

# Journal of Statistical Software

MMMMMM YYYY, Volume VV, Issue II.

doi: 10.18637/jss.v000.i00

# Making, Updating, and Querying Causal Models using CausalQueries

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#### Abstract

A guide to the  $\mathsf{R}$  package  $\mathsf{CausalQueries}$  for making, updating, and querying causal models

Keywords: causal models, stan, bayes.

#### 1. Introduction: Causal models

#### 1.1. What CausalQueries does

CausalQueries is an R package that lets users make, update, and query causal models. The base specification asks users to provide a statement that reports a set of binary variables and the relations of causal ancestry between them: which variables are direct causes of other variables, given the other variables in the model. Once provided to make\_model(), CausalQueries generates a set of parameters that fully describe all possible types of causal relations between variables ("causal types"), given the causal structure. Given a prior over distributions over causal types and data over some or all nodes, update\_model() deploys a stan model in order to generate a posterior distribution over parameters. The function query\_model() can then be used to ask any causal query of the model, using either the prior distribution, the posterior distribution, or a user specified candidate vector of parameters.

We illustrate these three core functions by showing how to use CuasalQueries to replicate

query	given	mean	sd	${\rm cred.low.} 2.5\%$	cred.high.97.5%
Y[X=1] - Y[X=0]	-	0.56	0.10	0.38	0.73
Y[X=1] - Y[X=0]	X==0 & Y==0	0.64	0.15	0.38	0.89
Y[X=1] - Y[X=0]	X[Z=1] > X[Z=0]	0.70	0.05	0.60	0.80

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

Rows 1 and 2 replicate results in Chickering and Pearl (1996); row 3 returns inferences for complier average effects.

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 treatment 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.

Our data on Z, X, and Y 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
                          12
                  ZXY
#> 7 Z0X1Y1
                  ZXY
                           0
#> 8 Z1X1Y1
                  ZXY
                          78
```

With CausalQueries, you can create the model, input data to update it, and then query the model for results.

```
R> make_model("Z -> X -> Y; X <-> Y") |>
+ update_model(lipids_data, refresh = 0) |>
+ 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. For example the data frame produced by the code above is shown in Table 1.

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.

#### 1.2. Connections to existing packages

- Embed the *software* into the respective relevant literature.
- compare with bareinboim package
- knox bounds package

#### 2. Statistical model

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

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

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

In the usual case we take the endogenous nodes to be binary.<sup>1</sup> 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 all possible ways that a node might respond to its parents. We refer to the ways that a node responds and the nodes "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  $m:=\prod_{i\in PA_j}k_i$ , then there are  $k_j^m$  different ways that a node 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",  $\theta$ .

The approach used by CausalQueries is to let the domain of  $\theta^{Y_j}$  be coextensive with the number of nodal types for  $Y_i$ . Function  $f^j$  then determines the value of y by simply reporting

<sup>&</sup>lt;sup>1</sup>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.

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,  $\lambda$ , 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  $\lambda^{j'} := \Pr(\theta^j = \theta^{j'})$ . From independence then we have that the probability of a given causal type  $\theta'$  is simply  $\prod_{i=1}^n \lambda^{i'}$ .

In cases in which there is confounding, the essential logic is the same except that we need to specify enough parameters to capture the joint distribution over nodal types for different nodes.

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

For concreteness: table ? illustrates these 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=1. Z.1 is the complementary probability that Z=1. Things are 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. This allows us to faithfully represent the full joint distribution of nodal types (see  $\mathbf{2Qeq-join}$ ).

$$\Pr(\theta^Z = \theta_1^Z, \theta^X = \theta_{10}^X, \theta^Y = \theta_{11}^Y) = \Pr(\theta^Z = \theta_1^Z) \Pr(\theta^X = \theta_{10}^X) \Pr(\theta^Y = \theta_{11}^Y | \theta^X = \theta_{10}^X)$$
 (1)

 $\{\#eq\text{-join}\}$ 

We see there are four sets of these parameters.

The final column shows a sample set of parameter values.

Together the parameters can describe a full joint probability distribution over types for Z, X and Y that is faithful to the graph.

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

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

 $p(D|\lambda')$  is calculated under the assumption that units are exchangeable and independently drawn, and of course, under the model. In practice this means that the probability that two

Table 2: Nodal types and parameters for Lipids model

node	nodal_type	param_set	param_names	param_value
${f Z}$	0	${f Z}$	Z.0	0.71
$\mathbf{Z}$	1	${f Z}$	Z.1	0.29
X	00	X	X.00	0.36
X	10	X	X.10	0.03
X	01	X	X.01	0.51
X	11	X	X.11	0.10
Y	00	Y.X.00	$Y.00_{X.00}$	0.43
Y	10	Y.X.00	$Y.10_{X.00}$	0.08
Y	01	Y.X.00	$Y.01_X.00$	0.34
Y	11	Y.X.00	$Y.11_X.00$	0.15
Y	00	Y.X.01	$Y.00_{X.01}$	0.43
Y	10	Y.X.01	$Y.10_{X.01}$	0.05
Y	01	Y.X.01	$Y.01_X.01$	0.39
Y	11	Y.X.01	$Y.11_X.01$	0.13
Y	00	Y.X.10	$Y.00_{X.10}$	0.24
Y	10	Y.X.10	$Y.10_X.10$	0.45
Y	01	Y.X.10	$Y.01_X.10$	0.12
Y	11	Y.X.10	$Y.11_X.10$	0.19
Y	00	Y.X.11	$Y.00_{X.11}$	0.61
Y	10	Y.X.11	$Y.10_X.11$	0.11
Y	01	Y.X.11	$Y.01_X.11$	0.03
Y	11	Y.X.11	Y.11_X.11	0.25

units have causal types  $\theta_i$  and  $\theta_j$  is simply  $\lambda_i'\lambda_j'$ . Since a causal type fully determines an outcome vector  $d = \{y_1, y_2, \dots, y_n\}$ , 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  $\lambda'$  we can calculate a vector of event probabilities,  $w(\lambda)$ , for each vector of outcomes, and under independence we have:

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

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

$$w(\lambda) = \begin{cases} w_{00} &=& \lambda_0^X (\lambda_{00}^Y + \lambda_{01}^Y) \\ w_{01} &=& \lambda_0^X (\lambda_{11}^Y + \lambda_{10}^Y) \\ w_{10} &=& \lambda_1^X (\lambda_{00}^Y + \lambda_{10}^Y) \\ w_{11} &=& \lambda_1^X (\lambda_{11}^Y + \lambda_{01}^Y) \end{cases}$$

The value of the CausalQueries package is to allow users to specify models of this form, figure out all the implied 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 a re function of the values or counterfactual values of nodes conditional on values or counterfactual values of nodes.

