A Quantitative Perspective on Values of Domain Knowledge for Machine Learning

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Abstract
With the exploding popularity of machine learning, domain knowledge in various forms has been playing a crucial role in improving the learning performance, especially when training data is limited. Nonetheless, there is little understanding of to what extent domain knowledge can affect a machine learning task from a quantitative perspective. To increase the transparency and rigorously explain the role of domain knowledge in machine learning, we study the problem of quantifying the values of domain knowledge in terms of its contribution to the learning performance in the context of informed machine learning. We propose a quantification method based on Shapley value that fairly attributes the overall learning performance improvement to different domain knowledge. We also present Monte-Carlo sampling to approximate the fair value of domain knowledge with a polynomial time complexity. We run experiments of injecting symbolic domain knowledge into semi-supervised learning tasks on both MNIST and CIFAR10 datasets, providing quantitative values of different symbolic knowledge and rigorously explaining how it affects the machine learning performance in terms of test accuracy.

1 Introduction
Machine learning has achieved great success in numerous fields, such as computer vision, natural language processing, security, and robotics. The current success of machine learning, or more generally artificial intelligence (AI), owes much to the huge amount of available data. That being said, a priori domain knowledge, which comes from various sources and has multiple forms, also plays an increasingly more crucial role in the development of machine learning and may lead to new breakthroughs [5, 46, 48].

Domain knowledge has already been playing a part in current machine learning pipelines in many real-world applications. Specifically, machine learning with domain knowledge injection (a.k.a informed machine learning [46]) can be accomplished in different ways. For example, in computer vision, image pre-processing such as flipping [4, 42], translation [4], cropping, [36], scaling [52] can help to augment data, which exploits the prior domain knowledge of image invariance. For another example, differential equations and logic rules from physical sciences and/or common knowledge provide additional constraints or new regularization terms for model training [3, 5, 34, 43, 49]. Moreover, knowledge graphs can provide relational knowledge for reasoning or feature representation in deep learning [9, 28]. In recent years, prior (domain) knowledge from one or more multiple teacher networks can also be injected into a learning task (i.e., student network) via distillation [24, 51]. As evidenced by many examples, such prior domain knowledge can effectively address the lack of labeled data commonly encountered in machine learning tasks, improving the learning performance in terms of various goals such as accuracy, generalization, and/or robustness.

In machine learning tasks, we need not only a model with good performance, but also model explainability [29, 33]. The model explainability can help us better understand the model, use the model with more trust, or more quickly debug the deployed model. There have been many prior studies to address model explainability (especially in the context of deep neural networks or DNNs) from various perspectives, such as model features [33], model inference [6], and contribution of individual data samples [16]. Nonetheless, despite the increasingly wider usage of informed machine learning and the clear advantages over its uninformed counterpart, a quantitative understanding of the actual contribution of domain knowledge injected into machine learning tasks has been lacking. This creates ambiguity about the role of domain knowledge in machine learning and decreases the explainability of the resulting models.

A foundation of domain knowledge explainability is to quantify the value or contribution of domain knowledge for machine learning tasks. In the first place, quantification of domain knowledge contribution gives us a better transparency of informed machine learning, which is part of the “right to explanation” legal requirement imposed in Europe for automated decision systems [19]. In addition, by domain knowledge quantification, we can know the actual contribution of different domain knowledge, which provides us with a principled guideline about what kind of domain knowledge is mostly needed to be collected in similar machine learning tasks. Last but not least, domain knowledge injected in machine learning may be implicit, inaccurate, and/or even corrupted. With domain knowledge quantification, we can make an informed decision as to which domain knowledge...
to utilize, since acquiring domain knowledge (e.g., coming from experts) may be quite expensive.

Nonetheless, it is non-trivial to quantify the value of domain knowledge in terms of its contribution of the performance of a learning task. First, domain knowledge has various forms and can be injected in machine learning in different ways [46]. Moreover, different domain knowledge is combined together and injected into a machine learning task, and the overall performance is typically not a simple linear combination of the performance corresponding to each piece of domain knowledge. Last but not least, we need to guarantee fairness for the quantification of domain knowledge in terms of its contribution to model performance.

