
Predicate Exchange: Inference with Declarative Knowledge

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Abstract

Programming languages allow us to express complex predicates, but existing inference methods are unable to condition probabilistic models on most of them. To support a broader class of predicates, we develop an inference procedure called *predicate exchange*, which softens predicates. A soft predicate quantifies the extent to which values of model variables are consistent with its hard counterpart. We substitute the likelihood term in the Bayesian posterior with a soft predicate, and develop a variant of replica exchange MCMC to draw posterior samples. We implement predicate exchange as a language agnostic tool which performs a nonstandard execution of a probabilistic program. We demonstrate the approach on sequence models of health and inverse rendering.

1. Introduction

Conditioning in Bayesian inference incorporates observed data into a model. In a broader sense, conditioning revises a model such that a predicate of uncertain truth becomes a fact. Conventionally, this predicate is the equality of observable variables to data. Predicates outside of this class have received significantly less attention, partly because it makes the inference problem significantly more challenging, and partly because conditioning on data accommodates many applications. Nevertheless, there are many more predicates outside this class than inside; our inability to condition on them is a major limitation.

The ability to condition on a broader class of predicates would enable us to incorporate more kinds of declarative domain knowledge into generative models. For example, probabilistic variants of inverse rendering (Marschner & Greenberg, 1998; Kulkarni et al., 2015) require a prior dis-

tribution over three dimensional scenes. Some forms of knowledge, such as the fact that rigid bodies do not intersect, are easier to express declaratively as predicates, than constructively in a generative model. Conditioning on predicates allows us to express what should be true without the burden of specifying how.

Predicates can also represent observations that restrict variables to sets rather than single values. For example, a medical practitioner may observe that a patient is hypoglycemic, i.e., that their glucose levels have fallen below a critical value. Given a model over time series of glucose levels (Levine et al., 2017; Murata et al., 2004), this observation can be realized as a predicate that maps the series to 1 if it falls below the threshold. Neither hypoglycemia nor any of the infinite number of predicates that can be expressed, need to exist in the generative model apriori.

Probability theory treats conditioning on predicates and concrete observations uniformly, but sampling from models conditioned on most predicates is challenging due to the lack of a tractable likelihood function. The likelihood function quantifies the extent to which values of latent variables are consistent with observations, and is deemed intractable if it is normalized by intractable integrals or summations. This can occur, for example, if we condition random variables that are deterministic transformations of other random variables (e.g., the occurrence of hypoglycemia in the example above, or the mean of a collection of variables). Alternatively, if the model is generative, i.e. specified as a stochastic simulation, the likelihood is not explicitly available even when the condition is a conventional observation. The numerous effective likelihood-based sampling (Andrieu et al., 2003) and variational (Jordan et al., 1999; Ranganath et al., 2014) methods are inapplicable as a result.

In this paper we present *predicate exchange*: a likelihood-free method to sample from distributions conditioned on predicates from a broad class. It is composed of two parts:

1. **Predicate Relaxation** constructs soft predicates which return values in a continuous Boolean algebra: the unit interval $[0, 1]$ with continuous logical connectives $\tilde{\wedge}$, $\tilde{\vee}$ and $\tilde{\neg}$. Softened predicates approximate their hard counterparts.
2. **Replica Exchange** is a Markov Chain Monte Carlo

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method that simulates Markov chains at different temperatures. Predicate relaxation is parameterized by a temperature which controls the amount of approximation introduced. We use replica exchange to draw samples from the unrelaxed model.

By returning a value in $[0, 1]$ instead of $\{0, 1\}$, a soft predicate quantifies the degree to which values of variables are consistent with the hard predicate. We concretize this concept in terms of distance: a realization of the model is almost consistent with a predicate if there is another realization that is both consistent with the predicate and close-by with respect to a metric.

Conventional predicates exist in a Boolean algebra; they can be conjoined, disjoined and negated. This allows us to use predicates to represent knowledge that has complex Boolean structure. Continuing the previous example, we may know that a person is *not* hypoglycemic, or that they are hypoglycemic *or* hyperglycemic, or *neither*. To be able to relax complex predicates, we construct a soft Boolean algebra with continuous counterparts to equality, inequalities and logical connectives.

To perform inference we replace the likelihood term in the Bayesian posterior with a soft predicate. This yields an *approximate posterior* which we sample from using Markov Chain Monte Carlo. However, relaxed predicates can still induce complex, multimodal posteriors. Increasing the temperature smooths the approximate posterior, but also causes it to diverge from the true posterior. We use replica exchange to mitigate the trade off. Replica exchange simulates high temperature chains – which explore vast regions of the sample space – in parallel with low temperature chain – which sample accurately from localized regions. We augment replica exchange with an accept-reject phase, which allows us to use approximate posteriors to sample from the true posterior.

