
Causal Shapley values

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Abstract

1 Explainability. Causal interpretation of Shapley values.

2 1 Introduction

3 Explainability. Attribution. Shapley. Conditioning or no conditioning.

4 2 A causal interpretation of Shapley values


5 Need more smooth talk.


6 We assume that we are given a set of features \mathbf{x} with corresponding model output $f(\mathbf{x})$. We compare
7 this output with the average output

$$f_0 = \mathbb{E}f(\mathbf{X}) = \int d\mathbf{X} P(\mathbf{X})f(\mathbf{X}) ,$$

8 with expectation taken over some (for now assumed to be known) probability distribution $P(\mathbf{X})$. We
9 would like to attribute the difference between $f(\mathbf{x})$ and f_0 in a sensible way to the different features
10 $i \in N$ with $N = \{1, \dots, n\}$ and n the number of features. That is, we would like to write

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^n \phi_i , \tag{1}$$

11 where we will refer to ϕ_i as the contribution of feature i to the output $f(\mathbf{x})$. Equation (1) is referred
12 to as the efficiency property, which appears to be a sensible desideratum for any attribution method
13  we here take as our starting point.

14 We can think of (at least) two  erent interpretations that, as we will see, will lead to two different
15 approaches for computing the contributions.

16 **Passive.** We interpret the feature vector \mathbf{x} as a passive observation. Feature values come in one after
17 the other and the contribution of feature i should reflect the difference in expected value of
18 $f(\mathbf{X})$ after and before *observing* its feature value x_i .

19 **Active.** We interpret the feature vector \mathbf{x} as the result of an action. Feature values are imposed one
20 after the other and the contribution of feature i relates to the difference in expected value of
21 $f(\mathbf{X})$ after and before *setting* its value to x_i .

22 Following the above reasoning, the contribution of each feature depends on the order π in which the
23 feature values arrive or are imposed. We write the contribution of feature i given the permutation π as

$$\phi_i(\pi) = v(\{j : j \preceq_{\pi} i\}) - v(\{j : j \prec_{\pi} i\}) , \tag{2}$$

24 with $j \prec_\pi i$ if j precedes i in the permutation π , if $\pi(j) < \pi(i)$, and where we define the value
 25 function

$$v(S) = \mathbb{E}[f(\mathbf{X}) | op(\mathbf{x}_S)] = \int d\mathbf{X}_{\bar{S}} P(\mathbf{X}_{\bar{S}} | op(\mathbf{X}_S = \mathbf{x}_S)) f(\mathbf{X}_{\bar{S}}, \mathbf{x}_S). \quad (3)$$

26 Here S is the subset of indices of features with known “in-coalition” feature values \mathbf{x}_S . To compute the
 27 expectation, we still need to average over the “out-of-coalition” feature values $\mathbf{X}_{\bar{S}}$ with $\bar{S} = N \setminus S$, the
 28 complement of S . The operator $op()$ specifies how the distribution of the “out-of-coalition” features
 29 $\mathbf{X}_{\bar{S}}$ depends on the “in-coalition” feature values \mathbf{x}_S . To arrive at the passive interpretation, we set
 30 $op()$ to conventional conditioning by observation, yielding $P(\mathbf{X}_{\bar{S}} | \mathbf{x}_S)$. For the active interpretation,
 31 we need to condition by intervention, for which we resort to Pearl’s *do*-calculus [6] and write
 32 $P(\mathbf{X}_{\bar{S}} | do(\mathbf{X}_S = \mathbf{x}_S))$. **Do we need a longer introduction/explanation of do-calculus?** A third option
 33 is to ignore the feature values \mathbf{x}_S and just take the unconditional, marginal distribution $P(\mathbf{X}_{\bar{S}})$. We
 34 will refer to the corresponding Shapley values as conditional, causal, and marginal, respectively.

