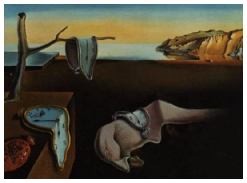


Journal of Statistical Software

MMMMMM YYYY, Volume VV, Issue II. *doi: 10.18637/jss.v000.i00*

Making, Updating, and Querying Causal Models using `CausalQueries`

Till Tietz
WZB

Lily Medina
University of California, Berkeley

Georgiy Syunyaev
Vanderbilt University

Macartan Humphreys
WZB

Abstract

The R package `CausalQueries` can be used to make, update, and query causal models defined on binary nodes. Users provide a causal statement of the form `X -> M <- Y; M <-> Y` which is interpreted as a structural causal model over a collection of binary nodes. `CausalQueries` can then (1) identify the set of principal strata—causal types—required to characterize all possible causal relations between nodes consistent with the causal statement (2) determine a set of parameters needed to characterize distributions over these types (3) update beliefs over distributions of causal types, using a `stan` model plus data and (4) pose a wide range of causal queries of the model, using either the prior distribution, the posterior distribution, or a user-specified candidate vector of parameters.

Keywords: causal model, Bayesian updating, DAG, Stan.

1. Introduction: Causal models

`CausalQueries` is an R package that lets users make, update, and query causal models. Users provide a statement that reports a set of binary variables and the relations of "causal ancestry" between them, that is, a statement indicating which variables are direct causes of other variables, given the other variables in the model. Once such a statement is provided to `make_model()`, `CausalQueries` generates a parameter vector that fully describes a probability distribution over all possible types of causal relations between variables ("causal types"). Given a prior over parameters and data over some or all nodes, `update_model()` deploys a Stan (Carpenter, Gelman, Hoffman, Lee, Goodrich, Betancourt, Brubaker, Guo, Li, and

Riddell 2017) model in order to generate a posterior distribution over causal models. The function `query_model()` can then be used to ask a wide range of causal queries of the model, using either the prior distribution, the posterior distribution, or a user-specified candidate vector of parameters.

In the next section we provide a motivating example. We then describe how the package relates to existing available software. Section 4 gives an overview of the statistical model behind the package. Section 5, Section 6, and Section 7 then describe the main functionality for the major operations using the package. We provide further computation details in the final section.

2. Motivating example

Before providing details on package functionality we illustrate these three core functions by showing how to use `CausalQueries` to replicate the analysis in (Chickering and Pearl 1996; see also Humphreys and Jacobs 2023). Chickering and Pearl (1996) seek to draw inference on causal effects in the presence of imperfect compliance. We have access to an instrument Z (a randomly assigned prescription for cholesterol medication), which is a cause of X (treatment uptake) but otherwise unrelated to Y (cholesterol). We imagine we are interested in three specific queries. The first is the average causal effect of X on Y. The second is the average effect for units for which $X = 0$ and $Y = 0$. The last is the average effect for "compliers": units for which X responds positively to Z. Thus two of these queries are conditional queries, with one conditional on a counterfactual quantity.

The data on Z, X, and Y is given in Chickering and Pearl (1996) but also included in `CausalQUeries`. The data is complete for all units and looks, in "compact form," as follows:

```
R> data("lipids_data")
R>
R> lipids_data
```

```
#>    event strategy count
#> 1 Z0X0Y0      ZXY   158
#> 2 Z1X0Y0      ZXY    52
#> 3 Z0X1Y0      ZXY     0
#> 4 Z1X1Y0      ZXY    23
#> 5 Z0X0Y1      ZXY    14
#> 6 Z1X0Y1      ZXY    12
#> 7 Z0X1Y1      ZXY     0
#> 8 Z1X1Y1      ZXY    78
```

Note that in compact form we simply record the number of units ("count") that display each possible pattern of outcomes on the three variables ("event").[1]

With `CausalQueries`, you can create the model, input data, and update the model thus.

```
R> lipids_model <-
```

[1]The "strategy" column records the set of variables for which data has been recorded. In this illustration the data is complete and so the implied strategy is `ZXY` for all units.

```
+  make_model("Z -> X -> Y; X <-> Y") |>
+  update_model(lipids_data, refresh = 0)
```

The model can then be queried thus:

```
R> lipids_queries <-
+  lipids_model  |>
+  query_model(query = "Y[X=1] - Y[X=0]",
+              given = c("All",  "X==0 & Y==0", "X[Z=1] > X[Z=0]"),
+              using = "posteriors")
```

The output is a data frame with estimates, posterior standard deviations, and credibility intervals. Table 1 shows the output from the analysis of the lipids data. In the table rows 1 and 2 replicate results in Chickering and Pearl (1996); row 3 returns inferences for complier average effects.

Table 1: Replication of Chickering and Pearl (1996).

query	given	mean	sd	cred.low	cred.high
Y[X=1] - Y[X=0]	-	0.55	0.10	0.37	0.73
Y[X=1] - Y[X=0]	X==0 & Y==0	0.64	0.15	0.37	0.89
Y[X=1] - Y[X=0]	X[Z=1] > X[Z=0]	0.70	0.05	0.59	0.80

As we describe below, the same basic procedure of making, updating, and querying models, can be used (up to computational constraints) for arbitrary causal models, for different types of data structures, and for all causal queries that can be posed of the causal model.

3. Connections to existing packages

The literature on causal inference and its software ecosystem is large, spanning the social and natural sciences as well as computer science and applied mathematics. Here we contextualize the scope and functionality of `CausalQueries` within the subset of the causal inference domain addressing the evaluation of causal queries on causal models encoded as directed acyclic graphs (DAGs) or structural equation models (SEMs). Table 2 provides an overview of relevant software and discusses key connections, advantages and disadvantages with respect to `CausalQueries`.

Table 2: Related software.

Software	Source	Language	Availability	Scope
`causalnex`	Beaumont, Horsburgh, Pilgerstorfer, Droth, Oentaryo, Ler, Nguyen, Ferreira, Patel, and Leong (2021)	Python	• pip	• causal structure learning • querying marginal distributions • discrete data
`pclag`	Kalisch, Mächler, Colombo, Maathuis, and Bühlmann (2012)	R	• CRAN • GitHub	• causal structure learning • ATEs under linear conditional expectations and no hidden selection
`DoWhy`	Sharma and Kiciman (2020)	Python	• pip	• identification • average and conditional causal effects • robustness checks
`autobounds`	Duarte, Finkelstein, Knox, Mummolo, and Shpitser (2023)	Python	• Docker • GitHub	• bounding causal effects • partial identification • DAG canonicalization • binary data
`causaloptim`	Sachs, Jonzon, Sjölander, and Gabriel (2023)	R	• CRAN • GitHub	• bounding causal effects • non-identified queries • binary data

`causalnex` is a highly comprehensive software in the causal modeling domain, offering a suite of functions rich in features and optimized for the learning, updating, and querying of causal models using discrete data. Its avoidance of the intricate model parametrization, characterized by principal strata (nodal types), enables `causalnex` to adeptly process non-binary data and scale to large causal models. This approach; however, significantly constrains the variety of feasible queries and the extent of prior knowledge that can be incorporated into models. In this capacity, `causalnex` mirrors machine learning strategies in causal inference, prioritizing the learning of causal structures in environments abundant with variables yet potentially

deficient in domain-specific knowledge; thus focusing on the assessment of basic queries over marginal distributions in learned DAGs. Conversely, the complex model structure utilized by `CausalQueries` is particularly advantageous for causal queries in settings where domain knowledge is more prevalent.

Like `causalnex`, `pclag` places particular emphasis on causal structure learning, utilizing the resultant DAGs to recover average treatment effects (ATEs) across all learned Markov-equivalent classes implied by observed data that satisfy linearity of conditional expectations. This approach again is more restrictive than `CausalQueries` in the DAGs and particularly the queries it allows.

`DoWhy` is a feature-rich, mature inference framework that emphasizes causal identification, causal effect estimation, and assumption validation. Given a user specified DAG, it deploys do-calculus to find expressions that identify desired causal-effects via Back-door, Front-door, IV and mediation identification criteria and leverages the identified expression and standard estimators to estimate the desired estimand. Following estimation, `DoWhy` deploys a comprehensive refutation engine implementing a large set of robustness tests. While this approach allows it to efficiently handle varied data types on large causal models, the decision to not parameterize the DAG itself places substantial limitations on the types of queries that can be posed.

The software bearing the highest resemblance to `CausalQueries` with respect to model definition are `autobounds` and `causaloptim`. Dealing with binary causal models, their definitions of principal strata (nodal types) and the resultant set of causal relations on the DAG (causal types) are very close to those of `CausalQueries`. Differences in model definition arise with respect to disturbance terms and confounding being defined implicitly via main nodes and edges in `CausalQueries` vs explicitly via separate disturbance nodes in `autobounds` and `causaloptim`. While `CausalQueries` assumes canonical form for input DAGs, `autobounds` and `causaloptim` facilitate canonicalization. The essential difference between the methods; however, lies in their approach to evaluating queries.

Both `autobounds` and `causaloptim` build on seminal approaches in Balke and Pearl (1997) to construct bounds of queries, using constrained polynomial and linear optimization respectively. In contrast, `CausalQueries` utilizes Bayesian inference to generate a posterior over the causal model which is then queried (consistent with Chickering and Pearl 1996; Zhang, Tian, and Bareinboim 2022). A key difference is the target of inference. The polynomial and linear programming approach to querying is in principle suited to handling larger causal models, though given their similarity in model parametrization, `autobounds`, `causaloptim` and `CausalQueries` face similar constraints induced by parameter spaces expanding rapidly with model size. The Bayesian approach to model updating and querying holds the efficiency advantage that a model can be updated once and queried arbitrarily, while expensive optimization runs are required for each separate query in `autobounds` and `causaloptim`.

Summarizing, the particular strength of `CausalQueries` is to allow users to specify arbitrary DAGs, to specify arbitrary queries defined on the DAG, and use the same canonical procedure to form Bayesian posteriors over those queries whether or not the queries are identified. Thus, for example, if researchers are interested in learning about a quantity like the local average treatment effect and their model in fact satisfies the conditions in Angrist, Imbens, and Rubin (1996), then updating will recover valid estimates as data grows even if researchers are

unaware that the local average treatment effect is identified and are ignorant of the estimation procedure proposed by Angrist *et al.* (1996).

There are two broad limitations on the sets of models handled natively by `CausalQueries`. First `CausalQueries` is designed for models with a relatively small number of binary nodes. Because there is no compromise made on the space of possible causal relations implied by a given model, the parameter space grows very rapidly with the complexity of the causal model. The complexity also depends on the causal structure and grows rapidly with the number of parents affecting a given child. A chain model of the form $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E$ has just 40 parameters. A model in which A, B, C, D are all direct ancestors of E has $65,544$ parameters. Moving from binary to non binary nodes has similar effects. The restriction to binary nodes is for computational and not conceptual reasons. In fact it is possible to employ `CausalQueries` to answer queries from models with non binary nodes but in general the computational costs make analysis of these models prohibitive.[2]

Second, the package is geared towards learning about populations from independently sampled units from populations. Thus the basic set up does not address problems of clustering, hierarchical structures, or purposive sampling. The broader framework can however be used for these purposes (see section 9.4 of Humphreys and Jacobs 2023). The targets of inference are usually case level quantities or population quantities and `CausalQueries` is not well suited for estimating sample quantities.

