}-\mathbf{w}} d\mu(\mathbf{X})$ is defined for all $\mathbf{x} \in (0, R)^n$. Then

$$\frac{\partial}{\partial x_i} \int p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \, \mathrm{d}\boldsymbol{\mu}(\boldsymbol{X}) = \int \frac{\partial}{\partial x_i} p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \, \mathrm{d}\boldsymbol{\mu}(\boldsymbol{X})$$
$$= \int (X_i - w_i) p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}[i \mapsto w_i+1]} \, \mathrm{d}\boldsymbol{\mu}(\boldsymbol{X})$$

holds and is defined for all $x \in [0, R)^n$ with $x_i > 0$.

Furthermore, suppose that the *i*-th component of μ is supported on \mathbb{N} , *i.e.* $\mu(S) = \mu(\{\mathbf{X} \in S \mid X_i \in \mathbb{N}\})$ for all measurable $S \subseteq \mathbb{R}^n_{\geq 0}$. Then the above claim even holds for all $\mathbf{x} \in [0, R)^n$, including $x_i = 0$, if the derivatives at zero are interpreted as right-hand derivatives.

Proof. Let $0 < \epsilon < R' < R$. We first prove $\partial_i \int p(\mathbf{X}) \mathbf{x}^{\mathbf{X}} d\mu(\mathbf{X}) = \int \partial_i p(\mathbf{X}) \mathbf{x}^{\mathbf{X}} d\mu(\mathbf{X})$ for any $x \in (\epsilon, R')$, using the Leibniz integral rule. For this purpose, we need to bound the derivative:

$$\begin{aligned} |\partial_i p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}}| &\leq |(X_i - w_i) p(\boldsymbol{X})| \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}[i \mapsto w_i+1]} \leq \frac{1}{x_i} X_i p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \\ &\leq \frac{1}{\epsilon} X_i p(\boldsymbol{X}) \max((R' \mathbf{1}_n)^{\boldsymbol{X}}, (\epsilon \mathbf{1}_n)^{-\boldsymbol{w}}) \end{aligned}$$

which is integrable as a function of X because $X_i(R')^{X_i} \leq R''^{X_i}$ for some R' < R'' < R and X_i sufficiently large, and $p(X)(R''\mathbf{1}_n)^X$ is integrable by assumption. Hence all conditions of the Leibniz integral rule are satisfied and interchanging differentiation and the integral is valid:

$$\partial_i \int p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \, \mathrm{d}\mu(\boldsymbol{X}) = \int \partial_i p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \, \mathrm{d}\mu(\boldsymbol{X})$$

$$= \int (X_i - w_i) p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X} - \boldsymbol{w}[i \mapsto w_i + 1]} \, \mathrm{d} \mu(\boldsymbol{X}).$$

Finally, we consider the second part of the lemma: $x_i = 0$. Note that $p(\mathbf{X}) = 0$ whenever $X_i \in \mathbb{N} \cap [0, w_i]$ because otherwise the integral would not be defined for $x_i = 0$ (the integrand would be infinite). The right-hand derivative is given by

$$\partial_i \int [X_j \in \mathbb{N}] p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X}-\boldsymbol{w}} \, \mathrm{d}\mu(\boldsymbol{X}) \bigg|_{x_i=0}$$

=
$$\lim_{h \searrow 0} \int [X_j \in \{w_i, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X}-\boldsymbol{w}} \frac{h^{X_i-w_i} - 0^{X_i-w_i}}{h} \, \mathrm{d}\mu(\boldsymbol{X})$$

Note that $\frac{h^{X_i-w_i}-0^{X_i-w_i}}{h} = \frac{1-1}{h} = 0$ if $X_i = w_i$ and $\frac{h^{X_i-w_i}-0^{X_i-w_i}}{h} = h^{X_i-w_i-1}$ if $X_i \ge w_i + 1$. Since in either case, the term is bounded by an integrable function for $h \in [0, \epsilon]$ for some $\epsilon > 0$, we can use the Dominated Convergence Theorem to interchange the limit and integral. Hence we find

$$\begin{split} \cdots &= \lim_{h \searrow 0} \int [X_j \in \{w_i + 1, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} h^{X_i - w_i - 1} \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int \lim_{h \searrow 0} [X_j \in \{w_i + 1, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} h^{X_i - w_i - 1} \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int [X_j \in \{w_i + 1, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} [X_i - w_i - 1 = 0] \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int [X_j \in \{w_i + 1, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} [X_i - w_i - 1 = 0] (X_i - w_i) \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int [X_j \in \{w_i, \dots\}] p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} (X_i - w_i) 0^{X_i - w_i - 1} \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} (X_i - w_i) x_i^{X_i - w_i - 1} \, \mathrm{d} \mu(\boldsymbol{X}) \\ &= \int p(\boldsymbol{X}) \boldsymbol{x}[i \mapsto 1]^{\boldsymbol{X} - \boldsymbol{w}} \partial_i x_i^{X_i - w_i} \, \mathrm{d} \mu(\boldsymbol{X}) \Big|_{x_i = 0} \\ &= \int \partial_i p(\boldsymbol{X}) \boldsymbol{x}^{\boldsymbol{X} - \boldsymbol{w}} \, \mathrm{d} \mu(\boldsymbol{X}) \Big|_{x_i = 0} \end{split}$$

as desired.

Corollary B.4. If the integral $\int \mathbf{x}^{\mathbf{X}} d\mu(\mathbf{X})$ for a measure μ on $\mathbb{R}^n_{\geq 0}$ is defined for all $\mathbf{x} \in [0, R)^n$, we have

$$\int \partial_{i_1} \cdots \partial_{i_m} \boldsymbol{x}^{\boldsymbol{X}} \, \mathrm{d} \boldsymbol{\mu}(\boldsymbol{X}) = \partial_{i_1} \cdots \partial_{i_m} \int \boldsymbol{x}^{\boldsymbol{X}} \, \mathrm{d} \boldsymbol{\mu}(\boldsymbol{X})$$

and both sides are defined for all $x \in (0, R)^n$.

Furthermore, suppose that for all $j \in \{1, ..., m\}$, the i_j -th component of μ is supported on \mathbb{N} , i.e. $\mu(S) = \mu(\{\mathbf{X} \in S \mid X_{i_j} \in \mathbb{N}\})$ for all measurable $S \subseteq \mathbb{R}^n_{\geq 0}$. Then the above claim even holds for all $\mathbf{x} \in [0, R)^n$ if the derivatives at zero are interpreted as right-hand derivatives.

