Quantifying and Visualizing Attribute Interactions

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Abstract

Interactions are the prototypical examples of unexpected and irreducible patterns in data that encompass several attributes. We attempt to unify the divergent definitions and conceptions of interactions present in the literature, and propose two separate conceptions of what interactions are: if a group of attributes interacts observationally, we cannot understand their relationship without looking at all the attributes simultaneously; if a group of attributes interacts representationally, we cannot create a model that would not include conditions involving all the attributes. Rather than test for interactions, we attempt to quantify them, and visually present the most important interactions of the data. Our quantification is based on how well we can approximate a joint probability distribution without admitting that there are interactions. Judging from these illustrations, most machine learning procedures are not treating interactions appropriately.

1 Introduction

The crux of intelligence is the ability to observe regularities in the environment, and create models through learning that facilitate informed decision-making. In noisy and uncertain environments, binary logic has proven to be of limited utility. A different way of expression of regularities is required, one that would be expressed in the language of probability, a proven framework for study of noise and uncertainty. In this text, we will adopt a strictly empirical stance, attempting to draw conclusions from data without assuming any background knowledge.

The most fundamental of regularities in probability is the concept of independence. A and B are independent if and only if \( P(A, B) = P(A)P(B) \). Independence also implies that A is irrelevant to B. However, independence is
not a stable relation: \( A \) may become dependent with \( B \) if we observe another attribute \( C \). For example, define \( C \) to be true when \( A \) and \( B \) are equal. Even if \( A \) and \( B \) are independent and random, they become dependent in the context of \( C \). Alternatively, \( A \) may become independent of \( B \) in the context of \( C \), even if they were dependent before: imagine that \( A \) and \( B \) are two independently sampled uncertain measurements of \( C \). Without \( C \), the measurements are similar, hence their dependence. With the knowledge of \( C \), however, the similarity between \( A \) and \( B \) disappears. It is hence difficult to systematically investigate dependencies.

Conditional independence was proposed as a solution to the above problem of flickering dependencies. Two attributes \( A \) and \( B \) are conditionally independent with respect to attribute \( C \) if and only if they are independent at every value of attribute \( C \). In probability theory, this can be expressed as \( P(A|B,C) = P(A|C) \). Hence, independence cannot be claimed unless it has been verified in the context of all other attributes. This helps us simplify the model of the environment. The most popular representation of the remaining dependencies is a Bayesian network \cite{BayesianNetworks}, which has several disadvantages:

- In a noisy environment, it is exceedingly rare to have perfect conditional independence. It is hence unclear what was the threshold used to determine whether a dependence was insignificant. The Bayesian network gives the false impression of perfection, even if it is an approximation. The Bayesian network does not disclose the loss in faithfulness to data incurred by the simplifying assumptions.

- The Bayesian network does not provide any insight into the importance of particular dependencies, that would help an analyst understand which connections are important and which are not.

- Although there were numerous problems analyzing a dependence between attributes in the context of all other attributes, or additional simplifying assumptions have been made, adding an additional unobserved attribute can change the network, just as \( C \) has affected the dependence between \( A \) and \( B \) in our earlier example. A Bayesian network is unstable with respect to introduction of additional attributes.

- Bayesian networks are ambiguous: multiple Bayesian networks may describe the same data. Furthermore, the direction of network edges is often arbitrary, and gives false impressions.

In this text, we endorse a different type of regularities, interactions. An interaction is the regularity present only in the whole set of attributes, but not in any subset. When there is such a regularity, we say that the attributes of the set interact. For example, a 2-way interaction between two attributes is the amount of their mutual dependence. A 3-way interaction between three attributes is that amount of their own mutual dependence that cannot be explained by 2-interactions among them. Interactions are local, meaning that they are only defined in the context of attributes they relate to. Interactions are stable, and
introduction of other attributes cannot change the interactions that already exist among the attributes. Interactions are unambiguous, meaning that the importance of a particular interaction is straightforward, easily quantifiable and simply visualized. Interactions are symmetric and undirected, so we do not need to infer causality as to explain directionality.

1.1 Overview of the Text
We attempt to capture the above intuitive view of probabilistic interactions by quantifying them with entropy-based interaction information. We note that the meaning of interactions is somewhat different in unsupervised and supervised learning. The rigorous interdisciplinary review of related work at the end of the section shows that virtually the same formulae have emerged independently a number of times in various disciplines, ranging from physics to psychology, adding weight to the worth of the idea.

We try to bridge the chasm between model performance measures and entropy in Section 3. We show that interaction information is merely a performance measure of specific models. For example, 3-way interaction information measures how well we describe a joint probability distribution of three attributes on the basis of joint probability distributions of all combinations of two attributes. We explain the relevance and limitations of other information theoretic heuristics, and how they deviate from reality. We provide a formal definition of observational interactions, one that fits naturally with the intuitions presented previously, and contrast it to better known representational interactions.

In Section 4 we show that assumptions made by several different popular machine learning algorithms can be easily expressed in terms of interactions, and that many heuristics in machine learning arise from quantifications of interaction magnitude. Using the connection between entropy and relative entropy, we are able to pinpoint certain fallacies of the heuristics.

We suggest a number of novel diagrams in Section 5 to visually present interactions in data, providing experimental justification for our approach to quantification. We observe that the data only rarely justifies the kind of conditional independence assumptions ubiquitously made in practice.

2 Quantifying Interactions with Entropy
Interactions are relationships that connect together a set of attributes. In other words, in an interacting set of attributes there is no attribute that can be declared to be independent of others. Instead of declaring a set of attributes as interacting or non-interacting, we will attempt to quantify the amount of interaction as the amount of information that is common to all the attributes, but not present in any subset.

The essence of learning is simplification of the joint probability distributions, achieved by exploiting certain regularities. A very useful discovery is that
$A$ and $B$ are independent, meaning that $P(A, B)$ can be approximated with $P(A)P(B)$. If so, we say that $A$ and $B$ do not 2-interact, or that there is no 2-way interaction between $A$ and $B$. Unfortunately, attribute $C$ may affect the relationship between $A$ and $B$ in a number of ways. Controlling for the value of $C$, $A$ and $B$ may prove to be dependent even if they were previously independent. Or, $A$ and $B$ may actually be independent when controlling for $C$, but dependent otherwise.

If the introduction of the third attribute $C$ affects the dependence between $A$ and $B$, we say that $A$, $B$ and $C$ 3-interact, meaning that we cannot decipher their relationship without considering all of them at once. Sudden appearance of a dependence is a type of positive interaction: positive interactions imply that the introduction of the new attribute increased the amount of dependence. A sudden disappearance of a dependence is a type of negative interaction: negative interactions imply that the introduction of the new attribute decreased the amount of dependence. If $C$ does not affect the dependence between $A$ and $B$, we say that there is no 3-interaction.

There are plenty of real-life examples of interactions. Negative interactions imply redundancy. For example, weather attributes rain and lightning are dependent, because they occur together. But the attribute storm interacts negatively with them, since it reduces their dependence. Storm somehow explains a part of their dependence. Should we wonder whether there is lightning, the information that there is rain would contribute no information if we already knew whether there is a storm.

Positive interactions imply synergy instead. For example, employment of a person and criminal behavior are relatively independent attributes, but adding the knowledge of whether the person has a new sports car suddenly makes these two attributes dependent: it is a lot more frequent that an unemployed person has a new sports car if he is involved in criminal behavior; the opposite is also true: it is somewhat unlikely that an unemployed person will have a new sports car if he is not involved in criminal behavior.

In real life, it is quite rare to have perfectly positive or perfectly negative interactions. Instead, we would like to quantify the magnitude and the type of an interaction. For this, we will employ entropy as a measure of uncertainty. A measure of mutual dependence can be constructed from an uncertainty measure, defining dependence as the amount of shared uncertainty.

Let us assume an attribute, $A$. We have observed its probability distribution, $P_A(a)$. Shannon’s entropy measured in bits is a measure of predictability of an attribute [50]:

$$H(A) \triangleq - \sum_{a \in A} P(a) \log_2 P(a) \quad (1)$$

The higher the entropy, the less reliable are our predictions about $A$. We can understand $H(A)$ as the amount of uncertainty about $A$, as estimated from its probability distribution. Although this definition is appropriate only for discrete sources, or discretized continuous sources, [50] also presents a direct definition for continuous ones.
2.1 Entropy Calculus for Two Attributes

Let us now introduce a new attribute, $B$. We have observed the joint probability distribution, $P_{AB}(a, b)$. We are interested in predicting $A$ with the knowledge of $B$. At each value of $B$, we observe the probability distribution of $A$, and this is expressed as a conditional probability distribution, $P_{AB}(a|b)$. Conditional entropy, $H(A|B)$, quantifies the remaining uncertainty about $A$ with the knowledge of $B$:

$$H(A|B) \triangleq - \sum_{a \in A, b \in B} P(a, b) \log_2 P(a|b) = H(A, B) - H(B)$$  \hspace{1cm} (2)

We quantify the 2-way interaction between the attributes with mutual information:

$$I(A; B) \triangleq \sum_{a \in A, b \in B} P(a, b) \log_2 \frac{P(a, b)}{P(a)P(b)} = H(A) + H(B) - H(A, B)$$

$$= H(A) - H(A|B) = I(B; A) = H(B) - H(B|A)$$  \hspace{1cm} (3)

In essence, $I(A; B)$ is a measure of correlation between attributes, which is always zero or positive. It is zero if and only if the two attributes are independent, when $P_{AB}(a, b) = P_A(a)P_B(b)$. If $A$ is the attribute and $L$ is the label attribute, $I(A; L)$ measures the amount of information provided by $A$ about $L$: in this context it is often called information gain.

