Learning a metric for class-conditional KNN

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Abstract—Naïve Bayes Nearest Neighbour (NBNN) is a simple and effective framework which addresses many of the pitfalls of K-Nearest Neighbour (KNN) classification. It has yielded competitive results on several computer vision benchmarks. Its central tenet is that during NN search, a query is not compared to every example in a database, ignoring class information. Instead, NN searches are performed within each class, generating a score per class. A key problem with NN techniques, including NBNN, is that they fail when the data representation does not capture perceptual (e.g. class-based) similarity. NBNN circumvents this by using independent engineered descriptors (e.g. SIFT). To extend its applicability outside of image-based domains, we propose to learn a metric which captures perceptual similarity. Similar to how Neighbourhood Components Analysis optimizes a differentiable form of KNN classification, we propose “Class Conditional” metric learning (CCML), which optimizes a soft form of the NBNN selection rule. Typical metric learning algorithms learn either a global or local metric. However, our proposed method can be adjusted to a particular level of locality by tuning a single parameter. An empirical evaluation on classification and retrieval tasks demonstrates that our proposed method clearly outperforms existing learned distance metrics across a variety of image and non-image datasets.

I. INTRODUCTION

Nearest Neighbour (NN) techniques for image classification have been overshadowed by parametric methods such as the bag-of-words method [11] combined with the spatial pyramid match kernel [2], and more recently, convolutional nets [3], [4]. However, Nearest Neighbour methods have several appealing properties: they are simple, they can handle a large number of classes that are not necessarily defined a priori, with no free parameters they cannot overfit, and they require no separate training phase.

An issue central to NN methods is the distance used to find neighbours. It is well known that Euclidean distance in pixel space is flawed. It is computationally expensive to compute on images of non-trivial size and it tends not to capture perceptual similarity, meaning that examples that humans perceive to be similar may not lie close together in Euclidean space. Modern NN methods [5], [6] rely on combinations of feature descriptors such as SIFT [7], luminance, color, and shape descriptors [8]. The downside of using such descriptors are that they are domain-specific and require engineering. They also tend to produce high-dimensional feature spaces. In the bag-of-words/spatial pyramid paradigm, descriptors are quantized. However, Boiman et al. argue in a seminal paper [5] that quantization, though significantly reducing dimensionality, leads to a severe degradation in the discriminative power of descriptors. Parametric methods can compensate by learning, but non-parametric methods are considerably weakened having essentially no way to correct.

A second issue hindering NN methods is the use of “image-to-image” rather than “image-to-class” distance. The former sees a query image compared to every other image in a database, selecting the $k$ nearest points. The latter sees a query image compared to each class in turn, selecting the $k$ nearest points in each class. This idea is key to a simple algorithm named Naïve-Bayes Nearest Neighbours (NBNN). The descriptors of the query image are strongly assumed to be independent by the model; however, the algorithm works well in practice and has seen several extensions which rival the state-of-the-art in object recognition [9], [6].

Returning to the central issue of distance in NN algorithms, an alternative to using descriptors is to learn a distance measure directly from data, exploiting distance information that is intrinsically available, for example, through class labels. Metric learning methods aim to learn a similarity measure that is both tractable to compute and perceptually coherent (i.e. observations that are perceptually similar will have a high measurable similarity).

Many distance metric learning methods are related to techniques for dimensionality reduction [10], [11], [12]. Simple methods like Locally Linear Embedding (LLE) [13] and Stochastic Neighbor Embedding (SNE) [14] depend on meaningful similarity in the input space. These approaches are not suitable for images unless they are perfectly registered and highly similar. Laplacian Eigenmaps [15] and other spectral methods do not require a meaningful metric in the input space, but they cannot cope with out-of-sample data because they do not learn a mapping[7]. This limits their applicability to retrieval.

A subset of approaches learn a function (mapping) from high-dimensional (i.e. pixel) space to low-dimensional “feature” space such that perceptually similar observations are mapped to nearby points on a manifold. Neighbourhood Components Analysis (NCA) [19] proposes a solution where quantization, though significantly reducing dimensionality, leads to a severe degradation in the discriminative power of descriptors. Parametric methods can compensate by learning, but non-parametric methods are considerably weakened having essentially no way to correct.