Proof. Follows inductively from Lemma B.3. Note that the shape of a single derivative $\int (X_i - w_i)p(\mathbf{X})\mathbf{x}^{\mathbf{X}-\mathbf{w}[i\mapsto w_i+1]} d\mu(\mathbf{X})$ again satisfies the requirements of the lemma for $\mathbf{x} \in (0, R)^n$, so can be iterated. For $x_i = 0$, note that the factor $X_i - w_i$ is 0 for $X_i = w_i$, so the polynomial $\tilde{p}(\mathbf{X}) := (X_i - w_i)p(\mathbf{X})$ is zero whenever $X_i \in \mathbb{N} \cap [0, w_i + 1)$, allowing the second part of the lemma to be iterated as well.

Remark B.1. As an example of what can go wrong with derivatives at zero if the measure is not supported on \mathbb{N} , consider the Dirac measure $\mu = \text{Dirac}(\frac{1}{2})$. It has the generating function $G(x) := \text{gf}(\mu)(x) = \sqrt{x}$ defined for $x \in \mathbb{R}_{\geq 0}$. Its derivative is $G'(x) := \frac{1}{2\sqrt{x}}$, which is not defined for x = 0.

С Details on implementation and optimizations

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Overview Our tool takes an SGCL program P with n variables as input, and a variable X_i whose posterior distribution is to be computed. It translates it to the GF $[P]_{gf}(1)$ according to the GF semantics and normalizes it: $G := \text{normalize}(\llbracket P \rrbracket_{ef}(1))$. This G is the GF of the posterior distribution of the program, from which it extracts the posterior moments of X_i and its probability masses (if X_i is discrete).

Computation of moments First, it computes the first four (raw) posterior moments from the factorial moments, which are obtained by differentiation of G:

$$\begin{split} M_{1} &:= \mathbb{E}[X_{i}] = \partial_{i}G(\mathbf{1}_{n}) \\ M_{2} &:= \mathbb{E}[X_{i}^{2}] = \mathbb{E}[(X_{i})(X_{i}-1)] + \mathbb{E}[X_{i}] = \partial_{i}^{2}G(\mathbf{1}_{n}) + \partial_{i}G(\mathbf{1}_{n}) \\ M_{3} &:= \mathbb{E}[X_{i}^{3}] = \mathbb{E}[X_{i}(X_{i}-1)(X_{i}-2)] + 3\mathbb{E}[X_{i}(X_{i}-1)] + \mathbb{E}[X_{i}] \\ &= \partial_{i}^{3}G(\mathbf{1}_{n}) + 3\partial_{i}^{2}G(\mathbf{1}_{n}) + \partial_{i}G(\mathbf{1}_{n}) \\ M_{4} &:= \mathbb{E}[X_{i}^{4}] = \mathbb{E}[X_{i}(X_{i}-1)(X_{i}-2)(X_{i}-3)] + 6\mathbb{E}[X_{i}(X_{i}-1)(X_{i}-2)] \\ &+ 7\mathbb{E}[X_{i}(X_{i}-1)] + \mathbb{E}[X_{i}] \\ &= \partial_{i}^{4}G(\mathbf{1}_{n}) + 6\partial_{i}^{3}G(\mathbf{1}_{n}) + 7\partial_{i}^{2}G(\mathbf{1}_{n}) + \partial_{i}G(\mathbf{1}_{n}) \end{split}$$

From the raw moments, it computes the first four (centered/standardized) moments, i.e. the expected value ($\mu := \mathbb{E}[X_i]$), the variance ($\sigma^2 := \mathbb{V}[X_i]$), the skewness ($\mathbb{E}[(X_i - \mu)^3]/\sigma^3$) and the kurtosis ($\mathbb{E}[(X_i - \mu)^4]/\sigma^4$):

$$\begin{split} \mu &:= \mathbb{E}[X_i] = M_1 \\ \sigma^2 &:= \mathbb{V}[X_i] = \mathbb{E}[(X_i - \mu)^2] = \mathbb{E}[X_i^2] - 2\mu \mathbb{E}[X_i] + \mu^2 = M_2 - \mu^2 \\ \operatorname{Skew}[X_i] &= \frac{\mathbb{E}[(X_i - \mu)^3]}{\sigma^3} = \frac{\mathbb{E}[X_i^3] - 3\mu \mathbb{E}[X_i^2] + 3\mu^2 \mathbb{E}[X_i] - \mu^3}{\sigma^3} \\ &= \frac{M_3 - 3\mu M_2 + 2\mu^3}{\sigma^3} \\ \operatorname{Kurt}[X_i] &= \frac{\mathbb{E}[(X_i - \mu)^4]}{\sigma^4} = \frac{\mathbb{E}[X_i^4] - 4\mu \mathbb{E}[X_i^3] + 6\mu^2 \mathbb{E}[X_i^2] - 4\mu^3 \mathbb{E}[X_i] + \mu^4}{\sigma^4} \\ &= \frac{M_4 - 4\mu M_3 + 6\mu^2 M_2 - 3\mu^4}{\sigma^4} \end{split}$$

Computation of probability masses If X_i is a discrete variable, the tool computes all the probability masses $\mathbb{P}[X_i = m]$ until the value of m such that the tail probabilities are guaranteed to be below a certain threshold, which is set to $\mathbb{P}[X_i \ge m] \le \frac{1}{256}$. This is achieved by setting $m := \mu + 4\sqrt[4]{\mathbb{E}[(X_i - \mu)^4]}$ where $\mu := \mathbb{E}[X_i]$. Then we find

$$\mathbb{P}[X_i \ge m] \le \mathbb{P}\left[|X_i - \mu| \ge 4\sqrt[4]{\mathbb{E}[(X_i - \mu)^4]}\right] = \mathbb{P}\left[(X - \mu)^4 \ge 256\mathbb{E}[(X_i - \mu)^4]\right] \le \frac{1}{256}$$

by Markov's inequality. Note that in practice, the tail probabilities are typically much smaller than $\frac{1}{256}$, usually in the order of 10^{-5} . For all $k \in \{0, \ldots, m\}$, the tool computes the posterior probability $\mathbb{P}[X_i = k]$ by marginalizing out all the other variables (substituting 1 for them) and computing the Taylor coefficient at $x_i = 0$:

$$\mathbb{P}[X_i = k] = \frac{1}{k!} \partial_i^k G(\mathbf{1}_n[i \mapsto 0]).$$

Implementation details The tool was implemented in Rust [16], a safe systems programming language, in order to have a tight control over memory usage and performance. In particular, optimizations to Taylor polynomial manipulations are crucial (see Appendix C.3). The coefficients of the Taylor polynomials are stored as 64-bit IEEE floating point numbers, in a multidimensional array provided by the ndarray library². Our implementation is available in the supplementary material and will be made available on Github after the review process.

²https://crates.io/crates/ndarray

C.1 Automatic differentiation and Taylor polynomials

The main difficulty in implementing the GF semantics is the computation of the (partial) derivatives. This seems to be a unique situation where we want to compute *d*-th derivatives where *d* is in the order of hundreds. The reason is that the observe $X_k = d$ construct is translated into a *d*-th (partial) derivative and if *d* is a real-world observation, it will not necessarily be small. We have not come across another application of automatic differentiation that required derivatives of a total order of more than 10.