2-way interaction helps reduce our uncertainty about either of the two attributes with the knowledge of the other one. We can calculate the amount of uncertainty remaining about the value of $A$ after introducing knowledge about the value of $B$. This remaining uncertainty is $H(A|B)$, and we can obtain it from mutual information, $H(A|B) = H(A) - I(A; B)$. Sometimes it is worth expressing it as a percentage. For example, after introducing attribute $B$, we have $100\% \cdot H(A|B)/H(A)$ percent of uncertainty about $A$ remaining. One attribute is usually better predictable than the other, percentage-wise. For two attributes, the above notions are illustrated in Fig. 1.

2.2 Entropy Calculus for Three Attributes

Let us now introduce the third attribute, $C$. We could now wonder how much uncertainty about $A$ remains after having obtained the knowledge of $B$ and $C$: $H(A|BC) = H(ABC) - H(BC)$. We might also be interested in seeing how $C$ affects the interaction between $A$ and $B$. This notion is captured with conditional mutual information:

$$I(A; B|C) \triangleq \sum_{a, b, c} P(a, b, c) \log_2 \frac{P(a, b|c)}{P(a|c)P(b|c)} = H(A|C) + H(B|C) - H(AB|C)$$

$$= H(A|C) - H(A|B, C) = H(AC) + H(BC) - H(C) - H(ABC)$$  \hspace{1cm} (4)
Figure 1: A graphical illustration of the relationships between information-theoretic measures on the joint distribution of attributes $A$ and $B$. The surface area of a section corresponds to the labeled quantity.

Conditional mutual information is always positive or zero; when it is zero, it means that $A$ and $B$ are unrelated given the knowledge of $C$, or that $C$ completely explains the association between $A$ and $B$. From this, it is sometimes inferred that $A$ and $B$ are both consequences of $C$. If $A$ and $B$ are conditionally independent, we can apply the naive Bayesian classifier for predicting $C$ on the basis of $A$ and $B$ with no remorse. Conditional mutual information is a frequently used heuristic for constructing Bayesian networks [10].

If conditional mutual information $I(A; B|C)$ describes the relationship between $A$ and $B$ in the context of $C$, we do not know the amount of influence resulting from the introduction of $C$. Hence, we could now introduce the measure of the intersection of all three attributes, or interaction information [40] or McGill’s multiple mutual information [22]:

$$I(A; B; C) \triangleq I(A; B|C) - I(A; B) = I(A, B; C) - I(A; C) - I(B; C)$$
$$= H(AB) + H(BC) + H(AC) - H(A) - H(B) - H(C) - H(ABC)$$

Like mutual information, interaction information is symmetric, meaning that $I(A; B; C) = I(A; C; B) = I(C; B; A) = \ldots$. Since interaction information may be negative, we will often refer to the absolute value of interaction information as interaction magnitude.

The concept of total correlation [56] describes the total amount of depen-
dence among the attributes:

\[ C(A, B, C) \triangleq H(A) + H(B) + H(C) - H(ABC) \]

\[ = I(A; B) + I(B; C) + I(A; C) + I(A; B; C) \] (6)

It is always positive, or zero if and only if all the attributes are independent, 

\[ P_{ABC}(a, b, c) = P_A(a)P_B(b)P_C(c). \]

However, it will not be zero even if only a pair of attributes are dependent. For example, if \( P_{ABC}(a, b, c) = P_{AB}(a, b)P_C(c) \), the total correlation will be non-zero, but only \( A \) and \( B \) are dependent. Hence, it is not justified to claim an interaction among all three attributes. For such a situation, interaction information will be zero, because \( I(A; B|C) = I(A; B) \).

### 2.2.1 Positive and negative interactions

Interaction information can either be positive or negative. Perhaps the best way of illustrating the difference is through the equivalence \( I(A; B; C) = I(A, B; C) - I(A; C) - I(B; C) \): Assume that we are uncertain about the value of \( C \), but we have information about \( A \) and \( B \). Knowledge of \( A \) alone eliminates \( I(A; C) \) bits of uncertainty from \( C \). Knowledge of \( B \) alone eliminates \( I(B; C) \) bits of uncertainty from \( C \). However, the joint knowledge of \( A \) and \( B \) eliminates \( I(A, B; C) \) bits of uncertainty. Hence, if interaction information is positive, we benefit from an unexpected synergy. If interaction information is negative, we suffer diminishing marginal returns by introducing attributes that partly contribute redundant information. The second interpretation, offered by [40], is as follows: Interaction information is the amount of information gained (or lost) in transmission by controlling one attribute when the other attributes are already known.

#### 2.3 Interactions and Supervised Learning

The objective of unsupervised machine learning is construction of a model which helps predict the value of any attribute with partial knowledge of other attribute values. Unsupervised models approximate the joint probability distribution \( P(A, B, C) \) with a joint probability distribution function \( \hat{P}(A, B, C) \). On the other hand, the objective of supervised learning is to predict the distinguished label attribute with the partial knowledge of other attributes. Supervised models attempt to describe the conditional probability distribution, distinguishing the label \( C \) from ordinary attributes \( A \) and \( B \). The conditional probability distribution can be modeled with informative models \( \hat{P}(A, B|C) \), or with discriminative models \( \hat{P}(C|A, B) \) [48]. For example, the naive Bayesian classifier is an informative model, while logistic regression is a discriminative model.

In supervised learning we are only interested in the interactions that involve the label: interactions between attributes that do not involve the label are rarely investigated. In fact, only those interactions that involve the label provide information about it. If there is no interaction with the label, there is no information about the label. As an example, we formulate the naive Bayesian
classifier as an approximation to the Bayes rule, introducing the assumption that $A$ and $B$ are independent given $C$, $P(a, b|c) \approx P(a|c)P(b|c)$:

$$P(c|a, b) = P(c) \frac{P(a, b|c)}{P(a, b)} \approx P(c) \frac{P(a|c)P(b|c)}{P(a, b)}$$  \hspace{1cm} (7)

The conditional independence assumption implies that for there does not exist any value of $C$, in the context of which $A$ and $B$ would 2-interact. We will refer to this type of interactions as informative conditional interactions, the interactions in informative probability distributions. For a label $C$ and attributes $X$ and $Y$, the 2-way informative conditional interaction information is $I(X; Y|C)$, the familiar conditional mutual information. It can be seen as the expected 2-way informative conditional interaction information between $A$ and $B$ over the values of $C$.

The relationship between the ordinary and the informative conditional interactions is easily seen from the definition of 3-way interaction information in (5): it is the difference between the two kinds of 2-way interaction information. It is quite easy to see that when $I(A; B|C) = 0$ the 3-way interaction information can only be zero or negative. When the 3-way interaction information is positive, the 2-way conditional interaction information is positive. However, when the 3-way interaction information is zero or negative, no specific conclusions can be made about the 2-way informative conditional interaction.

2.3.1 Limitations of conditional independence relations

If there is any conditional independence among the three attributes, the interaction cannot be positive. For an example, assume that $I(A; B|C) = 0$. Such a negative interaction can be perfectly represented with a Bayesian network [14]: $A \leftarrow C \rightarrow B$. If a pair of attributes are mutually independent, for example $I(A; B) = 0$, the interaction, if it exists, can only be positive. Such an interaction can be perfectly described with a Bayesian network, $A \rightarrow C \leftarrow B$.

Unfortunately, there are informative possibilities which cannot be unambiguously described with Bayesian networks. For example, in the case of $A = B \neq C$, where the attributes are binary, or the XOR problem, the mutual information between any pair of attributes is zero, yet the attributes are deterministically 3-way interacting. We can formally describe this with three consistent Bayesian networks: $A \rightarrow C \leftarrow B$, $A \rightarrow B \leftarrow C$ and $B \rightarrow A \leftarrow C$, but no network emphasizes the fact that there are no 2-way interactions. The interaction information in this case, however, is strictly positive.