#### TILL

- Embed the *software* into the respective relevant literature.
- For the latter both competing and complementary software should be discussed (within the same software environment and beyond), bringing out relative (dis)advantages. All software mentioned should be properly @cited'd.<sup>2</sup>

The particular strength of CausalQueries is to allow users to specify arbitrary DAGs, arbitrary queries over nodes in those DAGs, and use the same canonical procedure to learn about those queries whether or not the queries are identified. Thus is principle if researchers are interest 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 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 limitation on the sets of models handled natively by CausalQueries. First CausalQueries is designed for models with a relatively small number over 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  $A \to B \to C \to D \to E$  has just 40 parameters. A model in which A, B, C, D are all direct of E has 65544 parameters. Moving from binary to non binary nodes has similar effects. The restriction to binary nodes is for

<sup>&</sup>lt;sup>2</sup>See (Using BibTeX)[#sec-bibtex] for more details.

computational and not conceptual reasons. In fact there are ways to employ CausalQueries to answer queries from models with nonbinary nodes but in general the computational costs make analysis of these model prohibitive.

Second the package is geared for learning about populations from samples of units that are independent of each other and are independently randomly sampled from populations. This the basic set up does not address problems of sampling, clustering, hierarchical structures, or purposive sampling, for example. In section X we provide pointers to how all of these can be addressed.

## 3. Making models

A model is defined in one step using a dagitty syntax in which the structure of the model is provided as a statement.

For instance:

The statement in quotes, " $X \to M \to Y \leftarrow X$ ", 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:
  - $\begin{array}{ll} \bullet & Y = f(M,X,\theta^Y) \\ \bullet & M = f(X,\theta^M) \\ \bullet & X = \theta^X \\ \end{array}$
- 2. Distributions on  $\Theta$ :
  - $\Pr(\theta^i = \theta^i_k) = \lambda^i_k$
- 3. Independence assumptions:

• 
$$\theta_i \perp \!\!\!\perp \theta_i, i \neq j$$

where function f maps from the set of possible values of the parents of i to values of node igiven  $\theta^i$  as described above.

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

#### 3.1. 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 defined for the objects with class causal\_model produced by make\_model() function.

```
R> make_model("X -> M -> Y <- X; Z -> Y") |> + plot()
```

Alternatively you can provide a number of options to the plot() call that will be passed to CausalQueries:::plot\_dag via the method.

The graphs produced by the two calls above are shown in Figure 1. In both cases the resulting plot will have class c("gg", "ggplot") and so will accept any additional modifications available via ggplot2 package.

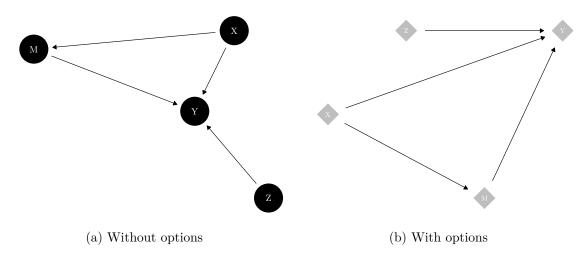


Figure 1: Examples of model graphs.

### 3.2. Model characterization

When a model is defined, a set of objects is generated. These are the key quantities that are used for all inference. The table below 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. nodes is simply a list of the node names in the model. Lastly, parents\_df, is a table listing the nodes, indicating if they are root nodes, and showing how many parents each node has.

The model includes additional elements, nodal\_types, parameters\_df, and causal\_types, which we explain later in detail.

Element Description A character string that describes directed causal relations statement between variables in a causal model, where arrows denote that one node is a potential cause of another. A data frame with columns 'parent' and 'children' indicating dag how nodes relate to each other. A list containing the nodes in the model. nodes 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 in the model. See Section 3.2.2 for more details. 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 3.2.1 for more details. A data frame listing causal types and the nodal types that causal\_types produce them. (See Causal Types Section) Should I include it? P: parameter matrix

Table 3: Core Elements of a Causal Model.

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 objects, which we refer to as stan\_objects. The stan\_objects will, at a minimum, include the distribution of nodal types and the data used for updating the model

Optionally, users can choose whether to keep and append additional elements to the stan\_objects. For instance, they can specify whether to include w, which maps parameters to event probabilities, as well as the stanfit object, the output generated by stan

The table below summarizes the objects attached to the model after updating.

Element	Description
posterior_distribution	The posterir distribution of the updated parameters generated
	by stan.
stan_objects	A list of objects, including, at a minimum,
	type_distribution and data.
data	The data used for updating the model, appended to
	stan_objects.
type_distribution	The updated distribution of the nodal types, appended to
	stan_objects.
W	A mapping from parameters to event probabilities, optionally
	appended to stan_objects.
stan_fit	The stanfit object generated by stan. This is optionally
	appended to stan_objects.

Table 4: Additional Elements.

#### 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 you generally have more parameters than nodal types.

#### For instance:

R> make\_model("X -> Y")\$parameters\_df

#>	#	A tibble: 6	x 8						
#>		param_names	node	gen	param_set	${\tt nodal\_type}$	given param_	value	priors
#>		<chr></chr>	<chr>&gt;</chr>	<int></int>	<chr></chr>	<chr></chr>	<chr></chr>	<dbl></dbl>	<dbl></dbl>
#>	1	X.0	X	1	X	0	" "	0.5	1
#>	2	X.1	X	1	X	1	" "	0.5	1
#>	3	Y.00	Y	2	Y	00	II II	0.25	1
#>	4	Y.10	Y	2	Y	10	11 11	0.25	1
#>	5	Y.01	Y	2	Y	01	11 11	0.25	1
#>	6	Y.11	Y	2	Y	11	11 11	0.25	1

Produces parameters data frame shown in Table 5. Each row in the data frame corresponds to a single parameter.

The columns of the parameters data frame are understood as follows:

param\_names gives the name of the parameter, in shorthand. For instance the parameter
 λ<sub>0</sub><sup>X</sup> = Pr(θ<sup>X</sup> = θ<sub>0</sub><sup>X</sup>) has par\_name X.0. See section @ref(notation) for a summary of
 notation.

param_names	node	gen	param_set	nodal_type	given	param_value	priors
X.0	X	1	X	0		0.50	1
X.1	X	1	X	1		0.50	1
Y.00	Y	2	Y	00		0.25	1
Y.10	Y	2	Y	10		0.25	1
Y.01	Y	2	Y	01		0.25	1
Y.11	Y	2	Y	11		0.25	1

Table 5: Example of Parameters Data Frame

- param\_value gives the (possibly default) parameter values. These are probabilities.
- 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  $\lambda_0^X + \lambda_1^X = 1$ .
- node indicates the node associated with the parameter. For parameter  $\mbox{\lambda^X_0}$  this is X.
- nodal\_type indicates the nodal types associated with the parameter.
- gen indicates the place in the partial causal ordering (generation) of the node associated with the parameter
- priors gives (possibly default) Dirichlet priors arguments for parameters in a set. Values of 1 (.5) for all parameters in a set implies uniform (Jeffrey's) priors over this set.