1Extensions of these techniques to cope with the out-of-sample problem have been proposed (c.f. [16], [17], [18]).
classification. While it is optimized for \( k = 1 \), using \( k > 1 \) tends to work better in practice, and a recent extension \[20\] derives a tractable way to optimize for \( k > 1 \) neighbours. NCA can be extended to the nonlinear case \[21\] by introducing intermediate representations and applying back-propagation. NCA is fundamentally “image-to-image” and training it requires a normalization over every pair of points.

In this paper, we introduce a smooth form of “image-to-class”-based Nearest Neighbour in which, in the spirit of NCA, distances are computed via a discriminatively learned embedding. In contrast to NCA, our algorithm makes local rather than global changes in its updates: nearest neighbours in the same class are pulled towards a point, while nearest neighbours in other classes are repelled. Far away points are unaltered. We show that the “image-to-class” paradigm works not just with engineered descriptors, but with learned distance metrics. Furthermore, learning the distance metric according to a “image-to-class” criterion is effective.

II. BACKGROUND

Before developing our technique, we first give a brief overview of Naïve Bayes Nearest Neighbour \[5\] and then Neighbourhood Components Analysis \[19\].

A. Naïve Bayes Nearest Neighbour

The goal of NBNN \[5\] is to classify a query image. Each such query image \( Q \) is classified as belonging to a class \( \hat{C} \) according to a maximum a posteriori estimation rule

\[
\hat{C} = \arg\max_{C} p(C|Q) . \tag{1}
\]

Assuming a uniform class prior and applying Bayes’ rule,

\[
\hat{C} = \arg\max_{C} \log p(Q|C) . \tag{2}
\]

In Naïve-Bayes Nearest Neighbours and its variants, a set of descriptors \( \{d_1, \ldots, d_n\} \) is extracted from each image. Assuming independence of the descriptors \( d_i \), given the class

\[
\hat{C} = \arg\max_{C} \log \prod_{i=1}^{n} p(d_i|C) = \arg\max_{C} \sum_{i=1}^{n} \log p(d_i|C) . \tag{3}
\]

Approximating \( p(d_i|C) \) by a Parzen window estimator with kernel \( K \) leads to

\[
\hat{p}(d_i|C) = \frac{1}{L} \sum_{j=1}^{L} K(d_i - d_j^C) , \tag{4}
\]

where \( L \) is the total number of descriptors over all images from class \( C \) in the training set and \( j \) indexes descriptors in class \( C \). This can be further approximated by only using the \( k \) nearest neighbour descriptors in class \( C \),

\[
p(d_i|C) \approx \hat{p}_k(d_i|C) = \frac{1}{L} \sum_{j=1}^{k} K(d_i - d_{NN}^C) , \tag{5}
\]

where \( d_{NN}^C \) is the \( j \)th nearest neighbour of \( d_i \) in class \( C \). By choosing a Gaussian kernel for \( K \) and substituting this into Eq.\[5\] the classification rule becomes

\[
\hat{C} = \arg\max_{C} \sum_{i=1}^{n} \log \left( \frac{1}{L} \sum_{j=1}^{k} \exp \left( -\frac{1}{\sigma^2} \|d_i - d_{NN}^C\|^2 \right) \right) . \tag{6}
\]

By setting \( k = 1 \), there is no longer a dependence on the kernel width \( \sigma \) and \( \log p(d_i|C) \) has a very simple form:

\[
\hat{C} = \arg\min_{C} \sum_{i=1}^{n} \|d_i - NN^C(d_i)\|^{2} , \tag{7}
\]

where \( \text{NN}^C(d_i) \) is the nearest neighbour to \( d_i \) in class \( C \). This is the setting used in \[5\] and \[6\].