4. Statistical model

The core conceptual framework is described in Pearl's *Causality* (Pearl 2009) but can be summarized as follows (using the notation proposed in Humphreys and Jacobs 2023):

Definition 1 *A "**causal model**" is:*

1. *an ordered collection of "endogenous nodes"* $Y = \{Y_1, Y_2, ..., Y_n\}$
2. *an ordered collection of "exogenous nodes"* $\Theta = \{\theta^{Y_1}, \theta^{Y_1}, ..., \theta^{Y_n}\}$
3. *a collection of functions* $F = \{f_{Y_1}, f_{Y_2}, ..., f_{Y_n}\}$ *specifying, for each* j*, how outcome* y_j *depends on* θ_j *and realizations of endogenous nodes prior to* j*.*
4. *a probability distribution over* Θ*,* λ*.*

By default, `CausalQueries` takes endogenous nodes to be binary.[3] When we specify a causal structure we specify which endogenous nodes are (possibly) direct causes of a node, Y_j, given other nodes in the model. These nodes are called the parents of Y_j, PA_j (we use upper case PA_j to indicate the collection of nodes and lower case pa_j to indicate a particular set of values that these nodes might take on). With discrete valued nodes, it is possible to identify

[2]For more on computation constraints and strategies to update and query large models see the associated package `CausalQueriesTools` available via `devtools::install_github("till-tietz/CausalQueriesTools")`. The core approach used here is to divide large causal models into modules, update on modules and reassemble to pose queries.

[3]`CausalQueries` can be used also to analyse non binary data though with a cost of greatly increased complexity. See section 9.4.1 of Humphreys and Jacobs (2023) for an approach that codes non binary data as a profile of outcomes on multiple binary nodes.

all possible ways that a node might respond to its parents. We refer to the ways that a node responds as "nodal type." The set of nodal types corresponds to principal strata familiar, for instance, in the study of instrumental variables (Frangakis and Rubin 2002).

If node Y_i can take on k_i possible values then the set of possible values that can be taken on by parents of j is $m_j := \prod_{i \in PA_j} k_i$. Then there are $k_j^{m_j}$ different ways that node j might respond to its parents. In the case of binary nodes this becomes $2^{\left(2^{|PA_j|}\right)}$. Thus for an endogenous node with no parents there are 2 nodal types, for a binary node with one binary parent there are four types, for a binary node with 2 parents there are 16, and so on.

The set of all possible causal reactions of a given unit to all possible values of parents is then given by its collection of nodal types at each node. We call this collection a unit's "causal type", θ.

The approach used by `CausalQueries` is to let the domain of θ^{Y_j} be coextensive with the number of nodal types for Y_j. Function f^j then determines the value of y by simply reporting the value of Y_j implied by the nodal type and the values of the parents of Y_j. Thus if $\theta^j_{pa_j}$ is the value for j when parents have values pa_j, then we have simply that $f_{Y_j}(\theta^j, pa_j) = \theta^j_{pa_j}$. The practical implication is that, given the causal structure, learning about the model reduces to learning about the distribution, λ, over the nodal types.

In cases in which there is no unobserved confounding, we take the probability distributions over the nodal types for different nodes to be independent: $\theta^i \perp\!\!\!\perp \theta^j, i \neq j$. In this case we use a categorical distribution to specify the $\lambda^j_x := \Pr(\theta^j = \theta^j_x)$. From independence then we have that the probability of a given causal type θ_x is simply $\prod_{i=1}^n \lambda^i_x$. For instance $\Pr(\theta = (\theta^X_1, \theta^Y_{01})) = \Pr(\theta^X = \theta^X_1)\Pr(\theta^Y = \theta^Y_{01}) = \lambda^X_1 \lambda^Y_{01}$.

In cases in which there is confounding, the logic is the same except that we need to specify enough parameters to capture the joint distribution over nodal types for different nodes. We do this making use of the causal structure.

As an example, for the Lipids model, the full joint distribution of nodal types can be simplified as in Equation 1.

$$\Pr(\theta^Z = \theta^Z_1, \theta^X = \theta^X_{10}, \theta^Y = \theta^Y_{11}) = \Pr(\theta^Z = \theta^Z_1)\Pr(\theta^X = \theta^X_{10})\Pr(\theta^Y = \theta^Y_{11}|\theta^X = \theta^X_{10}) \quad (1)$$

And so, for this model, λ would include parameters that represent $\Pr(\theta^Z)$ and $\Pr(\theta^X)$ but also the conditional probability $\Pr(\theta^Y|\theta^X)$:

$$\Pr(\theta^Z = \theta^Z_1, \theta^X = \theta^X_{10}, \theta^Y = \theta^Y_{11}) = \lambda^Z_1 \lambda^X_{10} \lambda^{Y|\theta^X_{10}}_{11} \quad (2)$$

Representing beliefs *over causal models* thus requires specifying a probability distribution over λ. This might be a degenerate distribution if users want to specify a particular model. `CausalQueries` allows users to specify parameters, α of a Dirichlet distribution over λ. If all entries of α are 0.5 this corresponds to Jeffreys priors. The default behavior is for `CausalQueries` to assume a uniform distribution – that is, that all nodal types are equally likely – which corresponds to α being a vector of 1s.

Updating is then done with respect to beliefs over λ. In the Bayesian approach we have simply:

$$p(\lambda|D) = \frac{p(D|\lambda)p(\lambda)}{\int_{\lambda'} p(D|\lambda')p(\lambda')}$$

where $p(D|\lambda')$ is calculated under the assumption that units are exchangeable and independently drawn. In practice this means that the probability that two units have causal types θ_i and θ_j is simply $\lambda'_i\lambda'_j$. Since a causal type fully determines an outcome vector $d = \{y_1, y_2, ..., y_n\}$, the probability of a given outcome ("event"), w_d, is given simply by the probability that the causal type is among those that yield outcome d. Thus from λ we can calculate a vector of event probabilities, $w(\lambda)$, for each vector of outcomes, and under independence we have:

$$D \sim \text{Multinomial}(w(\lambda), N)$$

Thus for instance in the case of a $X \rightarrow Y$ model, and letting w_{xy} denote the probability of a data type $X = x, Y = y$, the event probabilities are:

$$w(\lambda) = \begin{cases} w_{00} &= \lambda^X_0(\lambda^Y_{00} + \lambda^Y_{01}) \\ w_{01} &= \lambda^X_0(\lambda^Y_{11} + \lambda^Y_{10}) \\ w_{10} &= \lambda^X_1(\lambda^Y_{00} + \lambda^Y_{10}) \\ w_{11} &= \lambda^X_1(\lambda^Y_{11} + \lambda^Y_{01}) \end{cases}$$

For a more complex example Table 3 illustrates key values for the Lipids model. We see here that we have two types for node Z, four for X (representing the strata familiar from instrumental variables analysis: never takers, always takers, defiers, and compliers) and 4 for Y. For Z and X we have parameters corresponding to probability of these nodal types. For instance `Z.0` is the probability that $Z = 0$. `Z.1` is the complementary probability that $Z = 1$. Things are a little more complicated for distributions on nodal types for Y however: because of confounding between X and Y we have parameters that capture the conditional probability of the nodal types for Y *given* the nodal types for X. We see there are four sets of these parameters.

Table 3: Nodal types and parameters for Lipids model.

node	nodal_type	param_set	param_names	param_value	priors
Z	0	Z	Z.0	0.57	1
Z	1	Z	Z.1	0.43	1
X	00	X	X.00	0.24	1
X	10	X	X.10	0.30	1
X	01	X	X.01	0.20	1
X	11	X	X.11	0.27	1
Y	00	Y.X.00	Y.00_X.00	0.71	1
Y	10	Y.X.00	Y.10_X.00	0.19	1

Y	01	Y.X.00	Y.01_X.00	0.00	1
Y	11	Y.X.00	Y.11_X.00	0.10	1
Y	00	Y.X.01	Y.00_X.01	0.15	1
Y	10	Y.X.01	Y.10_X.01	0.40	1
Y	01	Y.X.01	Y.01_X.01	0.39	1
Y	11	Y.X.01	Y.11_X.01	0.06	1
Y	00	Y.X.10	Y.00_X.10	0.17	1
Y	10	Y.X.10	Y.10_X.10	0.65	1
Y	01	Y.X.10	Y.01_X.10	0.14	1
Y	11	Y.X.10	Y.11_X.10	0.04	1
Y	00	Y.X.11	Y.00_X.11	0.24	1
Y	10	Y.X.11	Y.10_X.11	0.71	1
Y	01	Y.X.11	Y.01_X.11	0.04	1
Y	11	Y.X.11	Y.11_X.11	0.01	1

The next to final column shows a sample set of parameter values. Together, the parameters describe a full joint probability distribution over types for Z, X and Y that is faithful to the graph.

From these we can calculate the probability of each data type. For instance the probability of data type $Z = 0, X = 0, Y = 0$ is:

$$w_{000} = \Pr(Z = 0, X = 0, Y = 0) = \lambda_0^Z \left(\lambda_{00}^X(\lambda_{00}^{Y|\lambda_{00}^X} + \lambda_{01}^{Y|\lambda_{00}^X}) + \lambda_{01}^X(\lambda_{00}^{Y|\lambda_{01}^X} + \lambda_{01}^{Y|\lambda_{01}^X})\right)$$

In practice `CausalQueries` generates a matrix, that maps from parameters into data types.

The value of the `CausalQueries` package is to allow users to specify *arbitrary* models of this form, figure out all the implied nodal types and causal types, and then update given priors and data by calculating event probabilities implied by all possible parameter vectors and in turn the likelihood of the data given the model. In addition, the package allows for arbitrary querying of a model to assess the values of estimands of interest that are a function of the values or counterfactual values of nodes, *conditional* on values or counterfactual values of nodes.

In the next sections we review key functionality for making, updating and querying causal models.

5. Making models

A model is defined in one step in `CausalQueries` using a `dagitty` syntax (Textor, van der Zander, Gilthorpe, Liśkiewicz, and Ellison 2016) in which the structure of the model is provided as a statement. For instance:

```
R> model <- make_model("X -> M -> Y <- X")
```

The statement in quotes, `"X -> M -> Y <- X"`, provides the names of nodes. An arrow ("`->`" or "`<-`") connecting nodes indicates that one node is a potential cause of another, i.e. whether a given node is a "parent" or "child" of another. Formally a statement like this is interpreted as:

1. Functional equations:
   - $Y = f(M, X, \theta^Y)$
   - $M = f(X, \theta^M)$
   - $X = \theta^X$
2. Distributions on Θ:
   - $\Pr(\theta^i = \theta^i_k) = \lambda^i_k$
3. Independence assumptions:
   - $\theta_i \perp\!\!\!\perp \theta_j, i \neq j$

Function f maps from the set of possible values of the parents of i to values of node i given θ^i as described above.

In addition, as we did in the Chickering and Pearl (1996) example, it is possible to use two headed arrows ("`<->`") to indicate "unobserved confounding", that is, the presence of an unobserved variable that might influence two or more observed variables. In this case condition 3 above is relaxed and the exogenous nodes associated with confounded variables have a joint distribution. We describe how this is done in greater detail in Section 5.3.2.

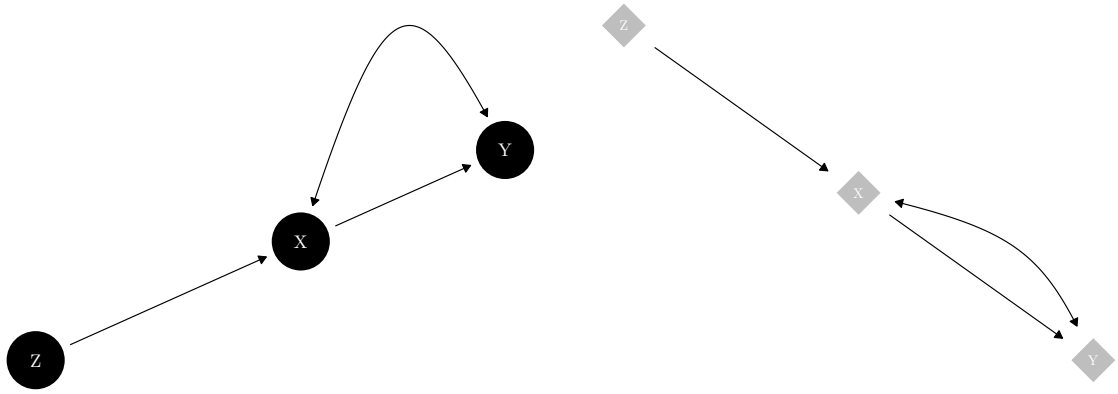
5.1. Graphing

Plotting the model can be useful to check that you have defined the structure of the model correctly. `CausalQueries` provides simple graphing tools that draw on functionality from the `dagitty`, `ggplot2`, and `ggdag` packages.

