Probabilistic Active Learning of Functions in Structural Causal Models

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Abstract

We consider the problem of learning the functions computing children from parents in a Structural Causal Model once the underlying causal graph has been identified. This is in some sense the second step after causal discovery. Taking a probabilistic approach to estimating these functions, we derive a natural myopic active learning scheme that identifies the intervention which is optimally informative about all of the unknown functions jointly, given previously observed data. We test the derived algorithms on simple examples, to demonstrate that they produce a structured exploration policy that significantly improves on unstructured base-lines.

1 Introduction

Large parts of the literature on causality are concerned with learning the causal graph of a system of random variables [Spirtes et al., 2000, Tong and Koller, 2001, Eberhardt, 2010, Hyttinen et al., 2013, Mooij et al., 2016]. Also known as causal discovery or causal inference, this problem is motivated by realistic problems in science: a biologist may wish to discover genes responsible for regulating other genes in a cell; a public health researcher may wish to know whether certain habits in a population (e.g. smoking) influence certain health outcomes (e.g. probability of developing lung cancer).

The starting point of this paper is to consider what should be done after the causal graph of a system of variables has already been identified (be it by causal discovery methods, or from prior knowledge). That is, it is known which variables are functions of which other variables, but the precise functional relationships are still unknown. Thus, although we understand the causal relationships in a coarse sense, we will not be able to accurately predict the result of an intervention to the system, possibly with implications for decision making.

For instance, suppose that in a cell, Gene A up-regulates Gene B and Gene B down-regulates Gene C. We know that reducing expression of Gene A will lead to a decrease in expression of Gene B which, in turn, will lead to an increase in expression of Gene C. However, without more precise knowledge of the relationships between genes, we will be unable to quantitatively predict the effect of applying a drug that reduces expression of Gene A by 20%. Similarly, if our goal is to reduce overall levels of lung cancer in the population, then knowing only that smoking causes cancer is insufficient to know what the best public health policy should be: would it be better if we could persuade 50% of smokers to stop smoking completely, or persuade every smoker to reduce their consumption by 50%?

For a passive agent supplied with data generated by the system, learning the functional relationships between parents and children reduces simply to separate regression problems—one for each unknown function—once the causal graph is known. Many knowledge acquisition problems, however, can be phrased as a sequential decision making process in which the data that is received at the next point in time is affected by a decision made based on the data that has already been observed. A biologist does not blindly perform a series of costly and time-consuming experiments, only looking at the generated data once the last is over; the data from each experiment would be analysed before the next is performed, thus informing which experiment would be best to perform next.
Below, we formalise this problem using the language of Structural Causal Models (SCMs), also known as Structural Equation Models [Pearl 2009, Bollen 2014]. An SCM, in essence, consists of functions connecting child variables with their causal parents, and is equipped with a notion of intervention in which a variable (or subset of variables) is externally forced to take a particular value (or values). We use these interventions as an idealised mathematical representation of performing an experiment. We take a Bayesian approach to estimating the functional relationships between parents and children, which naturally gives rise to an active learning algorithm to decide on the next ‘experiment’ to perform.

While our approach works with causal graphs that are arbitrary DAGs, the non-triviality of this problem is apparent even in the simple case of three variables whose causal graph is a chain (Figure 1). Our goal in this situation is, in a sense to be made precise later, to learn the functions $f_2$ and $f_3$. At each point in time, we must decide whether to perform one of the possible interventions or to passively observe the system, with each different action having some cost. If we make a passive observation, we will learn something about both $f_2$ and $f_3$, though only in areas where the distributions over $X_1$ and $X_2$ put probability mass. In the small sample setting, we are very unlikely to learn anything about the functions in areas of low probability of their inputs. If we intervene on $X_1$ and choose what value to set it to, we can decide precisely where we want to learn about $f_2$ and we will also learn about $f_3$ in some region, although we would be uncertain about where. If we intervene on $X_2$, we can learn a precise aspect of $f_3$, but will learn nothing about $f_2$. How should we decide which action to pick, given what we already know about $f_2$ and $f_3$?

The problem considered in this paper and our approach to solving it have a close connection to ideas in Bayesian optimization [Jones et al., 1998; Osborne et al., 2009; Shahriari et al., 2016]. In Bayesian optimization, the goal is to find the extremum of a function that is expensive to evaluate, possibly exploiting known structure to speed up the search. Due to this expense, the information obtained from each evaluation should be used efficiently. In contrast, however, in our setting we are not simply interested in finding the extremum of an unknown function, but rather to learn the entire function (or set of functions) in some sense. Tong and Koller [2000] considered a similar setting, but only treated discrete variables.

Below, we begin with a formal definition of Structural Causal Models (Section 2). Section 3 states the precise problem we are tackling. Section 4 provides a Bayesian formulation for inference in this setting, which is then complemented by an active learning scheme to guide exploration (Section 5). Section 6 provides empirical evaluations on synthetic toy examples.

2 Structural Causal Models

We now formally define Structural Causal Models (SCMs), the learning of which we will study in the remainder. For notational simplicity, our definition deviates from the wider literature by including the set of interventions modelled by the SCM.

**Definition 1.** Suppose that $X_1, \ldots, X_N, E_1, \ldots, E_N$ are variables with each $X_n$ and $E_n$ taking value in $\mathcal{X}_n = \mathbb{R}$ and $\mathcal{E}_n = \mathbb{R}$ respectively. We write $X = (X_n)_{n=1, \ldots, N}$ for the vector of variables, and $\mathcal{X} = \prod_{n=1, \ldots, N} \mathcal{X}_n$ for their domain, similarly for $E$ and $E$. A Structural Causal Model (SCM) $\mathcal{M} = (\mathcal{S}, \mathcal{I}, \mathbb{P}_E)$ is a tuple consisting of the following three quantities:

- $\mathcal{S}$ is a set of structural equations $X_n = f_n(X_{pa(n)}, E_n)$, where $pa(n) \subset \{1, \ldots, N\}$ and $X_{pa(n)}$ is the vector of variables $(X_m)_{m \in pa(n)}$. We call the $X_{pa(n)}$ the causal parents of $X_n$.
- $\mathcal{I}$ is a set of interventions. An intervention is a mathematical operation that replaces a subset of the equations in $\mathcal{S}$ with equations setting the variables to specific constants (e.g. $X_n = 3$). We write the intervention $i \in \mathcal{I}$ that intervenes on the subset of variables $X_{var(i)}$, $var(i) \subset \{1, \ldots, n\}$, setting them to values $x_{val(i)}$, as $do(X_{var(i)} = x_{val(i)})$ (we will often abuse notation by writing $do(i)$ instead). We write $\mathcal{S}^{do(i)}$ for the resulting equations.
The observational distribution of $M$ under the distribution $P$ is written as $P_{\mathcal{X}}^\text{do}(\emptyset)$ (where $\emptyset$ signifies the ‘empty’ intervention). Under each intervention, the resulting intervened structural equations $S_{\mathcal{X}}^\text{do}(i)$ are also acyclic. It follows by the same reasoning as above that the SCMs. In this case, given any fixed value $e$ of the variables $E$, there is a unique value $x \in \mathcal{X}$ such that each structural equation in $S$ is satisfied, thus $P_E$ induces a distribution over $\mathcal{X}$ via these unique solutions. We refer to this as the observational distribution of the SCM, and write it as $P_{\mathcal{X}}^\text{do}(\emptyset)$, where each equation is of the form $X_n = f_n(X_{pa(n)}) + E_n$, where each $E_n$ is a zero-mean Gaussian random variable.

This assumption could be relaxed to a more Bayesian approach involving a prior over the covariance matrix, which would reduce to running the algorithm derived in the following, but averaging its results over the posterior.

An important note is that once the graphical structure has been fixed, the parameters of the model $M$ are the functions $f_n$ and the distribution $P_E$ over the variables $E$. We will make the non-trivial assumption that the structural equations are non-linear with additive Gaussian noise, meaning that each equation is of the form $X_n = f_n(X_{pa(n)}) + E_n$, where each $E_n$ is a zero-mean Gaussian random variable.

### Example 1.

Consider the following SCM $M = (\mathcal{S}, \mathcal{I}, P_E)$ represented by Figure 7, where

$$
\mathcal{S} = \left\{ \begin{array}{l}
X_1 = 3 + E_1, \\
X_2 = X_1^2 + E_2, \\
X_3 = 2X_2 + \sin(X_2) + E_3
\end{array} \right\}, \quad \mathcal{I} = \{ \emptyset \} \cup \{ \text{do}(X_i = x_i) \mid x_i \in \mathbb{R}, \; i = 1, 2 \}, \\
E_n \sim \mathcal{N}(0, \sigma_n^2), \quad n = 1, 2, 3.
$$

The observational distribution of $M$ factorises as $P_{\mathcal{X}}^\text{do}(\emptyset) = P_{X_1}^\text{do}(\emptyset)P_{X_2}^\text{do}(\emptyset)P_{X_3}^\text{do}(\emptyset)$. Under, for instance, the intervention do$(X_2 = 0)$, the equation $X_2 = X_1^2 + E_2$ in $S$ is replaced by $X_2 = 0$.

Under the distribution $P_{X_1, X_2, X_3}^\text{do}(X_2=0)$, $X_1$ and $X_3$ are independent and $X_2$ is degenerate.

### Problem setup

Suppose there exists an SCM $M = (\mathcal{S}, \mathcal{I}, P_E)$ with $\mathcal{S} = \{ X_n = f_n(X_{pa(n)}) + E_n : n = 1, \ldots, N \}$ and $P_E \sim \mathcal{N}(0, \Lambda)$ where $\Lambda$ is diagonal. We assume that the graphical structure is known, but the functions $f_n$ themselves are not. For simplicity, we assume that $\Lambda$ is known.

We are given data $D$ drawn from the observational and a variety of interventional distributions of $M$; each element of $D$ is a tuple $(i, x)$, where $x$ is an independent draw from $P_{\mathcal{X}}^\text{do}(i)$. We are interested in two separate tasks.

#### Problem 1: Estimating $M$

Using $D$, learn functions $\hat{f}_n$ such that the estimated model $\hat{M} = (\mathcal{S}, \mathcal{I}, \hat{P}_E)$ with $\hat{S} = \{ X_n = \hat{f}_n(X_{pa(n)}) + E_n : n = 1, \ldots, N \}$ is ‘close’ to the true model $M$ in some sense. Part of this problem is to define a sensible notion of closeness between SCMs.

#### Problem 2: Active learning

We can select an intervention $i \in \mathcal{I}$ at some cost $c(i)$ and observe a single draw from $P_{\mathcal{X}}^\text{do}(i)$. Which $i$ should be selected to ensure the next estimate $\hat{M}$ after incorporating the new datum is as close to $M$ as possible?

The rest of this section is devoted to defining a risk functional to provide a notion of closeness between $\hat{M}$ and $M$. There may be no single best way to define this notion of closeness, as desirable properties may be dependent on particular use case.

Consider, for instance, the following scenarios in which the ultimate goal is to:

- Approximate each function $f_n$ so that a practitioner can visually interpret the relationship between predictors and response variables (e.g., identifying genes as ‘excitatory’ or ‘inhibitory’, or identifying a threshold dosage at which a drug under medical trial is considered toxic).
- Predict the result of an intervention that cannot be practically carried out, or is potentially dangerous to do so (e.g., raising interest rates, or giving a patient a drug).

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1. That is, the directed graph with nodes $\{1, \ldots, N\}$ with edges $n \rightarrow m$ if and only if $n \in pa(m)$ is a DAG.
2. That is, for any $e \in \mathcal{E}$, there is a unique $x \in \mathcal{X}$ such that $x_n = f_n(x_{pa(n)}, e_n)$ for each $n$. This can be seen to be true by explicitly writing each $x_n$ as a function of the $e_n$ by substituting the equations into one another.
3. This assumption could be relaxed to a more Bayesian approach involving a prior over the covariance matrix, which would reduce to running the algorithm derived in the following, but averaging its results over the posterior.
4. The same is true in the case of causal graph learning. See e.g. de Jongh and Druzdzel [2009].
• Better control a system in a variety of environments or conditions (e.g., learning the dynamics of a complex vehicle to be employed in variable conditions)