As a consequence, when we tried *pytorch*, a mature machine learning library implementing automatic differentiation, the performance for derivatives of high order was very poor. Therefore, we decided to implement our own automatic differentiation framework. Our approach is to compute the Taylor expansion in all variables up to some order d of the generating function instead of a symbolic expression of the d-th derivative. This has the advantage of growing polynomially in d, not exponentially. Contrary to [23], it is advantageous to use Taylor coefficients instead of the partial derivatives because the additional factorial factors are can easily lead to overflows.

Taylor polynomials More formally, we define the *Taylor polynomial* $\mathsf{Taylor}^d_{\boldsymbol{w}}(G)$ of a function $G : \mathbb{R}^n \to \mathbb{R}$ at $\boldsymbol{w} \in \mathbb{R}^n$ of order d as the polynomial

$$\mathsf{Taylor}^d_{\boldsymbol{w}}(G) := \sum_{\boldsymbol{\alpha} \in \mathbb{N}^n : |\boldsymbol{\alpha}| \leq d} \frac{1}{\boldsymbol{\alpha}!} \partial^{\boldsymbol{\alpha}} G(\boldsymbol{w}) \cdot (\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\alpha}}$$

where we used multi-index notation: $|\alpha|$ stands for $\alpha_1 + \cdots + \alpha_n$; α ! for $\alpha_1! \cdots \alpha_n!$; and ∂^{α} for $\partial_1^{\alpha_1} \dots \partial_n^{\alpha_n}$. The coefficients $c_{\alpha} := \frac{1}{\alpha!} \partial^{\alpha} G(w)$ are the *Taylor coefficients* of G at w and are stored in a multidimensional array in our implementation.

Operations The operations on generating functions (Appendix B) are implemented in terms of their effect on the Taylor expansions. Let $G, H : \mathbb{R}^n \to \mathbb{R}$ be two functions with Taylor expansions Taylor^{*d*}_{*w*}(*G*) = $\sum_{|\alpha| \leq d} g_{\alpha}(\boldsymbol{x} - \boldsymbol{w})^{\alpha}$ and Taylor^{*d*}_{*w*}(*H*) = $\sum_{|\alpha| \leq d} h_{\alpha}(\boldsymbol{x} - \boldsymbol{w})^{\alpha}$. Addition F = G + H of two generating functions is implemented by adding the coefficients: Taylor^{*d*}_{*w*}(*G* + *H*) = $\sum_{|\alpha| \leq d} (g_{\alpha} + h_{\alpha})(\boldsymbol{x} - \boldsymbol{w})^{\alpha}$. Scalar multiplication $F = c \cdot G$ is implemented by multiplying the coefficients: Taylor^{*d*}_{*w*}(*c*·*G*) = $\sum_{|\alpha| \leq d} (c \cdot g_{\alpha})(\boldsymbol{x} - \boldsymbol{w})^{\alpha}$. Multiplication $F = G \cdot H$ of two generating functions is implemented by the Cauchy product:

$$\mathsf{Taylor}_{\boldsymbol{w}}^{d}(G \cdot H) = \sum_{|\boldsymbol{\alpha}| \leq d} \left(\sum_{\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2 = \boldsymbol{\alpha}} g_{\boldsymbol{\alpha}_1} h_{\boldsymbol{\alpha}_2} \right) (\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\alpha}}$$

Division, exponentiation, logarithms, and powers can be implemented as well (see [11, Chapter 13] for details). Partial derivatives essentially correspond to shifting the index and a multiplication:

$$\mathsf{Taylor}_{\boldsymbol{w}}^{d-1}(\partial_k G) = \sum_{|\boldsymbol{\alpha}| \leq d-1} (\alpha_k + 1) g_{\boldsymbol{\alpha}[k \mapsto \alpha_k + 1]} \boldsymbol{x}^{\boldsymbol{\alpha}}$$

The most complicated case is composition/substitution, i.e. $F(\boldsymbol{x}) = G(\boldsymbol{x}[k \mapsto H(\boldsymbol{x})])$. For this, we let $\boldsymbol{w}' := \boldsymbol{w}[k \mapsto h_{\mathbf{0}}]$ where $\operatorname{Taylor}_{\boldsymbol{w}}^{d}(H) = \sum_{|\boldsymbol{\beta}| \leq d} h_{\boldsymbol{\beta}}(\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\beta}}$ and we let $\operatorname{Taylor}_{\boldsymbol{w}'}^{d}(G) = \sum_{|\boldsymbol{\alpha}| \leq d} g_{\boldsymbol{\alpha}}(\boldsymbol{x} - \boldsymbol{w}')^{\boldsymbol{\alpha}}$. Then we have (where "h.o.t." stands for "higher order terms")

$$G(\boldsymbol{x}[k \mapsto H(\boldsymbol{x})]) = G\left(\boldsymbol{x}\left[k \mapsto \sum_{|\boldsymbol{\beta}| \le d} h_{\boldsymbol{\beta}}(\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\beta}} + \text{h.o.t.}\right]\right)$$
$$= \sum_{|\boldsymbol{\alpha}| \le d} g_{\boldsymbol{\alpha}} \left(\boldsymbol{x}\left[k \mapsto h_{\boldsymbol{0}} + \sum_{1 \le |\boldsymbol{\beta}| \le d} h_{\boldsymbol{\alpha}}(\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\beta}} + \text{h.o.t.}\right] - \boldsymbol{w}'\right)^{\boldsymbol{\alpha}} + \text{h.o.t.}$$
$$= \sum_{|\boldsymbol{\alpha}| \le d} g_{\boldsymbol{\alpha}} \left((\boldsymbol{x} - \boldsymbol{w})\left[k \mapsto \sum_{1 \le |\boldsymbol{\beta}| \le d} h_{\boldsymbol{\alpha}}(\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\beta}}\right]\right)^{\boldsymbol{\alpha}} + \text{h.o.t.}$$

because by definition $\boldsymbol{x}[k \mapsto h_{0}] - w' = (\boldsymbol{x} - \boldsymbol{w})[k \mapsto 0]$. This means that we can obtain $\operatorname{Taylor}_{\boldsymbol{w}}^{d}(F)$ by substituting $\sum_{1 \leq |\boldsymbol{\beta}| \leq d} h_{\boldsymbol{\alpha}}(\boldsymbol{x} - \boldsymbol{w})^{\boldsymbol{\beta}}$ for $x_{k} - w'_{k}$ in $\operatorname{Taylor}_{\boldsymbol{w}'}^{d}(G)$.