Once defined, a model can be graphed by calling the `plot()` method on the objects with class `causal_model`. This method is a wrapper for the `plot_model()` function, and accepts additional options described in `?plot_model`.

Figure 1 shows figures generating by plotting `lipids_model` with and without options. The plots have class `c("gg", "ggplot")` and so will accept any additional layers available for the objects of class `ggplot`.

```
R> lipids_model |> plot()
R>
R> lipids_model |>
+  plot(x_coord = 1:3,
+       y_coord = c(3,2,1),
+       textcol = "white",
+       textsize = 3,
+       shape = 18,
+       nodecol = "grey",
+       nodesize = 12)
```



(a) Without options (b) With options

Figure 1: Examples of model graphs.

5.2. Model characterization

When a model is defined, a set of objects is generated. These are the key quantities that are used for all inferential tasks. Table 4 summarizes the core components of a model, providing a brief explanation for each one.

The first element is a `statement` which defines how the nodes in the model are related, specified by the user using `dagitty` syntax. The second element, `dag`, is a data frame that outlines the parent-child relationships within the model. The element `nodes` is simply a list of the names of the nodes in the model. Lastly, `parents_df`, is a table listing the nodes, indicating if they are "root" nodes (nodes with no parents among the set of specified nodes), and showing how many parents each node has.

The model includes additional elements, `nodal_types`, `parameters_df`, and `causal_types`, which we explain in detail later.

Table 4: Core Elements of a Causal Model.

Element	Description
`statement`	A character string using `dagitty` syntax that describes directed causal relations between variables in a causal model, where arrows denote that one node is a potential cause of another.
`dag`	A data frame with columns 'parent' and 'children' indicating how nodes relate to each other.
`nodes`	A list containing the nodes in the model.
`parents_df`	A table listing nodes, whether they are root nodes or not, and the number of parents they have.
`nodal_types`	A list with the nodal types of the model. See Section 5.2.2 for more details.

Element	Description
`parameters_df`	A data frame linking the model's parameters with the nodal types of the model, as well as the family to which they belong. See Section 5.2.1 for more details.
`causal_types`	A data frame listing causal types and the nodal types that produce them. (See Section 5.2.3.)

After updating a model, two additional components are attached to it:

- A posterior distribution of the parameters in the model, generated by Stan. This distribution reflects the updated parameter values.
- A list of other optional objects, `stan_objects`. The `stan_objects` can include the `stanfit` object and distributions over nodal types and event probabilities.

Table 5 summarizes the objects attached to the model after updating.

Table 5: Additional Elements.

Element	Description
`posterior_distribution`	The posterior distribution of the updated parameters generated by Stan.
`stan_objects`	A list of additional objects (see next rows).
`data`	The data used for updating the model, always included in `stan_objects`.
`type_distribution`	The updated distribution of the nodal types, appended to `stan_objects` by default.
`event_probabilities`	A mapping from parameters to event probabilities, optionally appended to `stan_objects`.
`stan_fit`	The `stanfit` object generated by Stan, optionally appended to `stan_objects`.

Parameters data frame

When a model is created, `CausalQueries` attaches a "parameters data frame" which keeps track of model parameters, which belong together in a family, and how they relate to causal types. This becomes especially important for more complex models with confounding that might involve more complicated mappings between parameters and nodal types. In the case with no confounding the nodal types *are* the parameters; in cases with confounding there are generally more parameters than nodal types. We already saw a segment of a parameters data frame for a model with confounding in Table 3. To access full parameters data frame we can call `grab()` function as follows

```
R> make_model("X -> Y") |>
+  grab("parameters_df")
```

```
#> Mapping of model parameters to nodal types:
#>
#> -----------------------------------------------------------------
#>
#>  param_names: name of parameter
#>  node: name of endogeneous node associated with the parameter
#>  gen: partial causal ordering of the parameter's node
#>  param_set: parameter groupings forming a simplex
#>  given: if model has confounding gives conditioning nodal type
#>  param_value: parameter values
#>  priors: hyperparameters of the prior Dirichlet distribution
#>
#> -----------------------------------------------------------------
#>
#>   param_names node gen param_set nodal_type given param_value priors
#> 1         X.0    X   1         X          0               0.50      1
#> 2         X.1    X   1         X          1               0.50      1
#> 3        Y.00    Y   2         Y         00               0.25      1
#> 4        Y.10    Y   2         Y         10               0.25      1
#> 5        Y.01    Y   2         Y         01               0.25      1
#> 6        Y.11    Y   2         Y         11               0.25      1
```

As in Table 3, each row in the parameters data frame corresponds to a single parameter. The `print()` method for the objects of `parameters_df` class also includes short description of each of the columns included in the data frame. More precisely, the columns of the parameters data frame are:

- `param_names` gives the name of the parameter, in shorthand. For instance the parameter $\lambda_0^X = \Pr(\theta^X = \theta_0^X)$ has `par_name X.0`.
- `node` indicates the node associated with the parameter.
- `gen` indicates the place in the partial causal ordering (generation) of the node associated with the parameter
- `param_set` indicates which parameters group together to form a simplex. The parameters in a set have parameter values that sum to 1. In this example $\lambda_0^X + \lambda_1^X = 1$.
- `nodal_type` indicates the nodal types associated with the parameter.
- `param_value` gives the (possibly default) parameter values (probabilities).
- `priors` gives (possibly default) Dirichlet priors arguments for parameters in a set. Values of 1 (.5) for all parameters in a set implies uniform (Jeffreys) priors over this set.

Nodal types

As described above, two units have the same *nodal type* at node Y, θ^Y, if their outcome at Y responds in the same ways to parents of Y.

A binary node with k binary parents has 2^{2^k} nodal types because there are 2^k possible values of the k parents and so 2^{2^k} ways to respond to these possible parental values.

When a model is created, the full set of nodal types is identified. These are stored in the

model. The labels for these nodal types indicate how the unit responds to values of parents. For instance, consider the model with two parents $X \rightarrow Y \leftarrow M$. In such a case, the nodal types of Y will have subscripts with four digits, with each digit representing one of the possible combinations of values that Y can take, given the values of its parents X and M. These combinations include the value of Y when:

- $X = 0$ and $M = 0$,
- $X = 0$ and $M = 1$,
- $X = 1$ and $M = 0$,
- $X = 1$ and $M = 1$.

As the number of parents increases, keeping track of what each digit represents becomes more difficult. For instance, if Y had three parents, its nodal types would have subscripts of eight digits, each associated with the value that Y would take for each combination of the three parents. The `interpret_type()` function provides a clear map to identify what each digit in the subscript represents. See the example below for a model with three parents.

The `interpret_type()` function can be called by the user to obtain interpretations for the nodal types of each node in the model.

```
R> make_model("X -> Y <- M; W -> Y") |>
+  interpret_type(nodes = "Y")
```

```
#> $Y
#>   node position     display            interpretation
#> 1    Y        1 Y[*]******* Y | M = 0 & W = 0 & X = 0
#> 2    Y        2 Y*[*]****** Y | M = 1 & W = 0 & X = 0
#> 3    Y        3 Y**[*]***** Y | M = 0 & W = 1 & X = 0
#> 4    Y        4 Y***[*]**** Y | M = 1 & W = 1 & X = 0
#> 5    Y        5 Y****[*]*** Y | M = 0 & W = 0 & X = 1
#> 6    Y        6 Y*****[*]** Y | M = 1 & W = 0 & X = 1
#> 7    Y        7 Y******[*]* Y | M = 0 & W = 1 & X = 1
#> 8    Y        8 Y*******[*] Y | M = 1 & W = 1 & X = 1
```

Causal types

Causal types are collections of nodal types. Two units are of the same *causal type* if they have the same nodal type at every node. For example in a $X \rightarrow M \rightarrow Y$ model, $\theta = (\theta_0^X, \theta_{01}^M, \theta_{10}^Y)$ is a type that has $X = 0$, M responds positively to X, and Y responds positively to M.

When a model is created, the full set of causal types is identified. These are stored in the model object:

```
R> lipids_model |>
+  grab("causal_types")
```

```
#>
#> Causal Types:
#> cartesian product of nodal types
#>
```

```
#>
#>  first 10 causal types:
#>            Z  X  Y
#> Z0.X00.Y00 0 00 00
#> Z1.X00.Y00 1 00 00
#> Z0.X10.Y00 0 10 00
#> Z1.X10.Y00 1 10 00
#> Z0.X01.Y00 0 01 00
#> Z1.X01.Y00 1 01 00
#> Z0.X11.Y00 0 11 00
#> Z1.X11.Y00 1 11 00
#> Z0.X00.Y10 0 00 10
#> Z1.X00.Y10 1 00 10
```

In the Lipids model there are $2 \times 4 \times 4 = 32$ causal types. A model with n_j nodal types at node j has $\prod_j n_j$ causal types. Thus the set of causal types can be large.

Knowledge of a causal type tells us what values a unit would take, on all nodes, whether or not there are interventions. For example for a model $X \to M \to Y$ a type $\theta = (\theta_0^X, \theta_{01}^M, \theta_{10}^Y)$ would imply data $(X = 0, M = 0, Y = 1)$ absent any intervention. (The converse of this, of course, is the key to updating: observation of data $(X = 0, M = 0, Y = 1)$ result in more weight placed on θ_0^X, θ_{01}^M, and θ_{10}^Y).) The general approach used by `CausalQueries` for calculating outcomes from causal types is given in Section 7.1.

Parameter matrix

The parameters data frame keeps track of parameter values and priors for parameters, but it does not provide a mapping between parameters and the probability of causal types. The parameter matrix—the "P matrix"—can be added to the model to provide this mapping. The P matrix has a row for each parameter and a column for each causal type. For instance:

```
R> make_model("X -> Y") |>
+  grab("parameter_matrix")
```

```
#>
#> Rows are parameters, grouped in parameter sets
#>
#> Columns are causal types
#>
#> Cell entries indicate whether a parameter probability isused
#> in the calculation of causal type probability
#>
#>      X0.Y00 X1.Y00 X0.Y10 X1.Y10 X0.Y01 X1.Y01 X0.Y11 X1.Y11
#> X.0       1      0      1      0      1      0      1      0
#> X.1       0      1      0      1      0      1      0      1
#> Y.00      1      1      0      0      0      0      0      0
#> Y.10      0      0      1      1      0      0      0      0
#> Y.01      0      0      0      0      1      1      0      0
```

```
#> Y.11      0      0      0      0      0      0      1      1
#>
#>
#>  param_set  (P)
#>
```

The probability of a causal type is given by the product of the parameter values for parameters whose row in the P matrix contains a 1. Later (e.g. in Section 5.3.2) we will see examples where the P matrix helps keep track of parameters that are created when confounding is added to a model.

The parameter matrix is generated on the fly as needed, but it can also be added to the model using `set_parameter_matrix()`, which can sometimes be useful to speed up operations:

```
R> make_model("X -> Y") |>
+  set_parameter_matrix()
```

5.3. Tailoring models

When a `dagitty` statement is provided to `make_data()` a model is formed with a set of default assumptions: in particular there are no restrictions placed on nodal types and flat priors are assumed over all parameters. These are features that can be adjusted after a model is formed.

Setting restrictions

Sometimes for theoretical or practical reasons it is useful to constrain the set of types. In `CausalQueries` this is done at the level of nodal types, with restrictions on causal types following from restrictions on nodal types.

To illustrate, in analyses of data with imperfect compliance, like we saw in our motivating Lipids model example, it is common to impose a monotonicity assumption: that X does not respond negatively to Z. This is one of the conditions needed to interpret instrumental variables estimates as (consistent) estimates of the complier average treatment effect. In `CausalQueries` we can impose this assumption as follows:

```
R> model_restricted <-
+  lipids_model |>
+  set_restrictions("X[Z=1] < X[Z=0]")
```

In words: we restrict by removing types for which X is decreasing in Z. If we wanted to retain only this nodal type, rather than remove it, we could do so by stipulating `keep = FALSE`. Users can use `grab(model, "parameter_matrix")` to view the resulting parameter matrix in which both the set of parameters and the set of causal types are restricted.