To address these challenges, we leverage a classic tool from game theory — Shapley value — which provides a fair distribution of total payoff among several participants [40]. Shapley value has been recently used in machine learning model explainability to quantify the contribution of features [44]. training data samples [16], algorithms [50], and neurons [17]. But, to our knowledge, quantifying the contribution of domain knowledge for machine learning is a novel perspective on model explainability that has not been considered. It will only become more important as informed machine learning becomes increasingly ubiquitous.

Our main contributions are summarized as follows.

- We formulate the problem of quantifying the value of domain knowledge in informed machine learning, with a focus on the common approach to using regularization for domain knowledge injection into machine learning tasks.
- We present a quantification method based on Shapley value to measure the value of domain knowledge in a fair manner. Additionally, we address the computational cost of Shapley value and give an approximated algorithm based on Monte-Carlo sampling, which achieves a polynomial time complexity.
- As examples of quantifying the value of domain knowledge, we perform experiments on image classification tasks using semi-supervised learning over datasets of MNIST [32] and CIFAR10 [10]. Specifically, we consider symbolic domain knowledge and inject it into a learning task by adding a knowledge-related loss to the learning objective. Our experiments show the performance improvement by injecting different combinations of domain knowledge, from which we calculate the value of each domain knowledge for quantitative explainability. Our results also quantify and explain the performance degradation due to imperfect domain knowledge (on MNIST).

2 Related Work

Explanation of DNN models. Since most of the current DNN models are black-box and hard to explain, model interpretability/explainability has attracted much attention from both academia and industry [29, 33]. The techniques to explain DNN or AI models can be broadly categorized into intrinsic interpretation techniques and post-hoc interpretation [33], depending on whether the adopted explainability method is integrated with the learning process and affects the model. Intrinsic explainability techniques usually rely on some explainable/interpretable models like regression models, decision tree [53], attention models [22], etc. More recently, intrinsic explainability techniques are also used in deep learning to achieve self-explanatory neural networks [1, 41]. Intrinsic explainability can have more accurate explanations for the output of DNN models, but it may also decrease the learning performance to some extent.

Unlike intrinsic explainability, post-hoc explainability uses a new explainable model to explain another more complex model after the model is trained. Many model-based methods have been proposed for post-hoc interpretability/explainability [20, 38, 39]. By contrast, explainability based on Shapley value is a model-free method and has been becoming increasingly popular for AI explanation due to its flexibility. Shapley value is proved to be the only method that satisfies a set of axioms of fairness in payoff distribution problems [40]. Among existing techniques based on Shapley value, [44] explains the features of model input, [16] studies the joint contribution of features of data samples, and [17] quantifies the contribution of domain knowledge in a novel perspective — quantifying the value of domain knowledge.

Informed Machine Learning Many techniques have been developed to inject domain knowledge in machine learning tasks [46, 48]. One naive approach is to generate additional synthetic training data based on domain knowledge. For example, samples generated from simulations or demonstration can help mitigate the data shortage problem in reinforcement learning [12, 15, 23, 27, 37]. Additionally, data can be generated by knowledge graphs [26], generative models [14], etc. Domain knowledge can also benefit machine learning tasks by choosing hypothesis sets like regression model and neural architectures. A good hypothesis set can improve the learning performance as well as reduce the training complexity. Examples include domain knowledge based neural architecture search [8, 45] and hyper-parameter tuning [31].

Injecting domain knowledge into machine learning tasks via a loss term in the training objective function is another common method. For example, AI models applied in real world are often trained on the optimization objective with constraints originated from domain knowledge [5, 34, 43]. Knowledge distillation from one or more multiple teacher networks also falls into this category of knowledge injection [24, 51]. Moreover, recent studies have shown that logical rules can also be integrated into machine learning by including a domain knowledge related loss term [23, 49].

To our knowledge, however, the values of domain knowledge injected into informed machine learning have not been rigorously or fairly quantified.