35 It is easy to check that the efficiency property (1) holds for any permutation π . So, for any distribution
 36 over permutations $w(\pi)$ with $\sum_\pi w(\pi) = 1$, the contribution

$$\phi_i = \sum_\pi w(\pi) \phi_i(\pi)$$

37 still satisfies (1). An obvious choice would be to take a uniform distribution $w(\pi) = 1/n!$. We then
 38 arrive at the standard definition of Shapley values:

$$\phi_i = \sum_{S \subseteq N \setminus i} \frac{|S|!(n - |S| - 1)!}{n!} [v(S \cup i) - v(S)],$$

39 where we use shorthand i for the singleton $\{i\}$. Besides efficiency, these Shapley values uniquely
 40 satisfy three other desirable properties [9].

41 **Linearity:** for two value functions v_1 and v_2 , we have $\phi_i(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 \phi_i(v_1) + \alpha_2 \phi_i(v_2)$.
 42 This guarantees that the Shapley value of a linear ensemble of models is a linear combination
 43 of the Shapley values of the individual models.

44 **Null player (dummy):** if $v(S \cup i) = v(S)$ for all $S \subseteq N \setminus i$, then $\phi_i = 0$. A feature that never
 45 contributes to the model output receives zero Shapley value.

46 **Symmetry:** if $v(S \cup i) = v(S \cup j)$ for all $S \subseteq N \setminus \{i, j\}$, then $\phi_i = \phi_j$. Symmetry holds for any
 47 of the three different ways (conventional conditioning, *do*-calculus, ignoring) to average
 48 over the “out-of-coalition” features.

49 Efficiency, linearity, and null player still hold for a non-uniform distribution of permutations, but
 50 symmetry is then typically lost.

51 **of the next two paragraphs probably to introduction.**

52 Janzing et al. [4] also argued for an active, interventional interpretation of Shapley values. They make
 53 a case for using the marginal instead of the (observational) conditional distribution to compute the
 54 Shapley values when dependencies between features are due to confounding. This follows directly
 55 from our reasoning, since in models with no causal links between the features and any dependen-
 56 cies only due to confounding, conditioning by intervention reduces to the marginal distribution:
 57 $P(\mathbf{X}_{\bar{S}} | do(\mathbf{X}_S = \mathbf{x}_S)) = P(\mathbf{X}_{\bar{S}})$ for any subset S .

58 Frye et al. [3] introduce asymmetric Shapley values as a way to incorporate causal information.
 59 Instead of taking a uniform distribution over all possible permutations, these asymmetric Shapley
 60 values only consider those permutations that are consistent with the causal structure between the
 61 features, i.e., are such that a known causal ancestor always precedes its descendants. Frye et al. apply
 62 conventional conditioning by observation to make sure that the resulting explanations respect the
 63 data manifold. This makes the approach somewhat of a mix between an active (incorporating causal
 64 structure) and a passive approach (conditioning by observation). In this paper, we suggest a more
 65 direct approach to incorporate causality, by replacing conditioning by observation with conditioning
 66 by intervention. This can, but does not have to be combined with the idea to make the permutations
 67 match the causal structure. We will illustrate the differences in the example below.

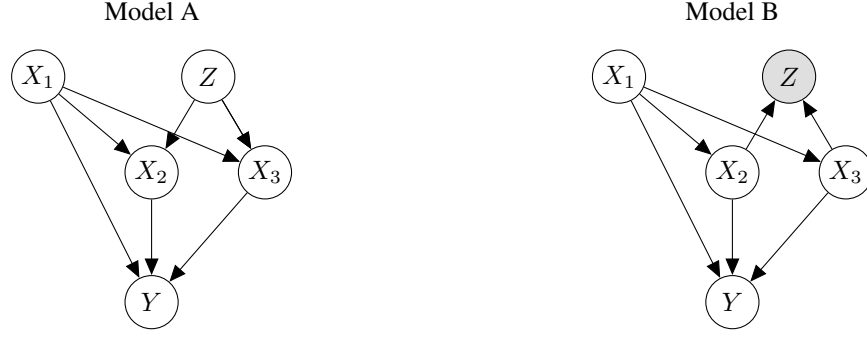


Figure 1: Two causal models. In both, X_1 causes X_2 and X_3 . In Model A the excess correlation between X_2 and X_3 is induced by a common confounder Z , in Model B by selection bias.