`CausalQueries` allows restrictions to be set in many other ways:

- Using nodal type labels

```
R> model <- lipids_model |>
+  set_restrictions(labels = list(X = "01", Y = c("00", "01", "11")),
+                   keep = TRUE)
```

- Using wildcards in nodal type labels

```
R> model <- lipids_model |>
+  set_restrictions(labels = list(Y = "?0"))
```

- In models with confounding, restrictions can be added to nodal types conditional on the values of other nodal types; this is done using a `given` argument.

```
R> model <- lipids_model |>
+  set_restrictions(labels = list(Y = c('00', '11')), given = 'X.00')
```

Setting restrictions sometimes involves using causal syntax (see Section 7.2 for a guide the syntax used by `CausalQueries`). Help file in `?set_restrictions` provides further details and examples on restrictions users can set.

Allowing confounding

Unobserved confounding between two (or more) nodes arises when the nodal types for the nodes are not independent. In the $X \rightarrow Y$ graph, for instance, there are 2 nodal types for X and 4 for Y. There are thus 8 joint nodal types (or causal types), as shown in Table 6.

Table 6: Nodal types in $X \rightarrow Y$ model.

	θ_0^X	θ_1^X	$\sum$
θ_{00}^Y	$\Pr(\theta_0^X, \theta_{00}^Y)$	$\Pr(\theta_1^X, \theta_{00}^Y)$	$\Pr(\theta_{00}^Y)$
θ_{10}^Y	$\Pr(\theta_0^X, \theta_{10}^Y)$	$\Pr(\theta_1^X, \theta_{10}^Y)$	$\Pr(\theta_{10}^Y)$
θ_{01}^Y	$\Pr(\theta_0^X, \theta_{01}^Y)$	$\Pr(\theta_1^X, \theta_{01}^Y)$	$\Pr(\theta_{01}^Y)$
θ_{11}^Y	$\Pr(\theta_0^X, \theta_{11}^Y)$	$\Pr(\theta_1^X, \theta_{11}^Y)$	$\Pr(\theta_{11}^Y)$
$\sum$	$\Pr(\theta_0^X)$	$\Pr(\theta_1^X)$	1

Table 6 has eight interior elements and so an unconstrained joint distribution would have 7 degrees of freedom. A no-confounding assumption means that $\Pr(\theta^X|\theta^Y) = \Pr(\theta^X)$, or $\Pr(\theta^X, \theta^Y) = \Pr(\theta^X)\Pr(\theta^Y)$. In this case we just put a distribution on the marginals and there would be 3 degrees of freedom for Y and 1 for X, totaling 4 rather than 7.

The parameters data frame for this model would have two parameter families for parameters associated with the node Y. Each family captures the conditional distribution of Y's nodal types, given X. For instance the parameter `Y01_X.1` can be interpreted as $\Pr(\theta^Y = \theta_{01}^Y|\theta^X = 1)$. See again Table 3 for an example of a parameters matrix with confounding.

The structure of confounding can have important effects for the number of parameters given the underlying DAG. Table 7 illustrates showing the number of independent parameters required given different types of confounding.

Table 7: Number of different independent parameters (degrees of freedom) for different three-node models.

Model	Degrees of freedom
`X -> Y <- W`	17
`X -> Y <- W; X <-> W`	18
`X -> Y <- W; X <-> Y; W <-> Y`	62
`X -> Y <- W; X <-> Y; W <-> Y; X <-> W`	63
`X -> W -> Y <- X`	19
`X -> W -> Y <- X; W <-> Y`	64
`X -> W -> Y <- X; X <-> W; W <-> Y`	67
`X -> W -> Y <- X; X <-> W; W <-> Y; X <-> Y`	127

Setting Priors

Priors on model parameters can be added to the parameters data frame and are interpreted as "alpha" arguments for a Dirichlet distribution. The Dirichlet distribution is a probability distribution over an $n-1$ dimensional unit simplex. It can be thought of as a generalization of the Beta distribution and is parametrized by an n-dimensional positive vector α. Thus for example a Dirichlet with $\alpha = (1, 1, 1, 1, 1)$ gives a probability distribution over all non negative 5-dimensional vectors that sum to 1, e.g. $(0.1, 0.1, 0.1, 0.1, 0.6)$ or $(0.1, 0.2, 0.3, 0.3, 0.1)$. This particular value for α implies that all such vectors are equally likely. Other values for α can be used to control the expectation for each dimension as well as certainty. Thus for instance the vector $\alpha = (100, 1, 1, 1, 100)$ would result in more weight on distributions that are close to $(0.5, 0, 0, 0, 0.5)$.

In `CausalQueries`, priors are generally specified over the distribution of nodal types (or over the conditional distribution of nodal types, when there is confounding). Thus for instance in an $X \rightarrow Y$ model we have one Dirichlet distribution over the two types for θ^X and one Dirichlet distribution over the four types for θ^Y.

Implicitly priors are independent across families. Thus for instance in an $X \rightarrow Y$ model we specify beliefs over λ^X and over λ^Y separately. `CausalQueries` does not let users specify correlated beliefs over these parameters.[4]

By default, prior hyperparameters are set to unity, corresponding to uniform priors. To retrieve the model's priors we can run the following code:

```
R> lipids_model |> grab("prior_hyperparameters", "X")
```

```
#>       Z.0       Z.1      X.00      X.10      X.01      X.11 Y.00_X.00 Y.10_X.00
#>         1         1         1         1         1         1         1         1
#> Y.01_X.00 Y.11_X.00 Y.00_X.01 Y.10_X.01 Y.01_X.01 Y.11_X.01 Y.00_X.10 Y.10_X.10
#>         1         1         1         1         1         1         1         1
#> Y.01_X.10 Y.11_X.10 Y.00_X.11 Y.10_X.11 Y.01_X.11 Y.11_X.11
```

[4]Of course, if a model involves possible confounding, users can specify beliefs about λ^Y given θ^X. But this is a statement about beliefs over a joint distribution not jointly distributed beliefs.

```
#>         1         1         1         1         1         1
```

Alternatively you could set Jeffreys priors using `set_priors()` as follows:

```
R> model <- lipids_model |>
+  set_priors(distribution = "jeffreys")
```

You can also add custom priors. Custom priors are most simply specified by being added as a vector of numbers using `set_priors()`. For instance:

```
R> lipids_model |>
+  set_priors(node = "X", alphas = 1:4) |>
+  grab("prior_hyperparameters", "X")
```

```
#>       Z.0       Z.1      X.00      X.10      X.01      X.11 Y.00_X.00 Y.10_X.00
#>         1         1         1         2         3         4         1         1
#> Y.01_X.00 Y.11_X.00 Y.00_X.01 Y.10_X.01 Y.01_X.01 Y.11_X.01 Y.00_X.10 Y.10_X.10
#>         1         1         1         1         1         1         1         1
#> Y.01_X.10 Y.11_X.10 Y.00_X.11 Y.10_X.11 Y.01_X.11 Y.11_X.11
#>         1         1         1         1         1         1
```

The priors here should be interpreted as indicating $\alpha_X = (1, 2, 3, 4)$, which implies a distribution over $(\lambda^X_{00}, \lambda^X_{10}, \lambda^X_{01}, \lambda^X_{11})$ centered on $\left(\frac{1}{10}, \frac{2}{10}, \frac{3}{10}\frac{4}{10}\right)$.

For larger models it can be hard to provide priors as a vector of numbers. For that reason `set_priors()` allows for more targeted modifications of the parameter vector. For instance:

```
R> lipids_model |>
+  set_priors(statement = "X[Z=1] > X[Z=0]", alphas = 3) |>
+  grab("prior_hyperparameters", "X")
```

```
#>       Z.0       Z.1      X.00      X.10      X.01      X.11 Y.00_X.00 Y.10_X.00
#>         1         1         1         1         3         1         1         1
#> Y.01_X.00 Y.11_X.00 Y.00_X.01 Y.10_X.01 Y.01_X.01 Y.11_X.01 Y.00_X.10 Y.10_X.10
#>         1         1         1         1         1         1         1         1
#> Y.01_X.10 Y.11_X.10 Y.00_X.11 Y.10_X.11 Y.01_X.11 Y.11_X.11
#>         1         1         1         1         1         1
```

Setting priors requires mapping alpha values to parameters, and so the problem of altering priors reduces to selecting rows of the `parameters_df` data frame at which to alter values. When specifying a causal statement as above, `CausalQueries` internally identifies nodal types that are consistent with the statement, which in turn identify parameters to alter priors for.

We can achieve the same result as above by specifying nodal types for which we would like to adjust the priors. Indeed, `set_priors()` allows for the specification of any non-redundant combination of arguments on the `param_names`, `node`, `nodal_type`, `param_set` and `given` columns of `parameters_df` to uniquely identify parameters to set priors for. Alternatively a fully formed subsetting statement may be supplied to `alter_at`. Since all these arguments get mapped to the parameters they identify internally they may be used interchangeably.[5] Thus the following two specifications of priors are equivalent:

[5]See `?set_priors` and `?make_priors` for many more examples.

While highly targeted prior setting is convenient and flexible, it should be used with caution. Setting priors on specific parameters in complex models, especially models involving confounding, may strongly affect inferences.

Furthermore, note that flat priors over nodal types do not necessarily translate into flat priors over queries. "Flat" priors over parameters in a parameter family put equal weight on each nodal type, but this in turn can translate into strong assumptions on causal quantities of interest. For instance in an $X \rightarrow Y$ model in which negative effects are ruled out, the average causal effect implied by "flat" priors is 1/3. This can be seen by querying the model as follows:

```
R> make_model("X -> Y") |>
+  set_restrictions(decreasing("X", "Y")) |>
+  query_model("Y[X=1] - Y[X=0]", using = "priors")
```

More subtly the *structure* of a model, coupled with flat priors, has substantive importance for priors on causal quantities. For instance with flat priors, priors on the probability that X has a positive effect on Y in the model $X \rightarrow Y$ is centered on 1/4. But priors on the probability that X has a positive effect on Y in the model $X \rightarrow M \rightarrow Y$ is centered on 1/8.

Again, you can use `query_model()` to figure out what flat (or other) priors over parameters imply for priors over causal quantities:

Caution regarding priors is particularly important when models are not identified, as is the case for many of the models considered here. In such cases, for some quantities, the marginal posterior distribution simply reflects the marginal prior distribution (Poirier 1998).

The crucial aspect we emphasize is the necessity of avoiding the misconception that "uninformative" priors are devoid of implications concerning the values of causal quantities of interest. In reality, these priors do carry certain presumptions. The impact of flat priors on causal quantities is contingent on the structural configuration of the model. Moreover for some inferences from causal models the priors can matter a lot even if you have a lot of data. In such cases it can be helpful to know what priors on parameters imply for priors on causal quantities of interest (by using `query_model()`) and to assess how much conclusions depend on priors (by comparing results across models that vary in their priors).

The following code gives an example where a change in model structure together with uniform priors implies different beliefs over causal quantities.

```
R> make_model("X -> Y") |>
+  query_model("Y[X=1] > Y[X=0]", using = "priors")
R>
R> make_model("X -> M -> Y") |>
+  query_model("Y[X=1] > Y[X=0]", using = "priors")
```

Setting Parameters

By default, models have a vector of parameter values included in the `parameters_df` data frame. These are useful for generating data, or for situations, such as process tracing, when one wants to make inferences about causal types (θ), given case level data, under the assumption that the model is known.

The logic for setting parameters is similar to that for setting priors: effectively we need to place values on the probability of nodal types. The key difference is that whereas the α value placed on a nodal types can be any positive number—capturing our certainty over the parameter value—the parameter values must lie in the unit interval, $[0, 1]$. In general if parameter values are passed that do not lie in the unit interval, these are normalized so that they do.

