Imitation Refinement

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Abstract

Many real-world tasks involve identifying patterns from data satisfying background and prior knowledge, for which the ground truth is not available, but ideal data can be obtained, for example using theoretical simulations. We propose a novel approach, imitation refinement, which refines imperfect patterns by imitating ideal patterns. The imperfect patterns are obtained for example using an unsupervised learner. Imitation refinement imitates ideal data by incorporating prior knowledge captured by a classifier trained on the ideal data: an imitation refiner applies small modifications to imperfect patterns, so that the classifier can identify them. In a sense, imitation refinement fits the data to the classifier, which complements the classical supervised learning task. We show that our imitation refinement approach outperforms existing methods in identifying crystal patterns from X-ray diffraction data in materials discovery. We also show the generality of our approach by illustrating its applicability to a computer vision task.

1 Introduction

Many real-world tasks involve identifying meaningful patterns from data, satisfying background and prior knowledge [Chapelle et al., 2009], for which not much labeled data are available. In such data-poor contexts, standard deep learning techniques are not effective, and therefore we need to rely on unsupervised learning. In many applications, ideal data can be obtained e.g., by synthesis and simulation [Rubin, 1993; Le Bras et al., 2014]. In this paper, we explore how to use ideal data to incorporate background and prior knowledge into learning tasks.

As an example, consider the following application in materials science, where we would like to discover new materials, which are characterized by their X-ray diffraction (XRD) patterns, based on real experimental data. This identification problem is challenging because real XRD patterns often mix with others and are further corrupted with noise. Nevertheless, an ideal XRD pattern for a known material can be synthesized using theoretical simulations that incorporate prior knowledge about materials. Can we take advantage of synthesized ideal patterns to help discover unknown patterns corresponding to new materials from real experiments?

We give an affirmative answer in this paper. We propose a novel approach called imitation refinement, which improves the quality of imperfect patterns to imitate patterns in the ideal dataset. Left: Refinement of XRD crystal patterns. Right: Refinement of hand-written digits.

Imitation refinement is related to data denoising [Xie et al., 2012] and data restoration [Dong et al., 2014], which improve noisy or corrupted data. One key difference is that imitation refinement does not require noisy data to be

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paired with its cleaned version while training. In fact, we directly train an imitation refiner on the imperfect dataset, for which we don’t know the ground truth. Also, the ideal dataset does not provide ground truth counterparts for the imperfect data. Our work is also related to style transfer [Gatys et al., 2015], which also requires paired images for the transformation. Besides, transfer learning [Pan and Yang, 2010] and domain adaptation [Glorot et al., 2011] modify models while the classifier here is fixed. Additionally, imitation refinement has notable differences with conventional inverse classification [Mannino and Koushik, 2000; Aggarwal et al., 2010], which uses inverted statistics to complete partial data or solve an optimization problem for each test sample respectively. Imitation refinement differs from these methods since it incorporates the knowledge embedded in a pre-trained classifier into the refiner, which can generalize to the unseen imperfect data. Further, imitation refinement allows for high-level data modification, while inverse classification often only changes data attributes. Finally, imitation refinement is different from GAN [Goodfellow et al., 2014] since its goal is not to refine imperfect data such that a discriminator cannot differentiate them from ideal data. Instead, imitation refinement only applies small modifications to the imperfect data to reflect the fundamental characteristics of the ideal data, captured by the classifier trained on them.

Our contributions can be summarized as follows: (i) we propose a novel framework of imitation refinement, which improves the quality of imperfect patterns, by mimicking the characteristics of ideal data. (ii) We show that imitation refinement can be trained with neural nets and in an end-to-end fashion. (iii) We demonstrate the effectiveness of imitation refinement on two real-world applications: in the first application, we show imitation refinement improves the quality of poorly written digits by imitating typesetting or well-written digits. In the second application, we show that imitation refinement improves the quality of identified crystal patterns from X-ray diffraction data in materials discovery.