Another example is the case of triplicated attributes, $A = B = C$. In this case, for all combinations of attributes, the conditional mutual information is zero. On the other hand, every pair of attributes is deterministically 2-way interacting. Again, the fact cannot be seen from any of the Bayesian networks consistent with the data: $A \leftarrow C \rightarrow B$, $A \leftarrow B \rightarrow C$ and $B \leftarrow A \rightarrow C$. The interaction information in this case is strictly negative.

These two were extreme examples, but having zero conditional mutual information is too an extreme example. Conditional or mutual information is rarely
zero, yet some are larger than others. The larger they are the more likely it is that the dependencies are not coincidental, and the more information we gain by not ignoring them.

2.4 Quantifying \( n \)-Way Interactions

In this section, we will generalize the above concepts to interactions involving an arbitrary number of attributes. Assume a set of attributes \( \mathcal{A} = \{X_1, X_2, \ldots, X_n\} \). A subset of \( \mathcal{A} \) is defined as \( S_i \subseteq \mathcal{A} \), where \( S_i = \{X_{i(1)}, X_{i(2)}, \ldots, X_{i(k)}\} \). Each attribute \( X \in \mathcal{A} \) has a set of associated values, \( \mathcal{X} = \{x_1, x_2, \ldots, x_p\} \). \( \mathcal{A} \) is the Cartesian product of the sets of attribute values, \( \mathcal{A} = \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n \). We also have a joint probability distribution, \( P(\vec{a}) \), where \( \vec{a} \in \mathcal{A} \).

We can define a marginal probability distribution for a subset of attributes \( S_i \):

\[
P(\vec{s}) \triangleq \sum_{\vec{a} \in \mathcal{A}, \vec{s}_j = \vec{a}_{(j)}, j = 1, 2, \ldots, k} P(\vec{a}). \tag{8}
\]

Next, we can define entropy for a subset of attributes:

\[
H(S) \triangleq -\sum_{\vec{v} \in \vec{S}} P(\vec{v}) \log_2 P(\vec{v}) \tag{9}
\]

We define \( k \)-way interaction information by generalizing from formulas for \( k = 3, 4 \) in \[40\]:

\[
I(S) \triangleq -\sum_{T \subseteq S} (-1)^{|S| - |T|} H(T) = I(S \setminus X | X) - I(S \setminus X), X \in S, \tag{10}
\]

where \( k \)-way multiple mutual information is closely related to lattice-theoretic derivation of multiple mutual information \( \Delta h(S) = -I(S) \) \[22\], to set-theoretic derivation of multiple mutual information \[59\] and co-information (which both use the same symbol) as \( I'(S) = (-1)^{|S|} I(S) \) \[5\].

We define \( k \)-way total correlation as \[56, 22\]:

\[
C(S) \triangleq \sum_{X \in S} H(X) - H(S) = \sum_{T \subseteq S, |T| \geq 2} I(T). \tag{11}
\]

We can see that it is possible to arrive at the estimate of total correlation by summing all the interaction information existing in the model. Interaction information can be hence seen as a decomposition of a \( k \)-way dependence into a sum of \( l, l \leq k \) dependencies.

2.5 Related Work

Although the idea of mutual information has been formulated (as ‘rate of transmission’) already by \[50\], the seminal work on higher-order interaction information was done by \[40\]. He was interested in analysis of contingency tables.
with the intention of identifying multi-way dependencies between a number of psychological variables. The analogy between variables and information theory was derived from viewing each variable as an information source. A slightly different approach to interactions has been recently described by [2] who decomposes relative entropy, entropy and information into a sum of non-negative quantities representing $k$-way interactions.

The concept of interaction information was also discussed in early textbooks on information theory, e.g. [13]. An important series of papers that encompassed a thorough study of the subject was concluded by [22]. A further discussion of mathematical properties of positive versus negative interactions appeared in [54]. The concept of co-information [4] is closely related to the Yeung’s notion of multiple mutual information, and suggested its usefulness in the context of dependent component analysis.

One of the first detailed discussions of total correlation was [56], even if the same concept had been described (but not named) previously by [40]. The properties of conditional mutual information as applied to conditional independence models appeared in [53]. They discussed total correlation, generalized it, and named it multiinformation. Multiinformation was used to show that conditional independence models have no finite axiomatic characterization. More recently, total correlation has been referred to as stochastic interaction [57], and as integration [52]. Total correlation has been compared with interaction information in the context of quantum information theory by [55]. In the field of neuroscience the utility of interaction information for three attributes was noted [8], and referred to as synergy. They used interaction information for observing relationships between neurons. Positive interactions have been referred to as synergy and negative as redundancy [17]. The similarity between total correlation and interaction information was investigated by [9].

The concept of interactions also appeared in cooperative game theory with applications in economics and law. The issue is observation of utility of cooperation to different players, for example, a coalition is an interaction which might either be of negative or positive value for those involved. The Banzhaf interaction index [20] proves to be a generalization of interaction information, if we adopt negative entropy as game-theoretic value, equate attributes with players, and disregard all other players while evaluating a coalition of a subset of them [26]. These notions have also been applied to rough set analysis [18].

### 2.5.1 The relationship between set theory and entropy

Interaction information is similar to the notion of intersection of three sets. It has been long known that these computations resemble the inclusion-exclusion properties of set theory [59]. We can view mutual information ($;$) as a set-theoretic intersection ($\cap$), joint entropy ($,$) as a set-theoretic union ($\cup$), and conditioning ($|$) as a set difference ($-$). The notion of entropy or information corresponds to $\mu$, a signed measure of a set, which is a set-additive function. Yeung defines $\mu$ to be an I-measure, where $\mu^*$ of a set is equal the entropy of the corresponding probability distribution, for example $\mu^*(\tilde{X}) = H(X)$. Yeung
refers to diagrammatic representations of a set of attributes as *information diagrams*, similar to Venn diagrams. Some think that using these diagrams for more than two information sources is misleading [36], for example because the set measures can be negative, because there is no clear concept of what the elements of the sets are, and because it is not always possible to keep the surface areas proportional to the actual uncertainty.

Via the principle of inclusion-exclusion, and understanding that multiple mutual information is equivalent to an intersection of sets, it is possible to arrive to a slightly different formulation of interaction information [59]. This formulation is the most frequent in recent literature, but it has a counter-intuitive semantics, as illustrated by [5]: *n*-parity, a special case of which is the XOR problem for $n = 2$, is an example of a purely $n$-way dependence. It has a positive co-information when $n$ is even, and a negative co-information when $n$ is odd. For that reason we decided to adopt the original definition [40].

### 2.5.2 Testing the significance of dependencies and interactions

Expressions involving entropy are closely associated with likelihood ratio [40]; total correlation and conditional mutual information follow a $\chi^2$ distribution for large samples. Asymptotical properties of interaction information are discussed in [22]. Hence, entropy is a very general statistic, useful for ascertaining significance of various forms of dependence or independence among attributes.

### 2.5.3 Total and partial correlation

Venn diagrams, such as the one in Fig. 1, are also an item of interest in statistics, where multiple correlation or the $R^2$ or $\eta^2$ statistics represents the total amount of variance in the dependent variable explained in the sample data by the independent variables. With this index, it is too possible to render Venn diagrams representing shared variance, even if these indices do not have as pleasant properties as entropy. Partial correlation quantifies the amount of variance in the dependent variable explained by only one independent variable, controlling for a set of other independent variables [60].

If correlation can be seen as a measure of dependence between a dependent variable and an independent variable, multiple correlation as a measure of dependence between a dependent variable and a number of independent variables, we can understand partial correlation as a quantification of conditional dependence for continuous variables.

Entropy is just a specific approach to quantification of variance, and the inferences we make have much in common with those based upon partial correlation. Our visualization methods would be equally suitable for presenting partial correlation among continuous variables.
3 Quantifying Interactions with Loss Functions

Hitherto, our discussion was based on entropy as a generic measure of uncertainty. As such, it might appear unrelated to the performance measures otherwise used in machine learning. In this section, we will note that interaction information is actually a performance measure which evaluates joint probability distribution approximations. The existence of an interaction among a set of attributes will be understood as a statement that their joint probability distribution cannot be factorized in a particular way, and the interaction information is the distance between the actual joint probability distribution and its factorization.

3.1 Relative Entropy

Kullback-Leibler divergence or relative entropy [35, 11] is a measure of similarity between two probability distribution functions $p$ and $q$, defined over the same alphabet $X$:

$$D(p \parallel q) \triangleq \sum_{x \in X} p(x) \log \frac{p(x)}{q(x)}$$

(12)

It is possible to show that $D(p \parallel q) \geq 0$, with equality iff $p(x) \equiv q(x)$. $D(p \parallel q) = +\infty$ when for some $x$, $p(x) > 0$ and $q(x) = 0$. For consistency with entropy, we used the logarithm of base 2, so relative entropy is too measured in bits. It is closely related to the Wilks likelihood ratio statistic $G^2$. It is not a metric, because it is not symmetric and does not satisfy the triangle inequality. It measures the excess in description length of a symbol encoded with $q$ in bits, where the true probability for the symbol was $p$. Hence, $D(p \parallel q)$ is the entropy gained (or information lost) when $q$ is used to approximate $p$.