We will suppose that for each function \( f_n \) with domain \( \mathcal{X}_{pa(n)} = \prod_{m \in pa(n)} \mathcal{X}_m \) we are supplied with a probability measure \( \Pi_n \) over \( \mathcal{X}_{pa(n)} \) specifying the importance of learning the pointwise value of \( f_n \) at each input \( x_{pa(n)} \in \mathcal{X}_{pa(n)}^{\alpha} \). That is, \( \Pi_n \) puts large amounts of mass in areas that we should learn \( \hat{f}_n \) precisely, small amounts of mass in areas that we should learn \( f_n \) only approximately, and zero mass in areas for which we do not care about learning \( f_n \) at all. For the (estimated) function \( \hat{f}_n \), we use the risk functional \( L_n \) below. The weighted sum of these according to the importance of each function gives rise to the total risk \( L \), where \( f = (f_n)_{n=1}^N \) and \( \hat{f} = (\hat{f}_n)_{n=1}^N \) are vectors of the functions \( f_n \) and \( \hat{f}_n \), respectively.

\[
L_n(\hat{f}_n||f_n) = \int_{\mathcal{X}_{pa(n)}} (f_n(x) - \hat{f}_n(x))^2 d\Pi_n(x), \quad L(f||f) = \sum_{n=1}^N \alpha_n L_n(\hat{f}_n||f_n), \quad \alpha_n \geq 0.
\]

We will assume for simplicity that \( \alpha_n = 1 \) for each \( n \). \( L_n \) is also known as the Mean Integrated Squared Error [Tsybakov, 2009] and in the case that \( \Pi_n = \mathbb{P}^{\text{do}(\varnothing)}_{X_{pa(n)}} \), this coincides with a typical objective that would be minimised in a classical non-parametric statistical learning setting [Györfi et al, 2006]. It is worth considering other possible risk functionals that could be used, since the presence of the measures \( \Pi_n \) is arguably somewhat arbitrary in the \( L \) that we consider. When learning the parameters of a statistical model, a commonly used objective with many separate justifications is to minimise the KL divergence \( \text{KL}[^{\mathbb{P}_X} ||^{\mathbb{P}_X}_X] \) between the true data distribution \( \mathbb{P}_X \) and that implied by the learned model, \( \mathbb{P}_X^{\text{MMD}} \). SCMs do not imply a single distribution over the variables \( X \), but rather a family of distributions, one for each intervention: \( \{\mathbb{P}_X^{\text{do}(i)} : i \in \mathcal{I} \} \). One may therefore wish to consider a separate loss for each interventional distribution and, for example, uniformly bound these losses over a subset of interventions \( \mathcal{I}' \subseteq \mathcal{I} \) of interest.

\[
L_{\text{KL}}^i(\hat{f}||f) = \text{KL}[^{\mathbb{P}_X^{\text{do}(i)}} ||^{\mathbb{P}_X^{\text{do}(i)}}_X], \quad L_{\text{KL}}^i(\hat{f}||f) = \sup_{i \in \mathcal{I}} L_{\text{KL}}^{\text{do}(i)}(\hat{f}||f).
\]

Alternatively, one could replace the KL divergence with a different divergence measure or metric on distributions. For instance, one could use the Maximum Mean Discrepancy (MMD) corresponding to a characteristic kernel \( l \) [Sriperumbudur et al, 2008]

\[
L_{\text{MMD}}^i(\hat{f}||f) = \text{MMD}[^{\mathbb{P}_X^{\text{do}(i)}} ||^{\mathbb{P}_X^{\text{do}(i)}}_X], \quad L_{\text{MMD}}^i(\hat{f}||f) = \sup_{i \in \mathcal{I}'} L_{\text{MMD}}^{\text{do}(i)}(\hat{f}||f).
\]

Though we do not analyse or derive active learning schemes for these risk functionals, they will be used in Section 6 to evaluate our algorithm. We leave their consideration for future work.

4 A probabilistic approach to learning \( f \)

By taking a Bayesian approach to learning the vector of unknown functions \( f \), Problem 1 can be reduced to a series of independent regression problems between input and output domains \( \mathcal{X}_{pa(n)} = \prod_{m \in pa(n)} \mathcal{X}_m \) for each \( n \). A common choice of prior when learning functions is a Gaussian Process (GP) [Rasmussen and Williams, 2005]. For each function \( f_n \), we will assume a zero mean GP prior with kernel \( k_n \) over the domain \( \mathcal{X}_{pa(n)} \)

\[
f_n \sim \mathcal{GP}(0, k_n).
\]

Recall that we are given a dataset \( D \) consisting of elements \( (i, x) \) where \( x \sim \mathbb{P}^{\text{do}(i)}_X \). Let \( D_n \) be the collection of marginal observations of \( (X_{pa(n)}, X_n) \) drawn from any distribution in which \( X_n \) is not intervened upon.\(^6\) Since by assumption \( X_n \sim f_n(X_{pa(n)}) + E_n \) where the distribution of \( E_n \sim N(0, \sigma_n^2) \) is known, each element \( (x_{pa(n)}, x_n) \) of \( D_n \) represents an evaluation of \( f_n \) at the input point \( x_{pa(n)} \) corrupted by Gaussian noise of known variance. Performing GP regression using

\(^5\)No specific assumptions will be made on the choice of \( k_n \), which can be freely chosen to incorporate prior knowledge about the functions (for instance, typical length scale of variation and magnitude). If \( X_n \) is parentless, \( f_n \) is an unknown constant for which we assume a 1-dimensional Gaussian prior with zero mean and variance \( k_n \).

\(^6\)That is, for any distribution \( \mathbb{P}^{\text{do}(i)}_X \) for which \( X_n \not\in \text{var}(i) \).
\(\mathcal{D}_n\) as the data gives the posterior distribution over \(f_n\). By properties of Gaussians, this is also a GP with distribution
\[
f_{n|\mathcal{D}_n} \sim \mathcal{GP}(\mu_{f_n|\mathcal{D}_n}, k_{f_n|\mathcal{D}_n}),
\]
where \(\mu_{f_n|\mathcal{D}_n}\) and \(k_{f_n|\mathcal{D}_n}(x,y)\) can be explicitly written in terms of \(k_n\) and the data \(\mathcal{D}_n\) (see Appendix for details). The above procedure can be applied for each \(f_n\) independently, giving a posterior distribution over the vector of functions \(f\).