2 Problem Formulation

In imitation refinement, we have an imperfect dataset \( A \), whose members come from post-processing a physical experiment or a complete unsupervised learning approach. Members in the imperfect dataset are defective because they fail to satisfy feasible conditions. On the other hand, we have an ideal dataset \( E \), whose members satisfy all physical constraints and prior knowledge. Our question is how to modify the members in the imperfect dataset \( A \) so that they imitate the characteristics of the members in the ideal dataset \( E \). For example, in our materials discovery application, the imperfect dataset \( A \) comprises of candidate patterns that are supposed to correspond to pure crystal structures that are obtained from real XRD data, using unsupervised learning. Each candidate pattern contains information of interest, but often it is mixed with other patterns or corrupted with background noise. On the other hand, we can obtain ideal XRD patterns for known materials from a dataset obtained using simulation. Such patterns are synthesized assuming ideal conditions. Our question is how we can fix the imperfect crystal structure patterns obtained by unsupervised learning to satisfy prior knowledge encapsulated in the ideal dataset.

Notice that we cannot complete this task by learning an one-to-one mapping between the imperfect dataset and the ideal dataset since the members of the imperfect dataset \( A \) and ideal dataset \( E \) refer to different entities. In our materials discovery application, members of the imperfect dataset \( A \) correspond to potentially unknown materials from real experiments, while members of \( E \) correspond to a restrictive set of theoretically synthesized and known materials. We cannot map any member in \( A \) directly to a member in \( E \). Instead, we modify members of the imperfect dataset \( A \) so they have similar characteristics to those in the ideal dataset \( E \).

We train an ideal classifier \( C \) to classify entities in the ideal dataset \( E \), which captures the prior knowledge from an idealized world. The imitation refinement problem is to modify examples from the imperfect dataset \( A \) so the classifier \( C \) identifies them. Formally, we search for an optimal refiner \( R \) to refine samples \( x \)’s drawn from the imperfect dataset \( A \), such that \( C \) has better performance on the refined dataset \( R(A) = \{R(x) | x \in A \} \). The performance of a classifier \( C \) is measured as its evaluation loss:

\[
\eta_C(A) := \mathbb{E}_{x \sim A} | \mathcal{H}(C(x)) |,
\]

where \( \mathcal{H}(\cdot) \) is a function giving a low score if the refined examples can be certainly classified in one category in the ideal world. For instance, \( \mathcal{H}(\cdot) \) can be the cross-entropy when the target categories are given when training, or be the entropy of predictions for some categories, which represents the uncertainty of the ideal classifier \( C \) on the refined dataset \( R(A) \), in the non-targeted case. We expect a low \( \eta_C(R(A)) \) after refinement. Imitation refinement can be interpreted as an inverse process of supervised learning, as shown in Figure 2. In imitation refinement, we modify imperfect data \( A \) to fit the classifier \( C \), instead of fitting a classifier to a fixed dataset.

Also, \( R \) should modify the original data as little as possible to accomplish its goal. We thus introduce a discrepancy distance:

\[
\delta_C(A, R(A)) := \mathbb{E}_{x \sim A} [\delta_C(x, R(x))]
\]

In general, \( \delta_C \) is a differentiable user-defined metric which measures the degree to which \( R \) modifies \( x \). One option is to use a metric on the input space such as \( \ell_p \) norm. In some
3 Neural Imitation Refinement

We propose an end-to-end neural network based framework to solve the imitation refinement problem (3). Figure 3 illustrates the basic structure. The classifier $C$ is pre-trained on the ideal dataset and is fixed during the training of refiner $R$, parameterized by $\theta$. $x$ is the imperfect data drawn from $A$ to be refined. It first passes the refiner and becomes the refined data $R_\theta(x)$. The evaluation loss $\eta_C$ given by $C$ is calculated on the input refined data $R_\theta(x)$. The discrepancy distance $\delta_C(x, R_\theta(x))$ is calculated by comparing the refined $R_\theta(x)$ with the original data $x$. In experiments, we first map both $x$ and $R_\theta(x)$ to a high dimensional space denoted by a high-level layer of the classifier $C$, and then use an $l_p$ norm in the high-level space to compute $\delta_C$. The total loss to minimize is a trade-off between the evaluation loss and the discrepancy distance, $L(\theta) = (1 - \lambda) \cdot \delta_C + \lambda \cdot \eta_C$. Assuming that the given classifier is differentiable, a neural refiner $R_\theta$ can be trained using stochastic gradient descent (see Algorithm 1).