3 Illustration

For illustration, we consider two causal models in Figure 1. They have a different causal structure, but the same dependency structure (all features are dependent) and we assume that the probability distribution $P(\mathbf{X})$ is exactly the same for Model A and Model B. Our estimate of the output Y is a linear function of the features:

$$f(\mathbf{x}) = \beta_0 + \sum_{i=1}^3 \beta_i x_i .$$

Too much detail in this section: move parts to supplement? If so, which parts? Combining (2) and (3), we obtain, after some rewriting

$$\phi_i(\pi) = \beta_i (x_i - \mathbb{E}[X_i | op(\mathbf{x}_{j:j \prec_{\pi} i})]) + \sum_{k \succ_{\pi} i} \beta_k (\mathbb{E}[X_k | op(\mathbf{x}_{j:j \preceq_{\pi} i})] - \mathbb{E}[X_k | op(\mathbf{x}_{j:j \prec_{\pi} i})]) .$$

For marginal Shapley values only the first term before the sum remains, yielding

$$\phi_i = \phi_i(\pi) = \beta_i (x_i - \mathbb{E}[X_i]) ,$$

as also derived in [1].

Analytically computing the conditional Shapley values is tedious, but conceptually straightforward. To write the equations in a compact form, we define $\bar{x}_{k|S} = \mathbb{E}[X_k | \mathbf{x}_S]$ and combine all expectations in a single matrix $\bar{\mathcal{X}}$:

$$\bar{\mathcal{X}} = \begin{pmatrix} x_1 & x_2 & x_3 \\ \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \\ \bar{x}_{1|2} & \bar{x}_{2|1} & \bar{x}_{3|1} \\ \bar{x}_{1|3} & \bar{x}_{2|3} & \bar{x}_{3|2} \\ \bar{x}_{1|2,3} & \bar{x}_{2|1,3} & \bar{x}_{3|1,2} \end{pmatrix} .$$

Taking a uniform distribution over permutations, the conditional Shapley values for any linear model with three variables can be written as


$$\phi^{\text{conditional}} = \mathcal{C}^{\text{conditional}} \times \text{vec}(\bar{\mathcal{X}} \times \text{diag}(\beta)) \quad (4)$$



with

$$\mathcal{C}^{\text{conditional}} = \frac{1}{6} \left(\begin{array}{ccccc|ccccc|ccccc} 6 & -2 & -1 & -1 & -2 & 0 & -2 & 2 & -1 & 1 & 0 & -2 & 2 & -1 & 1 \\ 0 & -2 & 2 & -1 & 1 & 6 & -2 & -1 & -1 & -2 & 0 & -2 & -1 & 2 & 1 \\ 0 & -2 & -1 & 2 & 1 & 0 & -2 & -1 & 2 & 1 & 6 & -2 & -1 & -1 & -2 \end{array} \right) .$$

Stop this explanation? The multiplication with the diagonal matrix of regression coefficients $\beta = (\beta_1, \beta_2, \beta_3)$ boils down to multiplying the i th column of $\bar{\mathcal{X}}$ with β_i . Vectorization then stacks the columns on top of one another to end up with a 15-dimensional column vector. The vertical bars in the matrix $\mathcal{C}^{\text{conditional}}$ indicate the three blocks, with the first 5 columns in the matrix mapping to the first column of $\bar{\mathcal{X}}$ with expectations of X_1 , the next 5 columns to the expectations of X_2 , and the final 5 columns to the expectations of X_3 .