**Which \(f\) should be chosen, given the posterior over \(f\)?** Problem 1 demands that a single choice \(\hat{f}\) be made when making the estimation \(\hat{M}\) of \(M\). For a fixed \(\hat{f}\), the total risk \(L(\hat{f}||f)\) is a random variable (the randomness coming from the uncertain belief over \(f\)). The expectation of this random variable can be calculated and expressed in terms of the posterior covariance and mean functions of each \(f_n\).

**Lemma 1.**
\[
\mathbb{E}_{f|\mathcal{D}}[L(\hat{f}||f)] = \sum_{n=1}^{N} \alpha_n \int_{X^{pa(n)}} \left( \hat{f}_n(x) - \mu_{f_n|\mathcal{D}_n}(x) \right)^2 + k_n|\mathcal{D}_n(x,x)d\Pi_n(x)
\]

See Appendix for proof. This immediately implies the following result.

**Lemma 2.** Let \(\mu_{f|\mathcal{D}}\) be the tuple of functions \((\mu_{f_n|\mathcal{D}_n})_{n=1,...,N}\). Then
\[
\mu_{f|\mathcal{D}} = \arg \min_{f} \mathbb{E}_{f|\mathcal{D}}[L(\hat{f}||f)]
\]

That is, choosing \(\hat{f}_n\) to be the posterior mean of \(f_n\) for each \(n\) minimises the expected total risk. The uncertain distribution over \(f\) directly yields an estimate of the total risk once the optimal \(\hat{f} = \mu_{f|\mathcal{D}}\) is chosen which, once the prior has been fixed, is purely a function of the data \(\mathcal{D}\). Denote by \(\mathcal{R}(\mathcal{D}) = \mathbb{E}_{f|\mathcal{D}}[L(\mu_{f|\mathcal{D}}||f)]\) this expected total risk. Choosing the intervention \(i\) for which \(\mathcal{R}(\mathcal{D} \cup \{(i,x)\})\) is expected to be smallest after making the new observation \(x\) from \(\mathbb{P}^{\text{do}(i)}_X\) forms the basis of the proposed active learning algorithm.

## 5 Active learning

In this section a myopic active learning algorithm is derived based on the GP belief of the functions \(f_n\) and the expected total risk \(\mathcal{R}(\mathcal{D})\) described above. At each step in time, we select an intervention \(i\) at cost \(c(i)\) and observe a single draw from the distribution \(\mathbb{P}^{\text{do}(i)}_X\). The goal is to select the intervention \(i \in \mathcal{I}\) which will reduce the expected total risk as much as possible, taking into account the cost \(c(i)\). This problem is non-trivial for two main reasons.

1. The true distributions \(\mathbb{P}^{\text{do}(i)}_X\) are unknown and therefore it is not possible to calculate the true expected reduction in expected total risk given a proposed intervention.
2. There is a potentially large set of interventions that must be searched over.

Consider the first issue above. How will the expected total risk change if the intervention \(i\) is chosen and a single new observation is drawn from \(\mathbb{P}^{\text{do}(i)}_X\)? If the new observation is \(x \in \mathcal{X}\), the new expected total risk will be \(\mathcal{R}(\mathcal{D} \cup \{(i,x)\})\). Define the value of the intervention \(i\) to be the expected reduction of \(\mathcal{R}\) after performing the intervention \(i\), divided by the cost of \(i\):
\[
V(i|\mathcal{D}) = \frac{\mathcal{R}(\mathcal{D}) - \mathbb{E}_{x \sim \mathbb{P}^{\text{do}(i)}_X}[\mathcal{R}(\mathcal{D} \cup \{(i,x)\})]}{c(i)}
\]

The goal is to find the intervention with the largest value, but since \(\mathbb{P}^{\text{do}(i)}_X\) is unknown it is not possible to calculate the right-hand term in the numerator of (1). It is possible, however, to estimate this by replacing \(\mathbb{P}^{\text{do}(i)}_X\) in the expectation with the belief of the distribution based on the uncertain estimates of each \(f_n\). In this next two parts of this section, two different methods are proposed that estimate the expected total risk after performing each intervention. The first uses sampling, and requires a brute-force search over the set of interventions. This may be appropriate when the set of possible interventions is small enough that this is feasible. The second uses a form of dynamic programming, enabling a search over a larger set of interventions more efficiently. The derived algorithm, however, makes specific assumptions on the graph of \(M\) and the set of interventions.
5.1 Sampling

Write $\mathbb{P}^{\text{do}(i)}_X$ for the belief of $\mathbb{P}^{\text{do}(i)}_X$, taking into account the full uncertainty over $f$.

Since the belief over each $f_n$ at each input $x_{pa(n)} \in X_{pa(n)}$ is Gaussian and the noise variables are additive and Gaussian, it is possible to efficiently sample from $\mathbb{P}^{\text{do}(i)}_X$. It is illustrated here how to draw from the estimated observational distribution $\mathbb{P}^{\text{do}(0)}_X$ for notational convenience, but the procedure for any other $\mathbb{P}^{\text{do}(i)}_X$ is essentially the same.

For any parentless variable, the structural equation is $X_n = f_n + E_n$ where $f_n \sim \mathcal{N}(\mu_n|D_n, k_n|D_n)$ and $E_n \sim \mathcal{N}(0, \sigma_n^2)$, and therefore $X_n \sim \mathcal{N}(\mu_n|D_n, k_n|D_n + \sigma_n^2)$.

For any variable with parents, the structural equation is $X_n = f_n(X_{pa(n)}) + E_n$ where $f_n \sim \mathcal{GP}(\mu_n|D_n, k_n|D_n)$ and $E_n \sim \mathcal{N}(0, \sigma_n^2)$. Therefore the conditional distribution of a variable given its parents is $X_n|X_{pa(n)} \sim \mathcal{N}(\mu_n|D_n, k_n|D_n)(X_{pa(n)}), k_n|D_n(X_{pa(n)}, X_{pa(n)}), \sigma_n^2)$. Observe that the joint distribution $\mathbb{P}^{\text{do}(0)}_X$ factorises as

$$\mathbb{P}^{\text{do}(0)}_X = \prod_{n:pa(n) = \emptyset} \mathbb{P}^{\text{do}(0)}_{X_n} \prod_{n:pa(n) \neq \emptyset} \mathbb{P}^{\text{do}(0)}_{X_n|X_{pa(n)}}.$$  

Since drawing from each of the above factors amounts to drawing from a Gaussian distribution, it is possible to efficiently sample from the entire joint distribution. By replacing $\mathbb{P}^{\text{do}(i)}_X$ with $\mathbb{P}^{\text{do}(0)}_X$ in Equation (4) above, we arrive at an estimate of the expected total risk which can be estimated using samples drawn from $\mathbb{P}^{\text{do}(0)}_X$:

$$\mathbb{E}_{x \sim \mathbb{P}^{\text{do}(0)}_X} \mathcal{R}(D \cup \{(i, x')\}) \approx \frac{1}{T} \sum_{t=1}^{T} \mathcal{R}(D \cup \{(i, x^t)\})$$

where each $x^t \sim \mathbb{P}^{\text{do}(0)}_X$ (see Algorithm 1). Finding the optimal intervention hence reduces to computing the above quantity for each $i \in I$ from which it is possible to estimate each $V(i|D)$.