**Classifiers** Our imitation refinement framework is highly flexible and can incorporate any classifiers that are differentiable. For the first handwritten digits application, we use a CNN-based model, LeNet [LeCun et al., 1998], as the classifier. For the second materials discovery application, we use an RNN-based classifier, LSTM [Hochreiter and Schmidhuber, 1997], which achieves the best empirical result.

**Refiners** The refiner improves the given imperfect input and produces a refined input to be fed into the classifier. An end-to-end model is ideal for this purpose. Here we employ U-Net [Ronneberger et al., 2015] to be our refiner (see Figure 3). The U-Net architecture is an encoder-decoder network which adds skip connections between encoder and decoder layers. The low-level and mid-level representations can be transferred to the decoders for up-sampling through these connections. We choose U-Net in our experiments because of good empirical performance. We expect other end-to-end models to work as well.

**Algorithm 1** Neural Imitation Refinement

Given the ideal classifier $C$ and the imperfect dataset $A$.

1. **for** number of training iterations **do**
2. Sample a minibatch $\{x^{(1)}, \ldots, x^{(m)}\}$ from $A$.
3. Calculate $\delta_C(x^{(i)}, R_\theta(x^{(i)}))$ and $\eta_C(R_\theta(x^{(i)}))$ for $i \in [m]$ to estimate of loss functions (2) and (1).
4. Update $R_\theta$ by descending its stochastic gradient:
   \[
   \nabla_\theta \frac{1}{m} \sum_{i=1}^{m} (1 - \lambda) \delta_C(x^{(i)}, R_\theta(x^{(i)})) + \lambda \eta_C(R_\theta(x^{(i)}))
   \]

**return** the refiner $R_\theta$

of good empirical performance. We expect other end-to-end models to work as well.

4 Experiments

4.1 Hand-Written Digits

In this experiment, we first investigate the following question: if we have the ideal digits typeset in different fonts, can the imitation refinement take advantage of these idealized digits to refine unseen handwritten digits?

**Idealized Digit Datasets** We generate ideal datasets which contain images of digits typeset in five different fonts respectively: Bradly Hand, Brush Script, Hanannotate, Times, and Typewriter. We augment images in each dataset by vertically and horizontally shifting at most two pixels, and also rotating in $\beta \in [-20^\circ, 20^\circ]$. Each dataset contains 10250 images of digits. We further add 10% non-digit (mixtures of digits, etc.) images into each dataset, to satisfy the closed-world assumption. We also merge these five datasets to make a dataset MixAll containing digits typeset in all these fonts.

**Handwritten Digits Datasets** The MNIST dataset [LeCun et al., 1998] is used as our imperfect dataset, which contains 60,000 handwritten digits for the training and validation and another 10,000 handwritten digits for the test. Some examples of digits in the ideal dataset and imperfect dataset are shown in the figure. Our goal is to refine handwritten digits by mimicking the characteristics of computer fonts.

**Classifiers Trained on Ideal Datasets** We first train the ideal classifiers on the idealized digit datasets. The classifiers should be able to classify instance in the idealized dataset into digits 0-9 and a non-digit category. The ideal classifiers are convolutional neural networks having the similar architecture
We show the improvement of the refiners with batch size 50 for total ten epochs.

The ideal classifier trained on the dataset MixAll achieves the best accuracy. The huge improvements of accuracies show the refined handwritten digits can be better identified by ideal classifiers.