In our approach, we propose to avoid the task of extracting descriptors and instead learn a functional mapping \( z = f(x) \), where \( x \) is a vector of the pixels of image \( Q \) and \( z \) is a vector representation in some feature space. Nearest neighbours are then found in this feature space. Before discussing this adaptation, we review Neighbourhood Components Analysis \[19\], a method which learns a functional mapping by optimizing a soft form of the KNN classification objective. Although NBNN is motivated from the standpoint of image classification, the idea of “image-to-class” comparison is broadly applicable to non-image modalities. Indeed, in our experiments, we consider non-image data. Additionally, once we have dropped the dependence on descriptors in favour of a single feature vector, we no longer rely on the Naïve-Bayes assumption. Therefore, in the remainder of the paper we will use the term “class-conditional” to refer to the “image-to-class” variant of KNN implied by NBNN.

B. Neighbourhood Components Analysis

NCA aims to optimize a distance metric under the objective of 1-NN classification accuracy. The form of the mapping \( f \) is not fundamental to the technique, only that it is differentiable and therefore trainable by gradient-based methods. To simplify our presentation and without loss of generality, we follow \[19\] and adopt a linear mapping \( z = Ax \). The distance between two vectors \( x \) and \( x' \) is then defined as

\[
g_A(x,x') = (x - x')^T A^T A (x - x') . \tag{8}
\]

This can be interpreted as first projecting points \( x \in \mathbb{R}^D \) into \( P \)-dimensional space using \( A \in \mathbb{R}^{P \times D} \) and then computing Euclidean distances in the \( P \)-dimensional space.

Optimizing \( A \) with respect to the KNN classification criterion is not differentiable because the objective is not a smooth function of \( A \). For example, making a small change to \( A \) may change the nearest-neighbour assignment, leading to a large change in the objective, whereas a large change to \( A \) may have negligible effect on the objective if it does not impact neighbour selection. Thus, NCA adopts a probabilistic view, in which a point \( i \) selects a point \( j \) to be its neighbour with
Algorithm 1: Mini-batch stochastic gradient descent training of Class Conditional Metric Learning (CCML).

\begin{algorithm}
\begin{algorithmic}
  \For{$m$ iterations do}
    \State Sample a mini-batch from the training data
    \State Compute the probability $p_i^C, \forall C$, using Eq. 10
    \State Compute the expectation in Eq. 11
    \State Update the parameters $A$ proportional to Eq. 12
  \EndFor
\end{algorithmic}
\end{algorithm}

a probability that is a function of their difference in feature space. The learning objective becomes the expected accuracy of a 1-NN classifier under the probability distribution,

$$L(A) = \sum_i \sum_{j \neq i} p_i(j) |C_i = C_j|,$$

where $p_i(j) \propto \exp(-||Ax_i - Ax_j||^2)$ is the probability that $i$ selects $j$ as its neighbour.

### III. CLASS CONDITIONAL METRIC LEARNING

Note that NCA takes essentially the “image-to-image” view, in which each point is compared to every other point based on its distance in projected space. Computing $p_i(j)$ is quadratic in the number of training points which severely limits its applicability to large datasets. In practice, NCA is often trained approximately using “mini-batch” gradient descent [21]. Inspired by NBNN, we propose an alternative objective to distance metric learning having two key properties: (i) nearest-neighbour finding is class-conditional; and (ii) only the $k$-nearest neighbours in each class contribute to the class decision. Let the probability of assigning point $i$ to class $C$ be a normalized function of the distances to its nearest neighbours in that class:

$$p_i^C = \frac{\exp\left(-\frac{1}{k} \sum_{j=1}^k ||Ax_i - \text{NN}_j^C(Ax_i)||^2\right)}{\sum_{C'} \exp\left(-\frac{1}{k} \sum_{j=1}^k ||Ax_i - \text{NN}_j^{C'}(Ax_i)||^2\right)},$$

where $\text{NN}_j^C(Ax_i)$ is the $j$th nearest neighbour, from class $C$, of the projection of $x_i$.

Similar to NCA, our objective is to maximize the expected accuracy of classification under this objective:

$$E(A) = \sum_i \sum_C p_i^C |C = C_i| = \sum_i p_i^C,$$

where $C_i$ is the class associated with point $x_i$. At each update, each data point will be attracted toward the $k$ nearest data points that share its class. This is equivalent to minimizing the mean distance between point $i$ and its $k$ nearest neighbours in the same class. This will encourage similar points in the same class to cluster. The denominator in Eq. 10 will locally repel nearby points not in the same class as $i$.