expectation	model A	model B
$\hat{x}_{1 2}$	\bar{x}_1	
$\hat{x}_{1 3}$		
$\hat{x}_{1 2,3}$		
$\hat{x}_{2 1}$	$\bar{x}_{2 1}$	
$\hat{x}_{2 3}$	\bar{x}_2	$\bar{x}_{2 3}$
$\hat{x}_{2 1,3}$	$\bar{x}_{2 1}$	$\bar{x}_{2 1,3}$
$\hat{x}_{3 1}$	$\bar{x}_{3 1}$	
$\hat{x}_{3 2}$	\bar{x}_3	$\bar{x}_{3 2}$
$\hat{x}_{3 1,2}$	$\bar{x}_{3 1}$	$\bar{x}_{3 1,2}$

Table 1:  **Intervening expectations under conditioning by intervention**, $\hat{x}_{i|S} = \mathbb{E}[x_i | do(\mathbf{X}_S = \mathbf{x}_S)]$, into expectations under conventional conditioning by observation, $\bar{x}_{i|S} = \mathbb{E}[x_i | \mathbf{X}_S]$, for the two models in Figure 1. **Needed? Can put it next to Figure 1 to save space.**

 **Additional** **this paragraph?** It is easy to check that efficiency indeed holds by summing every column of . The first column of each block (which relates to the feature values themselves) adds up to 1, the second (corresponding to the marginal expectations) to -1 , and the other three columns to zero, as they should. Since Shapley values are constructed by always comparing two (possibly) different expectations, each row within each block sums up to zero.

Putting X_1 before X_2 and X_3 , and X_2 and X_3 on equal footing, asymmetric Shapley values only consider the two permutations where x_1 is observed before x_2 and x_3 , leading to (we divide by 6 to make it easier to compare with the other Shapley values)

$$\mathcal{C}^{\text{asymmetric}} = \frac{1}{6} \left(\begin{array}{ccccc|ccccc|ccccc} 6 & -6 & 0 & 0 & 0 & 0 & -6 & 6 & 0 & 0 & 0 & 0 & -6 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 & 0 & -3 & 0 & -3 & 0 & 0 & 0 & 0 & -3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & 0 & 3 & 6 & 0 & -3 & 0 & -3 \end{array} \right).$$

Using the standard rules for *do*-calculus [6], we show in Table 1 how the expectations under conditioning by intervention reduce to expectations under conditioning by observation. Since in Model A the correlation between X_2 and X_3 is due to confounding, the interventional expectations and thus Shapley values simplify considerably:

$$\mathcal{C}^{\text{causal,A}} = \frac{1}{6} \left(\begin{array}{ccccc|ccccc|ccccc} 6 & -6 & 0 & 0 & 0 & 0 & -3 & 3 & 0 & 0 & 0 & 0 & -3 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 & -3 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & -3 & 3 & 0 & 0 \end{array} \right).$$

For Model B, on the other hand, features X_2 and X_3 do affect each other when intervened upon, which makes that compared to the conditional Shapley values only the first block changes:

$$\mathcal{C}^{\text{causal,B}} = \frac{1}{6} \left(\begin{array}{ccccc|ccccc|ccccc} 6 & -6 & 0 & 0 & 0 & 0 & -2 & 2 & -1 & 1 & 0 & -2 & 2 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 6 & -2 & -1 & -1 & -2 & 0 & -2 & -1 & 2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -1 & 2 & 1 & 6 & -2 & -1 & -1 & -2 \end{array} \right).$$