Below we will see examples where the parameter data frame helps keep track of parameters that are created when confounding is added to a model.

#### Nodal types

Two units have the same *nodal type* at node Y,  $\theta^Y$ , if their outcome at Y responds in the same ways to parents of Y.

A node with k parents has  $2^{2^k}$  nodal types. The reason is that with k parents, there are  $2^k$  possible values of the parents and so  $2^{2^k}$  ways to respond to these possible parental values. As a convention we say that a node with no parents has two nodal types (0 or 1).

When a model is created the full set of "nodal types" is identified. These are stored in the model. The subscripts become very long and hard to parse for more complex models so the model object also includes a guide to interpreting nodal type values. You can see them like this.

R> make\_model("X -> Y")\$nodal\_types

```
#> $X
#> [1] "0" "1"
#>
#> $Y
#> [1] "00" "10" "01" "11"
```

Note that we use  $\theta^j$  to indicate nodal types because for qualitative analysis the nodal types

are often the parameters of interest.

Alternatively, the interpret\_type function can be used to obtain interpretations for the nodal types of each node in the model. For instance, consider the model with two parents  $X \to Y \leftarrow M$ . 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 examples below for models with two and three parents.

```
R> interpretations <-
   make model("X -> Y <- M ") |>
   interpret_type()
R>
R> interpretations$Y
#>
     node position display
                               interpretation
                  1 Y[*]*** Y | M = 0 & X = 0
#> 1
#> 2
        Y
                 2 Y*[*]** Y | M = 1 & X = 0
#> 3
        Y
                 3 Y**[*]* Y | M = 0 & X = 1
#> 4
                  4 Y***[*] Y | M = 1 & X = 1
R> interpretations <-
   make_model("X -> Y <- M; W -> Y") |>
   interpret_type()
R>
R> interpretations$Y
#>
     node position
                        display
                                            interpretation
                  1 Y[*] ****** Y | M = 0 & W = 0 & X = 0
#> 1
                  2 Y*[*]****** Y | M = 1 & W = 0 & X = 0
#> 2
        Y
                  3 Y**[*]***** Y | M = 0 & W = 1 & X = 0
#> 3
        Y
#> 4
        Y
                  4 Y***[*]**** Y | M = 1 & W = 1 & X = 0
                  5 \ Y****[*]*** Y | M = 0 & W = 0 & X = 1
#> 5
        Y
#> 6
        Υ
                  6 \ Y*****[*]** Y | M = 1 & W = 0 & X = 1
#> 7
        Y
                  7 \ Y******[*]* Y | M = 0 & W = 1 & X = 1
                  8 Y*******[*] Y | M = 1 & W = 1 & X = 1
#> 8
        Y
```

LM: section on lookup types; interpret\_type EXAMPLE with maybe 2 parents

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  $X \to M \to Y$  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:

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. In the model  $(X \to M \to Y \leftarrow X)$  there are  $2 \times 4 \times 16 = 128$  causal types.

Knowledge of a causal type tells you what values a unit would take, on all nodes, absent an intervention. 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). (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  $\theta_0^X$ ,  $\theta_{01}^M$ , and  $\theta_{10}^Y$ ).)

# TILL: Show how realise\_outcomes connects causal types with data types: Show for something with a do operation and without a do operation; point out causal types on left

In effect; we can 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 functions achieves this by traversing the DAG, while recording for each node's nodal types, the values implied by realizations on the node's parents. By way of example, consider the first causal type of the  $X \to Y$  model above:

- 1. X is exogenous and has a realized value of 0
- 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 nodal types)

Recovering implied values on complex nodal types given parent realizations efficiently at scale, exploits the fact that nodal types are the Cartesian Product of possible parent realizations. Finding the index of a Node's realized value given parent realizations in a nodal type is equivalent to finding the row index in the Cartesian Product matrix corresponding to those parent realizations. By definition of the Cartesian product, the number of consecutive 0 or 1 elements in a given column is  $2^{columnindex}$ , when indexing columns from 0. Given a set of parent realizations R indexed from 0, the corresponding row index in the Cartesian Product Matrix indexed from 0 can thus be computed via:  $row = (\sum_{i=0}^{|R|-1} (2^i \times R_i))$ .

Calling realise\_outcomes on the above model thus yields:

with row names indicating nodal types and columns realized values. Intervening on X with do(X = 1) yields:

#### 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 (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") |> get_parameter_matrix()
#>
#> Rows are parameters, grouped in parameter sets
#>
#> Columns are causal types
#>
#> Cell entries indicate whether a parameter probability is used
#> in the calculation of causal type probability
#>
        XO.YOO X1.YOO XO.Y10 X1.Y10 XO.YO1 X1.Y01 XO.Y11 X1.Y11
#>
#> X.0
             1
                     0
                                    0
                                           1
                                                  0
                                                          1
                            1
#> X.1
             0
                     1
                            0
                                    1
                                           0
                                                  1
                                                          0
                                                                 1
#> Y.00
             1
                     1
                            0
                                    0
                                           0
                                                  0
                                                          0
                                                                 0
#> Y.10
             0
                     0
                                           0
                                                  0
                                                          0
                                                                 0
                            1
                                    1
```

```
#> Y.01
               0
                       0
                                        0
                                                                 0
                                                                         0
                                                1
                                                        1
#> Y.11
               0
                       0
                                        0
                                                                 1
                                                                         1
#>
#>
    param set
#>
```

The probability of a causal type is given by the product of the parameters values for parameters whose row in the P matrix contains a 1.

Below we will see examples where the P matrix helps keep track of parameters that are created when confounding is added to a model. CROSS REFERENCE

To speed up different operations it is sometimes useful to have P added to the model:

• set\_parameter\_matrix...

### 3.3. Tailoring models

 $Setting\ restrictions$ 

#### TILL: READ THROUGH

When a model is defined, the complete set of possible causal relations are worked out. This set can be very large.

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.

For instance to impose an assumption that Y is not decreasing in X we generate a restricted model as follows:

```
R> model <- make_model("X -> Y") |> set_restrictions("Y[X=1] < Y[X=0]")
or
R> model <- make_model("X -> Y") |> set_restrictions(decreasing("X", "Y"))
```

Viewing the resulting parameter matrix we see that both the set of parameters and the set of causal types are now restricted:

```
R> get_parameter_matrix(model)

#>
#> Rows are parameters, grouped in parameter sets
#>
#> Columns are causal types
#>
#> Cell entries indicate whether a parameter probability is used
#> in the calculation of causal type probability
#>
```

```
#>
        XO.YOO X1.YOO XO.YO1 X1.YO1 XO.Y11 X1.Y11
#> X.O
               1
                      0
                               1
                                       0
#> X.1
              0
                               0
                                               0
                      1
                                       1
                                                       1
#> Y.00
              1
                      1
                               0
                                       0
                                               0
                                                       0
#> Y.01
              0
                               1
                                       1
                                               0
                                                       0
                      0
#> Y.11
              0
                      0
                               0
                                       0
                                               1
                                                       1
#>
#>
#>
    param_set
                 (P)
#>
```

Here and in general, setting restrictions typically involves using causal syntax; see Section @ref(syntax) for a guide the syntax used by CausalQueries.

#### Note:

- Restrictions have to operate on nodal types: restrictions on *levels* of endogenous nodes aren't allowed. This, for example, will fail: make\_model("X -> Y") |> set\_restrictions(statement = "(Y == 1)"). The reason is that it requests a correlated restriction on nodal types for X and Y which involves undeclared confounding.
- Restrictions implicitly assume fixed values for *all* parents of a node. For instance: make\_model("A -> B <- C") |> set\_restrictions("(B[C=1]==1)") is interpreted as shorthand for the restriction "B[C = 1, A = 0]==1 | B[C = 1, A = 1]==1".
- To place restrictions on multiple nodes at the same time, provide these as a vector of restrictions. This is not permitted: set\_restrictions("Y[X=1]==1 & X==1"), since it requests correlated restrictions. This however is allowed: set\_restrictions(c("Y[X=1]==1", "X==1")).
- Use the keep argument to indicate whether nodal types should be dropped (default) or retained.
- Restrictions can be set using nodal type labels.

```
R> make_model("S -> C -> Y <- R <- X; X -> C -> R") |>
+ set_restrictions(labels = list(C = "1000", R = "0001", Y = "0001"),
+ keep = TRUE)
```

• Wild cards can be used in nodal type labels:

```
R> make_model("X -> Y") |>
+ set_restrictions(labels = list(Y = "?0"))
```

• adding "given" for restrictions with models with confounding

### Allowing confounding

(Unobserved) confounding between two nodes arises when the nodal types for the nodes are not independently distributed.

In the  $X \to Y$  graph, for instance, there are 2 nodal types for X and 4 for Y. There are thus 8 joint nodal types (or causal types):

param_names	node	gen	param_set	$nodal\_type$	given	param_value	priors
X.0	X	1	X	0		0.50	1
X.1	X	1	X	1		0.50	1
$Y.00_{X.0}$	Y	2	Y.X.0	00	X.0	0.25	1
$Y.10_{X.0}$	Y	2	Y.X.0	10	X.0	0.25	1
$Y.01_X.0$	Y	2	Y.X.0	01	X.0	0.25	1
$Y.11_X.0$	Y	2	Y.X.0	11	X.0	0.25	1
$Y.00_{X.1}$	Y	2	Y.X.1	00	X.1	0.25	1
$Y.10_X.1$	Y	2	Y.X.1	10	X.1	0.25	1
$Y.01_X.1$	Y	2	Y.X.1	01	X.1	0.25	1
Y.11_X.1	Y	2	Y.X.1	11	X.1	0.25	1

Table 7: Parameters Data Frame for Model with Confounding.

Table 6: Nodal Types in  $X \to Y$  Model.

$\theta^Y \setminus \theta^X$	0	1	Σ
00	$\Pr(\theta_0^X, \theta_{00}^Y)$	$\Pr(\theta_1^X, \theta_{00}^Y)$	$\Pr(\theta_{00}^{Y})$
10	$\Pr(\theta_0^X, \theta_{10}^Y)$	$\Pr(\theta_1^X, \theta_{10}^Y)$	$\Pr( heta_{10}^Y)$
01	$\Pr(\theta_0^X, \theta_{01}^Y)$	$\Pr(\theta_1^X, \theta_{01}^Y)$	$\Pr( heta_{01}^Y)$
11	$\Pr(\theta_0^X, \theta_{11}^Y)$	$\Pr(\theta_1^X, \theta_{11}^Y)$	$\Pr(\theta_{11}^{\tilde{Y}})$
$\sum$	$\Pr( heta_0^X)$	$\Pr( heta_1^X)$	1

This table has 8 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.

R> confounded <- make\_model("X -> Y ; X <-> Y")
R>

R> confounded\$parameters\_df

Table 7 shows the parameters data frame produced by the code above. We see here that there are now 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  $\Pr(\theta^Y = \theta_{01}^Y | X = 1)$ .

To see exactly how the parameters map to causal types we can view the parameter matrix:

#### R> get\_parameter\_matrix(confounded)

The output is shown in Table 8. Importantly, the P matrix works as before, despite confounding. We can assess the probability of causal types by multiplying the probabilities of the constituent parameters.

Unlike nodal restrictions, a confounding relation can involve multiple nodal types simultaneously. For instance make\_model("X -> M -> Y") |> set\_confound(list(X

	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
$Y.00_{X.0}$	1	0	0	0	0	0	0	0
$Y.10_{X.0}$	0	0	1	0	0	0	0	0
$Y.01_X.0$	0	0	0	0	1	0	0	0
$Y.11_X.0$	0	0	0	0	0	0	1	0
$Y.00_X.1$	0	1	0	0	0	0	0	0
$Y.10_X.1$	0	0	0	1	0	0	0	0
$Y.01_X.1$	0	0	0	0	0	1	0	0
Y.11_X.1	0	0	0	0	0	0	0	1

Table 8: Parameter Matrix for Model with Confounding.

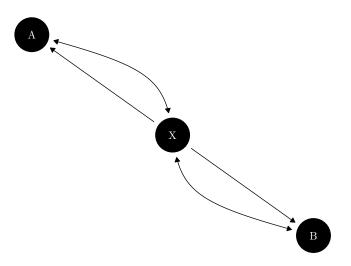


Figure 2: Graph of Model with Confounding.

- = "Y[X=1] > Y[X=0]")) allows for a parameter that renders X more or less likely depending on whether X has a positive effect on Y whether it runs through a positive or a negative effect on M.
- The parameters needed to capture confounding relations depend on the direction of causal arrows. For example compare:
  - make\_model("A -> W <- B ; A <-> W; B <-> W")\$parameters\_df |> dim In this case we can decompose shocks on A,B,W via:  $\Pr(\theta^A,\theta^B,\theta^W) = \Pr(\theta^W|\theta^A,\theta^A)\Pr(\theta^A)\Pr(\theta^B)$ , and we have 68 parameters.
  - make\_model("A <- W -> B ; A <-> W; B <-> W")\$parameters\_df |> dim In this case we have  $\Pr(\theta^A, \theta^B, \theta^W) = \Pr(\theta^A | \theta^W) \Pr(\theta^B | \theta^W) \Pr(\theta^W)$  and just has just 18 parameters.

Setting Priors

Priors on model parameters can be added to the parameters data frame. The priors 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 parameterized by an n-dimensional vector positive vector  $\alpha$ . 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  $\alpha$  implies that all such vectors are equally likely. Other values for  $\alpha$  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 (.5,0,0,0..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  $X \to Y$  model we have one Dirichlet distribution over the two types for  $\theta^X$  and one Dirichlet distribution over the four types for  $\theta^Y$ .

To retrieve the model's priors we can run the following code:

```
R> make_model("X -> Y") |> get_priors()
#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 1 1 1 1 1 1
```

Here the priors have not been specified and so they default to 1, which corresponds to uniform priors. Alternatively you could set Jeffreys priors using set\_priors as follows:

```
R> make_model("X -> Y") |>
+ set_priors(distribution = "jeffreys") |>
+ get_priors()

#> X.0 X.1 Y.00 Y.10 Y.01 Y.11

#> 0.5 0.5 0.5 0.5 0.5 0.5
```

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> make_model("X -> Y") |>
+ set_priors(1:6) |>
+ get_priors()

#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 1 2 3 4 5 6
```

The priors here should be interpreted as indicating:

- $\alpha_X=(1,2),$  which implies a distribution over  $(\lambda_0^X,\lambda_1^X)$  centered on (1/3,2/3).
- $\alpha_Y = (3, 4, 5, 6)$ , which implies a distribution over  $(\lambda_{00}^Y, \lambda_{10}^Y, \lambda_{01}^Y \lambda_{11}^Y)$  centered on (3/18, 4/18, 5/18, 6/18).

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> make_model("X -> Y") |>
+ set_priors(statement = "Y[X=1] > Y[X=0]", alphas = 3) |>
```

```
+ get_priors()
#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 1 1 1 1 3 1
```

As setting priors simply requires mapping alpha values to parameters, the process boils down to selecting rows of the parmeters\_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.

Note that there is nothing particularly unique about setting priors via causal syntax, as it is simply an abstract way of specifying how to subset the parameters\_df data frame. We can achieve the same result as above by specifying nodal type for which we would like to adjust the priors:

```
R> make_model("X -> Y") |>
   set_priors(nodal_type = "01", alphas = 3) |>
   get_priors()
    X.0 X.1 Y.00 Y.10 Y.01 Y.11
           1
                1
                      1
                           3
or even parameter names
R> make_model("X -> Y") |>
   set_priors(param_names = "Y.01", alphas = 3) |>
   get_priors()
#>
    X.0 X.1 Y.00 Y.10 Y.01 Y.11
#>
      1
           1
                1
                      1
                           3
```

As such 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 the identify internally they may be used interchangeably.<sup>3</sup>

```
R> make model("X -> M -> Y; X <-> Y") |>
   set_priors(node = "Y",
              nodal_type = c("01","11"),
+
+
              given = "X.1",
              alphas = c(3,2)) >
   get_priors()
                                             M.01
#>
                 X.1
                          M.00
                                                      M.11 Y.00 X.0 Y.10 X.0
        X.0
                                   M.10
#>
          1
                    1
                             1
                                                1
                                                          1
                                                                   1
                                       1
#> Y.01_X.0 Y.11_X.0 Y.00_X.1 Y.10_X.1 Y.01_X.1 Y.11_X.1
                    1
R> make_model("X -> M -> Y; X <-> Y") |>
+ set_priors(
```

<sup>&</sup>lt;sup>3</sup>See ?set\_priors and ?make\_priors for many more examples.

```
+
     alter_at =
       "node == 'Y' & nodal_type %in% c('01','11') & given == 'X.1'",
+
     alphas = c(3,2)) >
  get_priors()
        X.O
#>
                 X.1
                          M.00
                                   M.10
                                             M.01
                                                      M.11 Y.00_X.0 Y.10_X.0
#>
          1
                             1
                                                1
                                                                   1
  Y.01 X.0 Y.11_X.0 Y.00_X.1 Y.10_X.1 Y.01_X.1 Y.11_X.1
#>
```

It should be noted that while highly targeted prior setting is convenient and flexible; it should be done with caution. Setting priors on specific parameters in complex models; especially models involving confounding, may strongly affect inferences in intractable ways.

We additionally 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  $X \to Y$  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]", n_draws = 10000)
```

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  $X \to Y$  is centered on 1/4. But priors on the probability that X has a positive effect on Y in the model  $X \to M \to Y$  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:

```
R> make_model("X -> Y") |>
+ query_model("Y[X=1] > Y[X=0]", n_draws = 10000)
R>
R> make_model("X -> M -> Y") |>
+ query_model("Y[X=1] > Y[X=0]", n_draws = 10000)
```

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 can be the same as the marginal prior distribution (Poirier 1998).

The key point here is to make sure you do not fall into a trap of thinking that "uninformative" priors make no commitments regarding the values of causal quantities of interest. They do, and the implications of flat priors for causal quantities can depend on the structure 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).

#### Setting Parameters

By default, models have a vector of parameter values included in the parameters\_df dataframe. These are useful for generating data, or for situations, such as process tracing, when one wants to make inferences about causal types  $(\theta)$ , 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 *alpha* 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, X and 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") |>
+ get_parameters()

#> X.0 X.1 Y.00 Y.10 Y.01 Y.11
#> 0.50 0.50 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 .5, while the other nodal types of this parameter set were renormalized so that the parameters in the set still sum to one.

#### 3.4. 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.

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

Drawing data basics

By default, the parameters used are taken from model\$parameters\_df.

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

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

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 <-</pre>
   make_data(model,
             n = 8,
             nodes = list(c("X", "Y"), "M"),
             probs = list(1, .5),
             subsets = list(TRUE, "X==1 & Y==0"))
#> # A tibble: 2 x 5
     node names nodes
                           n_steps probs subsets
     <chr>
                 st>
                                    <dbl> <chr>
#>
                           <lgl>
#> 1 X, Y
                 <chr [2] > NA
                                          TRUE
#> 2 M
                 <chr [1] > NA
                                      0.5 X==1 & Y==0
R> sample_data_2
     X M Y
#> 1 0 NA 0
#> 2 0 NA 0
#> 3 0 NA 1
#> 4 0 NA 1
#> 5 0 NA 1
#> 6 0 NA 1
#> 7 0 NA 1
#> 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. CausalQueries includes functions that lets you move between these two forms in case of need.