Differentiating the expectation \[11\] with respect to the transformation matrix $A$ gives

$$\frac{\partial E}{\partial A} = -\frac{1}{k} \sum_i p_i^C (\beta^C_i - \sum_{C'} \beta^{C'} \exp\left(-\frac{1}{k} \sum_{j=1}^k ||Ax_i - \text{NN}_j^{C'}(Ax_i)||^2\right)),$$

where

$$\beta^C_i = \sum_{j=1}^k (Ax_i - \text{NN}_j^C(Ax_i)) x_i^T.$$

Our method, which we call Class Conditional Metric Learning (CCML) can be trained by mini-batch stochastic gradient descent\(^2\) using Eq. 12 to compute the gradient needed for the update to $A$.

Strictly speaking, NN(·) is a non-differentiable function, because its derivative is not defined at the boundaries between nearest neighbour assignments. However, in practice, we did not experience problems during optimization\(^3\). This is because most of the points lie on the interior of the nearest neighbour boundaries and the use of mini-batch SGD compensates when the gradients are averaged. A theoretically sound way to overcome this issue is by running SGD and ignoring the updates when we encounter a non-differentiable point [22].

#### A. Test time decision rule

At test time, we project each query, $z = Ax$ and apply the following decision rule, which we call Class Conditional KNN (CCKNN):

$$\hat{C} = \arg\min_C \left[ \sum_{j=1}^k ||z - \text{NN}_j^C(z)||^2 \right].$$

Eq. 14 has a similar form to NBNN (Eq. 7), except that for each class, we sum over the $k$ nearest neighbours of the projection of the query, $z$. This is consistent with Eq. 10, the probability of a query point $i$ being assigned to class $C$, $p_i^C \propto \exp\left(-\sum_{j=1}^k ||z_i - \text{NN}_j^C(z_i)||^2\right)$. The class with the highest probability under the “soft” decision rule is exactly the class selected by Eq. 14. We are explicit in differentiating the metric learning algorithm (CCML) from the nearest neighbour decision rule (CCKNN) so that we can evaluate their respective contributions in Section V.

Pseudo-code for training and testing our proposed model using CCML and CCKNN is shown in Algorithm 1 and 2, respectively.

\(^2\)In practice, we train with stochastic mini-batches, only performing the nearest neighbour search over the mini-batch.

\(^3\)We used the Theano library, specifically its auto-differentiation capabilities. We verified its stability of taking the gradient of NN(·) with the Theano development team (personal communication).
B. Towards a local search

For each query point, Eq. [10] implies a nearest neighbour search in each class. However, a query may have nearest neighbours in some classes that are globally very far away. Intuitively, it does not make sense to waste modeling power in repelling them further. We can capture this intuition while learning the distance metric by only considering the probability of a single event: the probability that a point is assigned to its true class. In other words, we do not need to explicitly formulate the probability of assignment to each class. We define the probability of “correct-class” assignment to be

\[
p_i^C = \exp \left( -\frac{1}{k} \sum_{j=1}^{k} ||Ax_i - \text{NN}_j^C(Ax_i)||^2 \right) \left[ \exp \left( -\frac{1}{k} \sum_{j=1}^{k} ||Ax_i - \text{NN}_j^C(Ax_i)||^2 \right) + \exp \left( -\frac{1}{k} \sum_{j=1}^{k} ||Ax_i - \text{NN}_j^C(Ax_i)||^2 \right) \right]^{-1}
\]

where \(\text{NN}_j^C(Ax_i)\) means that neighbours of \(Ax_i\) are chosen from all classes except \(C_i\). We still achieve the same effect if we replace Eq. [10] by Eq. [15] in Eq. [11], where neighbouring points of the same class are pulled together, and neighbouring points in different classes are repelled. Note that we cannot use this probability as part of a decision rule, since class labels are not available at test time. However, in practice, we use it in the objective for learning a distance metric and apply either Eq. [14] or the simple KNN rule in the projected space at test time. Of course, we expect (and verify in the experiments) that CCKNN improves performance.