Predicate exchange addresses a shortcoming of probabilistic programming languages, which have vastly expanded the class of probabilistic models that can be expressed, but still restrict the kinds of predicates that can be conditioned on to those which result in a tractable likelihood. In a similar vein to (Wingate et al., 2011) we provide a light-weight implementation that modulates the execution of a stochastic simulation based model to perform inference. This means predicate exchange is easily incorporated into existing probabilistic languages. For a concrete implementation, we build predicate exchange into the OMEGA probabilistic programming language¹ (Tavares et al., 2019),

In summary, we:

1. Formalize the desiderata for predicate relaxation (Section 2.1) and present relaxations of numerical and logical primitive functions.
2. Implement predicate exchange as nonstandard execution of a simulation based model (Section 3).
3. Evaluate our approach on examples, including case studies in inverse rendering and glycemic forecasting (Section 4).

2. Predicate Exchange

Given a model (a collection of random variables) $\mathbf{X} = (X_1, X_2, \dots, X_n)$ and a predicate ℓ which maps a model realization $\mathbf{x} = (x_1, x_2, \dots, x_n)$ to 0 or 1, predicate exchange samples from the posterior distribution of \mathbf{X} conditioned on ℓ through two steps:

1. **Predicate Relaxation** constructs a soft predicate $\tilde{\ell}$ from ℓ . $\tilde{\ell}$ maps a model realization \mathbf{x} in a realization space \mathcal{X} to a value in a continuous Boolean algebra: the unit interval $[0, 1]$ with continuous logical connectives $\tilde{\wedge}$, $\tilde{\vee}$ and $\tilde{\neg}$. $\tilde{\ell}$ is 1 iff ℓ is 1, but otherwise takes nonzero values denoting the degree to which ℓ is satisfied.
2. **Replica Exchange** is a Markov Chain Monte Carlo procedure that simulates several replicas of the model conditioned on $\tilde{\ell}$ at different temperatures, ultimately in order to condition on ℓ .

In this section we motivate and formalize the relaxation of predicates expressed as compositions of simple functions. In addition, the latter part of this section defines what it means to condition on a soft predicate. Together, these form the foundation of the relaxation and conditional sampling from probabilistic programs in Section 3.

2.1. Predicate Relaxation

Our objective is to construct a soft predicate $\tilde{\ell}$ that introduces approximations into ℓ to make inference more tractable. We refer to $\tilde{\ell}$ as a *relaxation* of ℓ . Informally, these approximations mean that while conditioning on ℓ eliminates a set of values, conditioning on $\tilde{\ell}$ makes them less likely.

A relaxation $\tilde{\ell}$ has a temperature parameter α that controls the fidelity of the approximation. There are three desiderata which govern this approximation. In particular, $\tilde{\ell}$ should (i) converge to ℓ as $\alpha \rightarrow 0$, (ii) converge to 1 as $\alpha \rightarrow \infty$, and (iii) be consistent with ℓ on 1, i.e., $\ell(\mathbf{x}) = 1$ iff $\tilde{\ell}(\mathbf{x}) = 1$ at all temperatures. Formally:

Definition 1. $\tilde{\ell} : \mathcal{X} \rightarrow [0, 1]$ parameterized by $\alpha \in [0, \infty)$ is a relaxation of $\ell : \mathcal{X} \rightarrow \{0, 1\}$ if for all $\mathbf{x} \in \mathcal{X}$:

- (i) $\lim_{\alpha \rightarrow 0} \tilde{\ell}(\mathbf{x}; \alpha) = \ell(\mathbf{x})$.

¹OMEGA is available at <http://github.com/zenna/Omega.jl>

- (ii) $\lim_{\alpha \rightarrow \infty} \tilde{\ell}(\mathbf{x}; \alpha) = 1$.
- (iii) for all $\alpha < \infty$, $\tilde{\ell}(\mathbf{x}; \alpha) = 1$ iff $\ell(\mathbf{x}) = 1$.

Similarity Based Satisfiability There is a straightforward, but generally incomputable, construction of ℓ that satisfies the relaxation axioms. Let ρ be a metric on \mathcal{X} , k_α be a relaxation kernel (described below) which maps distances in \mathbb{R} to similarities in $[0, 1]$, and $A = \{\mathbf{x} \mid \ell(\mathbf{x}) = 1\}$ be the satisfying set. The predicate $\tilde{\ell}_{\text{inf}}(\mathbf{x})$ is a relaxation of ℓ :

$$\tilde{\ell}_{\text{inf}}(\mathbf{x}) = k_\alpha(\rho(\mathbf{x}, A)) \quad (1)$$

The distance $\rho(\mathbf{x}, A) = \inf \{\rho(\mathbf{x}, a) \mid a \in A\}$ is the smallest distance between \mathbf{x} and any element of A .

Relaxation Kernels A relaxation kernel k_α maps a distance in \mathbb{R} to the unit interval, and is parameterized by temperature α . A relaxation kernel is valid if soft predicates constructed with it satisfy the aforementioned relaxation axioms. One such kernel, which we restrict our attention to, is the squared exponential kernel:

$$k_\alpha(r) = \exp\left(-\frac{r^2}{\alpha}\right) \quad (2)$$

Soft Primitives The distance $\rho(x, A)$ from a point to the satisfying set is in general incomputable. To relax complex programs we instead rely on composition, but first define relaxations for numerical and logical primitives. Soft equality is straightforward: $x \doteq y$ is defined as $k_\alpha(\rho(x, y))$. A soft inequality such as $x \gtrsim y$ is a function of the amount by which x must be increased (or y decreased) until $x > y$ is true. This is the distance between x and the interval $[y, \infty]$, where the distance between a point and any interval $[a, b]$ is the smallest distance between x and any element in $[a, b]$, and therefore 0 if $x \in [a, b]$:

$$\rho(x, [a, b]) = \begin{cases} a - x & \text{if } x < a \\ x - b & \text{if } x > b \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