To make this more concrete, let us assume that $P(\mathbf{X})$ follows a multivariate normal distribution corresponding to the causal model

$$X_1 \sim \mathcal{N}(0; 1) \text{ and } (X_2, X_3 | X_1) \sim \mathcal{N} \left((\alpha_2 X_1, \alpha_3 X_1); \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right),$$

where for notational convenience, we chose zero means and unit variance for all noise variables. The first feature drives the second and third feature with coefficients α_2 and α_3 . The confounding in Model A or selection bias in Model B leads to correlation ρ on top of the correlation induced by the joint dependence on the first feature. Straightforward calculations yield

$$\bar{\mathcal{X}} = \begin{pmatrix} x_1 & x_2 & x_3 \\ 0 & 0 & 0 \\ \frac{\alpha_2}{\sigma_2^2} x_2 & \alpha_2 x_1 & \alpha_3 x_1 \\ \frac{\alpha_3}{\sigma_3^2} x_3 & \frac{\gamma}{\sigma_3^2} x_3 & \frac{\gamma}{\sigma_2^2} x_2 \\ \frac{\delta_{23} x_2 + \delta_{32} x_3}{1 - \rho^2 + \delta_{23} \alpha_2 + \delta_{32} \alpha_3} & (\alpha_2 - \rho \alpha_3) x_1 + \rho x_3 & (\alpha_3 - \rho \alpha_2) x_1 + \rho x_2 \end{pmatrix}.$$

with $\delta_{ij} = \alpha_i - \rho\alpha_j$, $\sigma_i^2 = 1 + \alpha_i^2$ (the marginal correlation for feature i), and $\gamma = \rho + \alpha_2\alpha_3$ (the total correlation between the second and third feature). Plugging this and the expressions for the different \mathcal{C} matrices into (4), we obtain the asymmetric Shapley values

$$\begin{aligned}\phi_1^{\text{asymmetric}} &= \beta_1x_1 + (\alpha_2\beta_2 + \alpha_3\beta_3)x_1 \\ \phi_2^{\text{asymmetric}} &= \beta_2x_2 - \alpha_2\beta_2x_1 + \frac{\rho}{2}(\alpha_3\beta_2 - \alpha_2\beta_3)x_1 + \frac{\rho}{2}(\beta_3x_2 - \beta_2x_3) \\ \phi_3^{\text{asymmetric}} &= \beta_3x_3 - \alpha_3\beta_3x_1 + \frac{\rho}{2}(\alpha_2\beta_3 - \alpha_3\beta_2)x_1 + \frac{\rho}{2}(\beta_2x_3 - \beta_3x_2),\end{aligned}$$

and the causal Shapley values, for Model A,

$$\begin{aligned}\phi_1^{\text{causal,A}} &= \beta_1x_1 + \frac{1}{2}(\alpha_2\beta_2 + \alpha_3\beta_3)x_1 \\ \phi_2^{\text{causal,A}} &= \beta_2x_2 - \frac{1}{2}\alpha_2\beta_2x_1 \\ \phi_3^{\text{causal,A}} &= \beta_3x_3 - \frac{1}{2}\alpha_3\beta_3x_1.\end{aligned}$$

and, for Model B, (really ugly... can we prevent this?)

$$\begin{aligned}\phi_1^{\text{causal,B}} &= \beta_1x_1 + \frac{1}{2}(\alpha_2\beta_2 + \alpha_3\beta_3)x_1 - \frac{\rho}{6}(\alpha_3\beta_2 + \alpha_2\beta_3)x_1 - \frac{1}{6}\left(\frac{\alpha_3\delta_{23}}{\sigma_3^2}\beta_2x_3 + \frac{\alpha_2\delta_{32}}{\sigma_2^2}\beta_3x_2\right) \\ \phi_2^{\text{causal,B}} &= \beta_2x_2 - \frac{1}{2}\alpha_2\beta_2x_1 + \frac{\rho}{6}(2\alpha_3\beta_2 - \alpha_2\beta_3)x_1 + \\ &\quad \frac{1}{6}\left(2\frac{\alpha_2\delta_{32}}{\sigma_2^2}\beta_3x_2 - \frac{\alpha_3\delta_{23}}{\sigma_3^2}\beta_2x_3\right) + \frac{\rho}{2}(\beta_3x_2 - \beta_2x_3) \\ \phi_3^{\text{causal,B}} &= \beta_3x_3 - \frac{1}{2}\alpha_3\beta_3x_1 + \frac{\rho}{6}(2\alpha_2\beta_3 - \alpha_3\beta_2)x_1 + \\ &\quad \frac{1}{6}\left(2\frac{\alpha_3\delta_{23}}{\sigma_3^2}\beta_2x_3 - \frac{\alpha_2\delta_{32}}{\sigma_2^2}\beta_3x_2\right) + \frac{\rho}{2}(\beta_2x_3 - \beta_3x_2).\end{aligned}$$