<table>
<thead>
<tr>
<th>number of training examples</th>
<th>Bradly Hand</th>
<th>Brush Script</th>
<th>Hannotate</th>
<th>Times</th>
<th>Typewriter</th>
<th>MixAll</th>
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<tr>
<td>0</td>
<td>50.0%</td>
<td>29.72%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
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<td>1</td>
<td>70.14%</td>
<td>50.02%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
<tr>
<td>2</td>
<td>80.20%</td>
<td>50.02%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
<tr>
<td>3</td>
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<td>50.02%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
<tr>
<td>4</td>
<td>+50.03%</td>
<td>50.02%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
<tr>
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<td>50.02%</td>
<td>98.40%</td>
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<td>98.56%</td>
<td>98.27%</td>
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<td>98.49%</td>
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<td>50.02%</td>
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<td>98.27%</td>
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<td>50.02%</td>
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<tr>
<td>9</td>
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<td>50.02%</td>
<td>98.40%</td>
<td>98.49%</td>
<td>98.56%</td>
<td>98.27%</td>
</tr>
</tbody>
</table>

Table 1: The improvement of identifiability of handwritten digits after imitation refinement. The first and second rows show the rates of handwritten digits regarded as non-digits in the test set before and after refinement, respectively. The third and fourth rows show the test accuracies of ideal classifiers on the original and refined MNIST test dataset. The ideal classifier trained on the dataset MixAll achieves the best accuracy. The huge improvements of accuracies show the refined handwritten digits can be better identified by ideal classifiers.

Figure 4: The first row displays example digits in the ideal dataset. The second row shows examples of imitatively refining MNIST handwritten digits to have the characteristics of different fonts.

Figure 5: As the number of training examples from the MNIST dataset increases, the test accuracies of both ideal (MixAll) and real-world (No Prior) classifiers increase. However, when the number of the training examples is less than 300 (0.5% of MNIST), the captured prior knowledge can help the ideal classifier better recognize handwritten digits.

The power of prior knowledge. We compare a real world classifier directly trained on the MNIST dataset with a ideal classifier trained on the idealized dataset MixAll in terms of test accuracy. The results are shown in figure 5. As the number of training examples from the MNIST dataset increases, the test accuracies of both ideal (MixAll) and real-world (No Prior) classifiers increase. In the long term, both of them will achieve over 98% test accuracies. However, when the number of the training examples is less than 300, the captured prior knowledge can help the refiner improve handwritten digits, so that the ideal classifier can better recognize them than the classifier without any prior knowledge.

Visual effect of imitation refinement. To better illustrate the visual effect of imitation refinement, we also design a task to improve the poorly hand-written digits to mimic the well-written digits using imitation refinement. We use the same architectures for the classifier and refiner as in the previous setting. The ideal dataset contains the most representative well-written digits, which are manually selected from a sub-
Figure 6: Visual results of imitation refinement: (a) Selected examples of test results of targeted refinement on the imperfect hand-written digits. We set $\lambda = 0.55$ in the experiment to balance the discrepancy loss and the evaluation loss. In the first row, the target is “6” while the original imperfect digit is not complete. The refiner improves this digit by completing it. In the second row, the target is “7” while the original imperfect digit is like a “2”. The refiner corrects this digit by erasing its redundant part. A more interesting example of a batch of test results of non-targeted imitation refinement on the poorly written digits is shown in (b). The refiner modifies original ambiguous digits to the ones with higher classifier certainty. We set $\lambda = 0.15$ for this case. Since the process is non-targeted, it can creatively refine a digit to the less confusing one in the classifier’s sense. Four interesting instances are displayed in the left figure: 1) The first row shows an imperfect digit originally classified as “1”, being refined to a more idealized “7” by enhancing the horizontal line on the top, which corresponds with the human label. 2) The second row shows an imperfect digit correctly labeled originally as “4” but it may also be a “1” or “9”, since its left part is blurred. By erasing its left part, it becomes a more certain “1”. 3) An ambiguous digit which looks like “8”, “3” and “0” is shown in the third row, whose human label is “0”, while the classifier identifies it as “8”. To increase the certainty, its left connected line is erased after refinement, and it is more like a digit “3”. 4) In the last row, an imperfect digit “2” is so much like “7” that the classifier misclassified it. The refiner reinforces the classifier’s opinion by extending the vertical line in the middle and fading the connecting line.