Soft conjunction $\tilde{\wedge}$ and disjunction $\tilde{\vee}$ take the min and max respectively, which is standard. Soft negation, on the other hand, introduces complications. In continuous logics (Kimmig et al., 2012), the negation of $a \in [0, 1]$ is $1 - a$. However, as shown in Figure 1 (b), this violates criteria (iii) of predicate relaxation since there are values which satisfy the hard predicate $\neg(x > 0)$ which do take a value of 1 in $1 - (x \gtrsim 0)$. Figure 1 illustrates this issue.

The problem of negation arises because $\tilde{\ell}$ is consistent with ℓ at 1 but not at 0, i.e., $\tilde{\ell}(\mathbf{x}; \alpha) = 1$ iff $\ell(\mathbf{x}) = 1$ at all temperatures α . In other words, $\tilde{\ell}$ is a one-sided approximation. To resolve this, we use *two-sided* soft primitives which yield

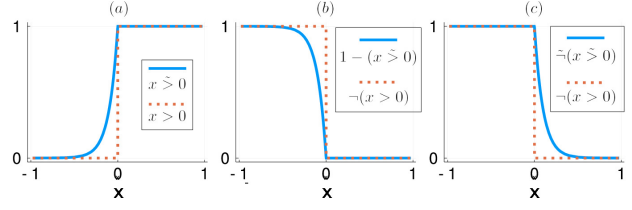


Figure 1. The problem of negation. All figures: soft (blue) and hard (red, dashed) predicates as a function of x . Left: $x > 0$ approximates $x > 0$. Middle: the standard approach to continuous negation ($1 - (x \gtrsim 0)$) violates relaxation criteria (iii). Right: the desired outcome of soft negation of $x \gtrsim 0$.

a pair (a_0, a_1) where $a_0, a_1 \in [0, 1]$. a_1 is consistent with ℓ on 1, just as before, while a_0 is consistent with $\neg \ell$ on 1. For example if $x \gtrsim 0$ evaluates to (a_0, a_1) , then a_1 is 1 iff $x > 0$ (Figure 1 (a)) and a_0 is 1 iff $x \leq 0$ (Figure 1 (c)). Two-sided soft equality and inequalities are defined as:

$$\begin{aligned} x \doteq y &= (a_0, k_\alpha(\rho(x, y))) \text{ where } a_0 = \begin{cases} \exp(1/\alpha) & \text{if } x = y \\ 1 & \text{otherwise} \end{cases} \\ x \gtrsim y &= (k_\alpha(\rho(x, [-\infty, y])), k_\alpha(\rho(x, [y, \infty]))) \\ x \lesssim y &= (k_\alpha(\rho(y, [x, \infty])), k_\alpha(\rho(y, [-\infty, x]))) \end{aligned} \quad (4)$$

Two-sided soft conjunction and soft disjunction follow De Morgan's laws, and soft negation simply swaps the elements of (a_0, a_1) to yield (a_1, a_0) :

$$\begin{aligned} (a_0, a_1) \tilde{\wedge} (b_0, b_1) &= (\max(a_0, b_0), \min(a_1, b_1)) \\ (a_0, a_1) \tilde{\vee} (b_0, b_1) &= (\min(a_0, b_0), \max(a_1, b_1)) \\ \neg(a_0, a_1) &= (a_1, a_0) \end{aligned} \quad (5)$$

Conditioning does not treat the outputs of a predicate symmetrically. Rather, it restricts the model to values which produce 1. Consequently, when used to condition in replica exchange, a_1 and not a_0 is used in the target density.

Composition of Soft Primitives We can construct $\tilde{\ell}$ from ℓ compositionally, by substituting primitive predicates (equality, inequalities and logical operators) with soft counterparts. For instance the predicate $(x > y) \vee \neg(x^2 = 2)$ is relaxed by $(x \gtrsim y) \tilde{\vee} \neg(x^2 \doteq 2)$.

Proposition 1. Relaxation criteria are preserved under composition. Let a and b be predicates, and \circ denote a binary logical operator. If \tilde{a} , \tilde{b} and $\tilde{\circ}$ are respective valid relaxations. Then $\tilde{a} \tilde{\circ} \tilde{b}$ is a relaxation of $a \circ b$.

2.2. Approximate Markov Chain Monte Carlo

We use soft predicates as approximate likelihoods for Markov Chain Monte Carlo sampling. MCMC algorithms

require a function f that is proportional to the target density. In Bayesian inference this is the posterior, dictated by Bayes’ theorem as the product of the likelihood and the prior. Approximate inference using soft predicates takes a similar form.