In this linear model, the asymmetric Shapley value for the first feature adds its indirect causal effects on the output through the second and third feature, $\alpha_2\beta_2x_1 + \alpha_3\beta_3x_1$, to its direct effect, β_1x_1 . The causal Shapley values for the first feature are somewhat more conservative: they essentially claim only half of the indirect effects through the other two features. **Move the rest of this paragraph elsewhere?** This is a direct consequence of taking a uniform distribution over all permutations: for any pair of features i and j , the feature value x_i is set before and after x_j for exactly half of the number of permutations. Which distribution over permutations to prefer, a uniform one or one that respects the causal structure, depends on the question the practitioner tries to answer and possibly on the application. For example, when a causal link represents a temporal relationship, it may make no sense to set a feature value before the values of all features preceding it in time have been set. In that case, it would be wise to consider a non-uniform distribution over permutations as in [3]. On the other hand, for causal models without temporal interpretation, e.g., describing presumed causal relationships between personal and biomedical variables related to Alzheimer [10] or between social and economic characteristics in census data [2], deviating from a uniform distribution over permutations (and hence sacrificing the symmetry property) seems unnecessary. With or without uniform distribution over permutations, applying *do*-calculus instead of conditioning by observation is a natural way to incorporate causal information.

The Shapley values for Model A are different from those for Model B, even though the observable probability distribution $P(\mathbf{X})$ is exactly the same. Those for Model A simplify a lot, because in this model any excess correlation between X_2 and X_3 beyond the correlation resulting from the common parent X_1 results from a confounder. This correlation vanishes when we intervene on either X_2 or X_3 . The contributions of the second and third feature are therefore just their direct effect, minus half of the indirect effect, which already has been attributed to the first feature. In Model B, on the other hand, for most expectations conditioning by intervention reduces to conditioning by observation on the same variables and does not further simplify to conditioning on less or even no variables as for Model A. Since the causal Shapley values consider all six permutations, in contrast to the asymmetric Shapley values which only consider two of them, expectations such as $\mathbb{E}[X_2|x_3]$ now also enter the equation, which considerably complicates the analytical expressions.

142 4 Causal chain graphs

143 This section may need some more “fluff” with Theorems and an algorithm or ??? All we use/need is
 144 in fact in [5]... Computing causal Shapley values not only requires knowledge of the probability
 145 distribution $P(\mathbf{X})$, but also of the underlying causal structure. And even then, there is no guarantee
 146 that any causal query is identifiable (see e.g., [7]). For example, if Model A or B also includes a
 147 causal link from X_2 to X_3 , even knowing the probability distribution $P(\mathbf{X})$ and the causal structure
 148 is insufficient: it is impossible to express, for example, $P(X_3|do(X_2 = x_2))$ in terms of $P(\mathbf{X})$,
 149 essentially because, without knowing the parameters of the causal model, there is no way to tell
 150 which part of the observed dependence between X_2 and X_3 is due to the causal link and which due
 151 to the confounding or selection bias.

152 Furthermore, and perhaps more importantly, requiring a practitioner to specify a complete causal
 153 structure, possibly even including some of its parameters, would be detrimental to the method’s
 154 generic applicability. We therefore follow the same line of reasoning as in [3] and assume that a
 155 practitioner may be able to specify a causal ordering, but not much more.