3.1.1 Approximating probability distributions

An important task in learning is approximating a probability distribution with a simpler probability distribution function, and we can apply relative entropy to investigate the quality of approximation. For example, to compare an approximation to $P(a, b)$ with the assumption of independence $\hat{P}(a, b) \triangleq P(a)P(b)$, we quickly find out that $D(P \parallel \hat{P}) = I(A; B)$. Hence, mutual information is nothing else than the loss we have incurred by assuming independence between a pair of attributes, or the gain we have achieved by assuming dependence.

For three attributes total correlation measures how well the joint probability distribution is approximated by probability distributions of individual attributes:

$$C(A, B, C) = D(P(a, b, c) \parallel P(a)P(b)P(c))$$

How well can be $P(a, b, c)$ approximated by including 2-way interactions into consideration? One approach is the Kirkwood superposition approximation [30], where properties of liquids are approximated in terms of 2-way interactions.
between molecules. The generalized Kirkwood superposition approximation for joint probability distributions of three attributes can be formulated as

\[ \hat{P}_K(a, b, c) \equiv \frac{P(a, b)P(b, c)P(a, c)}{P(a)P(b)P(c)} \]  

(13)

It is easy to show that

\[ D(P(a, b, c) \parallel \hat{P}_K(a, b, c)) = I(A; B; C). \]

The generalized Kirkwood superposition approximation for a \( n \)-attribute joint probability distribution \( P(\vec{a}) \), \( \vec{a} \in \vec{A} \) can be formulated as:

\[ \hat{P}_K(a_1, \ldots, a_n) \equiv \prod_{i_1 < \cdots < i_{n-1}} \frac{P(a_{i_1}, \ldots, a_{i_{n-1}})}{\prod_{i_1 < \cdots < i_{n-2}} P(a_{i_1}, \ldots, a_{i_{n-2}})} \]  

(14)

This time, the quality of the approximation is measured by \( n \)-way interaction information.

3.1.2 Normalizing probability distribution functions

\( n \)-way interaction information can be negative for \( n > 2 \), in seemingly paradoxical conflict with the non-negative property of relative entropy. The explanation is that \( \hat{P}_K(a, b, c) \) is not a proper probability distribution function, because it does not satisfy the normalization condition for all probability distribution functions \( p \), defined over an alphabet \( \mathcal{X} \):

\[ \sum_{x \in \mathcal{X}} p(x) = 1 \]  

(15)

Via counter examples, it is easy to see that the 3-way Kirkwood superposition approximation does not satisfy the normalization condition. When the sum is greater than 1, we may say that the approximation may be overfitting: it is boldly overestimating the probability in at least one case; When the sum is less than 1, we could say that the approximation could be underfitting: it is timidly underestimating the probability at least in one case.

Via relative entropy, it is also easy to illustrate why conditional mutual information verifies the core assumption of \( P(a, b|c) \approx P(a|c)P(b|c) \) in the naïve Bayesian classifier:

\[ I(A; B|C) = D(P(a, b|c) \parallel P(a|c)P(b|c)) = D \left( P(c|a, b) \middle\| P(c) \frac{P(a|c)P(b|c)}{P(a, b)} \right) \]

Knowing that \( P(a|c)P(c) = P(a, c) \), it is easy to see that approximating conditional probability distributions is just one approach to approximating joint probability distributions:

\[ I(A; B|C) = D \left( P(a, b, c) \middle\| \frac{P(a, c)P(b, c)}{P(c)} \right) \]

13
However, most naïve Bayesian classifier implementations are not based on (7), but arrive at the posterior label distribution by a slightly different means, merely by assuming \( P(c|a, b) \propto P(c)P(a|c)P(b|c) \), and normalizing the posterior label distribution through the law of total probability:

\[
\hat{P}_{NB}^N(c|a, b) \triangleq \frac{P(c)P(a|c)P(b|c)}{\sum_j P(c_j)P(a|c_j)P(b|c_j)} \quad (16)
\]

This assures that \( \hat{P}_{NB}^N \) always satisfies the normalization condition given any set of attribute values \( \{a, b\} \). The two forms of the naïve Bayesian classifier are not equivalent, and conditional mutual information often overestimates the actual quality of normalized naïve approximation: \( D(P(c|a, b) \parallel \hat{P}_{NB}^N(c|a, b)) \), as illustrated in Fig. 2. A similar technique can be applied to normalize the Kirkwood superposition approximation, normalizing it across all possible attribute values, and consequently eliminating negative interaction information, which some find problematic:

\[
\hat{P}_K^N(\vec{a}) \triangleq \frac{\hat{P}_K(\vec{a})}{\sum_{\vec{x} \in \vec{A}} P_K(\vec{x})} \quad (17)
\]

Figure 2: The conditional mutual information often tends to overestimate the loss in the approximation with the naïve Bayes classifier, because it does not take the loss-reducing normalization into consideration. The results correspond to all attribute pairs in the ‘mushroom’ data set.
3.1.3 Generalization

All we have done with relative entropy could be done with other loss measures. Interaction information is merely a measure of how well a particular model fits the data. Of course, other loss measures might not have certain useful properties, such as additivity of entropy of independent sources. Our visualization methods depend to some extent on these properties, especially since negative interactions would not exist otherwise.

Finally, relative entropy can be used to evaluate the generalization ability of a particular approximation function. Assume the available data $\mathcal{D}$ has been split into the training set $\mathcal{T}$ and the validation set $\mathcal{V}$, so that $\mathcal{D} = \mathcal{T} \cup \mathcal{V}$. Also assume an approximation function $f$, which estimates the joint probability distribution of attributes in a set of data with a probability distribution function. The generalization ability of the approximator can be estimated with $D(f(\mathcal{V}) \parallel f(\mathcal{T}))$. It is not hard to see that approximation with interactions of high order is usually less reliable than approximation with interactions of low order when data is scarce [39].

3.2 Formal Definitions of Interactions

To formalize and summarize our earlier intuitions and approximations, we will now present two definitions of interactions:

- **Observational interactions** indicate that the joint probability distribution of a number of attributes cannot be *predicted* without observing the values of all attributes simultaneously.

- **Representational interactions** indicate that the joint probability distribution of a number of attributes cannot be *modeled* with a function which is not observing the values of all the attributes simultaneously.

Our earlier discussion has been mostly focused on observational interactions, but representational interactions are more often discussed in learning.

3.2.1 Observational interactions

An *n-way observational interaction* exists in a set of attributes $\mathcal{A}, n = |\mathcal{A}|$ if and only if the joint probability distribution $P(\mathcal{A})$ cannot be described without observing the joint probability distribution directly.

Given a set of attributes $\mathcal{A}, n = |\mathcal{A}|$ and a loss function $L$, the interaction magnitude $I$ of the $n$-way interaction among $\mathcal{A}$ is the minimum loss in modeling of the joint probability distribution $P(\mathcal{A})$ with the set of joint probability distributions $\mathcal{S}_\mathcal{A} = \{P(\mathcal{X}), \mathcal{X} \subset \mathcal{A}\}$, but where the approximating procedure cannot observe $P(\mathcal{A})$ directly. Assume an approximating procedure $f : \mathcal{S}_\mathcal{A} \mapsto \hat{P}(\mathcal{A})$, we define the interaction magnitude to be:

$$I_L(\mathcal{A}) \triangleq L(P(\mathcal{A}) \parallel f(\mathcal{S}_\mathcal{A}))$$  \hspace{1cm} (18)
For example, assuming that our loss function is relative entropy \( I \), interaction magnitude is an approximation to \( M_{D} \), using the generalized Kirkwood superposition approximation \( (13) \) as the approximating procedure.

In supervised learning based on informative probability distributions, an example of which is \( P(A, B|C) \) with \( C \) as the label, the conditional interaction magnitude \( I(A, B|C) \) is instead of interest. It is defined for a loss function \( L \), an approximation function \( f \), a set of attributes \( A \) and the context \( C \) as:

\[
I_L(A|C) \equiv L(P(A|C) \parallel f(S_A|C)) \tag{19}
\]

The value of the loss function can be computed for a specific context, a certain assignment of values to label attributes in \( C \), or the expected value of the loss function can be computed over all the possible values of label attributes in \( \vec{C} \). An example of the former is \( I(A; B|C = 0) \), while an example of the latter is \( I(A; B|C) \).

Our definition of interactions has two useful properties. It is *stable*, meaning that observing additional attributes cannot invalidate interactions that already exist among them. It is also *unambiguous*, where only a single interaction magnitude is meaningful in a given situation. A more common conception of interactions, *representation interactions*, do not always have these properties.