Definition 2. Let \mathbf{X} be a model, ℓ be a predicate that conditions \mathbf{X} , and \mathbf{x} be a realization of \mathbf{X} . Assuming a prior density p , the approximate posterior f is the product:

$$f(\mathbf{x}) = p(\mathbf{x}) \cdot \tilde{\ell}(\mathbf{x}) \quad (6)$$

$\tilde{\ell}$ downweights parameter values which violate ℓ by the degree to which they violate it. This is modulated by the temperature α used in the relaxation kernels which constitute $\tilde{\ell}$. At maximum temperature $\tilde{\ell}$ has no effect, and the approximate posterior f is equal to the prior p . At zero temperature, f recovers the true posterior since parameter values which violate the condition are given zero weight.

For illustration, if $X_{1,2} \sim \mathcal{N}(0, 1)$ constitute a model conditioned on $X_1 + X_2 = 0$, the approximate posterior is:

$$f_\alpha(x_1, x_2) = \mathcal{N}_{0,1}(x_1) \cdot \mathcal{N}_{0,1}(x_2) \cdot k_\alpha(\rho(x_1 + x_2, 0)) \quad (7)$$

The temperature parameter trades off between tractability of inference and the fidelity of the approximation. If the temperature is too high $\tilde{\ell}$ will diverge too greatly from ℓ . If it is too low, convergence will be slow.

Balancing Different Constraints At a fixed, nonzero temperature, the scales of variables affects their influence on the conditional distribution. For instance, consider two uniformly distributed random variables $x \sim \text{Unif}(-1, 1)$ and $y \sim \text{Unif}(-10, 10)$, and predicates p_x, p_y defined as $x \doteq 0$ and $y \doteq 0$ respectively. The expectation of a soft predicate quantifies the degree to which it is true, and is a non-decreasing function of temperature. The prior expectation of p_x is significantly larger than that of p_y . because values far from zero are more likely under y .

This disparity persists if the model is conditioned. Figure 2 shows samples from the model conditioned on $p_x \tilde{\vee} p_y$, and a disparity in the histograms of the marginals of p_x and p_y . The disparity decreases with decreasing temperature, and disappears at zero. Still, it is undesirable in practice because it means that the approximation error is distributed unevenly.

To mitigate this issue, we minimize discrepancies between sample averages of constraints. Consider the case of two soft predicates p_1 and p_2 . We introduce a weight for all but the first constraint. In this case p_2 in the soft predicate is replaced by $\gamma_2 p_2$. The weight γ_2 should ensure that $\gamma_2 p_2$ has the same magnitude effect as p_1 on the energy function:

$$E_{p_{\alpha, \gamma_2}}[p_1] = E_{p_{\alpha, \gamma_2}}[\gamma_2 p_2]$$

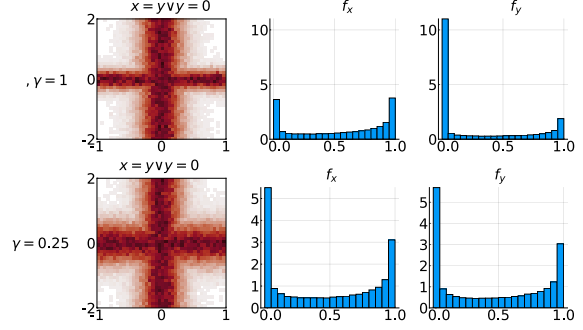


Figure 2. Magnitudes of variables can lead to uneven contributions to error if unadjusted. Top row: (left) samples from model, (middle and right) histograms of marginals. Bottom row is same model with weights adjusted to balance error.

In practice, we set γ_2 using an exponential moving average of the p_1 values over the p_2 values. Figure 2 visualizes the problem of unbalanced constraints, as well as corrections to γ .

2.3. Replica Exchange

Replica exchange (Swendsen & Wang, 1986) simulates M replicas of a model at different temperatures, and uses a Metropolis-Hastings update to periodically swap the temperatures of chains. Let f_{α_i} denote the approximate posterior function at temperature α_i , then two independent parallel chains simulating targets $f_{\alpha_1}(x), f_{\alpha_2}(y)$ follow a joint target $f_{\alpha_1, \alpha_2}(x, y) = f_{\alpha_1}(x)f_{\alpha_2}(y)$. Replica exchange swaps states between the chains while preserving the joint target. Swapping states is equivalent to swapping predicates, which motivates the name “predicate exchange”. Concretely, replica exchange proposes a swap from (x, y) to (y, x) , and accepts it with probability $\min(1, A)$, where:

$$A = \frac{f_{\alpha_1, \alpha_2}(y, x)}{f_{\alpha_1, \alpha_2}(x, y)} = \frac{f_{\alpha_1}(y)f_{\alpha_2}(x)}{f_{\alpha_1}(x)f_{\alpha_2}(y)} \quad (8)$$

We modify standard replica exchange in two ways: (i) for exact inference, states which violate the constraint are rejected, and (ii) unlike conventional replica exchange which draws samples only from the zero-temperature chain, we accept states from any chain so long as $f_{\alpha_i}(x) = 1$.

3. Implementation

In this section we describe a generic, lightweight implementation of predicate exchange. Our approach resembles (Wingate et al., 2011; Milch et al., 2007) as a language independent layer that can sit on top of existing programming languages and modeling formalisms. Our objective is twofold: (i) to compute the prior term p , approximate likelihood term $\tilde{\ell}$, and approximate posterior term f (Equation 7) from an arbitrary simulator π , and (ii) to perform replica

exchange MCMC to sample from the true posterior.