3 Informed Machine Learning

A key goal of machine learning is to find the intrinsic hypothesis for a learning task. Typically, a hypothesis h repre-
represents a mapping from an input variable \( X \) to an output variable \( Y \). In some cases, a hypothesis is a distribution over the mapping. In conventional machine learning, a training dataset \( D \) is provided and a hypothesis set \( \mathcal{H} \) is determined, usually by choosing a learning model \( h(X, \theta) \). With a certain loss function and learning algorithm, the model \( h(X, \theta) \) is learnt to approximate the optimal hypothesis \( h^* = h(X, \theta^*) \) which has the optimal performance among the chosen hypothesis set \( \mathcal{H} \). For example, given a performance metric \( R(h) \) (which can be risk, cost, or negative reward/utility), the optimal hypothesis in the chosen hypothesis set is \( h^* = \arg \min_{h \in \mathcal{H}} R(h) \). By training based on the dataset \( D \), we get a final hypothesis \( \hat{h}_D = h(X, \hat{\theta}_D) \).

For a machine learning task, various forms of domain knowledge from multiple sources can be integrated into the machine learning pipeline for improving the model performance. For example, domain knowledge can be used for data augmentation [46, 48] by generating synthetic data samples via simulations [12, 23, 27], data transforming [36, 52], and generative models [14, 18]. With more (independent) samples in the augmented dataset \([D, D_K]\), the generalization error can be reduced [21]. Also, domain knowledge is important for choosing a hypothesis set \( \mathcal{H} \). This is usually done by choosing a learning model \( h_K(X, \theta) \), such as knowledge-based neural architecture search [8] and hyper-parameter tuning [51]. Moreover, domain knowledge can be used to decide whether some final hypothesis should be discarded [40].

In this paper, we focus on another important approach to domain knowledge injection: adding knowledge-based constraints or loss terms as part of the objective function [5, 34, 43, 59]. Specifically, with a data-based loss \( L(h, D) \) used in conventional machine learning and a loss \( L_{K_n}(h, D_n) \) based on domain knowledge \( K_n \) applied to its corresponding (possibly unlabelled) dataset \( D_n \), for \( n = 1, \cdots, N \), the training objective based on domain knowledge can be expressed as

\[
\hat{h} = \arg \min_{h \in \mathcal{H}} L(h, D) + \sum_{n=1}^{N} \lambda_n L_{K_n}(h, D_n),
\]

where \( \lambda_n \geq 0 \) is used to balance the pure data-based loss and knowledge-based loss. In addition to knowledge-based constraints or losses, this formulation also applies to data augmentation based on domain knowledge: \( D_n \) is the synthetic training dataset generated based on domain knowledge \( K_n \) and we have \( L_{K_n}(h, D_n) = L(h, D_n) \) for \( n = 1, \cdots, N \).

Assume that \( R(h) \) is the performance metric of interest in a machine learning task given a set containing \( N \) pieces of domain knowledge \( \mathcal{K} = \{K_1, K_2, \cdots, K_N\} \). For conciseness, \( K_n \) represents the \( n \)-th domain knowledge as well as the corresponding (possibly unlabelled) dataset \( D_n \). With the final hypothesis \( \hat{h}_{D,K} \) learnt based on both training dataset \( D \) and domain knowledge in \( \mathcal{K} \), the learning performance is denoted as \( R(\hat{h}_{D,K}) \).

**4 The Value of Domain Knowledge**

For informed machine learning with domain knowledge, the model performance highly relies on the included domain knowledge information. Naturally, different domain knowledge can have different contributions to the learning performance, and the performance metric can change a lot by adding, removing or revising a subset of the domain knowledge. Thus, to explain the learnt model and achieve better transparency, it is crucial to quantify the value of each domain knowledge for the considered learning task in terms of the metric of interest. Moreover, the quantification of domain knowledge values should be *fair*. In this section, we give a set of axioms for fair quantification of domain knowledge values and propose a method based on Shapley value to achieve fair quantification.

**4.1 Axioms for Fairness**

If a set of knowledge \( \mathcal{K} = \{K_1, K_2, \cdots, K_N\} \), together with a labelled training dataset \( D \), jointly determines the model performance, the performance improvement contributed by the domain knowledge set \( \mathcal{K} \) is denoted as

\[
V(\mathcal{K}) = R(\hat{h}_D) - R(\hat{h}_{D,K}),
\]

where \( R(\hat{h}_D) \) is the performance without domain knowledge set \( \mathcal{K} \). Alternatively, if the domain knowledge is already included into a machine learning task, the performance improvement due to the specific domain knowledge set \( \mathcal{K} \) can be expressed as

\[
V(\mathcal{K}) = R(\mathbb{E}_K[\hat{h}_{D,K}]) - R(\hat{h}_{D,K}),
\]

where \( \mathbb{E}_K[\hat{h}_{D,K}] \) is the hypothesis averaged over all the possible domain knowledge.