Although both variants of CCML are bounded by the \(O(N^2)\) task of computing distances in projected space, we find that practically, sorting distances twice rather than per-class gives a modest speed-up. In addition, the burden of computing pairwise distances can be mitigated by employing an approximation method such as KD-trees or the AESA algorithm [23]. More important than the modest gain in speed, we find that this variant of CCML improves performance, which is consistent with the intuition above.

IV. Extension to the Convolutional Setting

Recently, convolutional neural networks have become much more popular due to their strong performance on vision benchmarks. These architectures naturally incorporate prior knowledge about the 2d structure of images. As in [24], we can construct a nonlinear variant of CCM by replacing the purely linear transformation by several convolutional layers, plus one or more fully-connected layers. The \(l^{th}\) convolutional and subsampling layer are formulated as

\[
x_j^{k(i)} = f \left( \sum_{j \in M_k} x_{j}^{(l-1)} * W_k^{(i)} + b_k^{(i)} \right)
\]

\[
x_j^{k(i)} = \text{down}(z_j^{(i)}) + c_j^{(i)}
\]

respectively, where \(*\) is the convolution operator, \(M_j\) is the selection of inputs from the previous layer (“input maps”), \(f\) is an activation function, and \(\{W_k, b_k, c_k\}\) are the parameters

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**Algorithm 2** Class Conditional K-Nearest Neighbour (CCKNN) test-time decision rule.

Partition the data by classes: \(x_{C_1}, x_{C_2}, \ldots, x_{C_n}\) where \(n\) is the number of classes.

Compute the class prior for \(C_i\) based on its frequency in the dataset \(D\): \(p(C_i) = \frac{\sum \text{number of } x_i \text{ belonging to } C_i}{\sum \text{number of } x_i \text{ belonging to } C_j}\)

for each class \(C_i\) do

Compute the distance between \(X_{\text{test}}\) and \(X_{C_i}^t\)

Find the \(k\)-nearest distances - and store in \(D_i\)

end for

Compute the variance of the distances, \(\sigma = \text{Var}[[D_1; D_2; \cdots; D_k]]\)

for each class \(C_i\) do

Compute the likelihood under a Gaussian distribution, \(p(x_{\text{test}}|C_i) = \mathcal{N}(D_{ij}[0, \sigma]) \forall j = 1, \ldots, k\)

Compute the score, which is proportional to the posterior probability, \(p(C_i|x_{\text{test}}) \propto p(x_{\text{test}}|C_i)p(C_i)\)

end for

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Fig. 1: Convolutional CCML with 2 convolution and subsampling layers. This architecture was used in our experiments.
of the model. The convolutional step (filtering) is expressed in Eq. [16]. Typically, the rectified linear (ReLU) or \( \tanh \) function are used as the activation function \( f \). The sub-sampling layer is expressed in Eq. [17] and we use max-pooling for the sub-sampling function \( \downarrow \), which selects the maximum value among the elements in each local \( n_p \times n_p \) region. In practice, the bias \( c_j^k \) is set to zero.

We can make a substitution in Eq. [15] replacing the input \( x_i \) by the flattened output of the last convolutional and sub-sampling stage. We use the same objective (Eq. [11]), backpropagating through all the fully-connected and convolutional layers. We denote the convolutional CCML as ConvCCML. The 2-layer ConvCCML architecture we used in our experiments is depicted in Fig. 1.

V. EXPERIMENTS

We evaluated CCML based on qualitatively assessing the distance metric by visualization using a synthetic dataset and quantitatively evaluating nearest neighbour classification and retrieval across four real datasets described below. In contrast to previous work on NBNN \([5]\), \([6]\), we avoid the use of computing descriptors. Instead, we compare NN or NBNN algorithms on raw pixels to learned representations obtained by distance metric learning.

A. Qualitative evaluation on synthetic data

![Fig. 2: CCML, NCA, and ITML embeddings of the Sandwich dataset. For CCML, various choices of \( k \) are used. Nearest neighbours are shown as links. Colour and symbol indicate class.]