R> sample\_data\_1 |> collapse\_data(model)

```
#>
      event strategy count
#> 1 XOMOYO
                  YMX
#> 2 X1MOY0
                  XMY
                           0
#> 3 XOM1YO
                  XMY
                           1
#> 4 X1M1Y0
                  XMY
#> 5 XOMOY1
                  XMY
#> 6 X1M0Y1
                  XMY
                           0
#> 7 XOM1Y1
                           3
                  XMY
#> 8 X1M1Y1
                           0
                  XMY
```

R> sample\_data\_2 |> collapse\_data(model)

```
#>
     event strategy count
#> 1
      XOYO
                  XY
#> 2
      X1Y0
                  XY
                          0
#> 3
      XOY1
                  XY
                          5
#> 4
      X1Y1
                  XY
                          1
```

In the same way it is possible to move from "compact data" to "long data" using expand data().

# 4. Updating models

The approach used by the CausalQueries package to updating parameter values given observed data uses stan and involves the following elements:

- Dirichlet priors over parameters,  $\lambda$  (which, in cases without confounding, correspond to nodal types)
- A mapping from parameters to event probabilities, w
- A likelihood function that assumes events are distributed according to a multinomial distribution given event probabilities.

We provide further details below.

#### 4.1. Data for stan

#### GS: general edit to this section

We use a generic stan model that works for all binary causal models. Rather than writing a new stan model for each causal model we send stan details of each particular causal model as data inputs.

In particular we provide a set of matrices that stan tailor itself to particular models: the parameter matrix (P) tells stan how many parameters there are, and how they map into causal types; an ambiguity matrix A tells **stan** how causal types map into data types; and an event matrix E relates data types into patterns of observed data (in cases where there are incomplete observations).

The internal function prep\_stan\_data prepares data for stan. You generally don't need to use this manually, but we show here a sample of what it produces as input for stan.

Note that NAs are interpreted as data not having been sought. So in this case the interpretation is that there are two data strategies: data on Y and X was sought in three cases; data on Y only was sought in just one case.

#### 4.2. How the stan model works

THIS DISCUSSION IS OUT OF DATE:

The stan model works as follows:

#### MH: ADD DISCUSSION OF parmap;

- We are interested in "sets" of parameters. For example in the  $X \to Y$  model we have two parameter sets (param\_sets). The first is  $\lambda^X \in \{\lambda_0^X, \lambda_1^X\}$  whose elements give the probability that X is 0 or 1. These two probabilities sum to one. The second parameter set is  $\lambda^Y \in \{\lambda_{00}^Y, \lambda_{10}^Y, \lambda_{01}^Y, \lambda_{11}^Y\}$ . These are also probabilities and their values sum to one. Note in all that we have 6 parameters but just 1+3=4 degrees of freedom.
- We would like to express priors over these parameters using multiple Dirichlet distributions (two in this case). In practice because we are dealing with multiple simplices of varying length, it is easier to express priors over gamma distributions with a unit scale parameter and shape parameter corresponding to the Dirichlet priors,  $\alpha$ . We make use of the fact that  $\lambda_0^X \sim Gamma(\alpha_0^X, 1)$  and  $\lambda_1^X \sim Gamma(\alpha_1^X, 1)$  then  $\frac{1}{\lambda_0^X + \lambda_1^X}(\lambda_0^X, \lambda_1^X) \sim Dirichlet(\alpha_0^X, \alpha_1^X)^4$
- For any candidate parameter vector  $\lambda$  we calculate the probability of causal types (prob\_of\_types) by taking, for each type i, the product of the probabilities of all parameters  $(\lambda_j)$  that appear in column i of the parameter matrix P. Thus the probability of a  $(X_0, Y_{00})$  case is just  $\lambda_0^X \times \lambda_{00}^Y$ . The implementations in stan uses prob\_of\_types\_[i] =  $\prod_j (P_{j,i}\lambda_j + (1-P_{j,i}))$ : this multiplies the probability of all parameters involved in the causal type (and substitutes 1s for parameters that are not). (P and not\_P (1-P) are provided as data to stan).
- The probability of data types, w, is given by summing up the probabilities of all causal types that produce a given data type. For example, the probability of a X = 0, Y = 0 case,  $w_{00}$  is  $\lambda_0^X \times \lambda_{00}^Y + \lambda_0^X \times \lambda_{01}^Y$ . The ambiguity matrix A is provided to stan to indicate which probabilities need to be summed.
- 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

<sup>&</sup>lt;sup>4</sup>For a discussion of implementation of this approach in stan see discussion (here)[https://discourse.mc-stan.org/t/ragged-array-of-simplexes/1382].

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. For example X is observed, but Y is not, then the probability of X = 0, Y = NA is  $w_{00} + w_{01}$ . The matrix E is passed to stan to figure out which event probabilities need to be combined for events with missing data.

• The probability of a dataset is then given by a multinomial distribution with these event probabilities (or, in the case of incomplete data, the product of multinomials, one for each data strategy).

#### GS: TO CHECK THE PATHS FUNCTIONALITY

#### 4.3. Implementation

To update a CausalQueries model with data use:

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

where the data argument is a dataset containing some or all of the nodes in the model.

As update\_model() calls rstan::sampling one can pass along all arguments in ... to rstan::sampling. For instance:

- iter sets the number of iterations and ultimately the number of draws in the posterior
- chains sets the number of chains; doing multiple chains in parallel speeds things up

#### 4.4. 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 2 updating processes with 3 parallel chains each simultaneously. More generally the number of parallel

processes at the upper level of the nested parallel structure are given by  $\left| \frac{cores}{chains+1} \right|$ .

```
+
       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
  )
+})
```

#### 4.5. Incomplete and censored data

CausalQueries assumes that missing data is missing at random, conditional on observed data. Thus for instance in a  $X \to M \to Y$  model one might choose 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 assessing 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  $X \neg Y$  has been censored then when we update we do not move towards a belief that X causes Y.

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

#### 4.6. Output

The primary output from update\_model() is a posterior distribution over model parameters, stored as a dataframe in model\$posterior\_distribution. However another of other objects are also optionally stored:

Models can be queried using the query\_distribution and query\_model functions. The difference between these functions is that query\_distribution examines a single query and returns a full distribution of draws from the distribution of the estimand (prior or posterior); query\_model takes a collection of queries and returns a dataframe with summary statistics on the queries.