5.2 Dynamic programming

If the set of interventions under consideration exhibits structure that coincides with that of the causal graph appropriately, it is possible to estimate the value of many interventions simultaneously. A specific example is provided here of how this can be done in the case that the causal graph is a chain $X_1 \rightarrow \ldots \rightarrow X_N$, and any intervention intervenes on one variable and everything upstream of it\(^7\). A similar example for chains in which all interventions intervene on exactly one variable is provided in the Appendix.

The crux of this approach is the fact that the posterior covariance function of a Gaussian Process is only a function of the inputs of the conditioning data, not of the outputs. That is, writing $\mathbb{P}^{\text{do}(i)}_X$, which is the estimated distribution once a particular choice for $f$ is made.

\(^7\)That is, any intervention is of the form do($X_n = x_n, n \leq m$) for some $m$. This is equivalent to the case that all interventions act on a single variable, but only variables downstream of this are observable.

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**Algorithm 1** Sampling to estimate expected risk after intervention

1. **Input:** Previously observed data $D$, GP kernels $k_n$, for prior on $f_n$, number of samples $T$, proposed intervention $i$.
2. **for** $i = 1, \ldots, T$ **do**
   3. Draw $x^t$ from predictive distribution $\mathbb{P}^{\text{do}(0)}_X$
   4. $s_t = \mathcal{R}(D \cup \{(i, x^t)\})$: expected loss given new $x^t$
   5. **end for**
5. **return** $\frac{1}{T} \sum_{t=1}^{T} s_t$: estimated expected loss after intervention $i$.

**Algorithm 2** Dynamic programming to estimate expected risk after interventions (chain, interventions on all $X_n \leq m$, some $m$)

1. **Input:** Previously observed data $D$, GP kernels $k_n$, discretisations $\tilde{X}_n$ of each $X_n$.
2. Pre-compute $U_n$ vectors and discrete approximations to conditional probability distributions:
3. **for** $n = 1, \ldots, N$ **do**
   4. If $n = 1$: $P^n_{x_1} \propto P(x_1)$ for $x_1 \in \tilde{X}_1$, else:
   5. $P_{x_{n-1}, x_n} \propto P(x_n|x_{n-1})$ for $x_{n-1} \in \tilde{X}_{n-1}, x_n \in \tilde{X}_n$
   6. $U^n_m = \mathcal{R}_n(D_n)$
   7. $U_n(x_{n-1})$ for $x_{n-1} \in \tilde{X}_{n-1}$
   8. **end for**
9. Calculate new expected risk for all interventions:
10. **for** $n = 1, \ldots, N$ **do**
   11. $V = 0$
   12. For $m = N - 1, \ldots, n + 1$
   13. $V = P^m(V + U_{m+1})$
   14. **end for**
15. Expected risk after intervention on variables $X_m, m \leq n$:
16. $E_{R_n} = V + U_1 + \ldots + U_n$
17. **end for**
18. **return** Vectors $E_{R_n}$ giving estimated expected risks after all interventions do($X_n = x_n, X_{n-1} = \ldots$)
Figure 2: The causal graphs of the SCMs (a) $\mathcal{M}_1$ and (b) $\mathcal{M}_2$ used in the experiments (Section 6).

$$\mathcal{R}_n(\mathcal{D}_n) = \mathbb{E}_{f_n|\mathcal{D}_n}[L_n(\mu_{f_n|\mathcal{D}_n}, f_n)] = \int X_{\text{pa}(n)} k_{n|\mathcal{D}_n}(x, x') d\Pi_n(x)$$ for the contribution to the expected total risk due to estimating function $f_n$, and writing $\mathcal{D}_n = \{(x^{s}_{\text{pa}(n)}, x^{s}_n) : s = 1 \ldots |\mathcal{D}_n|\}$, it follows that $\mathcal{R}_n$ is only actually a function of the $x^{s}_{\text{pa}(n)}$ (or, for parentless variables, just the size of the dataset $|\mathcal{D}_n|$). Consider the intervention $i = \text{do}(X_m = x_m, X_{m-1} = \ldots)$ that sets $X_m = x_m$ and all variables upstream of $X_m$ to arbitrary values. When a new observation $x \sim \mathbb{P}_X$ is made, this only provides new information about the functions $f_n$ for $n > m$, since $i$ intervenes on $X_n$ for $n \leq m$. Let $U^\text{curr}_n = \mathcal{R}_n(\mathcal{D}_n)$ for $n \leq m$ be the current contributions to the expected total risk. Define, for $n > m$, the following shorthand for the contribution to the new expected total risk function made by $f_n$ if a new observation of $f_n$ at the input point $x_{n-1}$ is made:

$$U_n(x_{n-1}) = \mathcal{R}_n(\mathcal{D}_n \cup \{(x_{n-1}, x_n)\}) \quad \text{for any value } x_n, n > m.$$ 

It follows that the estimated expected total risk after performing the intervention $i$ decomposes thus:

$$\mathbb{E}_{x \sim \tilde{\mathbb{P}}_{X|d_i}}[\mathcal{R}(\mathcal{D} \cup \{(i, x)\})] = \sum_{n=1}^{m} U^\text{curr}_n + \sum_{n=m+1}^{N} U_n(x_{n-1}).$$

By exploiting a factorisation of $\tilde{\mathbb{P}}_{X|d_i}$ similar to (1) and discretely approximating the continuous domains $\lambda_n$, it is possible to reduce evaluating the right hand side of (1) to a series of matrix multiplications and additions (see Appendix for details). This series of operations can be vectorised to allow calculation of (1) for many $x_m$ simultaneously. Moreover, many of the initial calculations can be cached and used to speed up calculation over different values of $m$. See Algorithm 2.