To quantify the contribution of individual domain knowledge, the performance improvement \( V(\mathcal{K}) \) should be attributed into individual contributions \( \phi(K_n), n = 1, 2, \cdots, N \) by different domain knowledge in the set \( \mathcal{K} \). Importantly, a *fair* attribution should meet the following basic axioms [16, 30].

**Axiom 1 (Efficiency)** The performance improvement contributed by the entire domain knowledge set \( \mathcal{K} \) is the sum of contributions by individual domain knowledge, i.e.

\[
V(\mathcal{K}) = \sum_{n=1}^{N} \phi(K_n).
\]

**Axiom 2 (Symmetry)** If two different domain knowledge \( K_n \) and \( K_m \) are exchangeable and not distinguishable in terms of the performance improvement, they should have equal contributions. Thus, for any knowledge subset \( \mathcal{K}' \subset \mathcal{K} \setminus \{K_n, K_m\} \), we have

\[
V(\mathcal{K}' \cup \{K_n\}) = V(\mathcal{K}' \cup \{K_m\}) \Rightarrow \phi(K_n) = \phi(K_m).
\]

**Axiom 3 (Null-player)** If individual domain knowledge \( K_n \) in \( \mathcal{K} \) in has no contribution to the performance improvement \( V(\mathcal{K}) \), the attributed contribution of \( K_n \) is zero. That is, for any domain knowledge subset \( \mathcal{K}' \in \mathcal{K} \setminus \{K_n\} \), we have

\[
V(\mathcal{K}' \cup \{K_n\}) = V(\mathcal{K}') \Rightarrow \phi(K_n) = 0.
\]


4.2 Domain Knowledge Shapley

Since domain knowledge in the set $\mathcal{K}$ combined together achieves performance improvement $V(\mathcal{K})$, it is non-trivial to find a contribution attribution method that satisfies all the above three axioms. To address this, we provide a attribution method based on Shapley value — Domain Knowledge Shapley — to quantify the contribution of different domain knowledge. Importantly, Shapley value, a classic tool from cooperative game theory, is proved to be the only method that satisfies the axioms (along with other properties) for fair attribution, as will be introduced in detail next [40].

In our problem, the performance improvement resulting from the domain knowledge set $\mathcal{K}$ can be seen as the total payoff to be distributed and each domain knowledge $K_n$ in the set $\mathcal{K}$ can be seen as a player in a cooperative game. Thus, domain knowledge contribution is also the payoff distributed to each player. Shapley value with respect to the $n$-th player representing domain knowledge $K_n$ is calculated as

$$\phi(K_n) = \frac{1}{N} \sum_{K' \subseteq \mathcal{K}\setminus\{K_n\}} \frac{V(\mathcal{K} \cup \{K_n\}) - V(\mathcal{K}')}{N - |\mathcal{K}'|}, \quad (7)$$

where $\binom{N - 1}{|\mathcal{K}'|}$ is the number of combinations with size $|\mathcal{K}'|$ from the total knowledge set $\mathcal{K}$, and $V(\mathcal{K} \cup \{K_n\}) - V(\mathcal{K}')$ is the marginal contribution of domain knowledge $K_n$ on the basis of a domain knowledge subset $\mathcal{K}'$. Intuitively, Shapley value quantifies the contribution of domain knowledge $K_n$ as the average marginal contribution of $K_n$ over all the possible $\mathcal{K}' \subseteq \mathcal{K}\setminus\{K_n\}$. The reason to average over the domain knowledge subset $\mathcal{K}'$ is fairness: the order of adding each domain knowledge for quantifying its marginal contribution should be equal for all domain knowledge.

4.3 Approximate Method

Although Shapley value is a provably fair in quantifying the contribution of domain knowledge, it needs $\Omega(|\mathcal{K}|^2)$ evaluations in total, accounting for different combinations of domain knowledge [40]. Thus, the computational cost of Shapley value is exponentially increasing with the size of the knowledge set $|\mathcal{K}|$, and can quickly become intolerable for some practical machine learning tasks that have both high training and testing costs. As a result, explaining DNN models (e.g., the contribution of training data samples [16]) based on Shapley value typically leverage approximate methods.