## 5. Queries

#### 5.1. Causal Syntax

Scholars typically explore a broad range of causal questions. CausalQueries provides syntax for the formulation of various causal queries, ranging from relatively straightforward queries, such as the proportion of units where Y equals 1 (expressed as "Y == 1"), to more detailed ones, such as questions about the types for which Y is greater when X equals 1 than when X equals 0 (expressed as "Y[X=1] > Y[X=0]").

This syntax enables users to write arbitrary causal queries to interrogate their models. For factual queries, users may employ logical statements to ask questions about observed conditions. 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.

Counterfactual queries can be expressed in CausalQueries by using square brackets []. Inside the brackets, variables that are to be intervened are specified. For instance, consider the counterfactual query that 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 factual condition, it is expressed as in the paragraph above using the logical operator ==. More precisely, such query can be written as "Y[X=0] == 1".

With the aid of logical operators such as ==, !=, >, >= <,<=, and the use of square brackets, users can formulate a broad range of queries. For example, they 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]". Alternatively, they can explore complex counterfactuals like "Y[M=M[X=0], X=1]==1". In this case, CausalQueries looks

<sup>&</sup>lt;sup>5</sup>CausalQueries also accepts = as a shorthand for ==. However, == is preferred as it is the conventional logical operator to express a condition of strict equality.

for 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.

One way to develop a clearer understanding of what types are being targeted with each query is using the function get\_query\_types. For instance, consider the model  $X \to Y \leftarrow M$  and the query "Y[X=1, M=1] > Y[X=0, M=0]".

In this case, the aim is to identify the types for which Y equals zero when X=0 and M=0, and Y equals 1 when X=1 and M=1. The specific values that Y takes for other combinations of X and M are not relevant for this query. Therefore, the types targeted in this query have a zero as the first digit of the subscript i.e., when X=0 and M=0, and a 1 as the last digit i.e., when X=1 and M=1, and any value in the second and third digits. The code and output below offer a more precise representation of this.

```
R> make_model('X -> M -> Y <- X') |>
   get_query_types(query = "Y[X=1, M=1] > Y[X=0, M=0]",
                   map = "nodal_type")
#>
#> Nodal types adding weight to query
#>
    query : Y[X=1,M=1] > Y[X=0,M=0]
#>
#>
#>
    0001
           0101
#>
    0011
           0111
#>
#>
    Number of nodal types that add weight to query = 4
#>
    Total number of nodal types related to Y = 16
```

#### LM: REVIEW AND FIX SECTION

WRITE SECTION DESCRIBING FACTUAL AND COUNTERFACTULA QUERIES AND THE SYNTAX INCLUDING Role of [] AND OF GIVEN

```
get_query_types
```

return sets; discuss how all queries related to these sets

start off with query Y==1 then Y[X=1] ==1 then Y[X=1] >= Y[X=0] then show linear functions possible Y[X=1] - Y[X=0]

#### 5.2. Query implementation

#### 5.3. Queries by hand

Queries can draw directly from the prior distribution of the posterior distribution provided by stan.

```
R> library(DeclareDesign)
```

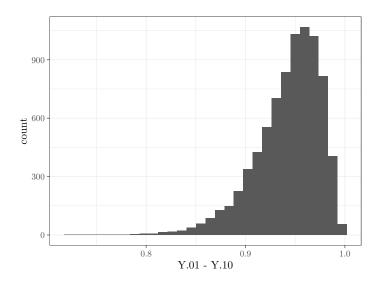


Figure 3: Posterior on 'Probability Y is increasing in X'

```
R> data <-
+ fabricate(N = 100, X = complete_ra(N), Y = X)
R>
R> model <-
+ make_model("X -> Y") |>
+ update_model(data, iter = 4000)
R>
R> model$posterior_distribution |>
+ ggplot(aes(Y.01 - Y.10)) + geom_histogram()
```

#### 5.4. Query distribution

query\_distribution works similarly except that distributions over queries are returned:

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

#### 5.5. Case level queries

Sometimes 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 lipds 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 |>
```

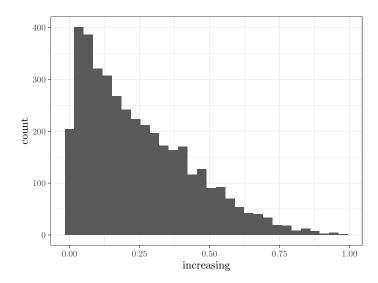


Figure 4: Prior on 'Probability Y is increasing in X'

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

Table 9: Case Level Quiry Example.

query	given	mean	$\operatorname{sd}$	${\rm cred.low.} 2.5\%$	cred.high.97.5%
Y[X=1] - Y[X=0]	X==1 & Y==1 & Z==1	0.95	0.04	0.87	1

The answer we get in Table 9 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.

Subtly though this is, in principle, different to what we would infer for a "new case" that we wonder about. When inquirying about a new case, the case level query *updates* on the given information observed in the new case. The resulting inference is different to the inference that would be made from the posterior *given* the features of the case.

To illustrate, consider a model for which we are quite sure that X causes Y but we do not know whether it works through two positive effects or two negative effects.

Thus we do not know if M=0 would suggest an effect or no effect. If asked what we would infer for a case that had M=0 we would not know whether M=0 information is consistent with a positive effect or not. However if provided with a randomly case and learn that it has M=0, then we update about the causal model and infer that there is an effect in this case (but that there wouldn't be were M=1).