6 Experiments

Figure 3 shows the results of running the proposed methods on two synthetic example SCMs $\mathcal{M}_1$ and $\mathcal{M}_2$, for which the graphs are given by Figures 2a and 2b, respectively. In each case, structural equations consisting of sines and cosines of the parent variables were fixed, giving two sets of structural equations $S_1$ and $S_2$. All noise variables in both SCMs were fixed to have variance 0.1. The interventions $I_1$ for the chain SCM $\mathcal{M}_1$ were chosen to be all interventions of the form $\text{do}(X_m = x_m, X_{m-1} = \ldots)$ with $x_m \in [-6, 6]$, such that $\mathcal{M}_1$ satisfies the conditions set out in the description of the dynamic programming algorithm. The interventions $I_2$ for the non-chain SCM $\mathcal{M}_2$ were defined to be all interventions on single variables $\text{do}(X_n = x_n)$ with $x_n \in [-6, 6]$. The total risk function for each experiment was chosen by setting $\Pi_n$ to be the uniform distribution on the domain $[-6, 6]^{\text{pa}(n)}$ and $a_n = 1$ for each $n$. All GP kernels used were Radial Basis Function kernels with bandwidth parameter 1. All costs $c(i)$ were assumed to be equal.

In each experiment, learning was initiated with no data. For learning $\mathcal{M}_1$, the proposed algorithms were compared against the strategies of only drawing from the observational distribution of $\mathcal{M}_1$ and of selecting an intervention uniformly at random. Since the dynamic programming algorithm could not be used for learning $\mathcal{M}_2$, we could only test the sampling algorithm. Uniform discretisations $I'_1$ and $I'_2$ of the intervention sets were made of total size 250 each. These were used as the sets of interventions to search over using the sampling algorithm.

The following quantities were used to evaluate the performance of the algorithms at each point in time: the true total risk incurred by choosing $\hat{f}$ to be the vector of GP posterior means; the maximum and median of the set of KL divergences $\text{KL}[\mathbb{P}_{\tilde{X}|d_i}||\mathbb{P}_{X|d_i}]$ calculated for each intervention $i \in I'_1$ in the discretised intervention sets; the maximum and median of the set of MMDs (corresponding to a Radial Basis Function kernel $l$ with bandwidth $1$) $\text{MMD}[\mathbb{P}_{\tilde{X}|d_i}||\mathbb{P}_{X|d_i}]$ calculated for each intervention $i \in I'_1$ in the discretised intervention sets. See Figure 3 for results.
Figure 3: Actively choosing informative interventions speeds up learning. The proposed methods (Algorithm 1, Algorithm 2) outperform only observing and randomly intervening by each metric of evaluation. Top and bottom row show results of experiments on learning $M_1$ and $M_2$ respectively. Experimental details described in Section 6. Each experiment was performed many times; faded lines represent results from single trials, bold lines represent averages of these single trials.

7 Discussion and future directions

There are many ways in which the work presented here could be incrementally furthered: it may be possible to find efficient ways to search over the set of interventions subject to less restrictive assumptions than those made for Algorithm 2; different distributions over the noise variables could be considered, in which case an approximation may need to be made when regressing to find the posterior distribution over each $f_n$; one could try to relax the additive noise assumption altogether. Other natural extensions include estimating the value of an intervention based on reasoning multiple steps into the future, or considering the implications of a constrained budget.

Although the proposed algorithms seem to perform well on the synthetic toy examples considered, it remains to be seen whether this method, suitably extended, would similarly perform well on a convincing real-world problem. It is hard to find suitable real-world problems where convincing ground truth (for the functional relationships) exists, which is why we believe that it is sensible to assay such methods on synthetic data where performance can be accurately measured.

A perhaps more fundamental issue that was raised and not tackled is the fact that it is not clear how best one should even define what it means to learn an SCM, or the parameters thereof. We proposed $\max_{i \in I'} L_{\text{KL}}(\hat{f} || f)$ and $\max_{i \in I'} L_{\text{MMD}}(\hat{f} || f)$ for a suitable set of interventions $I'$ as potentially more principled objectives to minimise than the total risk functional considered here. Interestingly, the derived algorithms do reduce these quantities in the experiments considered, though this was in no way an explicit objective. Future directions of research include trying to understand whether these, or other objectives, give rise to tractable methods for parameter estimation in causal models and for selecting interventions in active settings, and under what assumptions mathematical guarantees can be made.
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A Appendix

A.1 Posterior distribution of \( f_n \) given \( \mathcal{D}_n \)

The prior over \( f_n \) is a Gaussian Process with zero mean and covariance function \( k_n \)

\[
    f_n \sim \mathcal{GP}(0, k_n).
\]

Let \( \mathcal{D}_n = \{(x_{pa(n)}^s, x_n^s) : s = 1, \ldots, |\mathcal{D}_n|\} \) and let \( K \) be the matrix with entries

\[
    K_{st} = k_i(x_{pa(n)}^s, x_{pa(n)}^t).
\]

Suppose that the Gaussian noise variable \( \mathcal{E}_n \) has variance \( \sigma_n^2 \). Then the posterior mean function \( \mu_{f_n|\mathcal{D}_n} \) and posterior covariance function \( k_{f_n|\mathcal{D}_n} \) can be written in closed form as

\[
    \mu_{f_n|\mathcal{D}_n}(x) = \sum_{s,t=1}^{|\mathcal{D}_n|} K_{st} (x, x_{pa(n)}^s)(K + \sigma_n^2 I)^{-1} x_n^s,
\]

\[
    k_{f_n|\mathcal{D}_n}(x, y) = k_n(x, y) - \sum_{s,t=1}^{|\mathcal{D}_n|} K_{st} (x, x_{pa(n)}^s)(K + \sigma_n^2 I)^{-1} k_n(y, x_{pa(n)}^t).
\]