Monte-Carlo sampling is a common method to approximate the computation of Shapley values in the context of DNN explainability [42, 50]. Specifically, we denote $\varpi(\mathcal{K})$ as the set of permutations of $\mathcal{K}$ and rewrite domain knowledge Shapley in Eqn. (7) based on [7] as follows:

$$\phi(K_n) = \sum_{O \in \varpi(\mathcal{K})} \frac{1}{N!} [V(O_{\text{Pre}},n \cup \{K_n\}) - V(O_{\text{Pre}},n)] \quad (8)$$

where $O_{\text{Pre}},n$ is the set of predecessors of $K_n$ in a permutation $O$. Based on Eqn. (8), the domain knowledge Shapley for $K_n$ can be estimated by sampling from the permutation of domain knowledge set $\mathcal{K}$. The approximated knowledge Shapley algorithm is given in Algorithm 1. Critically, Shapley approximation based on Monte-Carlo sampling has a polynomial-time complexity and has been proven to have a bounded error with a high probability [30].

While Monte-Carlo sampling can effectively reduce the complexity, the evaluation for each marginal contribution $V(O_{\text{Pre}},n \cup \{K_n\}) - V(O_{\text{Pre}},n)$ can still be costly due to the requirement of calculating the values of $V(O_{\text{Pre}},n \cup \{K_n\})$ and $V(O_{\text{Pre}},n)$. To further reduce the cost of evaluating the learning performance with different combinations of domain knowledge, we can train the model over a smaller number of epochs and also use a smaller dataset for testing. Moreover, if the size of domain knowledge set is very large, we can also train an predictor for the learning performance that takes the domain knowledge subset as input and directly estimates the resulting learning performance without training. Such performance predictors are also used for avoiding the cost of model training for each architecture candidate and speeding up neural architecture search [11, 47].

Algorithm 1 Approximated Domain Knowledge Shapley

**Input:** Domain knowledge set $\mathcal{K}$, performance evaluation $V$

**Output:** Estimated domain knowledge Shapley $\hat{\phi}(K_n)$, $n = 1, \cdots, N$

**Initialization** count = 0, $\hat{\phi}(K_n) = 0$, $n = 1, \cdots, N$

while count < MaxIterNum do

Randomly generate a permutation $O$ of $\mathcal{K}$

for $n = 1, \cdots, N$ do

$O_{\text{Pre}},n$: set of predecessors of $K_n$.

$\phi(K_n) = \hat{\phi}(K_n) + [V(O_{\text{Pre}},n \cup \{K_n\}) - V(O_{\text{Pre}},n)]$

end for

count = count + 1

end while

$\hat{\phi}(K_n) = \phi(K_n)/\text{MaxIterNum}$, for $n = 1, \cdots, N$.

5 Experiments

In this section, we run experiments to quantify the values of domain knowledge for two image classification tasks under a semi-supervised setting for which domain knowledge can significantly improve the learning performance.

5.1 DNN with Symbolic Domain Knowledge

In our experiments, the domain knowledge comes from the symbolic label knowledge which can be expressed as a logical sentence [13, 49]. Specifically, a logical sentence is a set of assertions combined by relational expressions such as $\land$ (and), $\lor$ (or) and $\neg$ (not). For example, for states $S_1, S_2, S_3$, a logical sentence can be $\alpha = S_1 \lor (S_2 \land \neg S_3)$. Assume that for a logical sentence $\alpha$ and a state $S$, $S \models \alpha$ means that the state $S$ satisfies the logical knowledge $\alpha$, or in other words, the logical sentence $\alpha$ can be written as $\alpha = S \lor \cdots$. In the previous example, we have $S_1 \models \alpha$ and $(S_2 \lor \neg S_3) \models \alpha$.