### 3.2.2 Representation interactions

Most conceptions of interactions are based on restriction of expression rather than on the restriction of observation. For example, there is no 3-way interaction among nominal attributes \( A, B \) and \( C \) if there exist constants \( \alpha \) so that:

\[
\log \hat{P}_\alpha^{(2)}(A, B, C) = \sum_{a \in A} \alpha_a(A = a) + \sum_{b \in B} \alpha_b(B = b) + \sum_{c \in C} \alpha_c(C = c) - \alpha \\
+ \sum_{a \in A, b \in B} \alpha_{a,b}(A = a \land B = b) + \sum_{b \in B, c \in C} \alpha_{b,c}(B = b \land C = c) \\
+ \sum_{a \in A, c \in C} \alpha_{a,c}(A = a \land C = c) \tag{20}
\]

Here, log-linear modeling was used to approximate the true joint probability distribution, but limiting the terms to two attributes. However, it achieves this approximation by *observing* the full joint probability distribution.

If \( L \) is the loss function of interest, an optimal approximating function would seek \( \alpha \) as to minimize the loss of the approximation. The magnitude of a 3-way representational interaction in the above case would then be:

\[
I_L^{(2)}(A, B, C) \equiv \min_{\alpha} L(P(A, B, C) \parallel \hat{P}_\alpha^{(2)}(A, B, C))
\]

A general formal definition of representational interactions without assuming a particular approach to modeling would be intricate, but the idea of preventing the approximation function \( \hat{P}^{(\alpha-1)} \) from fitting terms that depend on
simultaneous appearance of particular values for more than \(n\) attributes, such as \(\alpha(A_1 = a_1 \land A_2 = a_2 \land \cdots \land A_n = a_n)\), is intuitively simple. Hence, a representational interaction does not exist among the attributes of the set \(\mathcal{A}\) if the joint probability distribution \(P(\mathcal{A})\) can be perfectly described with a representation that does not involve any conjunctions of simultaneous values of all the attributes. A representational interaction magnitude is the minimum loss achieved with approximations using such representations.

A further discussion of methods for representational interactions in statistics will appear in Sect. 4.4.1. Representational interactions have been applied to neuroscience \[27\], using log-linear models as approximation functions, and quantifying the 3-way interaction magnitude simply with the potentially ambiguous value of \(\alpha_{a,b,c}\). \[2\] gives a decomposition of a joint probability distribution into orthogonal dependencies of equal or lower orders using the information geometry. Analysis of multi-way interactions with log-linear models has also been applied to association rule induction \[58\].

There are several disadvantages of representational interactions in comparison with observational interactions. The representational interaction magnitude strongly depends on the approximation function. Because the joint probability distribution can be freely observed, the problem of overfitting becomes more distinct. We will provide two examples illustrating the pitfalls of ambiguity and instability, using multiple linear regression as the approximation function.

Linear regression is restricted to a linear model, but it is free to arbitrarily adjust the variable weights, observing all the variables. For example, if linear regression is executed on independent variables \(A, B\) and \(C\), and a dependent variable \(Y\), but where \(A\) and \(B\) are perfectly correlated, learning by only observing the correlations \((A, Y), (B, Y), \text{and} (C, Y)\), and averaging them to obtain the final model, we will find out that \(A\) and \(B\) are given \(2/3\) of the weight, even if they only deserved \(1/2\). If optimization was used, the weights \(a, b\) and \(c\) for each variable would be found, where \(c = 1/2\) but \(a + b = 1/2\). We would always be unsure about the exact value of \(a\) and \(b\), and therefore quantifying interaction magnitude on the basis of coefficient value is ambiguous. It would be possible to remedy this problem by measuring interaction magnitude using loss functions, rather than by observing arbitrary model coefficients. On the other hand, the approach based on interaction information would identify a 2-way interaction between \(A\) and \(B\), positive 3-way interactions between \((A, C, Y), (B, C, Y)\), and a negative 4-way interaction between all four, which declares that the two 3-way interactions are the same.

An inappropriate approach to interactions in linear regression might be unstable. For example, if linear regression is given independent binary variables \(A, B\) and the dependent variable \(C\), where \(C = A \neq B\), an interaction term between \(A\) and \(B\) will be found. But if another variable \(X\) is introduced, \(X = A \times B\), the interaction between \(A\) and \(B\) will no longer be found, since \(X\) carries that information. Nevertheless, the collinearity between variables \(X\) and \(A, B\) is nevertheless a well-documented problem in regression, because it causes numerical instability, and problems with interpretation of models and evaluation of individual variable significance. With our interaction information
approach, instead, a 3-way positive interaction will be found between $A, B$ and $C$, three 2-way interactions between $(X, C)$, $(A, X)$ and $(B, X)$, and a negative 4-way interaction which informs us that the 3-way interaction $(A, B, C)$ and the 2-way interaction $(X, C)$ are the same. The HWF models (Sect. 4.4.1) attempt to remedy the stability problem so that an outside attribute cannot affect the internal interactions.

4 Interactions in Common Machine Learning Procedures

In this section we will attempt to show that interactions, as they have been defined, are relevant to a number of supervised and unsupervised learning procedures. We will briefly survey several popular learning techniques in the light of interactions. We will see that the assumptions the learning algorithms make can be easily expressed in terms of assumptions about the number and magnitude of interactions.

4.1 Feature Selection, Construction and Discretization

Greedy feature selection and split selection heuristics are often based on various quantifications of 2-way interactions between the label and an attribute. The frequently used information gain heuristic is a simple example of how interaction magnitude has been used for evaluating attribute importance. Assume a label $D$ and an attribute $A$. The information gain is $I(A; D)$, indicating how much the two attributes deviate from independence. Had we used a loss measure $L$ instead of entropy, the generalization of information gain would have been $I_L(A; D)$: it is meaningful to use a single loss measure throughout the learning algorithm. It may be problematic to use a feature selection heuristic based on relative entropy just to evaluate the final model with a different loss function, such as classification accuracy.

The situation changes somewhat when we have more than a single attribute, as information gain is no longer a reliable measure. First, in positive interactions, information gain will underestimate the actual importance of attributes, since $I(A \times B; D) > I(A; D) + I(B; D)$, where $A \times B$ is the joint attribute, obtained by taking a Cartesian product. Second, in negative interactions information gain will overestimate the importance of attributes, because some of the information is duplicated, as can be seen from $I(A \times B; D) < I(A; D) + I(B; D)$.

The problems with positive interactions are known as myopia. Myopic feature selection evaluates an attribute’s importance independently of other attributes, and it is unable to appreciate their synergistic effect [34]. The disability of most feature selection algorithms to appreciate attributes involved in interactions was remedied with algorithms such as Relief [29, 47], which are usually based on instance-based heuristics. Besides, many learning algorithms are not able to take advantage of these synergies, and structured induction methods allow joint treatment of attributes, e.g. [51, 52].
Negative interactions, on the other hand, offer opportunity for eliminating unneeded redundant attributes. Conditional interaction information can also be applied as a feature selection heuristic. An attribute $B$ is a conditionally irrelevant source of information about the label $D$ given attribute $A$ if $I(B; D|A) = 0$, assuming that there are no other attributes positively interacting with the disposed attribute \[32\]. Another approach is based on minimizing mutual information among attributes, via eliminating $B$ if $I(A; B)$ is large \[21\], but this is merely an indirect approach to the same goal.

Feature selection algorithms are not the only algorithms in machine learning with myopia. Supervised discretization algorithms, e.g. \[14\], discretize one attribute at a time, determining the number of intervals with respect to the ability to predict the label. Such algorithms underestimate the number of intervals for positively interacting attributes, and it is better to use multivariate discretization algorithms \[4\]. Similarly, in negatively interacting groups of attributes, the total number of intervals may be excessive.

4.2 Classification Trees

The concept of interactions has been observed several times in machine learning, but with differing terminology and rarely formally defined. One of the first classification tree learning systems was Automatic Interaction Detector (AID) \[42\]. It no longer made the restrictive assumption of additivity or linearity of effects as does ordinary multiple regression.

The success in predicting the label $D$ from attributes $A$, $B$ and $C$ is much alike investigating the 2-way interaction between $P(D)$ and the joint probability distribution $P(A, B, C)$, which would be noted as $I(D; A \times B \times C)$, using the Cartesian product to form a joint attribute. If the attributes are useless to predicting the label, the interaction magnitude will be zero. Unfortunately, if the attributes are many, we seek a more effective representation of the attributes’ joint probability distribution.

Classification trees are an incremental approach to building the joint probability distribution. The information gain split selection heuristic, e.g. \[46\], essentially pursues the attribute $X$ with the highest interaction magnitude with the label $D$: $\arg \max_X I(D; X)$. Consequently, $X$ enters the joint probability distribution. In the second step, we pursue attribute $Y$, which will maximize the interaction magnitude between $Y$ and $D$, but in the context of the earlier attribute $X$: $\arg \max_X I(D; Y|X)$.