Example C.1 (Calculations with Taylor polynomials). Here we show how the expectation for Example 2.1 can be computed using Taylor polynomials. We use the same naming as in Example 3.1. Recall that to compute $\mathbb{E}[X]$, we need to evaluate $\partial_1 E(1, 1)$, so we compute the Taylor expansion of E at (1, 1) of order 1, i.e. $\text{Taylor}_{(1,1)}^1(E)$. To compute $E(x, y) = \frac{D(x,y)}{D(1,1)}$, we need D(x, y), so we need $\text{Taylor}_{(1,1)}^1(D)$. For $D(x, y) = \frac{1}{2!}y^2\partial_y^2 C(x, 0)$, we need the Taylor expansion of C at (1, 0) of order 1 + 2 = 3. For C(x, y) = B(x(0.1y + 0.9), 1), we need the Taylor expansion of B at $(1(0.1 \cdot 0 + 0.9), 1) = (0.9, 1)$ of order 3. Since $B(x, y) = \exp(20(x - 1)) = \exp(20((x - 0.9) - 0.1)) = \exp(20(x - 0.9) - 2)$, this Taylor expansion is

$$\mathsf{Taylor}^3_{(0.9,1)}(B) = e^{-2} + 20e^{-2} \cdot (x - 0.9) + 200e^{-2} \cdot (x - 0.9)^2 + \frac{4000}{3}e^{-2}(x - 0.9)^3 + \frac{1000}{3}e^{-2}(x - 0.9)^3 + \frac{1000}{3$$

Since C(1 + (x - 1), 0 + y) = B((1 + (x - 1))(0.1y + 0.9), 1) = B(0.9 + 0.9(x - 1) + 0.1y + 0.1(x - 1)y, 1), the Taylor expansion of C at (1, 0) is given by replacing (x - 0.9) with 0.9(x - 1) + 0.1y + 0.1(x - 1)y and we get

$$\begin{aligned} \mathsf{Taylor}^3_{(1,0)}(C) &= e^{-2} \left(1 + 2y + 2y^2 + \frac{4}{3}y^3 + 18(x-1) + 38(x-1)y + 40(x-1)y^2 \right. \\ &\qquad \qquad + 162(x-1)^2 + 360(x-1)^2y + 972(x-1)^3 \right) \end{aligned}$$

For $D(x, y) = \frac{1}{2!}y^2 \partial_y^2 C(x, 0)$, we compute the second partial derivative wrt. y, substitute y = 0 and then multiply by $y^2 = (1 + (y - 1))^2$, yielding

$$D(x,y) = \frac{1}{2!}y^2 e^{-2} (4 + 8y + 80(x - 1) + \text{higher order terms})|_{y=0}$$

= $e^{-2}(4 + 80(x - 1) + \text{higher order terms})(1 + (y - 1))^2$
= $e^{-2}(4 + 80(x - 1) + 8(y - 1) + \text{higher order terms})$

As a consequence, we find that $D(1,1) = 4e^{-2}$, so $\mathsf{Taylor}^{1}_{(1,1)}(E) = 1 + 20(x-1) + 2(y-1)$. So $\mathbb{E}[X] = \partial_x E(1,1) = 20$, as desired.

Memoizing intermediate results When computing the Taylor expansion of a function G, it is important to memoize the intermediate Taylor expansions of subexpressions of G because those may occur multiple times. For example, conditionals are translated to a generating function that uses the previous generating function twice. Evaluating it repeatedly would double the running time for each conditional. With memoization, it is possible to handle programs with lots of branching (e.g. > 2^{100} paths in the mixture model, cf. Table 4) in a reasonable amount of time.

C.2 Optimizing Observations from Compound Distributions

Observations from compound distributions are generally the bottleneck for the running time because the construct observe $d \sim D(X_k)$ is syntactic sugar for $X_{n+1} \sim D(X_k)$; observe $X_{n+1} = d$, which introduces a new variable, which is immediately discarded after the observation. This expansion has the semantics

$$\begin{split} \llbracket \text{observe} \, d \sim D(X_k) \rrbracket_{\mathsf{gf}}(G)(\boldsymbol{x}) &= \llbracket \text{observe} \, X_{n+1} = d \rrbracket_{\mathsf{gf}}(\llbracket X_{n+1} \sim D(X_k) \rrbracket_{\mathsf{gf}}(G))(x_1, \dots, x_{n+1}) \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} \llbracket X_{n+1} \sim D(X_k) \rrbracket_{\mathsf{gf}}(G)(x_1, \dots, x_{n+1}) \Big|_{x_{n+1} = 0} \end{split}$$

containing an extra variable x_{n+1} , which worsens the running time of the Taylor approach significantly. We can find more efficient ways of computing this semantics.

Theorem C.1. *Observing from compound binomial distributions can be implemented without introducing a new variable:*

$$[[\text{observe } d \sim \text{Binomial}(X_k, p)]]_{gf}(G) = \frac{1}{d!} (px_k)^d \cdot \partial_k^d G(\boldsymbol{x}[k \mapsto (1-p)x_k])$$

Proof. A proof for the discrete setting was given in [23]. In our setting, which allows continuous distributions, we cannot use the usual argument about power series anymore. Instead, we reason as follows:

$$\llbracket \mathsf{observe} \, d \sim \mathsf{Binomial}(X_k, p) \rrbracket_{\mathsf{gf}}(G)$$

$$= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} [\![X_{n+1} \sim \mathsf{Binomial}(X_k)]\!]_{\mathsf{gf}}(G)(x_1, \dots, x_{n+1})\Big|_{x_{n+1}=0}$$

$$= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} G(\mathbf{x}[k \mapsto x_k \cdot (px_{n+1}+1-p)])\Big|_{x_{n+1}=0}$$

$$\stackrel{*}{=} \frac{1}{d!} \partial^d_k G(\mathbf{x}[k \mapsto x_k \cdot (px_{n+1}+1-p)]) \cdot (px_k)^d\Big|_{x_{n+1}=0}$$

$$= \frac{1}{d!} (px_k)^d \partial^d_k G(\mathbf{x}[k \mapsto (1-p)x_k])$$

where * follows by iterating the following argument:

$$\frac{\partial}{\partial x_{n+1}} G(\boldsymbol{x}[k \mapsto x_k \cdot (px_{n+1}+1-p)])$$

$$= \partial_k G(\boldsymbol{x}[k \mapsto x_k \cdot (px_{n+1}+1-p)]) \cdot \frac{\partial (x_k \cdot (px_{n+1}+1-p))}{\partial x_{n+1}}$$

$$= \partial_k G(\boldsymbol{x}[k \mapsto x_k \cdot (px_{n+1}+1-p)]) \cdot px_k$$

which holds by the chain rule.