A common approach to injecting symbolic knowledge in DNNs is adding a knowledge-based loss in the train-
ing objective [49]. Consider a classification task where \( X \in X \) is the input and \( Y \in Y = \{1,2,\ldots,J\} \) is the label. We use a neural network \( h(X, \theta) \) as our classification model. Denote the output of \( h(X, \theta) \) as \( \hat{P}(X) = [\hat{P}_1(X), \hat{P}_2(X), \ldots, \hat{P}_J(X)] \) which is usually interpreted as the estimated probability that the corresponding label is the correct label. We include an additional loss term based on the symbolic knowledge as proposed in [49], which is the negative logarithm of the estimated probability that the knowledge is satisfied. If \( S \) represents a state of the sparse label space \( \{0,1\}^J \), given a domain knowledge \( K \) in the logical sentence form and an input \( X \), the knowledge-based loss can be expressed as

\[
L_K(X) = - \log \sum_{S \in K} \prod_{j:y=j} \hat{P}_j(X) \prod_{j:y \neq j} (1 - \hat{P}_j(X)).
\] (9)

For example, if the domain knowledge \( K \) means that only one label in \( Y \) is the correct output, then the knowledge-based loss is

\[
L_K(X) = - \log \sum_{j \in Y} \hat{P}_j(X) \prod_{i \neq j} (1 - \hat{P}_i(X)).
\] (10)

Similarly, if the knowledge \( K \) means that the correct label with respect to input \( X \) is one of the labels in the set \( J^' \subseteq Y \), the knowledge-based loss can be expressed as

\[
L_K(X) = - \log \sum_{j \in J^'} \hat{P}_j(X) \prod_{i \neq j} (1 - \hat{P}_i(X)).
\] (11)

The above domain knowledge injection method can be used to improve the learning performance for semi-supervised classification tasks. Specifically, we are given a training dataset \( D \) with input-label pairs as well as an unlabelled dataset \( D_N \). Denote \( L_{ce}(x,y) \) as the cross-entropy loss of an instance \( (x,y) \). The semi-supervised training objective with a set of knowledge \( K = \{K_1, \ldots, K_N\} \) is injected as

\[
L_{semi} = \sum_{(x,y) \in D} L_{ce}(x, y) + \sum_{n=1}^{N} \lambda_n \sum_{x \in D_N} L_{K_n}(x).
\] (12)

Given a test input \( x \in X \), the label is usually predicted as \( \hat{Y}(x) = \arg \max_{y} \hat{P}_y(x) \). While the performance of prediction can be evaluated by various metrics, we consider the widely-used top-1 accuracy, which can be formally expressed as \( acc = \mathbb{E}\left[1(\hat{Y} = \hat{Y}(X))\right] \). In practice, however, a test dataset \( D^T \) is usually used to empirically evaluate the accuracy, which is called the test accuracy:

\[
\hat{acc} = \frac{1}{|D^T|} \sum_{(x,y) \in D^T} 1(y = \hat{Y}(x)).
\] (13)

### 5.2 Results on MNIST

We begin our experiment of semi-supervised learning on a simple dataset — MNIST, which includes 60000 handwritten digit images with labels for training and 10000 images with labels for testing [32]. We use only 100 images (including 10 images for each digit) and their corresponding labels from the training dataset as labeled samples, and use the rest of images in the training dataset as unlabeled samples. The test accuracy is calculated on the entire testing dataset of 10000 images.

We consider a domain knowledge set \{One Hot, Constraint-I, Constraint-II\}. The knowledge One Hot as considered in [49] means that each input has only one correct label, whose knowledge-based loss is expressed in Eqn. (9). The knowledge Constraint-I specifies whether or not the digit of an image belongs to the interval \([0,3]\), while the knowledge Constraint-II informs us of whether or not the digit of an image is in the interval \([0,6]\). Additionally, we quantify the knowledge values under the setting where Constraint-II in the knowledge set is imperfect. Specifically, we consider that 10% of the unlabelled samples have wrong information about Constraint-II: if the true label of a sample with corrupted knowledge Constraint-II is in the interval \([0,6]\), the corrupted knowledge Constraint-II believes it is out of the interval \([0,6]\) and vice versa. The loss based on knowledge Constraint-I and Constraint-II can both be calculated according to Eqn. (10).

| Knowledge (Accurate) | Test Accuracy | Knowledge (Imperfect C-II) | Test Accuracy |
|----------------------|---------------|-----------------------------|---------------|
| No Knowledge         | 0.8372        | No Knowledge                | 0.8372        |
| One Hot              | 0.8725        | One Hot                     | 0.8725        |
| C-I                  | 0.9224        | C-I                         | 0.9224        |
| C-II                 | 0.9654        | C-II                        | 0.9425        |
| One Hot & C-I        | 0.9396        | One Hot & C-I               | 0.9396        |
| One Hot & C-II       | 0.9886        | One Hot & C-II              | 0.9590        |
| C-I & C-II           | 0.9733        | C-I & C-II                  | 0.9678        |
| One Hot & C-I & C-II | 0.9775        | One Hot & C-I & C-II        | 0.9687        |

Table 1: Test accuracy given different combinations of domain knowledge on MNIST. (C-I: Constraint-I; C-II: Constraint-II).