Consider the causal model below. It has two parameter sets, one for X and one for Y, with six nodal types, two corresponding to X and four corresponding to Y. The key feature of the parameters is that they must sum to 1 within each parameter set.

```
R> make_model("X -> Y") |>
+  grab("parameters")
```

```
#> Model parameters with associated probabilities:
#>
#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 0.5 0.5 0.25 0.25 0.25 0.25
```

The example below illustrates a change in the value of the parameter Y in the case it is increasing in X. Here nodal type `Y.Y01` is set to be 0.5, while the other nodal types of this parameter set were re-normalized so that the parameters in the set still sum to one.

```
R> make_model("X -> Y") |>
+  set_parameters(statement = "Y[X=1] > Y[X=0]", parameters = .7) |>
+  grab("parameters")
```

```
#> Model parameters with associated probabilities:
#>
#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 0.5 0.5 0.1 0.1 0.7 0.1
```

5.4. Drawing and manipulating data

Once a model has been defined it is possible to simulate data from the model using the `make_data()` function. This can be useful for instance for assessing the expected performance of a model given data drawn from some speculated set of parameter values.

Drawing data basics

Generating data requires a specification of parameter values. These can be provided by users; if not provided default values are used that place equal weight on all nodal types.

```
R> sample_data_1 <-
+  lipids_model |>
+  make_data(n = 4)
```

However you can also specify parameters directly or use parameter draws from a prior or posterior distribution. For instance:

```
R> lipids_model |>
```

```
+  make_data(n = 3, param_type = "prior_draw")
```

```
#>   Z X Y
#> 1 1 0 0
#> 2 1 0 0
#> 3 1 0 1
```

Note that the data is returned ordered by data type as in the example above.

Drawing incomplete data

CausalQueries can be used in settings in which researchers have gathered different amounts of data for different nodes. For instance gathering X and Y data for all units but M data only for some.

The function make_data allows you to draw data like this if you specify a data strategy indicating the probabilities of observing data on different nodes, possibly as a function of prior nodes observed.

```
R> sample_data_2 <-
+  lipids_model |>
+  make_data(n = 8,
+            nodes = list(c("Z", "Y"), "X"),
+            probs = list(1, .5),
+            subsets = list(TRUE, "Z==1 & Y==0"),
+            verbose = FALSE)
R>
R> sample_data_2
```

```
#>   Z  X Y
#> 1 0 NA 0
#> 2 0 NA 0
#> 3 0  1 0
#> 4 0 NA 0
#> 5 0 NA 1
#> 6 1 NA 1
#> 7 1 NA 0
#> 8 1 NA 1
```

Reshaping data

Whereas data naturally comes in long form, with a row per observation, as in the examples above, the data passed to Stan is in a compact form, which records only the number of units of each data type, grouped by data "strategy"—an indicator of the nodes for which data was gathered. CausalQueries includes functions that lets you move between these two forms in case of need.

```
R> sample_data_2 |> collapse_data(lipids_model)
```

```
#>     event strategy count
```

```
#> 1   Z0X0Y0      ZXY     0
#> 2   Z1X0Y0      ZXY     0
#> 3   Z0X1Y0      ZXY     1
#> 4   Z1X1Y0      ZXY     0
#> 5   Z0X0Y1      ZXY     0
#> 6   Z1X0Y1      ZXY     0
#> 7   Z0X1Y1      ZXY     0
#> 8   Z1X1Y1      ZXY     0
#> 9     Z0Y0       ZY     3
#> 10    Z1Y0       ZY     1
#> 11    Z0Y1       ZY     1
#> 12    Z1Y1       ZY     2
```

In the same way it is possible to move from "compact data" to "long data" using `expand_data()`. Note that `NA`'s are interpreted as data not having been sought. So in the case of `sample_data_2` the interpretation is that there are two data strategies: data on Y, M and X was sought in two cases only; data on Y and X only was sought in six cases.

6. Updating models

The approach used by the `CausalQueries` package to updating parameter values given observed data uses Stan (Carpenter *et al.* 2017).

Below we explain the data required by the generic Stan program implemented in the package, the structure of that program, and then show how to use the package to produce posterior draws of parameters.

6.1. Data for Stan

We use a generic Stan program that works for all binary causal models. The main advantage of the generic program we implement is that it allows us to pass the details of causal model as data inputs to Stan instead of generating individual Stan program for each causal model. The Stan model code can be found in Appendix B.

The data required by the Stan program includes vectors of observed data, and priors on parameters, as well as a set of matrices required for the mapping between events, data types, causal types and parameters. In addition, data includes counts of all relevant quantities as well as start and end positions of parameters pertaining to specific nodes and of distinct data strategies.

The internal function `prep_stan_data()` takes the model and data as arguments and produces a list with all objects that are required by the generic Stan program. Package users do not need to call the `prep_stan_data()` function directly.

6.2. How the Stan program works

The Stan model involves the following elements: (1) a specification of priors over sets of parameters, (2) a mapping from parameters to event probabilities, and (3) a likelihood function. Below we describe each of those elements in more details.

Probability distributions over parameter sets

The causal structure provided by a DAG allows us to reduce the problem of generating a probability distribution over all parameters to one of generating distributions over "sets" of parameters. In the absence of unobserved confounding, these sets correspond to the nodal types for each node: we have a probability distribution over the set of nodal types. In cases with confounding these are sets of nodal types for a given node *given* values of other nodes: we have to characterize the probability of each nodal type in a set given the values of nodal types for other nodes.

To illustrate, in the $X \rightarrow Y$ model we have two parameter sets. The first is $\lambda^X \in \{\lambda^X_0, \lambda^X_1\}$ whose elements give the probability that X is 0 or 1. These two probabilities sum to one. The second parameter set is $\lambda^Y \in \{\lambda^Y_{00}, \lambda^Y_{10}, \lambda^Y_{01}\lambda^Y_{11}\}$. These are also probabilities and their values sum to one. Note that we have 6 parameters but just $1 + 3 = 4$ degrees of freedom.

We express priors over these parameter sets using multiple Dirichlet distributions. Thus for instance we have $(\lambda^X_0, \lambda^X_1) \sim Dirichlet(\alpha^X_0, \alpha^X_1)$. Overall in $X \rightarrow Y$ we have a 2-dimensional Dirichlet distribution over the X nodal types (equivalently, a Beta distribution) and a 4-dimensional Dirichlet over the Y nodal types.

Event probabilities

For any candidate parameter vector λ we calculate the probability of "data types". This is done using a matrix that maps from parameters into data types. In cases without confounding there is a column for each data type; the matrix indicates which nodes in each set "contribute" to the data type, and the probability of the data type is found by summing within sets and taking the product over sets.

To illustrate we can examine the parameter mapping matrix for a simple model using the `grab` function:

```
R> make_model("X -> Y") |>
+  grab("parameter_mapping")
```

```
#>      X0Y0 X1Y0 X0Y1 X1Y1
#> X.0     1    0    1    0
#> X.1     0    1    0    1
#> Y.00    1    1    0    0
#> Y.10    0    1    1    0
#> Y.01    1    0    0    1
#> Y.11    0    0    1    1
#> attr(,"map")
#>      X0Y0 X1Y0 X0Y1 X1Y1
#> X0Y0    1    0    0    0
#> X1Y0    0    1    0    0
```

```
#> X0Y1     0     0     1     0
#> X1Y1     0     0     0     1
```

In this model, the probability of data type `X0Y0`, w_{00} is $\lambda_0^X \times \lambda_{00}^Y + \lambda_0^X \times \lambda_{01}^Y$. This formaula can be read from the parameter mapping matrix by combining a parameter vector with the first column of the matrix, taking the product of the probability of `X.0` and the *sum* of the probabilities for `Y.00` and `Y.01`.

In cases with confounding the approach is similar except that the parameter mapping matrix can contain multiple columns for each data type to capture non-independence between nodes.

In the case of incomplete data we first identify the set of "data strategies", where a collection of a data strategy might be of the form "gather data on X and M, but not Y, for n_1 cases and gather data on X and Y, but not M, for n_2 cases." The probability of an observed event, within a data strategy, is given by summing the probabilities of the types that could give rise to the incomplete data.

Data probability

Once we have the event probabilities in hand for each data strategy we are ready to calculate the probability of the data. For a given data strategy this is given by a multinomial distribution with these event probabilities. When there is incomplete data, and so multiple data strategies, this is given by the the product of the multinomial probabilities for each strategy.

6.3. Implementation

To update a `CausalQueries` model with data use:

```
R> model <- update_model(model, data)
```

The `data` argument provides a data frame containing some or all of the nodes in the model. The function `update_model()` relies on `rstan::sampling()` to draw from the posterior distribution and one can pass any additional arguments accepted by `rstan::sampling()` in `...` . Given that for complex models the model updating can sometimes be slow in Appendix A we show how users can utilize parallelization to improve computation speed. Appendix C provides an overview of model updating benchmarks, evaluating the effects of model complexity and data size on updating times.

6.4. Incomplete and censored data

`CausalQueries` assumes that missing data is missing at random, conditional on observed data. For instance in an $X \rightarrow M \rightarrow Y$ model, a researcher might have chosen to observe M in a random set of cases in which $X = 1$ and $Y = 1$. In that case if there are positive relations at each stage you may be more likely to observe M in cases in which $M = 1$. However observation of M is still random conditional on the observed X and Y data. The Stan model in `CausalQueries` takes account of this kind of sampling naturally by asseevent_probabilitiesssing the probability of observing a particular pattern of data within each data strategy. For a discussion see Section 9.2.3.2 of Humphreys and Jacobs (2023).

In addition, it is possible to indicate when data has been censored and for the Stan model to take this into account also. Say for instance that we only get to observe X in cases where $X = 1$ and not when $X = 0$. This kind of sampling is non random conditional on observables. It is taken account however by indicating to Stan that the probability of observing a particular data type is 0, regardless of parameter values. This is done using the `censored_types` argument in `update_model()`.

To illustrate, in the example below we observe perfectly correlated data for X and Y. If we are aware that data in which $X \neq Y$ has been censored then when we update we do not move towards a belief that X causes Y.

```
R> data <- data.frame(X = rep(0:1, 5), Y = rep(0:1, 5))
R>
R> list(
+  uncensored =
+    make_model("X -> Y") |>
+    update_model(data),
+  censored =
+    make_model("X -> Y") |>
+    update_model(data, censored_types = c("X1Y0",  "X0Y1"))
+  ) |>
+
+  query_model(te("X", "Y"), using = "posteriors")
```

Table 8: Posterior inferences taking account of censoring and not.

model	query	mean	sd
uncensored	(Y[X=1] - Y[X=0])	0.59	0.20
censored	(Y[X=1] - Y[X=0])	0.02	0.32

6.5. Output

The primary output from `update_model()` is a model with an attached posterior distribution over model parameters, stored as a data frame in the model list. This posterior distribution can be directly accessed using `grab(model, "posterior_distribution")`.

```
R> make_model("X -> Y")  |>
+  update_model() |>
+  grab("posterior_distribution")
```

In addition, a distribution of causal types is stored by default; the `stanfit` object and a distribution over event probabilities are optionally saved as follows.

```
R> lipids_model <-
+  lipids_model |>
+  update_model(keep_fit = TRUE,
+               keep_event_probabilities = TRUE)
```

The summary of the Stan model evaluated by the call to `update_model()` can be accessed using `grab()` function and is saved regardless of other options. This provides two measures to help assess convergence.

```
R> make_model("X -> Y")  |>
+  update_model(keep_type_distribution = FALSE) |>
+  grab("stan_summary")
```

```
#> Inference for Stan model: simplexes.
#> 4 chains, each with iter=2000; warmup=1000; thin=1;
#> post-warmup draws per chain=1000, total post-warmup draws=4000.
#>
#>             mean se_mean   sd   2.5%   25%   50%   75% 97.5% n_eff Rhat
#> X.0         0.51    0.01 0.28   0.03  0.26  0.51  0.75  0.97  2921    1
#> X.1         0.49    0.01 0.28   0.03  0.25  0.49  0.74  0.97  2921    1
#> Y.00        0.25    0.00 0.19   0.01  0.09  0.20  0.37  0.70  2198    1
#> Y.10        0.25    0.00 0.20   0.01  0.09  0.21  0.37  0.72  4235    1
#> Y.01        0.25    0.00 0.20   0.01  0.09  0.21  0.38  0.71  4414    1
#> Y.11        0.25    0.00 0.19   0.01  0.10  0.21  0.37  0.70  4395    1
#> lp__       -7.53    0.05 1.66 -11.72 -8.35 -7.16 -6.30 -5.43  1284    1
#>
#> Samples were drawn using NUTS(diag_e) at Wed Apr 17 18:13:54 2024.
#> For each parameter, n_eff is a crude measure of effective sample size,
#> and Rhat is the potential scale reduction factor on split chains (at
#> convergence, Rhat=1).
```

This summary provides information on the distribution of parameters as well as convergence diagnostics, summarized in the `Rhat` column. The last row shows the unnormalized log density on Stan's unconstrained space which, as described in Stan documentation is intended to diagnose sampling efficiency and evaluate approximations. This summary can also include summaries for the transformed parameters, if users opt to retain these (see Table 5 for options).