Theorem C.2. *Observing from compound Poisson distributions can be implemented without introducing a new variable:*

$$[\![\text{observe } d \sim \text{Poisson}(\lambda X_k)]\!]_{\text{gf}}(G) = \frac{1}{d!} D^d_{k,\lambda}(G)(\boldsymbol{x}[k \mapsto e^{-\lambda} x_k])$$

where

$$D_{k,\lambda}(G)(\boldsymbol{x}) := \lambda x_k \cdot \partial_k G(\boldsymbol{x}).$$

Proof. Let $F : \mathbb{R}^n \to \mathbb{R}$ be a smooth function. Then

$$\frac{\partial}{\partial x_{n+1}} F(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}]) \\
= \partial_k F(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}]) \cdot x_k e^{\lambda(x_{n+1}-1)} \cdot \lambda \\
= D_{k,\lambda}(F)(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}]).$$

Inductively, we get

$$\frac{\partial^d}{\partial x_{n+1}^d} G(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}]) = D_{k,\lambda}^d(G)(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}])$$

Substituting $x_{n+1} \mapsto 0$ in the final expression and dividing by d! yields:

$$\begin{split} & [\![\text{observe } d \sim \text{Poisson}(\lambda X_k)]\!]_{\text{gf}}(G) \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} [\![X_{n+1} \sim \text{Poisson}(\lambda X_k)]\!]_{\text{gf}}(G)(x_1, \dots, x_{n+1})\Big|_{x_{n+1}=0} \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} G(\boldsymbol{x}[k \mapsto x_k \cdot e^{\lambda(x_{n+1}-1)}])\Big|_{x_{n+1}=0} \\ &= \frac{1}{d!} D_{k,\lambda}^d(G)(\boldsymbol{x}[k \mapsto e^{-\lambda} x_k]) \end{split}$$

Theorem C.3. *Observing from compound negative binomial distributions can be implemented without introducing a new variable:*

$$[\![\text{observe } d \sim \mathsf{NegBinomial}(X_k, p)]\!]_{\mathsf{gf}}(G) = \frac{1}{d!} \sum_{i=0}^d \partial_k^i F(\boldsymbol{x}[k \mapsto p \cdot x_k]) \cdot p^i x_k^i \cdot (1-p)^d L_{d,i}$$

where the numbers $L_{d,i}$ are known as Lah numbers and defined recursively as follows:

$$\begin{array}{ll} L_{0,0} := 1 \\ L_{d,i} := 0 & \quad \text{for } i < 0 \text{ or } d < i \\ L_{d+1,i} := (d+i)L_{d,i} + L_{d,i-1} & \quad \text{for } 0 \leq i \leq d+1 \end{array}$$

Proof. Let $F : \mathbb{R}^n \to \mathbb{R}$ be a smooth function and $y : \mathbb{R} \to \mathbb{R}$ given by $y(z) := \frac{1}{1-(1-p)z}$. Then $y'(x) = -\frac{1}{1-(1-p)x} \cdot (-(1-p)) = (1-p)y(x)^2$ and

$$\frac{\partial}{\partial x_{n+1}} F(\boldsymbol{x}[k \mapsto \frac{x_k \cdot p}{1 - (1 - p)x_{n+1}}])$$

= $\partial_k F(\boldsymbol{x}[k \mapsto x_k p \cdot y(x_{n+1})]) \cdot px_k \cdot (1 - p)y(x_{n+1})^2$

We claim that we can write

$$\frac{\partial^a}{\partial x_{n+1}^d} F(\boldsymbol{x}[k \mapsto \frac{px_k}{1 - (1 - p)x_{n+1}}])$$

= $\sum_{i=0}^d \partial_k^i F(\boldsymbol{x}[k \mapsto x_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^d L_{d,i} \cdot y(x_{n+1})^{d+i}.$

The claim is proved by induction. First the case d = 0:

$$F(\boldsymbol{x}[k \mapsto \frac{px_k}{1 - (1 - p)x_{n+1}}]) = F(\boldsymbol{x}[k \mapsto \frac{px_k}{1 - (1 - p)x_{n+1}}]) \cdot (1 - p)^0 x_k^0 L_{0,0} \cdot y(x_{n+1})^0$$

Next, the induction step:

$$\begin{split} &\frac{\partial^{d+1}}{\partial x_{n+1}^{d+1}} F(\mathbf{x}[k \mapsto \frac{px_k}{1 - (1 - p)x_{n+1}}]) \\ &= \frac{\partial}{\partial x_{n+1}} \left(\sum_{i=0}^d \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^d L_{d,i} \cdot y(x_{n+1})^{d+i} \right) \\ &= \sum_{i=0}^d \partial_k^{i+1} F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot px_k y'(x_{n+1}) \cdot p^i x_k^i (1 - p)^d L_{d,i} y(x_{n+1})^{d+i} \\ &+ \sum_{i=0}^d \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i (1 - p)^d \cdot L_{d,i} (d + i) y(x_{n+1})^{d+i-1} \cdot y'(x_{n+1}) \\ &= \sum_{i=0}^d \partial_k^{i+1} F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^{i+1} x_k^{i+1} \cdot (1 - p)^{d+1} y(x_{n+1})^2 \cdot L_{d,i} y(x_{n+1})^{d+i} \\ &+ \sum_{i=0}^d \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^{d+1} y(x_{n+1})^2 \cdot (d + i) L_{d,i} y(x_{n+1})^{d+i-1} \\ &= \sum_{i=0}^{d+1} \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^{d+1} L_{d,i-1} y(x_{n+1})^{d+i+1} \\ &+ \sum_{i=0}^{d+1} \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^{d+1} (d + i) L_{d,i} y(x_{n+1})^{d+i+1} \\ &= \sum_{i=0}^{d+1} \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^{d+1} ((d + i) L_{d,i} + L_{d,i-1}) y(x_{n+1})^{d+i+1} \\ &= \sum_{i=0}^{d+1} \partial_k^i F(\mathbf{x}[k \mapsto px_k \cdot y(x_{n+1})]) \cdot p^i x_k^i \cdot (1 - p)^{d+1} L_{d+1,i} y(x_{n+1})^{d+i+1} \end{split}$$

Substituting $x_{n+1} \mapsto 0$ in the final expression and dividing by d! yields:

$$\begin{split} \llbracket \text{observe } d &\sim \text{NegBinomial}(X_k, p) \rrbracket_{\text{gf}}(G) \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} \llbracket X_{n+1} \sim \text{NegBinomial}(X_k, p) \rrbracket_{\text{gf}}(G)(x_1, \dots, x_{n+1}) \Big|_{x_{n+1}=0} \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} G(\boldsymbol{x}[k \mapsto \frac{x_k \cdot p}{1 - (1 - p)x_{n+1}}]) \Big|_{x_{n+1}=0} \\ &= \frac{1}{d!} \sum_{i=0}^d \partial_k^i F(\boldsymbol{x}[k \mapsto p \cdot x_k]) \cdot p^i x_k^i \cdot (1 - p)^d L_{d,i} \end{split}$$