Our training setting follows [49]. Specifically, we consider a DNN with four fully-connected hidden layers having 1000, 500, 250, 250 hidden neurons respectively, a batch normalization layer and a dropout layer with dropout probability 0.5. The weight to balance the cross-entropy loss and the knowledge-based loss is 0.1. During training, each batch has 16 images with corresponding labels and 16 images without labels (100 labeled images are reused to balance the number of labeled and unlabeled examples). Adam optimizer with learning rate \(10^{-3}\) is used for updating weights followed by a tuning phase with learning rates \(5 \times 10^{-5}, 10^{-5}, 5 \times 10^{-6}\) and \(10^{-6}\). Note that since we only have three different pieces of domain knowledge and our DNN has a reasonably low training cost, we re-train the DNN given each combination of domain knowledge without Monte-Carlo sampling.

The test accuracies given each combination of domain knowledge are shown in Table 1. Based on the accuracy results, we calculate the value of each domain knowledge in
In this paper, we study valuation of domain knowledge and provide a first step towards quantitative understanding of contribution of domain knowledge injected into informed machine learning. Specifically, we propose domain knowledge Shapley to quantify the values of domain knowledge in terms of the learning performance improvement for machine learning tasks in a fair manner. We run experiments on both MNIST and CIFAR10 datasets using semi-supervised learning and quantitatively measure the fair value of different domain knowledge. Our results also quantify the extent to which imperfect domain knowledge can affect the learning performance (for the MNIST dataset).

### 5.3 Results on CIFAR10

We also run experiments on the CIFAR10 dataset, which includes images with $32 \times 32$ pixels and 10 classes (airplane, automobile, bird, cat, deer, dog, frog, horse, ship, truck) in the label space. It has 50000 training samples and 10000 test examples. We use only 10% of the training images with labels (5000 labeled images), and another 15000 training images without labels for training. For testing, we use all the 10000 test images in the test dataset.

Our domain knowledge set has three different types of symbolic knowledge $\{\text{One Hot}, \text{Animal}, \text{Mammal}\}$. The knowledge One Hot provides the information that each image has only one correct label, whose knowledge-based loss is expressed in Eqn. (9). The knowledge Animal provides the information whether or not the label of an image belongs to animals. With the knowledge Animal, we can decide if the label of an input is in the label subset $\{\text{bird, cat, deer, dog, frog, horse}\}$, even though the exact label is unknown. The knowledge Mammal provides information of whether or not the label of a training image belongs to mammals. Similarly, the knowledge Mammal specifies whether the label of a training image is in the label subset $\{\text{cat, deer, dog, horse}\}$. The loss based on knowledge Animal and Mammal can be calculated by Eqn. (10).

In our experiment, Ladder Net [35, 49] is used as the neural architecture. The weight to balance the cross entropy loss and knowledge-based loss is set as 0.1. A batch of 512 inputs consists of both labeled images and unlabeled images are used for each weight update. To balance the number of labeled and unlabeled inputs, the labeled inputs are reused. Training is performed by the momentum algorithm with a learning rate of 0.1, followed by a tuning phase with learning rates 0.05, 0.01 and 0.0001.

After training the neural network with different combinations of domain knowledge, we evaluate the test accuracy as shown in Table 2. The domain knowledge Shapley in terms of the test accuracy improvement is calculated and shown in Fig. 1(c). We can see that the knowledge Mammal is the most informative one and hence has the largest contribution to the test accuracy, while the common-sense knowledge One Hot contributes the least to the test accuracy improvement. The knowledge Animal has a contribution between the other two knowledge.

### 6 Conclusion

In this study, we provide a rigours quantification of values of different domain knowledge. Our results also quantify the extent to which imperfect domain knowledge can affect the learning performance (for the MNIST dataset).
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