A.2 Proof of Lemma 1

Proof: The expected total risk can be written in full form as

\[
    \mathbb{E}_{f|\mathcal{D}} \left[ L(\hat{f}||f) \right] = \mathbb{E}_{f|\mathcal{D}} \left[ \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \left( \hat{f}_n(x) - f_n(x) \right)^2 d\Pi_n(x) \right]
\]

\[
    = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \mathbb{E}_{f_n|\mathcal{D}_n} \left[ \left( \hat{f}_n(x) - f_n(x) \right)^2 \right] d\Pi_n(x)
\]

\[
    = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \mathbb{E}_{f_n|\mathcal{D}_n} \left[ \left( \hat{f}_n(x) - f_n(x) \right)^2 \right] d\Pi_n(x).
\]

Under the posterior distribution given \( \mathcal{D}_n \), we can decompose \( f_n \) as the sum of its posterior mean and a zero mean Gaussian Process:

\[
    f_n|\mathcal{D}_n = \mu_{f_n|\mathcal{D}_n} + g_n, \quad g_n \sim \mathcal{GP}(0, k_{f_n|\mathcal{D}_n}).
\]

We can therefore rewrite the expected total risk as

\[
    \mathbb{E}_{f|\mathcal{D}} \left[ L(\hat{f}||f) \right] = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \mathbb{E}_{g_n|\mathcal{D}_n} \left[ \left( \hat{f}_n(x) - \mu_{f_n|\mathcal{D}_n}(x) - g_n(x) \right)^2 \right] d\Pi_n(x)
\]

\[
    = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \mathbb{E}_{g_n|\mathcal{D}_n} \left[ \left( \hat{f}_n(x) - \mu_{f_n|\mathcal{D}_n}(x) + g_n(x) \right)^2 \right] d\Pi_n(x)
\]

\[
    = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \left( \hat{f}_n(x) - \mu_{f_n|\mathcal{D}_n}(x) \right)^2 d\Pi_n(x)
\]

\[
    = \sum_{n=1}^{N} \alpha_n \int_{X_{pa(n)}} \left( \hat{f}_n(x) - \mu_{f_n|\mathcal{D}_n}(x) \right)^2 + k_{f_n|\mathcal{D}_n}(x, x) d\Pi_n(x).
\]

A.3 Derivation of Algorithm 2

Under the intervention \( i = \text{do}(X_m = x_m^*, X_{m-1} = \ldots) \), the distribution \( \overline{\mathbb{P}}^{\text{do}(i)}_{X} \) factorises as:

\[
    \overline{\mathbb{P}}^{\text{do}(i)}_{X} = \prod_{n \leq m} \delta_{X_n = x_n^*} \prod_{n \geq m+1} \overline{\mathbb{P}}_{X_n|X_{n-1}}.
\]
where
\[ X_n | X_{n-1} \sim N \left( f_n(X_{n-1}), \sigma_n^2 \right) \]
\[ \sim N \left( \mu_{f_n|X_n}(X_{n-1}), k_{f_n|X_n}(X_{n-1}, X_n) + \sigma_n^2 \right). \]

The quantity we are trying to calculate can hence be written
\[ E_{x \sim \mathcal{P}^{do(i)}}[R(\mathcal{D} \cup \{(i,x)\})] = \sum_{n=1}^{m} U_n^{\text{sur}} + E_{x \sim \mathcal{P}^{do(i)}} \left[ \sum_{n=m+1}^{N} U_n(x_{n-1}) \right] \]
\[ = \sum_{n=1}^{m} U_n^{\text{sur}} + \int_{X} \sum_{n=m+1}^{N} U_n(x_{n-1}) \, d\overline{\mathcal{P}}^{do(i)}(x) \]
\[ = \sum_{n=1}^{m} U_n^{\text{sur}} + \sum_{n=m}^{N-1} \int_{X} U_{n+1}(x_n) \, d\overline{\mathcal{P}}^{do(i)}(x_n). \]

Now, since \( \overline{\mathcal{P}}^{do(i)}_{X_m} = \delta_{X_m=x^*_m} \), observe that we can write
\[ \int_{X_m} U_{m+1}(x_m) \, d\overline{\mathcal{P}}^{do(i)}_{X_m}(x_m) = U_{m+1}(x^*_m). \]

For any \( n > m \), we have
\[ \int_{X_n} U_{n+1}(x_n) \, d\overline{\mathcal{P}}^{do(i)}(x_n) \]
\[ = \int_{X_m} \ldots \int_{X_n} U_{n+1}(x_n) \, d\overline{\mathcal{P}}^{do(i)}_{X_{n}|X_{n-1}}(x_n|x_{n-1}) \ldots d\overline{\mathcal{P}}^{do(i)}_{X_{m+1}|X_m}(x_{m+1}|x_m) d\overline{\mathcal{P}}^{do(i)}_{X_m}(x_m). \]

Hence if we define the following quantities recursively
\[ V_{N-1}(x_{N-2}) = \int_{X_{N-1}} U_N(x_{N-1}) \, d\overline{\mathcal{P}}^{do(i)}_{X_{N}|X_{N-2}}(x_{N}|x_{N-2}), \]
\[ V_n(x_{n-1}) = \int_{X_n} V_{n+1}(x_n) + U_{n+1}(x_n) \, d\overline{\mathcal{P}}^{do(i)}_{X_{n+1}|X_n}(x_{n+1}|x_n) \quad n = N-2, \ldots, m+1, \]
it follows that
\[ V_{m+1}(x^*_m) = \sum_{n=m}^{N-1} \int_{X_n} U_{n+1}(x_n) \, d\overline{\mathcal{P}}^{do(i)}_{X_m}(x_n). \]

We can approximate calculation of \( V_{m+1}(x^*_m) \) for many \( x^*_m \) simultaneously by discretising each \( X_n \) into a set of points \( x_n^1, x_n^2, \ldots, x_n^{D_n} \). Define \( P^n \) to be the matrix with normalised rows such that \( P^n_{ij} \propto \overline{\mathcal{P}}^{do(i)}_{X_n|x_{n-1}}(x_n^i|x_n^{i-1}) \), where \( \overline{\mathcal{P}}^{do(i)} \) is the density of \( \mathcal{P}^{do(i)} \) with respect to the Lebesgue measure on \( X \). Define \( u^n \) to be the vector with entries \( u^n_i = U_n(x_n^{i-1}) \). Then, if we recursively define
\[ v^{N-1} = P^{N-1} u_N, \]
\[ v^n = P^n (v^{n+1} + u_{n+1}) \quad n = N-2, \ldots, m+1, \]
it follows that \( v^{m+1}_i \approx V_{m+1}(x^*_i) \).