Figure 7: Materials discovery task: Each blue dot is a sample. $\alpha, \beta, \gamma$ represent different phases/compounds. The XRD pattern at each sample point is given, potentially a mixture of $\alpha, \beta, \gamma$. The goal is to obtain the unknown pure XRD patterns of $\alpha, \beta, \gamma$. A typical materials discovery task is to find the unknown pure XRD patterns of $\alpha, \beta, \gamma$. The set of the MNIST dataset. We also manually select poor digits from another subset of the MNIST dataset, and the ground truths of these imperfect digits are unknown. When training, the discrepancy distance is the same as that in the previous setting. And the evaluation loss has two configurations: when the labels of digits are given when training the refiner (targeted case), it is the negative log-likelihood. Notice that it does not mean we know the ground truths of poor handwritten digits in terms of shape. The idealized well-written counterparts of the digits are still unknown. When the labels of the digits are not given (non-targeted case), it is the entropy of the prediction to be a digit, since we expect a poorly written digit to not be a non-digit, and increase the classifier’s certainty after refinement. We show visual results in figure 6.

4.2 Materials Discovery
Motivations and Modeling
In this second application, we further apply imitation refinement to a scientific task in materials discovery.

High throughput combinatorial materials discovery is a materials science task whose intent is to discover new materials using a variety of methods including X-ray diffraction pattern analysis [Green et al., 2017]. Figure 7 shows a typical physically meaningful material system. In a ternary material composition space, different ratios of three metallic elements are mixed together to form different crystalline materials. At each elemental composition, also called sample, a different material is formed, which can be composed of a single crystalline compound, or a mixture of several compounds. The
X-ray diffraction (XRD) pattern at each sample is given. The goal is to unveil the XRD pattern of each single compound, which is also referred to as ”phase”.

The above task can be modeled as a typical pattern decomposition problem under constraints, which was explored in recent work [Long et al., 2009; Ermon et al., 2015; Xue et al., 2017; Suram et al., 2016; Bai et al., 2017]. Though these methods produce estimated patterns for each phase that are usually quite similar to the expected patterns of corresponding pure phases, they typically include a fraction of the patterns belonging to other phases, as well as background and experimental noise. This leads to errors in explaining the structure of the materials system, and the goal of this application is to refine each imperfect pattern to more correctly estimate that of the corresponding pure phase.

The ideal dataset \( E \) in this application is composed of physically meaningful synthetic pure phases and mixtures from the Materials Project [Jain et al., 2013]. The Materials Project provides crystal structure information and energy of formation using density functional theory for each phase. XRD patterns are calculated for each constituent using pymatgen [Ong et al., 2013]. In this database, approximately 3000 synthetic material systems contain over 30,000 pure phases and 32,000 mixtures. 95% of the 3000 systems provide pure phases and mixtures used for creating the ideal dataset \( E \) for training the classifier \( C \) to discriminate between pure phases and mixtures. Among these systems, 80% are picked randomly for training \( (E_{\text{train}}) \), while 10% are left for validation \( (E_{\text{valid}}) \) and another 10% for testing \( (E_{\text{test}}) \).

The imperfect dataset \( A \) is derived from the remaining 135 systems. For each system, non-negative matrix factorization (NMF) [Lee and Seung, 2001] decomposed all the XRDs into phases that are supposed to be pure. Note however that typically they differ from the expected pure phases, as described above. These imperfect phases form the imperfect dataset \( A \), which should be refined to be more pure. We randomly split \( A \) into training set \( A_{\text{train}} \) (80%), validation set \( A_{\text{valid}} \) (10%) and test set \( A_{\text{test}} \) (10%). We assume that the imperfect patterns \( x \) in \( A \) are pure phases, since they are the factors produced by NMF. Nevertheless, the ground-truth mapping \( G(x) \), which matches each imperfect phase to the corresponding ground-truth pure phase, is not known during the training of the refiner. To simulate the real materials discovery where we explore new systems without ground truths based on known systems, \( E \) contains all the known systems while \( A \) comprises of unknown systems, which means \( G(A_{\text{train}}) \) is unused in training and \( G(A_{\text{test}}) \) is used only for evaluation.

\[ \delta_{C}(x, R(x)) = \text{KL divergence}, \quad D_{KL}(R(x)||x), \quad \eta_{C}(R(A)) = \text{negative log-likelihood given by } C. \]

A network similar to the previous application is used here except that \( C \) is an LSTM and \( R \) is adapted to process 1-d input.