We used a synthetic dataset called “Sandwich” in order to visualize the behaviour of CCML embedding, with respect to the choice of \( k \). Fig. 2 shows the embedding at various settings of \( k \), with nearest neighbour points as linked and colours/symbols indicating class. In the input space, we can see that every data point is linked with a data point in another class, which indicates that the Euclidean metric is a poor choice for this dataset. However, even after just using \( k = 1 \) for learning the metric, CCML alleviates the problem. We see that for small values of \( k \), data points are clustered locally with other points from the same class. As we increase \( k \), the clustering becomes more global. This implies that, compared to NCA, the scale of the clustering can be controlled with the choice of \( k \). This illustrates that our metric can be tuned to learn a local or global distance metric depending on the data (e.g. whether the data is highly multi-modal or not). The data points projected by NCA (\( k = 1 \)) and Information-Theoretic Metric Learning (ITML) \([25]\) are also shown.

B. Datasets

Here we will describe the four datasets that were considered in the experiments described in the remainder of this section. The UCI wine dataset contains 178 examples. We took the standard approach (e.g. as used by \([26]\)) of randomly separating the data into 70% training examples. The data consists of three different types of wines with 13 attributes that describe each wine. Although the dataset is small both in number of examples and dimensionality, we included it because of its common use in the distance metric learning literature (c.f. \([25]\), \([27]\), \([28]\), \([26]\)).

The MNIST dataset contains 60,000 training and 10,000 test images that are \( 28 \times 28 \) pixel images of handwritten digits from the classes 0 to 9. From the 60,000 training examples, we used 10,000 as validation examples to tune the hyper-parameters in our model.

The ISOLET dataset contains 7,797 instances and 617 features. The task is to predict which letter-name was spoken from various people, and the features include: spectral coefficients, contour features, pre-sonorant features, and post-sonorant features. From the 7,797 examples, the dataset is pre-split into 6,238 (80%) training examples and 1,559 (20%) test examples.

The small NORB dataset contains 24,300 training examples and 24,300 test examples that are stereo pairs of \( 32 \times 32 \) images. It consists of 50 toy objects from five different classes: four-legged animals, humans, airplanes, trucks, and cars. Objects are captured under different lighting conditions, elevation, and azimuth to assess the invariance properties of classifiers.

C. Classification Performance

We now compare several metric learning techniques based on nearest neighbour classification. With the exception of the convolutional models, we applied principal component analysis (PCA) before training to reduce the dimensionality of the data, retaining 99% of the variance. For the NORB dataset, we preprocessed with Local Contrast Normalization \([30]\). For all other datasets, we used raw pixels as input. We used the usual training and test splits for ISOLET, MNIST, and NORB. For the wine dataset, we ran 10-fold cross-validation to obtain the results. Hyperparameters \( k \), learning rate, weight-decay cost, batch size, and size of the projected dimension were selected from discrete ranges and chosen based on a held-out validation set.

For classification, we measured accuracy using Euclidean distance on the original space and transformed space via PCA, NCA, ITML \([25]\), NCMC \([29]\), LMNN \([26]\), and CCML. Results are shown in Table 1 and more details on each of the baselines are given in Section VI. We applied both KNN and CCKNN to each metric, in an attempt to separate the gain from the type of NN decision rule to the gain from the particular distance metric used. The results illustrate that employing the

\(^4\text{Code can be found at } https://github.com/jiwoongim/CCML\)
TABLE I: Classification error rates across datasets. After learning or selecting a metric, we apply either a standard (KNN) or class-conditional (CCKNN) decision rule. For the Euclidean metric, we considered two feature representations: PCA retaining 99% of the variance, and PCA with an optimal number of components selected on a validation set in parentheses. Note that the convolutional models were only applied to image-based datasets.

| Metric | WINE | ISOLET | MNIST | NORB |
|--------|------|--------|-------|------|
|        | KNN  | CCKNN  | KNN   | CCKNN | KNN  | CCKNN |
| Euclidean (PCA w/ 99% variance) | 3.99 | 3.29   | 8.79  | 7.12  | 2.91 | 2.71  |
| Euclidean (PCA w/ optimal # of comp.) | 4.31 (6) | 3.67 (6) | 8.66 (300) | 6.80 (200) | 2.48 (20) | 2.19 (10) |
| ITML [25] | 4.44 | 3.71   | 9.49  | 7.45  | 2.93 | 2.75  |
| NCMC [26] | 3.51 | 2.96   | 5.13  | 5.06  | 3.21 | 3.09  |
| LMNN [26] | 2.59 | 2.59   | 5.33  | 5.38  | 2.11 | 2.1   |
| NCA [19] | 2.74 | 2.60   | 4.24  | 4.05  | 2.65 | 2.45  |
| CCML | 2.13 | 2.04   | 3.66  | 3.60  | 1.91 | 1.77  | 12.15 | 11.89 |