We define a simulator π as a program composed of deterministic and stochastic procedures, but where all randomness comes from a set of known random primitives. Primitives correspond to primitive parametric distribution families, such as the uniform or normal distribution. Let \mathcal{T} be a set of primitive types. Each type $\tau \in \mathcal{T}$ must support (i) evaluation of the conditional density $p_\tau(x \mid \theta_1, \dots, \theta_n)$, and (ii) sampling from the distribution. Concretely, π is any nullary program that contains the statements:

1. $\text{rand}(n, \tau, \theta_1, \dots, \theta_n)$ returns a random sample from $p_\tau(\cdot \mid \theta_1, \dots, \theta_n)$. n is a unique name described below.
2. $\text{cond}(y)$ conditions π . It throws an error if $y \in \{0, 1\}$ is 0, and otherwise allows simulation to resume with no effect.

Example Program 1 illustrates a simple conditioned model.

Names Names (e.g. n_x) passed to rand are not the same as variable names (e.g. x) in the host programming language. If two distinct names are used, the samples output from rand will be independent or conditionally independent. Care must be taken when a program has loops to avoid inadvertently reusing the same name. A simple solution is to append the loop counter to the name.

3.1. Tracked Soft Execution

Predicate exchange relies on `softexecute` (Algorithm 3), which formalizes the soft execution of a program π in the context of dictionary \mathbb{D} , at temperature α . \mathbb{D} is a mutable mapping from a set of names to values. In the context of a particular dictionary, the simulation of a program is deterministic. This allows the simulation of π to be modulated by controlling the elements of \mathbb{D} .

`softexecute` computes the prior term p as the product of random choices in the program. That is, let $\pi_k \mid x_1, \dots, x_{k-1}$ be the k 'th random primitive encountered in while executing π , x_k be the value it takes, and x denote the set of all values of all random primitives constructed in the simulation of π , $p(x)$ is then the product:

$$p(x) = \prod_{k=1}^K p_\tau(x_k \mid \theta_1, \dots, \theta_n) \quad (9)$$

The parameters $\theta_1, \dots, \theta_n$ may be fixed values or depend on values of other random primitives π .

`softexecute` executes π but within a context where (i) variables $\ell_{\mathbb{D}}$ and $p_{\mathbb{D}}$ accumulate prior and approximate posterior values, and (ii) the following operators are redefined:

Example Program 1

```
x = rand(n_x, N, 0, 1)
y = rand(n_y, N, 0, 1)
cond(x > y)
Return: (x, y)
```

Example Program 2

```
x = rand(n_x, N, 0, 1)
if x > 0 then
  cond(x = 1)
else
  cond(x = -100)
end if
Return: x
```

1. $\text{rand}(\tau, n, \theta_1, \dots, \theta_n)$ returns $\mathbb{D}(n)$ if $n \in \mathbb{D}$, and in compliance with Equation 9 updates $p_{\mathbb{D}}$ with the conditional density. If n is not a key in \mathbb{D} , the distribution is sampled from and $\mathbb{D}(n)$ is updated with this value.
2. $a \text{ op } b$ and $\text{op } a$ for $\text{op} \in \{>, <, =, \wedge, \vee, \neg\}$ are replaced with the softened counter-parts $\tilde{\text{op}} \in \{\tilde{>}, \tilde{<}, \tilde{=}, \tilde{\wedge}, \tilde{\vee}, \tilde{\neg}\}$.
3. $\text{cond}(y)$ updates $\tilde{\ell}_{\mathbb{D}}$ with $\tilde{\ell}_{\mathbb{D}} \tilde{\wedge} y$. y will be a soft Boolean value rather than a Boolean due to substitution of primitives with soft primitives.

`softexecute` returns a real value for the approximate posterior of f as a function of the dictionary \mathbb{D} .

Control Flow Programs may have control flow, such as if-then-else statements. If a branch condition depends on an uncertain value, there may be unexplored paths which would, if explored, produce values that are closer to the satisfying set. `softexecute` is ignorant of these other possibilities. For illustration, if $x = -1$ in Example Program 2, the condition fails, and `softexecute` will yield $x \tilde{=} -100$. This is significantly larger than if the true branch were taken.

3.2. Replica Exchange

`predexchange` (Algorithm 4) performs replica exchange using `softexecute` to compute approximate posterior values. It takes as input an MCMC algorithm, which simulates a Markov Chain by manipulating elements of the \mathbb{D} .

4. Experiments

Experimental Setup Replica exchange requires a within chain MCMC algorithm. For finite dimensional continuous models we use the No U-Turn Sampler (Hoffman & Gelman, 2014), a variant of Hamiltonian Monte Carlo (HMC).