If users are require more advanced diagnostics of performance they can retain and access the `raw` stan output.

```
R> model <- make_model("X -> Y") |>
+  update_model(refresh = 0, keep_fit = TRUE)
```

Note that the raw output uses labels from the generic `stan` model: `lambda` for the vector of parameters, corresponding to the parameters in the parameters dataframe (`grab(model, "parameters_df")`), and , if saved, a vector `types` for the causal types (see `grab(model, "causal_types")`) and `event_probabilities` for the event probabilities (`grab(model, "event_probabilities")`).

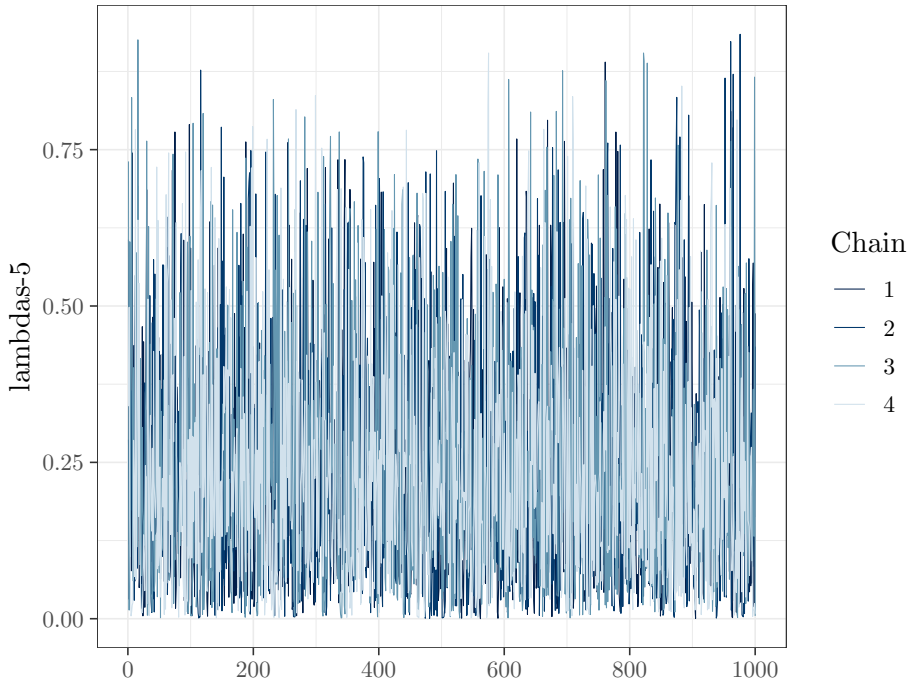
```
R> model |> grab("stan_fit")
```

```
#> Inference for Stan model: simplexes.
#> 4 chains, each with iter=2000; warmup=1000; thin=1;
#> post-warmup draws per chain=1000, total post-warmup draws=4000.
#>
```

```
#>             mean se_mean   sd   2.5%   25%   50%   75% 97.5% n_eff Rhat
#> lambdas[1]  0.50    0.01 0.29   0.03  0.26  0.51  0.75  0.97  2831    1
#> lambdas[2]  0.50    0.01 0.29   0.03  0.25  0.49  0.74  0.97  2831    1
#> lambdas[3]  0.25    0.00 0.19   0.01  0.09  0.21  0.37  0.71  1940    1
#> lambdas[4]  0.25    0.00 0.19   0.01  0.09  0.20  0.37  0.70  3752    1
#> lambdas[5]  0.25    0.00 0.19   0.01  0.09  0.20  0.37  0.71  4425    1
#> lambdas[6]  0.25    0.00 0.19   0.01  0.09  0.21  0.38  0.71  4746    1
#> types[1]    0.13    0.00 0.13   0.00  0.03  0.08  0.19  0.50  2317    1
#> types[2]    0.13    0.00 0.13   0.00  0.03  0.08  0.18  0.48  2243    1
#> types[3]    0.12    0.00 0.13   0.00  0.03  0.08  0.18  0.50  3462    1
#> types[4]    0.12    0.00 0.13   0.00  0.02  0.08  0.18  0.48  3095    1
#> types[5]    0.12    0.00 0.13   0.00  0.03  0.08  0.18  0.48  3494    1
#> types[6]    0.12    0.00 0.13   0.00  0.03  0.08  0.18  0.47  3526    1
#> types[7]    0.13    0.00 0.14   0.00  0.03  0.08  0.18  0.49  3495    1
#> types[8]    0.12    0.00 0.13   0.00  0.03  0.08  0.18  0.48  3774    1
#> lp__       -7.55    0.04 1.64 -11.53 -8.44 -7.21 -6.29 -5.45  1490    1
#>
#> Samples were drawn using NUTS(diag_e) at Wed Apr 17 18:13:59 2024.
#> For each parameter, n_eff is a crude measure of effective sample size,
#> and Rhat is the potential scale reduction factor on split chains (at
#> convergence, Rhat=1).
```

Users can then use diagnostic packages such as `bayesplot`.

```
R> np <- model |> grab("stan_fit") |> bayesplot::nuts_params()
R>
R> model |> grab("stan_fit") |>
+  bayesplot::mcmc_trace(pars = "lambdas[5]", np = np) +
+  ylab("lambdas-5")
```



7. Queries

`CausalQueries` provides functionality to pose and answer elaborate causal queries. The key approach is to code causal queries as functions of causal types and return a distribution over the queries that is implied by the distribution over causal types.

7.1. Calculating factual and counterfactual quantities

A key step in the calculation of most queries is the assessment of what outcomes will arise for causal types given different interventions on nodes. In practice, we map from causal types to data types by propagating realized values on nodes forward in the DAG, moving from exogenous or intervened upon nodes to their descendants in generational order. The `realise_outcomes()` function achieves this by traversing the DAG, while recording for each node's nodal types, the values implied by realizations on the node's parents.

To illustrate, consider the first causal type of a $X \rightarrow Y$ model:

1. θ_0^X implies that, absent intervention on X, X has a realized value of 0; θ_{00}^Y implies that, absent intervention on Y, Y has a realized value of 0 regardless of X
2. We substitute for Y the value implied by the 00 nodal type given a 0 value on X, which in turn is 0 (see Section 5.2.2).

Calling `realise_outcomes()` on this model yields the outcomes implied by all causal types:

```
R> make_model("X -> Y") |> realise_outcomes()
```

```
#>      X Y
#> 0.00 0 0
#> 1.00 1 0
#> 0.10 0 1
#> 1.10 1 0
#> 0.01 0 0
#> 1.01 1 1
#> 0.11 0 1
#> 1.11 1 1
```

In the output above, row names indicate nodal types and columns realized values. Intervening on X (see Pearl 2009) with $do(X = 1)$ yields:

```
R> make_model("X -> Y") |> realise_outcomes(dos = list(X = 1))
```

```
#>      X Y
#> 0.00 1 0
#> 1.00 1 0
#> 0.10 1 0
#> 1.10 1 0
#> 0.01 1 1
#> 1.01 1 1
#> 0.11 1 1
#> 1.11 1 1
```

In the same way `realise_outcomes()` can return the realized values on all nodes for each causal type given arbitrary interventions.

7.2. Causal Syntax

`CausalQueries` provides syntax for the formulation of various causal queries including queries on all rungs of the "causal ladder" (Pearl 2009): prediction, such as the proportion of units where Y equals 1; intervention, such as the probability that $Y = 1$ when X is *set* to 1; counterfactuals, such as the probability that Y would be 1 were $X = 1$ given we know Y is 0 when X was observed to be 0. Queries can be posed at the population level or case level and can be unconditional (e.g. what is the effect of X on Y for all units) or conditional (for example, the effect f X on Y for units for whom Z affects X). This syntax enables users to write arbitrary causal queries to interrogate their models.

The heart of querying is figuring out which causal types correspond to particular queries. For factual queries, users may employ logical statements to ask questions about observed conditions, without any intervention. Take, for example, the query mentioned above about the proportion of units where Y equals 1, expressed as `"Y == 1"`. In this case the logical operator `==` indicates that `CausalQueries` should consider units that fulfill the condition of strict equality where Y equals 1.[6] When this query is posed, the `get_query_types()` function identifies all types that give rise to $Y = 1$, absent any interventions.

[6] `CausalQueries` also accepts = as a shorthand for ==. However, == is preferred as it is the conventional logical operator to express a condition of strict equality.

```
R> make_model("X -> Y")  |> get_query_types("Y==1")

#>
#> Causal types satisfying query's condition(s)
#>
#>  query =  Y==1
#>
#> X0.Y10  X1.Y01
#> X0.Y11  X1.Y11
#>
#>
#>  Number of causal types that meet condition(s) =  4
#>  Total number of causal types in model =  8
```

The key to posing causal queries is being able to ask about values of variables given that the values of some other variables are "controlled". This corresponds to application of the `do` operator in Pearl (2009). In `CausalQueries` this is done by putting square brackets `[ ]` around variables that should be intervened upon.

For instance, consider the query `Y[X=0]==1`. This query asks about the types for which Y equals 1 when X is set to 0. In this case, since X is being intervened to be zero, X is placed inside the brackets. Given that Y equaling 1 is a condition about potentially observed values, it is expressed as using the logical operator `==`. The set of causal types that meets this query is quite different:

```
R> make_model("X -> Y")  |> get_query_types("Y[X=1]==1")

#>
#> Causal types satisfying query's condition(s)
#>
#>  query =  Y[X=1]==1
#>
#> X0.Y01  X1.Y01
#> X0.Y11  X1.Y11
#>
#>
#>  Number of causal types that meet condition(s) =  4
#>  Total number of causal types in model =  8
```

When a node has multiple parents it is possible to set the values of none, some or all of the parents. For instance if $X1$ and $X2$ are parents of Y then `Y==1`, `Y[X1 = 1]==1`, and `Y[X1 = 1, X2 = 1]==1` queries cases for which $Y = 1$ when, respectively, neither parents values are controlled, when $X1$ is set to 1 but $X2$ is not controlled, and when both $X1$ and $X2$ are set to 1. For example we can have:

```
R> make_model("X1 -> Y <- X2")  |>
+  get_query_types("X1==1 & X2==1 & (Y[X1=1, X2=1] > Y[X1=0, X2=0])")

#>
#> Causal types satisfying query's condition(s)
#>
```

```
#>  query =  X1==1&X2==1&(Y[X1=1,X2=1]>Y[X1=0,X2=0])
#>
#> X11.X21.Y0001  X11.X21.Y0101
#> X11.X21.Y0011  X11.X21.Y0111
#>
#>
#>  Number of causal types that meet condition(s) =  4
#>  Total number of causal types in model =  64
```

In this case, the aim is to identify the types for which $X1 = X2 = 1$ *and at the same time* $Y = 0$ when $X1 = X2 = 0$, and $Y = 1$ when $X1 = X2 = 1$.

In general, the variables to be intervened upon, as if conducting an experiment, are placed inside square brackets, followed by an equal sign and the value to which we want to set them, either 1 or 0. The variable whose value is observed should be placed before the square brackets. Thus `"Y[X=1]"` queries the values of Y when X is set to 1. Finally, conditions related to observed or potentially observed values, in the context of an intervention, are expressed outside the brackets, along with the logical condition that defines the observed values, as in `"Y==1"`, `"Y[X=1]==1` or `"Y[X=1] > Y[X=0]"`.