### A.4 Another Dynamic Programming Algorithm: chain, single variable interventions.

Similar reasoning to the above can be used to derive a dynamic programming scheme to calculate the estimated total risk after a proposed intervention \( i = do(X_n = x^*_n) \) (i.e. intervening on a single variable) for many \( x^*_m \) simultaneously. This is summarised by Algorithm 3.

Under this intervention, the joint distribution factorises as
\[ \overline{\mathcal{P}}^{do(i)}_{X_m} = \overline{\mathcal{P}}_{X_1} \prod_{n=2}^{m-1} \overline{\mathcal{P}}_{X_n|X_{n-1}} \delta_{X_m=x^*_m} \prod_{n=m+1}^{N} \overline{\mathcal{P}}_{X_n|X_{n-1}}. \]
When we intervene on a single variable $X_m$, we learn something new about all functions except $f_m$. We can write the expected new total risk, the quantity we want to evaluate, as

$$\mathbb{E}_{x \sim \tilde{p}^{do(i)}(\cdot, X)}[\mathbb{R}(D \cup \{(i, x)\})] = U_1 + \mathbb{E}_{x \sim \tilde{p}^{do(i)}(\cdot, X)} \left[ \sum_{n=2}^{m-1} U_n(x_{n-1}) \right] + U_{m-1} + \mathbb{E}_{x \sim \tilde{p}^{do(i)}(\cdot, X)} \left[ \sum_{n=m+1}^{N} U_n(x_{n-1}) \right].$$

Each of the expectations above can be calculated recursively in a similar fashion to the strategy employed above. If we define

$$V_{N-1}(x_{N-2}) = \int_{X_{N-1}} U_N(x_{N-1}) \tilde{p}^{do(i)}_{X_{N-1}|X_{N-2}}(x_{N-1}|x_{N-2}),$$

$$V_n(x_{n-1}) = \int_{X_n} V_{n+1}(x_n) + U_{n+1}(x_n) \tilde{p}^{do(i)}_{X_{n}|X_{n-1}}(x_n|x_{n-1}), \quad n = N - 2, \ldots, m + 1,$$

it follows that

$$V_{m+1}(x_m) = \mathbb{E}_{x \sim \tilde{p}^{do(i)}(\cdot, X)} \left[ \sum_{n=m+1}^{N} U_n(x_{n-1}) \right].$$

Similarly, defining

$$V_{m-2}(x_{m-3}) = \int_{X_{m-2}} U_{m-1}(x_{m-2}) \tilde{p}^{do(i)}_{X_{m-2}|X_{m-3}}(x_{m-2}|x_{m-3}),$$

$$V_n(x_{n-1}) = \int_{X_n} V_{n+1}(x_n) + U_{n+1}(x_n) \tilde{p}^{do(i)}_{X_{n}|X_{n-1}}(x_n|x_{n-1}), \quad n = m - 3, \ldots, 2,$$

$$V_1 = \int_{X_1} V_2(x_1) + U_2(x_1) \tilde{p}^{do(i)}_{X_2}(x_1),$$

it follows that

$$V_1 = \mathbb{E}_{x \sim \tilde{p}^{do(i)}(\cdot, X)} \left[ \sum_{n=2}^{m-1} U_n(x_{n-1}) \right].$$

As before, we can approximate calculation of $V_{m+1}(x_m)$ for many $x_m$ simultaneously by discretising each $X_n$ into a set of points $x_1^i, x_2^i, \ldots, x_{D_n}^i$. Define $P^n$ to be the matrix with normalised rows such that $P^n_{ij} \propto \tilde{p}^{do(i)}_{X_n|X_{n-1}}(x_n^i|x_{n-1}^j)$ for $n > 1$, where $\tilde{p}^{do(i)}$ is the density of $\tilde{p}^{do(i)}$ with respect to the Lebesgue measure on $X$. Define $P^1$ to be the normalised vector with $P^1_i \propto \tilde{p}_{X_1}(x_1^i)$. Define $u^n$ to be the vector with entries $u^n_i = U_n(x_{n-1}^i)$. Then, if we recursively define

$$v^{N-1} = P^{N-1} u_N,$$

$$v^n = P^n (v^{n+1} + u_{n+1}) \quad n = N - 2, \ldots, m + 1,$$

it follows that $v^{m+1} \approx V_{m+1}(x_m)$. We must also estimate $V_1$. If we define

$$v^{m-2} = P^{m-2} u_{m-2},$$

$$v^n = P^n (v^{n+1} + u_{n+1}) \quad n = m - 3, \ldots, 2,$$

$$v^1 = P^1 v + u_2$$

then it follows that $v^1 \approx V_1$. 
Algorithm 3 Dynamic programming to estimate expected risk after interventions (chain, interventions on single variable \( X_m \))

1: **Input:** Previously observed data \( D \), GP kernels \( k_n \), discretisations \( \hat{X}_n \) of each \( X_n \).
2: Pre-compute \( U_n \) vectors and discrete approximations to conditional probability distributions:
3: \( \text{for } n = 1, \ldots, N \) do
4: \( P_{n,n-1}^m \propto P(x_n | x_{n-1}) \) for \( x_{n-1} \in \hat{X}_{n-1}, x_n \in \hat{X}_n \)
5: \( U_n^m = R_n(D_n) \)
6: \( U_n(x_{n-1}) \) for \( x_{n-1} \in \hat{X}_{n-1} \)
7: end for
8: Calculate expected loss for all interventions on each variable in turn:
9: \( \text{for } m = 1, \ldots, N \) do
10: \( V = 0 \)
11: \( \text{for } n = N - 1, \ldots, m + 1 \) do
12: \( V = P^n(V + U_n) \)
13: end for
14: \( V' = 0 \)
15: \( \text{for } n = m - 1, \ldots, 2 \) do
16: \( V' = P^n(V' + U_n) \)
17: end for
18: Expected risk after intervention on variable \( m \): \( ER_m = V + V' + U_1 + U_{\text{curr}}^m \)
19: end for
20: **return** Vectors \( ER_n \) giving estimated expected risks after interventions for all interventions on \( X_n \).