Algorithm 3 Soft Execution: $\text{softexecute}(\pi, \alpha, \mathbb{D})$

Input: program π , temperature α , dictionary \mathbb{D}
 Initialize $\tilde{\ell}_{\mathbb{D}} = 1, p_{\mathbb{D}} = 1$
 Simulate π with following subroutines redefined as:
subroutine $\text{rand}(n, \tau, \theta_1, \dots, \theta_n)$
 if $n \in \mathbb{D}$ **then**
 $x \stackrel{d}{=} \mathbb{D}(n)$
 else
 $x \stackrel{d}{=} \text{sample from } p_{\tau}(x \mid \theta_1, \dots, \theta_n)$
 Update dictionary: $\mathbb{D}(n) \stackrel{d}{=} x$
 end if
 $p_{\mathbb{D}} \stackrel{d}{=} p_{\mathbb{D}} \cdot p_{\tau}(x \mid \theta_1, \dots, \theta_n)$
 Return from subroutine: x
end subroutine

subroutine $\text{cond}(y)$
 $\tilde{\ell}_{\mathbb{D}} \stackrel{d}{=} \tilde{\ell}_{\mathbb{D}} \tilde{\wedge} y$
end subroutine

subroutine $\text{op}(x, \dots)$ for $\text{op} \in \{>, <, =, \wedge, \vee, \neg\}$
 Return from subroutine: $\tilde{\text{op}}(x, \dots)$
end subroutine

Return: $p_{\mathbb{D}} \cdot \tilde{\ell}_{\mathbb{D}}$

We use reverse-mode automatic differentiation (Griewank & Walther, 2008) to compute the negative log gradient of f , which is required for HMC. For other models we use standard Metropolis Hastings by defining proposals on elements in the dictionary. In particular we use the single site Metropolis Hastings (SSMH) (Wingate et al., 2011) which modifies a single random variable at a time.

Replica exchange has a number of hyper-parameters: the number of parallel chains, the corresponding temperatures, the swapping schedule. Several good practices are outlined in (Earl & Deem, 2005). In practice, we logarithmically space α between a lower and upper bound (e.g., $\log_{10}(\alpha_1) = 5$ to $\log_{10}(\alpha_M) = -5$), and swap states of chains that are adjacent in temperature (α_1 with α_2 , α_2 with α_3 , etc) periodically.

Small Models In Figure 4 we use conditioning to truncate a normal distribution. Figure 3 shows histograms of samples from a uniform prior $[-1, 1]^2$ conditioned on a variety of predicates. While simple, these examples can be challenging due to discontinuities in the approximate posterior.

Inverse Ray Tracing In this example we sample from a posterior distribution over scenes conditioned on an observed rendering. A scene s is a set of $n \sim \text{poisson}(\lambda = 3)$ spheres. A sphere is parameterized by color, reflectance, emission color, transparency, radius and position, all with

Algorithm 4 Predicate Exchange: predexchange

Input: program π , temperatures $\alpha_1, \dots, \alpha_m$, nsamples n
Input: mcmc, nsamples between swaps q
 Initialize $\mathcal{D} = \text{empty collection of dictionaries}$
 Initialize $\mathbb{D}_1^{\text{init}}, \dots, \mathbb{D}_m^{\text{init}}$ empty dictionaries
 Define $f_{\alpha_i}(\mathbb{D}) = \text{softexecute}(\pi, \alpha_i, \mathbb{D})$
repeat
 for $i = 1$ **to** M **do**
 $\mathbb{D}_1, \dots, \mathbb{D}_q \stackrel{d}{=} q$ mcmc samples at temp α_i , from $\mathbb{D}_i^{\text{init}}$
 $\mathbb{D}_i^{\text{init}} \stackrel{d}{=} \mathbb{D}_q$
 for $j = 1$ **to** q **do**
 if $f_{\alpha_i}(\mathbb{D}_j) = 1$ **then**
 append \mathbb{D}_j to \mathcal{D}
 end if
 end for
 end for
 for $i = m$ **down to** 2 **do**
 $j \stackrel{d}{=} i - 1$
 $p \stackrel{d}{=} f_{\alpha_i}(\mathbb{D}_j) f_{\alpha_j}(\mathbb{D}_i) / f_{\alpha_i}(\mathbb{D}_i) f_{\alpha_j}(\mathbb{D}_j)$
 if $p > \text{random sample in } [0, 1]$ **then**
 swap α_i with α_j
 end if
 end for
until \mathcal{D} has n elements
Return: \mathcal{D}

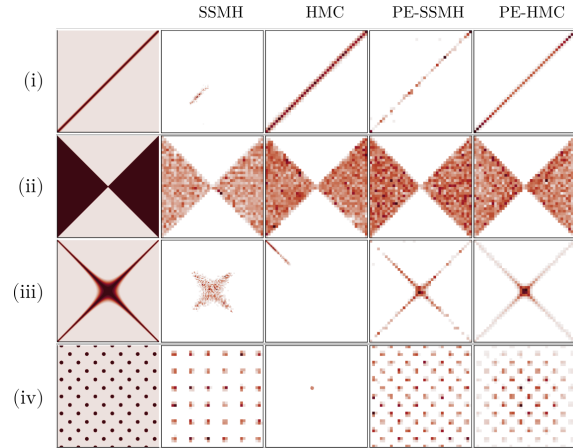


Figure 3. Samples from models using different procedures. Each model is $x, y \sim \text{Unif}(-1, 1)$ conditioned on (i) $x \doteq y$, (ii) $|x| \gtrsim |y|$, (iii) $x^2 \doteq y^2$ and (iv) $\sin(kx) \cos(kx) \gtrsim 0.9999$. Inference procedures are: Single Site Metropolis Hastings (SSMH), Hamiltonian Monte Carlo (HMC), and Predicate-Exchange (PE) using HMC and SSMH within chain.