Theorem C.4. Observing from compound Bernoulli distributions can be implemented without introducing a new variable:

$$\llbracket \text{observe } d \sim \text{Bernoulli}(X_k) \rrbracket_{\text{gf}}(G) = \begin{cases} G(\boldsymbol{x}[k \mapsto 1]) - x_k \partial_j G(\boldsymbol{x}[k \mapsto 1]) & d = 0\\ x_k \cdot \partial_j G(\boldsymbol{x}[k \mapsto 1]) & d = 1\\ 0 & otherwise \end{cases}$$

Proof. We argue as follows:

$$\begin{split} \llbracket \mathsf{observe} \, d &\sim \mathsf{Bernoulli}(X_k) \rrbracket_{\mathsf{gf}}(G)(\mathbf{x}) \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} \llbracket X_{n+1} \sim \mathsf{Bernoulli}(X_k) \rrbracket_{\mathsf{gf}}(G)(x_1, \dots, x_{n+1}) \Big|_{x_{n+1}=0} \\ &= \frac{1}{d!} \frac{\partial^d}{\partial x_{n+1}^d} \left(G(\mathbf{x}) + x_k(x_{n+1}-1) \cdot \partial_k G(\mathbf{x}) \right) \Big|_{x_{n+1}=0} \end{split}$$

If d = 0, the right-hand side is $G(\mathbf{x}) - x_k \partial_k G(\mathbf{x})$. If d = 1, the right-hand side is $x_k \partial_k G(\mathbf{x})$. For larger $d \ge 2$, the *d*-th derivative vanishes, which completes the proof.

C.3 Analysis of the running time

If the program makes observations (or compares variables with constants) d_1, \ldots, d_m , the running time of the program will depend on these constants. Indeed, each observation of (or comparison of a variable with) d requires the computation of the d-th partial derivative of the generating function. In our Taylor polynomial approach, this means that the highest order of Taylor polynomials computed will be $d := \sum_{i=1}^{m} d_i$. If the program has n variables, storing the coefficients of this polynomial alone requires $O(d^n)$ space. This can be reduced if the generating function is a low-degree polynomial, in which case we do not store the zero coefficients of the terms of higher order.

Naively, the time complexity of multiplying two such Taylor polynomials is $O(d^{2n})$ and that of composing them is $O(d^{3n})$. However, we can do better by exploiting the fact that the polynomials are sparse. In the generating function semantics, we never multiply two polynomials with n variables. One of them will have at most two variables. This brings the running time for multiplications down to $O(d^{n+2})$. Furthermore, the GF semantics has the property that when composing two generating functions, we can substitute variables one by one instead of simultaneously, bringing the running time down to $O(d^{2n})$. Even more, the substituted terms have at most two variables, which brings the running time down to $O(d^{n+3})$.

Theorem C.5. Our exact inference method can evaluate a generating function in $O(s \cdot d^{n+3})$, and $O(sd^3)$ for n = 1, where s is the number of statements, d (for data) is the sum of all values that are observed or compared against in the program, and n is the number of variables of the program. To evaluate a d'-th derivative of the generating function, d' has to be added to d in the above equation.

Proof. The above arguments already analyze the bottlenecks of the algorithm. But for completeness' sake, we consider all operations being performed on generating functions and their Taylor expansions (cf. Appendix C.1).

The maximum order of differentiation needed is d (potentially including the additional d' if computing the d'-th derivative of the GF) and since there are n variables, the maximum number of Taylor coefficients that need to be stored is $O(d^n)$. Addition of two such Taylor polynomials and scalar multiplications trivially take $O(d^n)$ time. Since in the GF semantics, a GF is only ever multiplied by one with at most two variables, the multiplications take $O(d^{n+2})$ time. Division only happens with a divisor of degree at most 1, which can also be implemented in $O(d^{n+1})$ time [11, Chapter 13]. Exponentiation $\exp(\ldots)$, logarithms $\log(\ldots)$, and powers $(\ldots)^m$ are only performed on polynomials with one variable, where they can be implemented in $O(d^2)$ time [11, Table 13.2]. Finally, the only substitutions that are required are ones where a term with at most two variables is substituted for a variable, i.e. of the form $p(\boldsymbol{x}[k \mapsto q(x_1, x_2)])$ where $p(\boldsymbol{x}) = \sum_{|\boldsymbol{\alpha}| < d} p_{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}}$. Then

$$p(\boldsymbol{x}[k \mapsto q(x_1, x_2)]) = p_0(\boldsymbol{x}) + q(x_1, x_2) \cdot (p_1(\boldsymbol{x}) + q(x_1, x_2) \cdot (p_2(\boldsymbol{x}) + \cdots))$$

where $p_i(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha}:\alpha_k=i} p_{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}[k\mapsto 0]}$. This needs d multiplications of $q(x_1, x_2)$ in 2 variables and a polynomial in n variables, each of which takes $O(d^{n+2})$ time. In total, the substitution can be performed in $O(d^{n+3})$ time. Finally, if there is only one variable, the substitution can be performed in $O(d^3)$ time because q can only have one variable.

In summary, the input SGCL program has s statements, and each of them is translated to a bounded number of operations on generating functions. These operations are performed using Taylor expansions of degree at most d, each of which takes at most $O(d^{n+3})$ time (and at most $O(d^3)$ time for n = 1). So overall, the running time is $O(s \cdot d^{n+3})$ (and $O(sd^3)$ for n = 1).

Performance in practice Note that, for many programs, the running time will be better than the worst case. Indeed, substitutions are the most expensive operation, if the substitute expression is of high degree. For some models, like the population model, the substitutions take the form of Theorem C.1, i.e. $G(\boldsymbol{x}[k \mapsto (1-p)x_k])$, which is of degree 1. Such a substitution can be performed in $O(d^n)$ time, because one simply needs to multiply each coefficient by a power of (1-p). This explains why the population model is so fast in the experimental section (Section 5). In other cases as well, we can often make use of the fact that the polynomials are sparse (few variables or low degree) to reduce the space needed to store the coefficients and to speed up the operations.

C.4 Numerical issues

As our implementation uses 64-bit floating point numbers, there is the possibility of rounding errors and numerical instabilities, which could invalidate the results. To guard against this, we implemented an option in our tool to use interval arithmetic in the computation: instead of a single (rounded) number, it keeps track of a lower and upper bound on the correctly rounded result. If this interval is very wide, it indicates numerical instabilities. In this way, we verified the experimental results to be correct up to at least 6 significant digits.