Conditional queries

Many queries of interest are "conditional" queries. For example the effect of X on Y for units for which $W = 1$. Or the the effect of X on Y for units for which Z has a positive effect on X. Such conditional queries are posed in `CausalQueries` by providing a `given` statement in addition to the `query` statement. The full query then becomes: for what units does the `query` condition hold among those units for which the `given` condition holds. The two parts can each be calculated using `get_query_types`. Thus for instance in an $X \rightarrow Y$ model the probability that X causes Y given $X = 1 \& Y = 1$ is the probability of causal `X1.Y11` type divided by the sum of the probabilities of types `X1.Y11` and `X1.Y01`. In practice this is done automatically for users when they call `query_model()` or `query_distribution()`.

Complex expressions

Many queries involve complex statements over multiple sets of types. These can be formed with the aid of relational operators. For example, you can make queries about cases where X has a positive effect on Y, i.e., whether Y is greater when X is set to 1 compared to when X is set to 0, expressed as `"Y[X=1] > Y[X=0]"`. The query "X has some effect on Y" is given by `"Y[X=1] != Y[X=0]"`.

Linear operators can also be used over set of simple statements. Thus `"Y[X=1] - Y[X=0]"` returns the average treatment effect. In essence rather than returning a `TRUE` or `FALSE` for the two parts of the query, the case memberships are forced to numeric values (1 or 0) and the differences are taken, which can be a 1, 0 or -1 depending on the causal type. Averaging in effect averages over the share of cases with positive effects, less the share of cases with negative effects.

```
R> make_model("X -> Y")  |> get_query_types("Y[X=1] - Y[X=0]")
```

```
#> X0.Y00 X1.Y00 X0.Y10 X1.Y10 X0.Y01 X1.Y01 X0.Y11 X1.Y11
#>      0      0     -1     -1      1      1      0      0
```

Nested queries

`CausalQueries` lets users pose nested "complex counterfactual" queries. For instance `"Y[M=M[X=0], X=1]==1"` queries the types for which Y equals 1 when X is set to 1, while keeping M constant at the value it would take if X were 0.

7.3. Quantifying queries

Giving a *quantitative* answer to a query requires placing probabilities over the causal types that correspond to a query.

Queries by hand

Queries can be calculated directly from the prior distribution or the posterior distribution provided by Stan. For example the following call plots the posterior distribution for the query that probability of Y is increasing in X for the $X \rightarrow Y$ model. The resulting plot is shown in Figure 2.

```
R> data  <- data.frame(X = rep(0:1, 50), Y = rep(0:1, 50))
R>
R> model <-
+  make_model("X -> Y") |>
+  update_model(data, iter  = 4000, refresh = 0)
R>
R> model |> grab("posterior_distribution")  |>
+  ggplot(aes(Y.01 - Y.10)) + geom_histogram()
```

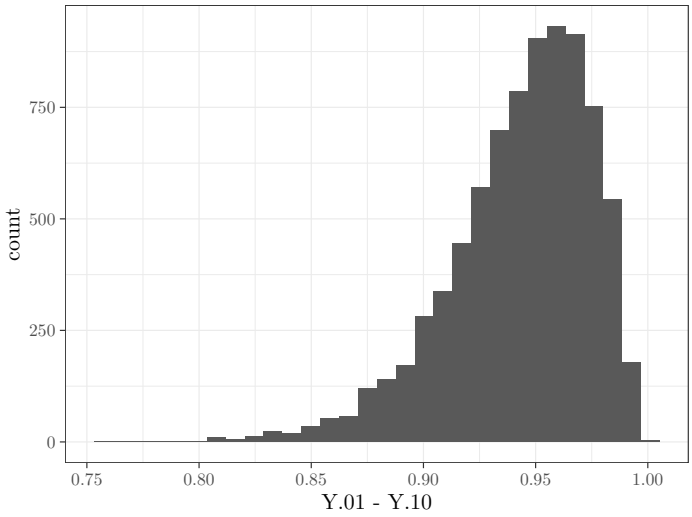


Figure 2: Posterior on "Probability Y is increasing in X".

Query distribution

It is generally useful to use causal syntax to define the query and calculate the query with respect to the prior or posterior probability distributions. This can be done for a list of queries using `query_distribution()` function as follows:

```
R> make_model("X -> Y") |>
+  query_distribution(
+    query = list(increasing = "(Y[X=1] > Y[X=0])"),
+    using = "priors")
```

`query_distribution()` can also be used when one is interested in assessing the value of a query for a *particular case*. In a sense this is equivalent to posing a conditional query, querying conditional on values in a case. For instance we might consult our posterior for Lipids model and ask about the effect of X on Y for a case in which $Z = 1$, $X = 1$ and $Y = 1$.

```
R> lipids_model |>
+    query_model(query = "Y[X=1] - Y[X=0]",
+                given = "X==1 & Y==1 & Z==1",
+                using = "posteriors")

#>
#> Causal queries generated by query_model (all at population level)
#>
#> |query           |given              |using      |  mean|    sd| cred.low| cred.high|
#> |:---------------|:------------------|:----------|-----:|-----:|--------:|---------:|
#> |Y[X=1] - Y[X=0] |X==1 & Y==1 & Z==1 |posteriors | 0.954| 0.036|    0.862|     0.997|
```

The result is what we now believe for all cases in which $Z = 1$, $X = 1$ and $Y = 1$. It is in fact the expected average effect among cases with this data type and so this expectation has an uncertainty attached to it.

This is, in principle, different to what we would infer for a "new case" that we wonder about. When inquiring about a new case, the case level query *updates* on the given information observed in the new case. The resulting inference can be different to the inference that would be made from the posterior *given* the features of the case. If `case_level = TRUE` is specified, this new case level inference is calculated. For a query Q and given D this returns the value $\frac{\int \pi(Q\&D|\lambda_i)p(\lambda_i)d\lambda_i}{\int \pi(D|\lambda_i)p(\lambda_i)d\lambda_i}$ which may differ from the mean of the distribution $\frac{\pi(Q\&D|\lambda)}{\pi(D|\lambda)}$, $\int \frac{\pi(Q\&D|\lambda_i)}{\pi(D|\lambda_i)}p(\lambda_i)d\lambda_i$.

To simplify, consider a model where it is clear that X causes Y, but it is uncertain if this is through two positive or two negative effects. If we encounter a case with $M = 0$, it is unclear if this indicates an effect or not. However, if we randomly find a case with $M = 0$, our understanding of the causal model evolves, leading us to believe there is an effect in this specific case, which would not be the case if $M = 1$. In this case, the case level query gives a single value without posterior standard deviation, representing the belief about this new case. The non-case level query summarizes the posterior distribution for cases with similar data.

```
R> # "Results for a case level query"
R>
R> make_model("X -> M -> Y") |>
+  update_model(data.frame(X = rep(0:1, 8), Y = rep(0:1, 8)), iter = 4000) |>
+  query_model("Y[X=1] > Y[X=0]",
+              given = "X==1 & Y==1 & M==1",
+              using = "posteriors",
+              case_level = c(TRUE, FALSE))

#>
#> Causal queries generated by query_model
#>
#> |query           |given              |using      |case_level |  mean|    sd| cred.low|
#> |:---------------|:------------------|:----------|:----------|-----:|-----:|--------:|-
#> |Y[X=1] > Y[X=0] |X==1 & Y==1 & M==1 |posteriors |TRUE       | 0.674|    NA|    0.674|
#> |Y[X=1] > Y[X=0] |X==1 & Y==1 & M==1 |posteriors |FALSE      | 0.429| 0.327|    0.004|
```

Batch queries

The function `query_model()` is perhaps the most important function for querying models. The function takes as input a list of models, causal queries, and conditions. It then calculates population or case level estimands given prior or posterior distributions and reports summaries of these distributions. The result is a data frame that can be displayed as a table or used for graphing.

Table 9 returns to the Lipids data and shows output from a single call to `query_model()` with the `expand_grid` argument set to `TRUE` to generate all combinations of list elements.

```
R> models <- list(
+  A = lipids_model |>
+    update_model(data = lipids_data, refresh = 0),
+  B = lipids_model |> set_restrictions("X[Z=1] < X[Z=0]") |>
```

```
+    update_model(data = lipids_data, refresh = 0))
R>
R> queries <-
+  query_model(
+  models,
+  query = list(ATE = "Y[X=1] - Y[X=0]",
+               POS = "Y[X=1] > Y[X=0]"),
+  given = c(TRUE,  "Y==1 & X==1"),
+  case_level = c(FALSE, TRUE),
+  using = c("priors", "posteriors"),
+  expand_grid = TRUE)
```

Table 9: Results for two queries on two models.

model	query	given	using	case_level	mean	sd
A	ATE	-	priors	FALSE	0.01	0.20
B	ATE	-	priors	FALSE	0.00	0.22
A	ATE	-	posteriors	FALSE	0.55	0.10
B	ATE	-	posteriors	FALSE	0.56	0.10
A	ATE	Y==1 & X==1	priors	FALSE	0.50	0.22
B	ATE	Y==1 & X==1	priors	FALSE	0.50	0.24
A	ATE	Y==1 & X==1	posteriors	FALSE	0.95	0.04
B	ATE	Y==1 & X==1	posteriors	FALSE	0.95	0.04
A	POS	-	priors	FALSE	0.25	0.12
B	POS	-	priors	FALSE	0.25	0.13
A	POS	-	posteriors	FALSE	0.61	0.10
B	POS	-	posteriors	FALSE	0.61	0.10
A	POS	Y==1 & X==1	priors	FALSE	0.50	0.22
B	POS	Y==1 & X==1	priors	FALSE	0.50	0.24
A	POS	Y==1 & X==1	posteriors	FALSE	0.95	0.04
B	POS	Y==1 & X==1	posteriors	FALSE	0.95	0.04
A	ATE	-	priors	TRUE	0.01	NA
B	ATE	-	priors	TRUE	0.00	NA
A	ATE	-	posteriors	TRUE	0.55	NA
B	ATE	-	posteriors	TRUE	0.56	NA
A	ATE	Y==1 & X==1	priors	TRUE	0.50	NA
B	ATE	Y==1 & X==1	priors	TRUE	0.50	NA
A	ATE	Y==1 & X==1	posteriors	TRUE	0.95	NA
B	ATE	Y==1 & X==1	posteriors	TRUE	0.95	NA
A	POS	-	priors	TRUE	0.25	NA
B	POS	-	priors	TRUE	0.25	NA
A	POS	-	posteriors	TRUE	0.61	NA
B	POS	-	posteriors	TRUE	0.61	NA
A	POS	Y==1 & X==1	priors	TRUE	0.50	NA

B	POS	Y==1 & X==1	priors	TRUE	0.50	NA
A	POS	Y==1 & X==1	posteriors	TRUE	0.95	NA
B	POS	Y==1 & X==1	posteriors	TRUE	0.95	NA

Computational details and software requirements

Version	• 1.21 |
Availability	• Stable Release: https://cran.rstudio.com/web/packages/CausalQueries/index.html • Development: https://github.com/integrated-inferences/CausalQueries
Issues	• https://github.com/integrated-inferences/CausalQueries/issues
Operating Systems	• Linux • MacOS • Windows
Testing Environments OS	• Ubuntu 22.04.2 • Debian 12.2 • MacOS • Windows
Testing Environments R	• R 4.3.1 • R 4.3.0 • R 4.2.3 • r-devel
R Version	• R(>= 3.4.0)
Compiler	• either of the below or similar: • g++ • clang++
Stan requirements	• inline • Rcpp (>= 0.12.0) • RcppEigen (>= 0.3.3.3.0) • RcppArmadillo (>= 0.12.6.4.0) • RcppParallel (>= 5.1.4) • BH (>= 1.66.0) • StanHeaders (>= 2.26.0) • rstan (>= 2.26.0)
R-Packages Depends	• dplyr • methods
R-Packages Imports	• dagitty (>= 0.3-1) • dirmult (>= 0.1.3-4) • stats (>= 4.1.1) • rlang (>= 0.2.0) • rstan (>= 2.26.0) • rstantools (>= 2.0.0) • stringr (>= 1.4.0) • ggdag (>= 0.2.4) • latex2exp (>= 0.9.4) • ggplot2 (>= 3.3.5) • lifecycle (>= 1.0.1)

The results in this paper were obtained using R~3.4.1 with the **MASS**~7.3.47 package. R itself

and all packages used are available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/.