a uniform prior. Let r be a ray tracing function that maps scenes to image, i_{obs} be an observed image, and nointersect be a predicate that maps a scene to 1 iff any spheres intersect. The prior s is conditioned on the conjunction of the inverse

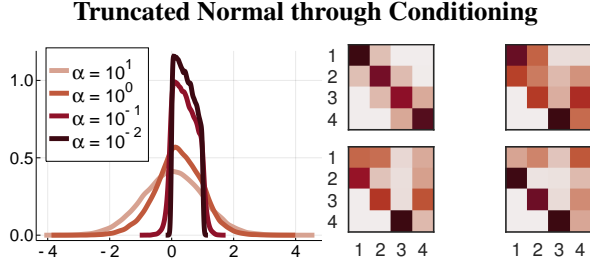


Figure 4. Left: Kernel density estimation from samples of Gaussian truncated to $[0, 1]$ through conditioning. Shown at different temperatures. Right: transitions between different temperatures of replica exchange. For each matrix, value in row i and column j is the fraction of times replica exchange swapped a state at temperature i to temperature j . Temperature is lowest at 4 and increases exponentially to 1. Clockwise, starting top-left: transition counts are accumulated for the first, second, third and fourth quarters of simulation.

rendering and the no-intersection constraints:

$$(r(s) = i_{obs}) \wedge \text{nointersect}(s) \quad (10)$$

Figure 5 visualizes conditional samples.

Glucose Model Type 2 diabetes is a prevalent and costly condition. Keeping blood glucose within normal limits helps prevent the long-term complications of Type 2 diabetes like diabetic neuropathy and diabetic retinopathy (Brownlee & Hirsch, 2006). Models to predict the trajectories of blood glucose aid in keeping glucose within normal limits (Zeevi et al., 2015). Traditional models have been built from compositions of differential equations (Albers et al., 2017; Levine et al., 2017) whose parameters are estimated separately for each patient. An alternative approach would be to use a flexible sequence model like an RNN. The problem with this approach is that an RNN can extrapolate to glucose values incompatible with human physiology. This is especially a problem where we have patients with only a few blood glucose measurements. To build an RNN model that respects physiology, we condition on it.

We compare the independent RNN model to the one with declarative knowledge on a second patient from Physionet (Moody et al., 2001). Figure 6 plots the results performed on more than 300 pairs of patients. We see that the conditional model simulates more realistic glucose dynamics for the patient with only a short observed time-series.

Benchmarks To quantitatively compare predicate exchange with existing approaches we constructed an artificial problem that scales in difficulty. Let $X_i \sim \mathcal{N}(0, 1)$ in a d -dimensional model $\mathbf{X} = (X_1, \dots, X_d)$ conditioned on

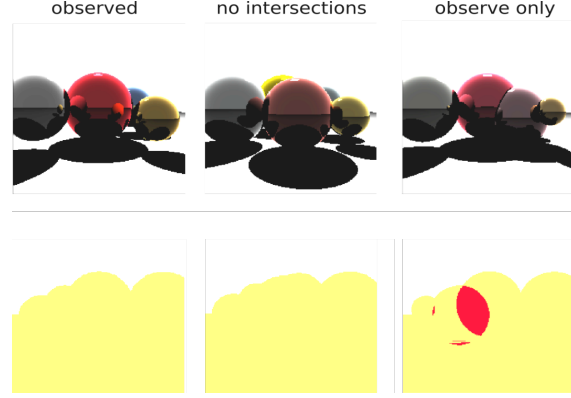


Figure 5. Inverse rendering with and without no-intersection constraints. Top row: raytraced scenes. Bottom row: red pixels denote the existence of an intersection between spheres at that point. (middle) and (right) scenes are samples from posterior over scenes having observed image on left. The observed scene has no intersections. Without the no-intersection condition (right), intersections occur. Conditioning on intersection eliminates intersections (middle).

an ϵ -thick ring:

$$\ell_\epsilon(\mathbf{x}) = 1 < |\mathbf{x}| < 1 + \epsilon \quad (11)$$

Table 4 compares the sample average of particle Gibbs (PG), sequential Monte Carlo (SMC), rejection sampling (RS) and predicate exchange (PE), varying both ϵ and d . The theoretical expectation of all models is 0. Among these methods, predicate exchange is unique in its support for inference with predicates, which makes direct comparison difficult. For all inference procedures we use predicate relaxation to compute $d = \ell_\epsilon(\mathbf{x})$, and sample from \mathbf{X} conditioned on $\mathcal{N}(d, 1/(2\alpha)) = 1$, where α is the lowest temperature used in predicate exchange. Predicate exchange compares favourably in most scenarios.