Initially, we observed large numerical errors (caused by catastrophic cancelation) for probabilistic programs involving continuous distributions. The reason for this turned out to be the term $\log(x)$ that occurs in the PGF of the continuous distributions. The Taylor coefficients of $\log(x)$ at points 0 < z < 1 are not well-behaved:

$$\log(x) = \log(z) + \sum_{n=1}^{\infty} \frac{(-1)^n z^{-n}}{n} (x - z)^n$$

because the coefficients grow exponentially for z < 1 (due to the term z^{-n}) and the alternating sign exacerbates this problem by increasing the likelihood of catastrophic cancelations.

To fix this problem, we adopted a slightly modified representation. Instead of computing the Taylor coefficients of the GF G directly, we compute those of the function $H(\mathbf{x}) := G(\mathbf{x}')$ where $x'_i := x_i$ if X_i is discrete and $x'_i := \exp(x_i)$ if X_i is continuous, thus canceling the logarithm.³ (The reason we don't use $\mathbf{x}' := \exp(\mathbf{x})$ for all variables is that for discrete variables, we may need to evaluate

³Note that this boils down to using the moment generating function (MGF) $\mathbb{E}[\exp(x_i X_i)]$ for continuous variables X_i and the probability generating function (PGF) $\mathbb{E}[x_i^{X_i}]$ for discrete variables X_i . In mathematics, the MGF is more often used for continuous distributions and the PGF more commonly for discrete ones. It is interesting to see that from a numerical perspective, this preference is confirmed.

Table 4: Summary of the benchmarks: n is the number of variables, o is the number of observations, d is the sum of all the observed values, i.e. the total order of derivatives that needs to be computed, s is the number of statements, and p the number of program paths.

Benchmark	n	0	d	s	p	continuous priors?
population model (Fig. 1a)	1	4	254	13	1	no
population (modified, Fig. 1b)	1	4	254	21	16	no
population (two types, Fig. 1c)	2	8	277	30	1	no
switchpoint (Fig. 2a)	2	109	188	12433	111	yes
mixture model (Figs. 2b and 2c)	2	218	188	329	$2^{109} \approx 6 \cdot 10^{32}$	no
HMM (Fig. 2d)	3	60	51	152	$2^{30} \approx 10^9$	no

at $x'_i = 0$, corresponding to $x_i = -\infty$, which is impossible.) It is straightforward to adapt the GF semantics to this modified representation. Due to the technical nature of the adjustment (case analysis on whether an index corresponds to a discrete variable or not), we do not describe it in detail. With this modified representation, we avoid the catastrophic cancelations and obtain numerically stable results for programs using continuous distributions as well.

D Details on the Empirical Evaluation

Experimental setup As explained in Section 5, we ran several of Anglican's inference algorithms. Each algorithm was run with a sampling budget of 1000 and 10000. The precise settings we used are the following:

- Importance Sampling (IS): has no settings
- Lightweight Metropolis Hastings (LMH): has no settings
- Random-Walk Metropolis Hastings (RMH): has two settings: the probability α of using a local MCMC move and the spread σ of the local move. We used the default $\alpha = 0.5, \sigma = 1$ and another setting facilitating local moves with $\alpha = 0.8, \sigma = 2$.
- Sequential Monte Carlo (SMC): number of particles $\in \{1, 1000\}$. The default is 1 and we also picked 1000 to see the effect of a larger number of particles while not increasing the running time too much.
- Particle Gibbs (PGibbs): number of particles $\in \{2, 1000\}$. The default is 2 and we also picked 1000 as the other setting for the same reason as for SMC.
- Interacting Particle MCMC (IPMCMC): it has the settings "number of particles per sweep", "number of nodes running SMC and CSMC", "number of nodes running CSMC", and "whether to return all particles (or just one)". We left the last three settings at their defaults (32 nodes, 16 nodes running CSMC, return all particles). For the number of nodes and the number of nodes we chose the default setting (2) and a higher one (1000) for the same reason as SMC.

A full list of Anglican's inference algorithms and their settings can be found at https://probprog. github.io/anglican/inference. Each inference algorithm was run 20 times on each benchmark to reduce noise. This took around an hour per benchmark. The experiments were run on a laptop computer with a Intelő Core i5-8250U CPU @ 1.60GHz Œ 8 processor and 16 GiB of RAM, running Ubuntu 22.04.2.

D.1 Benchmarks

A summary with important information on each benchmark can be found in Table 4, including some statistics about the probabilistic programs. We describe each benchmark in more detail in the following.

Population models The probabilistic program for the original population model from [22] is shown in Fig. 6a. This program can also be written without the extra variable *New* by writing the two statements involving it as $N + \sim \text{Poisson}(\lambda_1)$. Here we used the same parameter values as [22]: $\delta = 0.2636$, $\lambda = \Lambda \cdot (0.0257, 0.1163, 0.2104, 0.1504, 0.0428)$, and $\Lambda = 2000$ is the population size

	$N := Poisson(\lambda_0);$	$N_1 \sim Poisson(\lambda_0^{(1)});$ $N_2 \sim Poisson(\lambda_0^{(2)});$
$N := Poisson(\lambda_0);$ $N \sim Binomial(N, \delta);$ $New \sim Poisson(\lambda_1);$ $N := New + N;$ $observe \ y_1 \sim Binomial(N, \rho);$	$\begin{split} N &\sim Binomial(N, \delta);\\ Disaster &\sim Bernoulli(0.1);\\ \text{if } Disaster &= 1 \left\{ &\\ N + &\sim Poisson(\lambda_1') \\ \right\} \text{ else } \left\{ &\\ N + &\sim Poisson(\lambda_1) \\ \right\}\\ \text{observe } y_1 &\sim Binomial(N, \rho); \end{split}$	$\begin{split} N_2 & + \sim Binomial(N_1, \gamma); \\ N_1 & \sim Binomial(N_1, \delta_1); \\ N_2 & \sim Binomial(N_2, \delta_2); \\ N_1 & + \sim Poisson(\lambda_1^1); \\ N_2 & + \sim Poisson(\lambda_1^2); \\ observe \ y_1^{(1)} & \sim Binomial(N_1, \rho); \\ observe \ y_1^{(2)} & \sim Binomial(N_2, \rho); \end{split}$
÷	÷	:

(a) Original model from [22]. (b) Randomly modified arrival rate. (c) Two interacting populations.

Figure 6: The program code for the population model variations.

parameter. Note that the largest population size considered by [22] is $\Lambda = 500$. For the observation rate ρ , Winner and Sheldon [22] consider values from 0.05 to 0.95. For simplicity, we set it to $\rho = 0.2$. The y_k are k = 4 simulated data points: (45, 98, 73, 38) for $\Lambda = 2000$.

The modified population example is shown in Fig. 6b, where the arrival rate is reduced to $\lambda' := 0.1\lambda$ in the case of a natural disaster, which happens with probability 0.1. The rest of the model is the same.