156 In the special case that a complete causal ordering of the features can be given and that all causal
 157 relationships are unconfounded, $P(\mathbf{X})$ satisfies the Markov properties associated with a directed
 158 acyclic graph (DAG) and can be written in the form

$$P(\mathbf{X}) = \prod_{j \in N} P(X_j | \mathbf{X}_{pa(j)}) ,$$

159 with $pa(j)$ the parents of node j . If no further conditional independences are assumed, the parents of
 160 j are all nodes that precede j in the causal ordering. For causal DAGs, we have the interventional
 161 formula [5]:

$$P(\mathbf{X}_{\bar{S}} | do(\mathbf{X}_S = \mathbf{x}_S)) = \prod_{j \in \bar{S}} P(X_j | \mathbf{X}_{pa(j) \cap \bar{S}}, \mathbf{x}_{pa(j) \cap S}) , \quad (5)$$

162 with $pa(j) \cap T$ the parents of j that are also part of subset T . The interventional formula can be used
 163 to answer any causal query of interest. We will often approximate the expectations needed to compute
 164 the Shapley values through sampling, which is particularly straightforward for causal DAGs under
 165 conditioning by intervention. Variables are sampled consecutively by following the causal ordering.
 166 The probability distribution for a feature then only depends on the values of its parents, which by
 167 then is either sampled or fixed. Since the intervention blocks the influence of all descendants, there is
 168 no need for an MCMC approach such as Gibbs sampling: the values of all features can be sampled in
 169 a single pass through the graph.

170 If we only consider permutations that follow the causal ordering, as with asymmetric Shapley values,
 171 conditioning by intervention reduces to conditioning by observation.

172 We may not always be willing or able to give a complete ordering between the individual variables, but
 173 rather a partial ordering as, for example, in Figure 1 where we have the partial ordering $(\{1\}, \{2, 3\})$:
 174 the first feature precedes the second and third feature in the causal ordering, with the second and third
 175 feature on equal footing, i.e., without specifying whether the second causes the third or vice versa.
 176 Here causal chain graphs [5] come to the rescue. A causal chain graph has directed and undirected
 177 edges. All features that are treated on an equal footing are linked together with undirected edges
 178 and become part of the same chain component. Edges between chain components are directed and
 179 represent causal relationships. The probability distribution $P(\mathbf{X})$ now factorizes as a “DAG of chain
 180 components”:

$$P(\mathbf{X}) = \prod_{\tau} P(\mathbf{X}_{\tau} | \mathbf{X}_{pa(\tau)}) ,$$

181 with each τ corresponding to a chain component, consisting of all features that are treated on an
 182 equal footing.

183 How to compute the effect of an intervention now depends on the interpretation of the generative
 184 process leading to the undirected part of the probability distribution. One possible interpretation is
 185 that the undirected part corresponds to the equilibrium distribution of a dynamic process resulting
 186 from interactions between the variables within a component [5]. In this case, setting the value of a
 187 feature does affect the distribution of the variables within the same component and the interventional

188 formula reads

$$P(\mathbf{X}_{\bar{S}}|do(\mathbf{X}_S = \mathbf{x}_S)) = \prod_{\tau} P(\mathbf{X}_{\tau \cap \bar{S}}|\mathbf{X}_{pa(\tau) \cap \bar{S}}, \mathbf{x}_{pa(\tau) \cap S}, \mathbf{x}_{\tau \cap S}).$$

189 That is, in the observational distribution we need to condition on intervened features that are parents
190 and those that are within the same component. The same interventional formula applies when the
191 dependencies within a component are the result of a selection bias as in Model B in Figure 1.