In case of negative interactions between $X$ and $Y$, the classification tree learning method will also appropriately adjust the $Y$’s usefulness in the context of $X$, because $I(Y; D|X) < I(Y; D)$. Using the context we are also able to appreciate positive interactions, but only if just one of the attributes is outside the context. For example, if $X$ and $Y$ interact positively, $I(Y; D|X) > I(Y; D)$. We only need to achieve that $B$ somehow finds its way into the model. The multidimensional relational projection algorithm \[45\] is intended for discovering and resolving complex $n$-way interactions in classification problems.

The classification tree learning approach has the advantages of managing
negative and positive interactions, and not assuming that \( n \)-way interactions do not exist. Unfortunately, it makes an assumption that there is only a \textit{single} interaction in the data. Consequently, the method is incapable of simplifying the learning problem to the study of several interactions of lower order.

A symptom of trying to capture all regularities with a single interaction fragments the data, making it difficult to employ all the available information. Recently, several possibilities with improved performance have emerged, mainly based on ensembles: aggregations of simple classifiers. For example, random forests aggregate the votes arising from a large number of small trees, where each tree can be imagined to be focusing on a single interaction. A recent survey of interactions in machine learning noted that interactions are interesting for an observer, that interactions make learning harder, and that interactions can be resolved via feature construction.

### 4.3 Na"ive Bayesian Classifier

As we have seen in Sect. 2.3, the na"ive Bayesian classifier makes the conditional independence assumption. In other words, it assumes that for every subset \( S \) of the set of attributes, \( S \subseteq \{A, B, C\} \), the interaction magnitude of \( S \) in the context of the label \( D \) is zero: \( I(S|D) = 0 \).

When the data does not correspond to the above assumption, a number of methods have been proposed to improve performance by joint treatment of contextually dependent attributes. Conditional interaction information \( I(A;B|D) \) has been used as a heuristic for detecting the problems associated with the assumption of conditional independence. Of course, the heuristic only works perfectly when there are three attributes: if there are more, it will not detect complex dependencies between them. For example, parity among four binary attributes is an example of a domain where conditional interaction information among all triples of attributes will be zero: there is only a single 4-way positive interaction.

Conditional mutual information is based on a slightly different application of the Bayes rule. Namely, na"ive Bayesian classifier normalizes the posterior label probability distribution, while the approximation corresponding to conditional mutual information does not. In Fig. 2 we saw that conditional mutual information usually overestimates the performance loss arising from the conditional independence assumption. In summary, normalization allows the na"ive Bayesian classifier to perform better than we would expect from the violations of the conditional independence assumption.

### 4.4 Interactions in Statistics

The concepts we discussed earlier have been known in statistics for a very long time. Nevertheless, the meaning of the term ‘interaction’ differs among the branches of statistics, as does the term: other expressions are moderator or moderating effects. We will briefly survey the concepts, only providing an overall topography. The focus of statistical analysis of interactions is testing whether
interactions among variables exist or not. In the first conception of these tests, we are testing whether a model that takes interaction effects into consideration is better in predicting the dependent variable than a model that does not: resembling the earlier representational interactions. In the second conception, we are testing directly whether the relationship between two variables remains constant regardless of the value of the third variable: resembling the earlier notion of observational interactions.

4.4.1 Interactions improve models

An interaction is defined to be significant when models that use a particular interaction term are significantly better than models not using them. Hence, we determine the existence of an interaction with model selection techniques.

Most statistical models where interactions are of concern are additive, attempting to approximate the label as closely as possible with a function \( f(\vec{X}) = \sum_i t(X_i) \) for some vector of variables \( \vec{X} \). An interaction between \( X_i \) and \( X_j \) exists in this context if a model involving a higher-order interaction term \( t(X_i, X_j) \) is better than a model not involving it. This notion, however, needs a better definition. One possibility is by using hierarchically well-formulated (HWF) models [25, 31]. A HWF model contains all the lower-order components of a higher-order interaction term. To evaluate the interaction between \( X, Y \) and \( Z \), we then compare the model using the terms \( X, Y, Z, XY, YZ, XZ \) and the model using the terms \( X, Y, Z, XY, YZ, XZ, XYZ \). If the extended model is significant, the interaction too is significant. By filling them model, we have prevented the second model from capturing any information that was not already captured by a simpler model. By only including the lower-order components, we have assured stability.

It is not hard to see that the evaluation of an interaction needs to be performed outside the context of other variables. If, unbeknownst to the analyst, a third variable \( Z \) contains the extra information gained from the interaction between \( X \) and \( Y \), the model involving the two-factor interaction term \( XY \) will not be any better if \( Z \) is included. On the other hand, such an interaction is not useful if our only purpose is effective prediction of the dependent variable.

Another pitfall is the method used for fitting the model. An implicit assumption of the above approach is that a HWF model achieves a better fit than any model containing only a subset of the HWF’s terms. This is true when using the ordinary least-squares optimization which minimizes variance, where the fit is assessed on the very data that was used for fitting, and where the quality of the model is assessed only through the quantity minimized in the procedure.

A very important issue is the definition of the interaction term \( t(X_1, X_2) \). If \( X_1 \) and \( X_2 \) are categorical variables, \( t \) is often merely an introduction of a new variable with the Cartesian product of the two original variables’ domains as the new domain. For continuous variables, however, \( t \) is often an arithmetic product multiplied by some scalar: \( \alpha X_1 X_2 \). This solution is not particularly satisfying, since a product cannot capture all possible regularities.
4.4.2 Interactions as deviations from conditional invariance

In analysis of contingency tables [1], terms of conditional and marginal dependence are often used. Quantifications of dependence are referred to as measures of association [19]. There are many such measures and some of them are based also on entropy, such as the various uncertainty coefficients. A rather similar concept are the measures of agreement.

In addition to the known concepts of marginal and conditional independence, there is a situation called homogeneous association between three factors, defined to exist when all pairs of factors are pairwise associated, yet the association between the pair does not vary with the third factor. When a triple is homogeneously associated, we say that there is no interaction between two factors with respect to their effects on the third factor [1]. In other words, all pairs must be conditionally independent of the remaining variable.

If we adopt correlation as the measure of association, we come up with operational definition of interactions [6]: 'A first-order interaction of two independent variables \(X_1\) and \(X_2\) on a dependent variable \(Y\) occurs when the relation between either of the \(X\)'s and \(Y\) (as measured by the slope) is not constant for all values of the other independent variable.'

In analysis of variance (ANOVA), interactions are sometimes defined to be differences in mean differences, implementing the above notion of conditional invariance [24]. For some dependent variable \(Y\) and two binary independent variables \(X_1\) and \(X_2\), we test the two hypotheses:

\[
H_0 : (\mu_{X_1=0,X_2=0} - \mu_{X_1=1,X_2=0}) - (\mu_{X_1=0,X_2=1} - \mu_{X_1=1,X_2=1}) = 0
\]
\[
H_1 : (\mu_{X_1=0,X_2=0} - \mu_{X_1=1,X_2=0}) - (\mu_{X_1=0,X_2=1} - \mu_{X_1=1,X_2=1}) \neq 0
\]

Here, \(\mu_{X_1=0,X_2=0}\) indicates the mean of variable \(Y\) given the two independent variable values. The first hypothesis tests for non-existence of interaction, the second hypothesis tests for existence of interaction.

5 Visualizing Interactions

We will now apply the tools of visualization to present the most important interactions in the data. Entropy and interaction information yield easily to graphical presentation, as they are both measured in bits. Nonetheless, all the visualization methods could be easily used with the loss-based or even representational measures of interaction magnitude.

The optimal type of visualization method depends on the type of learning it supports. In unsupervised learning, we are interested in general relationships between attributes. In supervised learning, we are particularly interested in the relevance of individual attributes to predictions about the label.

In our analysis, we have used several problem domains from the UCI repository [23]. In all cases, maximum likelihood probability estimates were used.
5.1 Unsupervised Visualization

We can illustrate the interaction quantities we discussed with interaction diagrams [26]. For clarity, we deviated from Venn diagrams and instead adopted an ordinary graph, where the surface area of each node identifies the amount of uncertainty. White circles will indicate the ‘gain’ of the model, the entropy that was eliminated in the joint model. Gray circles will indicate the individual entropy of attributes that we have started with, and the negative interactions that quantify redundancy of the model. The total entropy is obtained by summing all the gray areas and subtracting all the white areas. We start with a simple example involving two attributes from the ‘census/adult’ data set, illustrated in Fig. 3. The instances of the data set are a sample of adult population from a census database.