The model of two interacting populations (multitype branching process) is programmed as shown in Fig. 6c, where $\lambda^{(1)} := 0.9\lambda$, $\lambda^{(2)} := 0.1\lambda$, $\gamma := 0.1$. In this model, some individuals of the first kind (i.e. in N_1) can turn into individuals of the second kind and are added to N_2 . An example of this would be healthy cells mutating into cancer cells. The other parameters of this model are the same as before. The data points are $y^{(1)} = (35, 83, 78, 58)$ and $y^{(2)} = (3, 6, 10, 4)$.

In fact, this program can be rewritten to the more efficient form shown in Fig. 7b, to minimize the number of variables needed.

Mixture model In the binary mixture model, the frequency events are observed from an equalweight mixture of two Poisson distributions with different parameters Λ_1 , Λ_2 , which are in discrete steps of 0.1. This is implemented by imposing a geometric prior and multiplying the rate by 0.1 in the Poisson distribution: Poisson $(0.1 \cdot \Lambda_1)$. The data is the same as for the switchpoint model. The task is to infer the first rate Λ_1 . The probabilistic program is shown in Fig. 8a.

Hidden Markov model The hidden Markov example is based on [18, Section 2.2]. The hidden state Z can be 0 or 1 and transitions to the other state with probability 0.2. The rate of the Poisson-

```
\Lambda \sim \mathsf{Exponential}(1);
                                                                            if 1 \sim \text{Bernoulli}(1/m) {
                                                                                    observe y_1 \sim \mathsf{Poisson}(\Lambda);
       T \sim \mathsf{Uniform}\{1..n\};
                                                                                    \Lambda \sim \mathsf{Exponential}(1);
       \Lambda_1 \sim \mathsf{Exponential}(1);
                                                                                    observe y_2 \sim \mathsf{Poisson}(\Lambda);
       \Lambda_2 \sim \mathsf{Exponential}(1);
       if 1 < T {
           y_1 \sim \mathsf{Poisson}(\Lambda_1);
                                                                                    observe y_m \sim \mathsf{Poisson}(\Lambda);
       } else {
                                                                                   T := 1;
           y_1 \sim \mathsf{Poisson}(\Lambda_2);
                                                                             } else { if 1 \sim \text{Bernoulli}(1/(m-1)) {
                                                                                    observe y_1 \sim \mathsf{Poisson}(\Lambda);
        }
                                                                                    observe y_2 \sim \mathsf{Poisson}(\Lambda);
                                                                                    \Lambda \sim \mathsf{Exponential}(1);
       if n < T {
                                                                                    observe y_3 \sim \mathsf{Poisson}(\Lambda);
           y_n \sim \mathsf{Poisson}(\Lambda_1);
       } else {
           y_n \sim \mathsf{Poisson}(\Lambda_2);
                                                                                    observe y_m \sim \mathsf{Poisson}(\Lambda);
       }
                                                                                    T := 2;
                                                                            } else {
(a) Switchpoint model from [19].
                                                                                     ٠.
                                                                            }}
```

 $T \sim \mathsf{Uniform}\{1..n\};$

(b) More efficient version of the switchpoint model.

Figure 7: The program code for the Bayesian switchpoint analysis.

Z := 1;

```
\Lambda_1 \sim \text{Geometric}(0.1);
   \Lambda_1 \sim \text{Geometric}(0.1);
                                                                                     \Lambda_2 \sim \text{Geometric}(0.1);
   \Lambda_2 \sim \text{Geometric}(0.1);
                                                                                    if Z = 0 {
   if 1 \sim \text{Bernoulli}(0.5) {
                                                                                            observe y_1 \sim \mathsf{Poisson}(0.1 \cdot \Lambda_1);
      observe y_1 \sim \mathsf{Poisson}(0.1 \cdot \Lambda_1)
                                                                                            Z \sim \text{Bernoulli}(0.2);
   } else {
                                                                                    } else {
      observe y_1 \sim \mathsf{Poisson}(0.1 \cdot \Lambda_2)
                                                                                            observe y_1 \sim \mathsf{Poisson}(0.1 \cdot \Lambda_2);
   }
                                                                                            Z \sim \mathsf{Bernoulli}(0.8); \}
   if 1 \sim \text{Bernoulli}(0.5) {
                                                                                    if Z = 0 {
      observe y_m \sim \mathsf{Poisson}(0.1 \cdot \Lambda_1)
                                                                                            observe y_m \sim \mathsf{Poisson}(0.1 \cdot \Lambda_1);
   } else {
                                                                                            Z \sim \text{Bernoulli}(0.2);
      observe y_m \sim \mathsf{Poisson}(0.1 \cdot \Lambda_2)
                                                                                     } else {
   }
                                                                                            observe y_m \sim \mathsf{Poisson}(0.1 \cdot \Lambda_2);
                                                                                            Z \sim \mathsf{Bernoulli}(0.8); \}
(a) Program code for the mixture model.
```

(b) Program code for the HMM.

Figure 8: The program code for the mixture and HMM model.



Figure 10: Comparison of moments for the modified population model.

distributed number of observed events depends on the state Z and is $0.1 \cdot \Lambda_1$ or $0.1 \cdot \Lambda_2$, where we impose a geometric prior on Λ_1 and Λ_2 . As for the mixture model, this discretizes the rates in steps of 0.1. The inference problem is to infer the first rate Λ_1 . The probabilistic program is shown in Fig. 8b, where y_k are m = 30 simulated data points from the true rates $\lambda_1 := 0.5$ and $\lambda_2 := 2.5$. Concretely, we have y = (2, 2, 4, 0, 0, 0, 0, 0, 1, 1, 0, 2, 4, 3, 3, 5, 1, 2, 3, 1, 3, 3, 0, 0, 2, 0, 0, 2, 6, 1).

D.2 Additional results

In the main text, the data we presented was mainly in form of the total variation distance (TVD) between the true posterior (computed by our method) and the approximated posterior (computed by Anglican's inference algorithms). In this section, we present additional evidence in two forms:

- errors of the posterior moments (mean, standard deviation, skewness, and kurtosis) in Figs. 9 to 14, and
- histograms (Fig. 15) of the sampled distribution produced by the best MCMC algorithm, where the sampling budget is picked such that the running time is close to that of our method (e.g. 1000 for the (fast) population model and 10000 for the (slower) mixture model).

The additional plots confirm the conclusions from Section 5.



Figure 11: Comparison of moments for the two-type population model.



Figure 12: Comparison of moments for the switchpoint model.



Figure 13: Comparison of moments for the mixture model.



(a) Error of the mean

(b) Error of the standard de- (c) Error of the skewness viation

(d) Error of the kurtosis

Figure 14: Comparison of moments for the HMM.



Figure 15: Histograms of the exact distribution and the MCMC samples with the lowest TVD and similar running time to our exact method.

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