Acknowledgments

We thank Ben Goodrich who provided generous insights on using `stan` for this project. We thank Alan M Jacobs for key work developing the framework underlying the package. Our thanks to Cristian-Liviu Nicolescu who provided wonderful feedback on use of the package and a draft of this paper. Our thanks to Jasper Cooper for contributions generating a generic function to create Stan code, to Clara Bicalho who helped figure out the syntax for causal statements, to Julio S. Solís Arce who made many key contributions figuring out how to simplify the specification of priors, and to Merlin Heidemanns who figured out the `rstantools` integration and made myriad code improvements.

References

Angrist JD, Imbens GW, Rubin DB (1996). "Identification of Causal Effects Using Instrumental Variables." *Journal of the American Statistical Association*, **91**(434), 444–455. doi:10.1080/01621459.1996.10476902.

Balke A, Pearl J (1997). "Bounds on Treatment Effects from Studies with Imperfect Compliance." *Journal of the American Statistical Association*, **92**(439), 1171–1176. doi:10.1080/01621459.1997.10474074.

Beaumont P, Horsburgh B, Pilgerstorfer P, Droth A, Oentaryo R, Ler S, Nguyen H, Ferreira GA, Patel Z, Leong W (2021). "**CausalNex**." URL https://github.com/quantumblacklabs/causalnex.

Carpenter B, Gelman A, Hoffman MD, Lee D, Goodrich B, Betancourt M, Brubaker MA, Guo J, Li P, Riddell A (2017). "**Stan**: A Probabilistic Programming Language." *Journal of Statistical Software*, **76**, 1. doi:10.18637/jss.v076.i01.

Chickering DM, Pearl J (1996). "A Clinician's Tool for Analyzing Non-Compliance." In *Proceedings of the National Conference on Artificial Intelligence*, pp. 1269–1276. URL https://cdn.aaai.org/AAAI/1996/AAAI96-188.pdf.

Duarte G, Finkelstein N, Knox D, Mummolo J, Shpitser I (2023). "An Automated Approach to Causal Inference in Discrete Settings." *Journal of the American Statistical Association*, pp. 1–16. doi:10.1080/01621459.2023.2216909.

Frangakis CE, Rubin DB (2002). "Principal Stratification in Causal Inference." *Biometrics*, **58**(1), 21–29. doi:10.1111/j.0006-341X.2002.00021.x.

Humphreys M, Jacobs AM (2023). *Integrated Inferences: Causal Models for Qualitative and Mixed-Method Research*. Cambridge University Press. doi:10.1017/9781316718636.

Kalisch M, Mächler M, Colombo D, Maathuis MH, Bühlmann P (2012). "Causal Inference Using Graphical Models with the R Package **pcalg**." *Journal of Statistical Software*, **47**, 1–26. doi:10.18637/jss.v047.i11.

Pearl J (2009). *Causality*. Cambridge University Press. ISBN 978-0-521-89560-6.

Poirier DJ (1998). "Revising Beliefs in Nonidentified Models." *Econometric Theory*, **14**(4), 483–509. doi:10.1017/S0266466698144043.

Sachs MC, Jonzon G, Sjölander A, Gabriel EE (2023). "A General Method for Deriving Tight Symbolic Bounds on Causal Effects." *Journal of Computational and Graphical Statistics*, **32**(2), 567–576. doi:10.1080/10618600.2022.2071905.

Sharma A, Kiciman E (2020). "DoWhy: An End-to-End Library for Causal Inference." *arXiv preprint arXiv:2011.04216*.

Textor J, van der Zander B, Gilthorpe MS, Liśkiewicz M, Ellison GT (2016). "Robust Causal Inference Using Directed Acyclic Graphs: the R Package **dagitty**." *International Journal of Epidemiology*, **45**(6), 1887–1894. doi:10.1093/ije/dyw341.

Zhang J, Tian J, Bareinboim E (2022). "Partial Counterfactual Identification from Observational and Experimental Data." In *Proceedings of the 39th International Conference on Machine Learning*, pp. 26548–26558. PMLR. URL https://proceedings.mlr.press/v162/zhang22ab.html.

Appendix A: Parallelization

If you have multiple cores you can do parallel processing by including this line before running `CausalQueries`:

```
R> library(parallel)
R>
R> options(mc.cores = parallel::detectCores())
```

Additionally parallelizing across models or data while running MCMC chains in parallel can be achieved by setting up a nested parallel process. With 8 cores one can run two updating processes with three parallel chains each simultaneously. More generally the number of parallel processes at the upper level of the nested parallel structure are given by $\lfloor \frac{cores}{chains+1} \rfloor$.

```
R> library(future)
R> library(future.apply)
R>
R> chains <- 3
R> cores <- 8
R>
R> future::plan(list(
+      future::tweak(future::multisession,
+                    workers = floor(cores/(chains + 1))),
+      future::tweak(future::multisession,
+                    workers = chains)
+    ))
R>
R> model <- make_model("X -> Y")
R> data <- list(data_1, data_2)
R>
R> future.apply::future_lapply(data, function(d) {
+  update_model(
+    model = model,
+    data = d,
+    chains = chains,
+    refresh = 0
+  )
+})
```

Appendix B: Stan code

Updating is performed using a generic Stan model. The data provided to Stan is generated by the internal function `prep_stan_data()` which returns a list of objects that Stan expects to receive. The code for the Stan model is shown below. After defining a helper function, the code starts with a block declaring what input data is to be expected. Then there is a characterization of parameters and the transformed parameters. Then the likelihoods and priors are provided. At the end there is a block for generated quantities which can be used

to append a posterior distribution of causal types to the model.

```
S4 class stanmodel 'simplexes' coded as follows:
functions{
  row_vector col_sums(matrix X) {
    row_vector[cols(X)] s ;
    s = rep_row_vector(1, rows(X)) * X ;
    return s ;
  }
}
data {
int<lower=1> n_params;
int<lower=1> n_paths;
int<lower=1> n_types;
int<lower=1> n_param_sets;
int<lower=1> n_nodes;
array[n_param_sets] int<lower=1> n_param_each;
int<lower=1> n_data;
int<lower=1> n_events;
int<lower=1> n_strategies;
int<lower=0, upper=1> keep_type_distribution;
vector<lower=0>[n_params] lambdas_prior;
array[n_param_sets] int<lower=1> l_starts;
array[n_param_sets] int<lower=1> l_ends;
array[n_nodes] int<lower=1> node_starts;
array[n_nodes] int<lower=1> node_ends;
array[n_strategies] int<lower=1> strategy_starts;
array[n_strategies] int<lower=1> strategy_ends;
matrix[n_params, n_types] P;
matrix[n_params, n_paths] parmap;
matrix[n_paths, n_data] map;
matrix<lower=0,upper=1>[n_events,n_data] E;
array[n_events] int<lower=0> Y;
}
parameters {
vector<lower=0>[n_params - n_param_sets] gamma;
}
transformed parameters {
vector<lower=0, upper=1>[n_params] lambdas;
vector<lower=1>[n_param_sets] sum_gammas;
matrix[n_params, n_paths] parlam;
matrix[n_nodes, n_paths] parlam2;
vector<lower=0, upper=1>[n_paths] w_0;
vector<lower=0, upper=1>[n_data] w;
vector<lower=0, upper=1>[n_events] w_full;
// Cases in which a parameter set has only one value need special handling
// they have no gamma components and sum_gamma needs to be made manually
```

```
for (i in 1:n_param_sets) {
  if (l_starts[i] >= l_ends[i]) {
    sum_gammas[i] = 1;
    // syntax here to return unity as a vector
    lambdas[l_starts[i]] = lambdas_prior[1]/lambdas_prior[1];
    }
  else if (l_starts[i] < l_ends[i]) {
    sum_gammas[i] =
    1 + sum(gamma[(l_starts[i] - (i-1)):(l_ends[i] - i)]);
    lambdas[l_starts[i]:l_ends[i]] =
    append_row(1, gamma[(l_starts[i] - (i-1)):(l_ends[i] - i)]) /
      sum_gammas[i];
    }
  }
// Mapping from parameters to data types
// (usual case): [n_par * n_data] * [n_par * n_data]
parlam  = rep_matrix(lambdas, n_paths) .* parmap;
// Sum probability over nodes on each path
for (i in 1:n_nodes) {
 parlam2[i,] = col_sums(parlam[(node_starts[i]):(node_ends[i]),]);
 }
// then take product  to get probability of data type on path
for (i in 1:n_paths) {
  w_0[i] = prod(parlam2[,i]);
 }
 // last (if confounding): map to n_data columns instead of n_paths
 w = map'*w_0;
  // Extend/reduce to cover all observed data types
 w_full = E * w;
}
model {
// Dirichlet distributions
for (i in 1:n_param_sets) {
  target += dirichlet_lpdf(lambdas[l_starts[i]:l_ends[i]]  |
    lambdas_prior[l_starts[i] :l_ends[i]]);
  target += -n_param_each[i] * log(sum_gammas[i]);
 }
// Multinomials
// Note with censoring event_probabilities might not sum to 1
for (i in 1:n_strategies) {
  target += multinomial_lpmf(
  Y[strategy_starts[i]:strategy_ends[i]] |
    w_full[strategy_starts[i]:strategy_ends[i]]/
     sum(w_full[strategy_starts[i]:strategy_ends[i]]));
 }
}
// Option to export distribution of causal types
```

```
generated quantities{
vector[n_types] types;
if (keep_type_distribution == 1){
for (i in 1:n_types) {
   types[i] = prod(P[, i].*lambdas + 1 - P[,i]);
}}
 if (keep_type_distribution == 0){
    types = rep_vector(1, n_types);
 }
}
```

Appendix C: Benchmarks

We present a brief summary of model updating benchmarks. The first benchmark considers the effect of model complexity on updating time. The second benchmark considers the effect of data size on updating time. We run 4 parallel chains for each model. Results of the benchmarks are presented in Table 11 and Table 12 respectively.

Table 11: Benchmark 1.

Model	Number of Model Parameters	`update_model()` Runt-Time (seconds)
$X1 \rightarrow Y$	6	10.85
$X1 \rightarrow Y \leftarrow X2$	20	15.79
$X1 \rightarrow Y \leftarrow X2; X3 \rightarrow Y$	262	77.56

Table 12: Benchmark 2.

Model	Number of Observations	`update_model()` Run-Time (seconds) |
$X1 \rightarrow Y$	10	9.04
$X1 \rightarrow Y$	100	9.31
$X1 \rightarrow Y$	1000	10.56
$X1 \rightarrow Y$	10000	14.57
$X1 \rightarrow Y$	100000	17.25

Increasing the number of parents in a model greatly increases the number of parameters and computational time. The growth of the parameter space with increasing model complexity places limits on feasible computability without further recourse to specialized methods for handling large causal models. Data size increases here have a more modest effect on computation time.

Affiliation:

Till Tietz
IPI
Reichpietschufer 50
Berlin Germany
E-mail: ttietz2014@gmail.com
URL: https://github.com/till-tietz

Lily Medina
E-mail: lily.medina@berkeley.edu
URL: https:/lilymedina.github.io/

Georgiy Syunyaev
E-mail: g.syunyaev@vanderbilt.edu
URL: https://gsyunyaev.com/

Macartan Humphreys
IPI
Reichpietschufer 50
Berlin Germany
E-mail: macartan.humphreys@wzb.eu
URL: https://macartan.github.io/

Journal of Statistical Software http://www.jstatsoft.org/
published by the Foundation for Open Access Statistics http://www.foastat.org/
MMMMMM YYYY, Volume VV, Issue II *Submitted:* yyyy-mm-dd
doi:10.18637/jss.v000.i00 *Accepted:* yyyy-mm-dd