ConvNet (1-layer) 1.13  9.25
ConvNet (2-layer) 1.12  7.96
ConvCCML (1-layer) 1.36  1.30  6.84  6.80
ConvCCML (2-layer) 0.91  0.83  6.59  6.65

Fig. 3: Retrieval quality w.r.t. the number of images retrieved using KNN on the ISOLET, MNIST, and NORB datasets.

CCKNN classifier, rather than KNN, consistently achieves better performance. Moreover, the distance metric learned by NCA improves accuracy, but applying CCML improves accuracy by a bigger margin. As expected, the learned CCML metric combined with a CCKNN decision rule achieves the best performance. Our method outperforms NCA, ITML, NCMC, and LMNN\(^5\) across all datasets.

For the image-based datasets, we evaluated a convolutional version of our model, comparing it to an identical convolutional architecture trained discriminatively (denoted ConvNet). The 1 and 2-convolutional layer variants of CCML are denoted “convCCML(1-layer)” and “convCCML(2-layer)” in Table I. The simplest architecture, convCCML(1-layer) used 10 5 × 5 filters. The other architecture, convCCML(2-layer), used 10 filters for each layer with 5 × 5 filters on the first convolutional layer and 3 × 3 filters on the second layer. The pooling size was 2 by 2 for all convolutional architectures. ConvCCML significantly outperformed the baseline ConvNet, as well as the vector-based metric learning techniques.

D. Data retrieval

Distance metric learning is frequently used for the retrieval of relevant examples, such as images or documents. In this section, we explore the performance of various distance metric learning methods using a KNN rule for retrieval. Retrieval quality was measured using normalized Discounted Cumulative Gain (nDCG), where \(\text{DCG}_k = \sum_{i=1}^{k} \frac{2^{r_i} - 1}{\log_2(i+1)}\), \(\text{nDCG}_k = \frac{\text{DCG}_k}{\text{IDCG}_k}\) and \(\text{IDCG}_k\) is the maximum possible (ideal) DCG for a given set of queries. nDCG, commonly used in information retrieval, measures the performance of retrieved data quality based on the graded relevance of the retrieved entities. We use a binary indicator of class match as a relevance score. This task focuses more on evaluating the individual returned examples from the database, rather than their aggregate vote. This is a more explicit form of evaluating the ability of the learned distance metric to capture perceptual similarity than classification.

For each of the datasets (ISOLET, MNIST, and NORB), we reported the fraction that were from the true class (Fig. 5). Note that CCKNN cannot be employed in the retrieval task since CCKNN compares each item to a class, returning a class decision. Here, we want to compare the query example to each individual item in the database and return the most relevant item. The results on all three datasets illustrate that retrieval using a distance metric significantly outperforms retrieval using a Euclidean distance, and it consistently shows a large relative gain between CCML and other methods like NCA or LMNN. We also evaluated the retrieval quality of convolutional variants of CCML. The more flexible convCCML was shown to significantly outperform the other methods.

Fig. 4 visualizes retrieval and failure modes. Each row shows the five nearest neighbours to the query using the

\(^5\)According to [26], the MNIST classification error on LMNN is 1.31%. We were unable to reproduce these results, even using the authors’ code.
Euclidean, CCML and convCCML distance metrics. Both MNIST and NORB target samples in the first four rows of Fig. 4 were incorrectly classified by KNN, but correctly classified by KNN after being transformed by CCML. The first, second, third, and fourth rows of Fig. 4 are dominated by images of ‘sixes’, ‘sevens’, ‘zeros’, and ‘sevens’, even though the query images were ‘eight’, ‘nine’, ‘two’, and ‘two’. Although performance improves with CCML, it still produces a few errors: not all of the five nearest neighbors share a class with the query. Indeed, this is amended by using convCCML, where all five nearest neighbors are correct.