Figure 3: Education and occupation do have something in common: they interact because the area of the white circle, indicating the mutual information \( I(\text{education}; \text{occupation}) \), is non-zero. This is a 2-way interaction, since two attributes are involved in it. The areas of the gray circles quantify entropy of individual attributes: \( H(\text{education}) \) and \( H(\text{occupation}) \).

The occupation is slightly harder to predict a priori than the education because occupation entropy is larger. Because the amount of mutual information is fixed, this means that knowledge of occupation will eliminate a larger proportion of uncertainty about education than vice versa, but there is no reason for asserting directionality merely from the data, especially as such predictive directionality could be mistaken for causality.

5.1.1 A negative interaction

The relationship between three characteristics of animals in the ‘zoo’ database is rendered in Fig. 4. All three attributes are 2-interacting, but there is duplication between them, indicated by a negative interaction. It is illustrated as the gray circle, connected to the 2-way interactions, which means that they have a shared quantity of information. It would be wrong to subtract all the 2-way interactions from the sum of individual entropies to estimate the complexity of the triplet, as we would underestimate it. For that reason, the 3-way negative interaction acts as a correcting factor.

This model is also applicable to supervised learning. If we were interested in whether an animal breathes, while knowing whether it has milk and whether...
it lays eggs, we would obtain the residual uncertainty $H(\text{breathes}|\text{eggs}, \text{milk})$ by the following formula:

$$H(\text{breathes}) - (I(\text{breathes}; \text{eggs}) + I(\text{breathes}; \text{milk}) + I(\text{breathes}; \text{eggs}; \text{milk})).$$

This domain is better predictable than the one from Fig. 3, since the 2-way interactions are comparable in size to the prior attribute entropies. It is quite easy to see that knowing whether an animal lays eggs provides us pretty much all the evidence whether it has milk: namely, mammals don’t lay eggs. Of course, such deterministic rules are not common in natural domains.

Furthermore, the 2-way interactions between breathing and eggs and between breathing and milk are very similar in magnitude to the 3-way interaction, but opposite in sign, meaning that they cancel each other out. Using the relationship between conditional mutual information and interaction information from (5), we can conclude that:

$$I(\text{breathes}; \text{eggs}|\text{milk}) \approx 0$$
$$I(\text{breathes}; \text{milk}|\text{eggs}) \approx 0$$

Therefore, if the 2-way interaction between such a pair is ignored, we need no 3-way correcting factor. Bayesian networks represent the two models, each assuming that a certain 2-way interaction does not exist in the context of the remaining attribute:

breathes ← milk → eggs
breathes ← eggs → milk

If we were using the naïve Bayesian classifier for predicting whether an animal breathes, we might also find out that feature selection would eliminate one of the attributes: Trying to decide whether an animal breathes, and knowing that the animal lays eggs, most of the information contributed by the fact that the animal doesn’t have milk is redundant.
5.1.2 A positive interaction

Most real-life domains are difficult. The dependencies between the attributes are weak, but the importance of correct predictions is high. One such problem domain is a potential customer’s credit risk estimation. The ‘German credit’ domain describes credit risk for a number of customers. Fig. 5 describes a relationship between the riskiness of a customer and two of his characteristics.

Figure 5: An example of a 3-way positive interaction between the customer’s credit risk, his purpose for applying for a credit and his employment status.

The mutual information between all attribute pairs are very low, indicating difficult prediction. The interesting aspect is the positive 3-interaction, which additionally reduces the entropy of the model. We emphasize the positivity by painting the circle corresponding to the 3-way interaction white, and by connecting it to the attributes rather than to the 2-way interactions.

It is not hard to understand its significance. On average, unemployed applicants are riskier as customers than employed ones. Also, applying for a credit to finance a business is riskier than applying for purchasing a TV set. But if we heard that an unemployed person is applying for a credit to finance purchasing a new car, it would provide much more information about risk than if an employed person has given the same purpose. The corresponding reduction in credit risk uncertainty is a sum of all three interactions connected to it, on the basis of employment, on the basis of purpose, and on the basis of employment and purpose simultaneously.

5.1.3 Interactions with zero interaction information

The first explanation for a situation with zero 3-way interaction information is that an attribute \( C \) does not affect the relationship between attributes \( A \) and \( B \), thus explaining the zero interaction information \( I(A; B|C) = I(A; B) \Rightarrow I(A; B; C) = 0 \). A homogeneous association among three attributes is described by all the attributes 2-interacting, yet not 3-interacting. This would mean that
their relationship is fully described by a loopy set of 2-way marginal associations. Although one could imagine that Fig. 6 describes such a homogeneous association, there is an another possibility.

![Figure 6: An example of an approximate homogeneous association between body mass, and insulin and glucose levels in 'pima' data set. All the attributes are involved in 2-way interactions, yet the negative 3-way interaction is very weak, either indicating that all the 2-way interactions are independent, or indicating that there is a mixture of a positive and a negative interaction.](image)

Imagine a situation which is a mixture of a positive and a negative interaction. Three attributes \( A, B, C \) are taking values from \( \{0, 1, 2\} \). The permissible events are \( \{ A = B + C \mod 2, A = B = C = 2 \} \). The first event denotes a positive interaction, the familiar XOR problem. The second event denotes a negative interaction, again the familiar example of perfectly correlated attributes. In an appropriate mixture between these two events, the interaction information \( I(A; B; C) \) is zero, because the interaction information is an average of interaction information across all the possible combinations of attribute values. The benefit of joining the three attributes and solving the XOR problem exactly matches the loss caused by duplicating the dependence between the three attributes.

Hence, 3-way interaction information should not be seen as a full description of the 3-way interaction but as the interaction information averaged over the attribute values, even if we consider interaction information of lower and higher orders. These problems are not specific only to situations with zero interaction information, but generally. If a single attribute contains information about complex events, much information is blended together, which should rather be kept apart. To solve this problem, we represent a many-valued attribute \( A \) with a set of binary attributes, each corresponding to one of the values of \( A \).
5.1.4 Managing complexity

If the number of attributes under investigation is increased, the combinatorial complexity of interaction information may quickly get out of control. Fortunately, interaction information is often low for most combinations of unrelated attributes. We have also observed that the average interaction information of a certain order is decreasing with the order in a set of attributes.

Although an interactive tool for exploring interactions in large domains would be best, a simple approach is to identify $N$ interactions with maximum interaction magnitude among the $n$. For performance and reliability, we also limit the maximum interaction order to $k$, meaning that we only investigate $l$-way interactions, $2 \leq l \leq k \leq n$. Namely, it is difficult to reliably estimate joint probability distributions of high order. The estimate of $P(x)$ is often far more robust than the estimate of $P(x, y, z, w)$ given the same number of instances.

A larger scale interaction diagram with a selection of interactions in the ‘mushroom’ domain is illustrated in Fig. The informativity of the stalk shape attribute towards mushroom’s edibility is very weak, but this attribute has a massive synergistic effect if accompanied with the stalk root shape attribute. We can describe the situation with the term moderation: stalk shape ‘moderates’ the effect of stalk root shape on edibility. Stalk shape is hence a moderator variable. It is easy to see that such a situation is problematic for feature selection: if our objective was to predict edibility, a myopic feature selection algorithm would eliminate the stalk shape attribute, before we could take advantage of it in company of stalk root shape attribute.

Because the magnitude of the mutual information between edibility and stalk root shape is similar in magnitude to the negative interaction among all three, we can conclude that there is a conditional independence between edibility of a mushroom and its stalk root shape given the mushroom’s odor. A useful term for such a situation is mediation: odor ‘mediates’ the effect of stalk root shape on edibility.

The 4-way interaction information involving all four attributes was omitted from the diagram, but it is distinctly negative. This can be understood by looking at the information gained about edibility from the other attributes and their interactions with the actual entropy of edibility: we cannot explain 120% of entropy, unless we are counting the evidence twice. The negativity of the 4-way interaction indicates that a certain amount of information provided by the stalk shape, stalk root shape and their interaction is also provided by the odor attribute.

5.2 Supervised Visualization

The objective of supervised learning is acquiring information about a particular label attribute from the other attributes in the domain. In such circumstances, we are interested only in those relationships between attributes that involve the label. Figuratively, we place ourselves into the label and view the other attributes from this perspective. It enables us to simplify the earlier diagrams
Figure 7: A selection of important interactions in the 'mushroom' domain. We have not rendered the 4-way interaction and the interactions with low absolute interaction information.

considerably, which, in turn, permits the application of the interaction analysis methodology to exploratory data analysis.

There are several types of inter-attribute relationships which can be of interest. Interaction graphs [27] disclose 2-way and 3-way interactions involving the label in a domain. Interaction dendrograms [28] are a compact summary of proximity between attributes with respect to the similarity (or synergy) of the information they provide about the label. Conditional interaction graphs attempt to illustrate the magnitude of unwanted dependencies which affect the performance in learning algorithms that make the conditional independence assumption.