192 However, if we assume that the undirected part of the probability distribution is the consequence of
193 marginalizing out a common confounder, we should take

$$P(\mathbf{X}_{\bar{S}}|do(\mathbf{X}_S = \mathbf{x}_S)) = \prod_{\tau} P(\mathbf{X}_{\tau \cap \bar{S}}|\mathbf{X}_{pa(\tau) \cap \bar{S}}, \mathbf{x}_{pa(\tau) \cap S}),$$

194 i.e., we should only condition on the parent components, not on the intervened variables within the
195 same component. This interpretation is consistent with [4] and Model A in Figure 1.

196 So, to be able to compute the expectations in the Shapley equations under an interventional interpretation,
197 we need to specify (1) a partial order and (2) whether any dependencies between features that
198 are treated on an equal footing are most likely the result of mutual interaction or selection, or of a
199 common confounder. Based on this information, any expectation by intervention can be translated to
200 an expectation by observation.

201 To compute these expectations, we can rely on the various methods that have been proposed to
202 compute conditional Shapley values [1, 3]. Following [1], we will assume a multivariate Gaussian
203 distribution for $P(\mathbf{X})$ that we estimate from the training data. Alternative proposals include assuming
204 a Gaussian copula distribution, estimating from the empirical (conditional) distribution (both from [1])
205 and a variational autoencoder [3].

206 5 Experiments

207 From here on just rough text and ideas.

208 Show that it works. For now: example on bike rental. Do we predict more bike shares on a warm,
209 but cloudy day in August because of the season or because of the weather? ADNI as another
210 example? Tried German Credit Data, but hard to see differences between causal and conditioning,
211 mainly because the features, such as gender and age, that can be considered causes of some of the
212 others, hardly affect the prediction. Other suggestions? Currently using a relatively straightforward
213 adaptation of the code of [1]. How to describe this? Do we need to publish the code? Do we need to
214 show results for asymmetric Shapley values as well? If so, need to dig deeper into the code. Also:
215 currently no code for handling discrete variables. Could connect to Ruifei's Gaussian copula's for
216 mixed missing data, if needed?

217 6 Discussion

218 Which Shapley value to use depends on interpretation: what happens if we set the features to their
219 values compared to what happens to when we observe that features obtain their values. Both interpretations
220 are fine. In most cases the causal interpretation seems to be the one to prefer/implicitly
221 implied.

222 Marginal fine when dependencies are purely the result of confounding, as Janzing argued. However,
223 when there actually are causal relationships between the features and/or the dependencies between features
224 results from selection bias or mutual feedback, expectations under conditioning by intervention
225 do not simplify to marginal expectations.

226 Novel algorithm, based on causal chain graphs. All that a practitioner needs to provide is a partial
227 causal order (as for asymmetric Shapley) and how to interpret dependencies between features that are
228 on the same footing. Conditioning by intervention becomes conditioning by observation, but only on
229 ancestors and possibly, depending on the interpretation, features within the same component. Any
230 existing approach for conditional Shapley values can be easily adapted: if anything the expectations
231 simplify, since no conditioning on descendants.

232 Provides an interpretation for asymmetric Shapley values: for all permutations that are consistent
 233 with the causal ordering, conditioning by intervention boils down to conditioning by observation.
 234 However, current definition [3] implicitly assumes that dependencies between features that are on the
 235 same footing is due to mutual feedback or selection bias, not common confounding. Whether or not
 236 to only consider permutations that match the causal ordering depends on application and possibly
 237 taste. This paper shows that it is unnecessary to give away symmetry in order to arrive at a causal
 238 interpretation of Shapley values. Roughly speaking, asymmetric (causal/conditioning) Shapley values
 239 attribute all indirect effects of a causal variable through a mediator on the output to the causal variable
 240 (is this the right term?), subtracting it from the Shapley value of the mediator (since efficiency should
 241 hold). Symmetric Shapley values are more conservative and attribute only half to the causal variable.

242 Discuss non-manipulable causes as in [8]?

243 Mention that it's easy to combine with any of TreeSHAP, KernelShap, and so on?

244 Compare with counterfactual explanations?

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