5. Related Work

Demand for likelihood-free inference emerged in genetics ecology. Tavaré et al. (1997) filtered samples from a stochastic simulator to only those which matched (according to summary statistics) observed data. Weiss et al. (1998) extended this with a tolerance term, so that simulations sufficiently close to the data were accepted. A variety of approaches in this general regime (Beaumont et al., 2002; Sisson et al., 2007) fall under the heading of Approximate Bayesian Computation (ABC). Marjoram et al. (2003) simulated Markov Chains according to the prior, but applied the same summary statistic based filtering to yield approximate posterior samples. A small tolerance leads to a high rate of rejected simulations, whereas a large tolerance results in an unacceptable approximation error. Among several solutions are dynamically decreasing the tolerance (Toni et al., 2008),

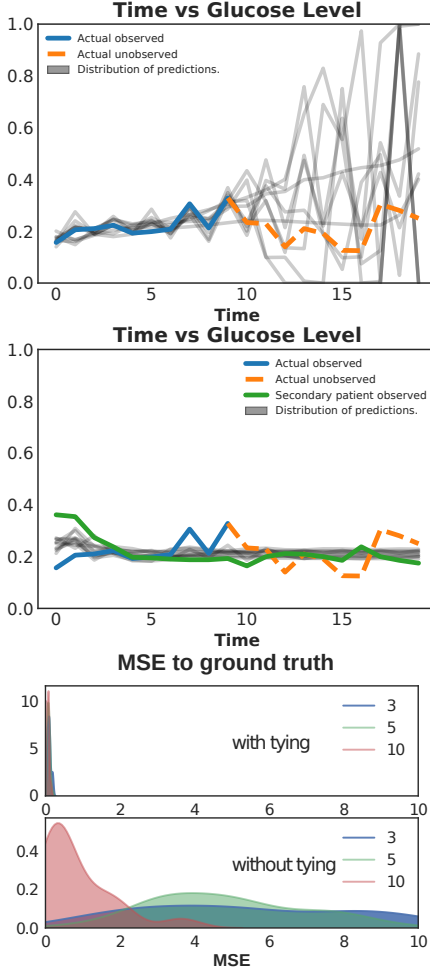


Figure 6. Top: Actual (dotted) and predicted trajectories that were learned using a partial trajectory. Center: Distribution of predicted trajectories learned only using the first ten data points and a tie with a secondary patient. Bottom, top: MSE when tie is present. Bottom, bottom: without tie. Tying expectations has dramatic influence on prediction error, while as more data is observed, the effect of tying decreases.

importance reweighting samples based on distance (Wegmann et al., 2009), adapting the tolerance based on distance (Del Moral et al., 2012; Lenormand et al., 2013), as well as annealing the tolerance as a temperature parameter (Albert et al., 2015). Predicate exchange targets simulation models and uses distance metrics, but does not require summary statistics.

Probabilistic logics such as ProbLog (Richardson & Domingos, 2006) and Markov logic networks (De Raedt et al., 2007) extend first order logic to express both models and conditions. Of particular note, probabilistic soft logic (PSL) (Brocheler et al., 2012; Kimmig et al., 2012) uses continuous logic to encode graded beliefs. For example, $\text{isfriend}(\text{Alice}, \text{Bob}) \rightarrow 0.9$ denotes a strong friendship between Alice and Bob. The primary distinction between

d, ϵ	$1, 10^{-1}$	$1, 10^{-5}$	$100, 10^{-1}$	$100, 10^{-5}$
PE	0.0054	0.4735	-0.00037	0.00854
SMC	0.06	-0.226	-0.018	0.09
PG	-0.029	0.239	-0.03	0.03
RS	0.003	timeout	timeout	timeout

Figure 7. Comparison of expectations of samples from d dimensional ring. Theoretical value is 0 in all cases.

PSL and predicate exchange is in the semantics of the soft predicates. In predicate exchange, relaxation is used solely to make inference more tractable; soft Boolean values are used only within the sampling process and do not appear in the resulting samples themselves. In addition, predicate exchange is motivated by probabilistic programming languages for generative models, such as (Milch et al., 2007; Wood et al., 2014; Mansinghka et al., 2014; Goodman et al., 2008), rather than purely declarative logic based languages.

Several continuous (Levin, 2000) and fuzzy (Klir & Yuan, 1995) logics apply model-theoretic tools to metric structures. Continuous logics replace the Boolean structure $\{T, F\}$, quantifiers $\forall x$ and $\exists x$, and logical connectives with continuous counter-parts. Semantically, our approach remains within measure theoretic foundations, which relies on hard predicates to condition.

6. Discussion

In this work we expanded the class of predicates that probabilistic models can be conditioned on in practice. This pushes predicates exchange into the domain of constraint solvers. However, it remains difficult to delineate which predicates are amenable to our method.

Equality conditions on continuous variables indicate sets of zero measure. This is problematic because the probability of proposing a satisfying state in a Markov chain becomes zero. In these cases predicate exchange must sample at a minimum temperature strictly greater than zero, which is approximate.

Control flow remains a challenge, and is related to the path explosion problem in program analysis (Cadaru et al., 2008; Sen et al., 2005). Future work is to adapt program analysis solutions to this problem.

Hard predicates provide a single bit of information. Predicate relaxation effectively increases the quantity of information available to inference procedures to a single real value. We anticipate that increasing this further would lead to novel approaches to inference.

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