5.2.1 Interaction dendrograms

In initial phases of exploratory data analysis, we might not be interested in detailed relationships between attributes, but merely to discover groups of mutually interacting attributes. In supervised learning, we are not investigating the relationships between attributes themselves (where mutual information would have been the metric of interest), but rather the relationships between the mutual information of either attribute with the label. In other words, we would like to know whether two attributes provide similar information about the label, or whether there is synergism between attributes’ information about the label. This way, we can identify clusters of attributes whose relationships should be investigated more closely.

We can summarize the above information by introducing a distance measure between attributes. With respect to the amount of interaction, interacting attributes will hence appear close to one another; non-interacting attributes will appear far from one another. One possible distance measure $d_{mn}$ between two attributes $X, Y$ with respect to the amount of their interaction with the label
Figure 8: An interaction dendrogram illustrates which attributes interact, positively or negatively, with the label in the ‘census/adult’ data set. The label indicates the individual’s salary. The number of asterisks indicates the amount of mutual information between an attribute and the label.

\[ d_{m}(X, Y) \triangleq \begin{cases} |I(X; Y; C)|^{-1} & \text{if } |I(X; Y; C)|^{-1} < K, \\ K & \text{otherwise.} \end{cases} \]  

(21)

To prevent attribute independence from disproportionately affecting the graphical representation, we used \( K = 1000 \) as the upper bound for distance. To present the function \( d_{m} \) to a human analyst, we tabulate it in a dissimilarity matrix. We can apply the techniques of clustering or multi-dimensional scaling to graphically summarize the dissimilarity matrix.

In the example in Fig. 8, we used the Ward’s method for agglomerative hierarchical clustering for summarizing the dissimilarity matrix. The summary does not retain all the information, and an attribute’s membership in a cluster merely indicates its average relationship with other cluster members. The interaction dendrogram is an approach to variable clustering, which is normally applied to numerical variables outside the context of supervised learning.

We can observe that there are two distinct clusters of attributes. One cluster contains attributes related to the lifestyle of the person: age, family, working hours, sex. The second cluster contains attributes related to the occupation and education of the person. There are several attributes that appear in between both clusters, such as native country, race and work class.

Interaction diagrams may be useful for feature selection. The fnlwgt attribute in Fig. 8 is both unrelated to other attributes, so it does not participate
Figure 9: An interaction graph containing eight of the 3-way interactions with the largest interaction magnitude in the ‘adult/census’ domain. All interactions are negative.

in any positive interactions, and is marked as uninformative: a natural candidate for elimination during feature selection. There is a considerable amount of redundancy in each cluster of attributes. For example, older people tend to be married, and highly educated people spent many years in school. In aggressive feature selection, we could hence simply pick the individually best attributes from each cluster. In our example, these would be marital status and education.

5.2.2 Interaction graphs

Many interesting relationships are not visible in detail in the dendrogram because of compactness. To drill deeper into the relationships among a group of attributes, we can apply interaction graphs. There, individual attributes are represented as graph nodes and 3-way interactions as edges. To limit the complexity arising from a combinatorial explosion of the number of interactions in a domain with many attributes, we restrict the number of interactions illustrated only to those with the largest magnitude, and to those that involve the label.

Nodes and edges of an interaction graph are labeled numerically. The percentage in the node expresses the amount of label’s uncertainty eliminated by the node’s attribute. For example, in Fig. 9 the most informative attribute is relationship, and the mutual information between the label and relationship amounts to 20.7% of salary’s entropy.

The dashed edges indicate negative interactions that involve the two connected attributes and the label. The edge between relationship and marital status is labeled with $-19\%$, implying that the negative interaction between the two attributes comprises 19% of the label’s entropy. If we wanted to know
Figure 10: An interaction graph containing eight of the positive and eight of the negative 3-way interactions with the largest interaction magnitude in the ‘mushroom’ domain. The positive interactions are indicated by solid arrows.

how much information we gained about the salary from these two attributes, we would sum up the mutual information for both 2-way interactions and the 3-way interaction information: $20.7 + 19.6 - 19 = 21.3\%$ of entropy was eliminated using both attributes. Once we knew the relationship of a person, the marital status further eliminated only $0.6\%$ of the salary’s entropy.

The interaction graph is an approximation to the true relationships between attributes, as only a part of 3-way interactions are drawn, without regard to interactions of higher order. The number of interactions illustrated was determined merely on the basis of graph clarity: if the graph became cluttered, we reduced the number of interactions shown. Therefore, we should be careful when generalizing the above entropy computations to more than three attributes. Nevertheless, we have observed that negative interactions, viewed as relations, tend to be transitive, but not positive interactions.

As an example of a more complex interaction graph we illustrate the familiar ‘mushroom’ domain in Fig. 10. As an example, let us consider the positive interaction between stalk and stalk root shape. Individually, stalk root shape eliminates $13.4\%$, while stalk shape only $0.75\%$ of edibility entropy. If we exploit the synergy, we gain additional $55.5\%$ of entropy. Together, these two attributes eliminate almost $70\%$ of our uncertainty about a mushroom’s edibility.

5.2.3 Conditional interaction graphs

The visualization methods described in previous sections are unsupervised in sense that they describe 3-way interactions outside any context. They were merely customized for the properties of analysis specific to supervised learning. We now focus on conditional interactions that affect model selection in supervised learning. These are useful for verifying the grounds for taking the
conditional independence assumption in the naïve Bayesian classifier. Such assumption may be problematic if there are informative conditional interactions between attributes with respect to the label.

In Fig. 11 we have illustrated the informative conditional interactions with large magnitude in the ‘adult/census’ data set, with respect to the label – the salary attribute. Learning with the conditional independence assumption would imply that these interactions are ignored. The negative 3-way conditional interaction with large magnitude involving education, years of education and occupation offers a possibility for simplifying the domain. There are some other attributes in the domain, but they were not interacting, except for race and native country attributes, and were left out from the chart.

6 Summary and Discussion

Interactions are unexpected and irreducible relationships between attributes. We have distinguished two types of interactions. The joint probability distribution of observationally interacting attributes cannot be predicted without observing the actual distribution. The observational interaction is a formalization of unexpected holistic relationships between attributes. The joint probability distribution of representationally interacting attributes cannot be represented without at least one term that would involve a conjunction of values of all the attributes. The representational interactions formalize the notion of irreducible holistic relationships between attributes. In certain cases, interactions among attributes in controlled contexts may also be relevant, and in this case
conditional probability distributions are used instead of joint probability distributions.

The question of whether there is an interaction is often less useful than attempting to quantify the magnitude of interaction. We have proposed a method for quantifying interactions using the notions of an approximation to the probability distribution and a loss function. The observational approximation is made without observing the joint probability distribution. The representational approximation may not observe all attributes simultaneously when making the prediction, but it can access the joint probability distribution to calibrate the approximation.

If we adopt relative entropy as the loss function, and the Kirkwood superposition approximation function, we are able to explain several properties of interaction information, one of the most frequent information-theoretic quantifications of interaction that has arisen independently in several fields of science. We have also provide a rigorous survey of the topic, attempting to unify several approaches.

We have proposed a number of novel visualization methods that attempt to present interactions present in data, given some quantification of interactions. On examples we show that the above quantifications often confirm the intuitions, and that today’s learning algorithms are not able to model interactions as they appear in the data. The unsupervised learning algorithms disregard interactions, while the supervised learning methods often fall into two extremes. One extreme, epitomized by classification trees, assumes only a single interaction in the data. The second extreme, exemplified by the naïve Bayesian classifier, assumes that there are no conditional interactions in the data, conditioning for the label value. Perhaps this dichotomy explains why the middle way, such as ensembles of classifiers, performs better than either extreme. Also, we show that feature selection and discretization are based upon limited notions of 2-way interactions, and would benefit from a more general view.

Pursuing interactions in data is complementary to pursuit of independence, but from the opposite direction. Starting with a simple model with no dependencies, we gradually build a complex one by successively introducing important interactions. Interaction models are stable in sense that adding new attributes does not eliminate interactions that previously existed, but may only introduce new interactions of higher order that affect them. The focus of interaction analysis is quantification of interactions and their presentation. There are further epistemological connections: If conditional independence is the instrument of causality, interactions could be the instrument of synchronicity.

We have neglected to discuss several important issues. The order of interactions in an approximation is associated with the complexity of the model. One can expect that restricting the order of interactions effectively restricts the complexity of the model. We are investigating when it makes sense to assume the existence of an interaction and when it does not, depending on the amount of available data. We are examining learning algorithms that are not sidetracked by or blind of interactions. For example, feature construction seems to be an appropriate method for capturing positive interactions. Somewhat surprisingly,
for simpler and frequent negative interactions, we have not been able to find learning methods that would work consistently. Finally, we have only focused on nominal attributes in this text.

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