We also show visual retrieval performance on the NORB dataset (Fig. 4b). Discrimination among the five different categories of 3D objects is more difficult than with MNIST, because images from the same category can significantly differ in appearance. This is reflected in their pixel-space distances. The last row in both the MNIST and NORB retrieval examples show failure modes of convCCML. Even though the retrieved images are incorrectly classified, we can see that the images retrieved using the convCCML distance measure do capture some sort of similarity in terms of geometry. Qualitatively, among the misclassified examples, images retrieved using convCCML appear to be more sensible.

VI. RELATED WORK

Many metric learning methods, particularly k-NN, have been proposed for non-parametric classification. A large number of these methods attempt to learn a Mahalanobis distance. A well-known example is Neighbourhood Components Analysis (NCA), which learns an optimal Mahalanobis distance for 1-NN [19]. It maximizes a stochastic variant of the leave-one-out criterion, and it is trained through stochastic gradient descent. Since our work is inspired by NCA, we have already discussed its formulation in Section II-B.

Salakhutdinov and Hinton extended NCA to the non-linear setting by incorporating a multi-layer neural network into the embedding and training it with backpropagation [21]. They incorporated unsupervised pre-training [31] into their formulation and regularized with an auto-encoder objective. In a similar manner, we demonstrate the extension of our method to the non-linear setting by utilizing an embedding based on convolutional neural networks.

One drawback of the NCA criterion is that it only finds the best metric for a 1-NN classifier since it stochastically selects a single neighbour per point. Tarlow et al. address this issue by extending to stochastic k-neighbourhood selection [20]. Though this method is theoretically sound, in practice, optimization is complicated. Moreover, the technique is memory-intensive in the case of large datasets, and as a result, it is not as straightforward to extend to non-linear mappings.

Another well-known metric learning algorithm is Large Margin Nearest Neighbour (LMNN) [26], which also learns a Mahalanobis distance for k-NN by maximizing a hinge loss function. The optimization is formulated as a semi-definite programming problem, which is convex. However, it does not permit non-linear embeddings as in [21] or the present work.

Mensink et al. proposed a non-parametric classification method called the nearest class mean classifier (NCMC).
Superficially, this algorithm may appear similar to ours, but operationally, it is not. NCMC is a prototype-based algorithm that compares the distance between a point to the mean over all points from each class. On the other hand, our method discriminates classes based on computing the average of $k$ all points from each class. Optimizing for NCMC and CCKNN is not the same (see Section III-A). An advantage of our method is its local to global scaling (as shown in Fig. 2). Moreover, NCMC learns from image descriptors such as SIFT, whereas our proposed metric learns features from pixels.

Other types of metric learning were also explored in the learning literature, including Information-Theoretic Metric Learning [25, ITML]. ITML minimizes the log determinant divergence subject to linear constraints based on Bregman optimization, which is convex like LMNN. Also, other variants of ITML that use Bregman optimization exist, such as [32], [33] or generalized maximum entropy [34, 35]. Though these methods have compelling theoretical results, none have emerged as dominant in practice.

VII. CONCLUSION

Inspired by Neighbourhood Components Analysis which optimizes a distance metric for 1-nearest neighbour classification, we show how to learn a distance metric optimized for class-conditional nearest neighbour. Its benefit is twofold: i) we show improved performance over existing metric learning methods, including ITML, NCMC, LMNN, and NCA; and ii) by removing the dependency on engineered descriptors, we extend the method’s applicability to non-image domains.

We demonstrated linear and nonlinear versions of our technique, the latter based on convolutional neural networks. For non-signal type data, i.e. data inappropriate for convnets, any nonlinear function can be used, as long as it is differentiable. CCML is trained by gradient descent (applying backpropagation in the case of multi-layer mappings) and it is suitable for batch or online learning. Moreover, it can be adjusted to be more local or global by tuning a single parameter.

Due to the nature of our decision rule, our metric learning approach is limited to datasets which have pre-defined class labels. We intend to investigate whether the approach can be extended to weaker forms of labeling.

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