### Training and Results

Each XRD pattern is of length 2000 and is further dissected into 50 segments, each of length 40. A simple one-layer LSTM with dropout 0.5 and hidden size 64 is used here for classification. The final output feature of cell state is fed into a softmax layer for classification. The batch size for training is 64. The LSTM gives 94.93% prediction accuracy on \( E_{\text{test}} \).

<table>
<thead>
<tr>
<th>Methods</th>
<th>AgileFD</th>
<th>IAFD</th>
<th>NMF</th>
<th>IR</th>
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<td>44.2320</td>
<td>45.7362</td>
<td>45.4367</td>
<td><strong>45.9345</strong></td>
</tr>
<tr>
<td>( l_2 )</td>
<td>0.1430</td>
<td>0.1373</td>
<td>0.1197</td>
<td><strong>0.1197</strong></td>
</tr>
<tr>
<td>( KL \text{ div} )</td>
<td>76.8572</td>
<td>74.7262</td>
<td>78.1946</td>
<td><strong>74.5778</strong></td>
</tr>
</tbody>
</table>

Table 2: Comparisons with the ground-truth phases. For \( l_1 \) loss, \( l_2 \) loss and \( KL \text{ divergence} \), the smaller, the better. The best result for each measure is in **bold**. Imitation refinement (IR) uses NMF for generating imperfect dataset \( A \).

The confidence of being recognized as pure phase by the classifier \( C \) is its purity. Figure 8 shows the purity before and after refinement: all the phases from \( A_{\text{test}} \) get improved dramatically, except one in the upper-right corner. Even in the case where the initial purity is small indicating that the raw phase is not pure, many phases are still improved significantly (see the left upper corner in the figure).

We also evaluate the performance of the refiner \( R \) directly by the classification output of \( C \). Initially, \( C \) classified only 36.54% of the examples in \( A_{\text{test}} \), but after refinement, this percentage goes to 88.46%.

We also evaluate the refined phases \( R(A_{\text{test}}) \) by comparing with the ground-truth \( G(A_{\text{test}}) \), using the \( l_1 \) loss, \( l_2 \) loss, KL divergence. Recall that neither \( C \) nor \( R \) were trained with paired imperfect and ground truth data, and \( R \) was trained only to increase purity as represented by \( C \). This evaluation is therefore much more challenging in that the refiner is not directly trained to minimize the difference, but the evaluation is also more relevant to the scientific discovery goals.

Imitation refinement is compared with NMF and another two state-of-art methods, AgileFD [Suram et al., 2016] and IAFD [Bai et al., 2017] on the quality of phases. The phases produced by these methods are compared with the corresponding ground truth. Different measurements are taken to evaluate them. For each type of measurement, the sum over the distances for all the testing phases are shown in the Table 2. Imitation refinement (IR) outperforms other methods or is at least as competitive as the others.

### 5 Discussion and Future Work

**Imitation refinement** improves the quality of imperfect data by imitating ideal data. Using the prior knowledge captured by an ideal classifier trained on an ideal dataset, a refiner learns to apply modifications to imperfect data, such that the ideal classifier can better recognize them. A general end-to-end neural framework is proposed to address the underlying optimization problem and it is further exemplified by two applications: handwritten digits and XRD patterns in materials discovery. Imitation refinement improves readability and accuracy of identifying hand-written digits when complementing a small training dataset (0.3% of MNIST) with computer generated data. It also improves the quality of crystal phases produced by an unsupervised learner (NMF), a promising result in scientific discovery. Imitation refinement is easily extensible with different ways of producing and refining the imperfect data. For example, imperfect data may result from crowdsourcing tasks to non-experts and other supervised models can be used. Imitation refinement is a promising approach for incorporating prior and background knowledge.
into learning tasks. We hope that this work will stimulate additional imitation refinement efforts.

References