```
R> # DO ALL THIS IN ONE TABLE
R>
R> set.seed(1)
R> model <-</pre>
```

```
make model("X -> M -> Y") |>
    update_model(data.frame(X = rep(0:1, 8), Y = rep(0:1, 8)), iter = 10000)
+
R>
    Q \leftarrow "Y[X=1] > Y[X=0]"
   G <- "X==1 & Y==1 & M==1"
R>
    \label{eq:QG <- "(Y[X=1] > Y[X=0]) & (X==1 & Y==1 & M==1)"}
R>
R>
   # In this case these are very different:
R.>
R>
   query_distribution(model, Q, given = G, using = "posteriors")[[1]] |> mean()
    query_distribution(model, Q, given = G, using = "posteriors",
    case_level = TRUE)
R>
R> # These are equivalent:
R> # 1. Case level query via function
R>
    query_distribution(model, Q, given = G,
     using = "posteriors", case_level = TRUE)
+
R>
   # 2. Case level query by hand using Bayes
R.>
    distribution <- query_distribution(</pre>
R>
     model, list(QG = QG, G = G), using = "posteriors")
+
R>
R>
    mean(distribution$QG)/mean(distribution$G)
```

#### 5.6. Batch queries

The query\_model() function takes causal queries and conditions (given) and specifies the parameters to be used. The result is a data frame which can be displayed as a table.

Table 10: Results for Two Queries on Two Models.

model	query	given	using	case_level	mean	$\operatorname{sd}$
1	ATE	-	parameters	FALSE	0.00	NA
2	ATE	-	parameters	FALSE	0.33	NA

1	ATE	_	priors	FALSE	0.00	0.32
2	ATE	_	priors	FALSE	0.33	0.32 $0.23$
1	ATE	Y==1 & X==1	parameters	FALSE	0.50	NA
$\frac{1}{2}$	ATE	Y==1 & X==1 Y==1 & X==1	parameters	FALSE	0.50	NA
1	ATE	Y==1 & X==1 Y==1 & X==1	parameters	FALSE	0.50	0.29
	ATE		-			
2		Y = = 1 & X = = 1	priors	FALSE	0.49	0.29
1	POS	-	parameters	FALSE	0.25	NA
2	POS	-	parameters	FALSE	0.33	NA
1	POS	-	priors	FALSE	0.25	0.20
2	POS	-	priors	FALSE	0.33	0.23
1	POS	Y = = 1 & X = = 1	parameters	FALSE	0.50	NA
2	POS	Y = =1 & X = =1	parameters	FALSE	0.50	NA
1	POS	Y==1 & X==1	priors	FALSE	0.50	0.29
2	POS	Y==1 & X==1	priors	FALSE	0.49	0.29
1	ATE	-	parameters	TRUE	0.00	NA
2	ATE	-	parameters	TRUE	0.33	NA
1	ATE	-	priors	TRUE	0.00	NA
2	ATE	-	priors	TRUE	0.33	NA
1	ATE	Y==1 & X==1	parameters	TRUE	0.50	NA
2	ATE	Y==1 & X==1	parameters	TRUE	0.50	NA
1	ATE	Y==1 & X==1	priors	TRUE	0.50	NA
2	ATE	Y==1 & X==1	priors	TRUE	0.49	NA
1	POS	-	parameters	TRUE	0.25	NA
2	POS	-	parameters	TRUE	0.33	NA
1	POS	-	priors	TRUE	0.25	NA
2	POS	-	priors	TRUE	0.33	NA
1	POS	Y==1 & X==1	parameters	TRUE	0.50	NA
2	POS	Y==1 & X==1	parameters	TRUE	0.50	NA
1	POS	Y==1 & X==1	priors	TRUE	0.50	NA
2	POS	Y==1 & X==1	priors	TRUE	0.49	NA

# Computational details and software requirements

Version	• 1.0.0
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	• Linux
Systems	• MacOS
	• Windows

	TTI 22.04.0
Testing	• Ubuntu 22.04.2
Environments	• Debian 12.2
OS	• MacOS
T	• Windows
Testing	• R 4.3.1
Environments	• R 4.3.0
R	• R 4.2.3
R Version	<ul> <li>r-devel</li> <li>R(&gt;= 3.4.0)</li> </ul>
Compiler Compiler	<ul> <li>h(&gt;= 5.4.0)</li> <li>either of the below or similar:</li> </ul>
Compiler	
	• g++
Stan	• clang++ • inline
requirements	• Rcpp ( $>= 0.12.0$ )
requirements	• RcppEigen (>= 0.3.3.3.0)
	7
	• RcppArmadillo (>=
	0.12.6.4.0
	• RcppParallel (>= $5.1.4$ )
	• BH $(>= 1.66.0)$
	• StanHeaders ( $>= 2.26.0$ )
D D 1	• rstan (>= $2.26.0$ )
R-Packages	• dplyr
Depends	• methods
R-Packages	• dagitty ( $>= 0.3-1$ )
Imports	• dirmult ( $>= 0.1.3-4$ )
	• stats ( $>= 4.1.1$ )
	• rlang ( $>= 0.2.0$ )
	• rstan ( $>= 2.26.0$ )
	• rstantools ( $\geq 2.0.0$ )
	• 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

The approach to generating a generic stan function that can take data from arbitrary models was developed in key contributions by Jasper Cooper and Georgiy Syunyaev. Lily Medina did magical work pulling it all together and developing approaches to char-

acterizing confounding and defining estimands. Clara Bicalho helped figure out the syntax for causal statements. Julio Solis made many key contributions figuring out how to simplify the specification of priors. Merlin Heidemanns figured out the <code>rstantools</code> integration and made myriad code improvements. Till Tietz revamped the entire package and improved every part of it.

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#### More technical details

Appendices can be included after the bibliography (with a page break). Each section within the appendix should have a proper section title (rather than just *Appendix*). For more technical style details, please check out JSS's style FAQ at [https://www.jstatsoft.org/pages/view/style#frequently-asked-questions] which includes the following topics:

- Title vs. sentence case.
- Graphics formatting.
- Naming conventions.
- Turning JSS manuscripts into R package vignettes.
- Trouble shooting.
- Many other potentially helpful details...

# Using BibTeX

References need to be provided in a BibTeX file (.bib). All references should be made with @cite syntax. This commands yield different formats of author-year citations and allow to include additional details (e.g.,pages, chapters, ...) in brackets. In case you are not familiar with these commands see the JSS style FAQ for details.

Cleaning up BIBTEX files is a somewhat tedious task – especially when acquiring the entries automatically from mixed online sources. However, it is important that informations are complete and presented in a consistent style to avoid confusions. JSS requires the following format.

- item JSS-specific markup (\proglang, \pkg, \code) should be used in the references
- item Titles should be in title case.
- item Journal titles should not be abbreviated and in title case.
- item DOIs should be included where available.
- item Software should be properly cited as well. For R packages citation("pkgname") typically provides a good starting point.

# 6. Appendix: stan code

prep\_stan\_data then returns a list of objects that stan expects to receive. These include indicators to figure out where a parameter set starts (l\_starts, l\_ends) and ends and where a data strategy starts and ends (strategy\_starts, strategy\_ends), as well as the matrices described above.

#### MOVE TO APPENDIX? ADD DISCUSSION OF PARMAP

Below we show the stan code. This starts off with a block saying 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. stan takes it from there and generates a posterior distribution.

```
#> 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_transformed;
#> 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]) {</pre>
#>
       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 (earlier versions used gamma)
#> 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] prob_of_types;
#> if (keep_transformed == 1){
#> for (i in 1:n_types) {
#> prob_of_types[i] = prod(P[, i].*lambdas + 1 - P[,i]);
#> }}
#> if (keep_transformed == 0){
#> prob_of_types = rep_vector(1, n_types);
#> }
#> }
```

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

Submitted: yyyy-mm-dd Accepted: yyyy-mm-dd