DNet-kNN: A Deep Non-Linear Feature Mapping for Large-Margin kNN Classification

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kNN Classification with Metric Learning

- KNN is popular in almost all fields of data analysis: simple and effective
- When kNN fails:
  - A lot of class-irrelevant features present
  - Bad distance metric adopted
- Distance Metric Learning required for good performance
  - Linear feature transformation is widely used, but it is incapable of capturing higher-order statistics hidden in input feature vector components
  - Non-Linear feature transformation using a kernel trick has also been tried, but it is not scalable to large datasets
  - Neural Networks has also been used to learn non-linear mappings to improve kNN classification, but the neural networks used are often shallow.
Why deep and non-linear feature mapping

- The difference between statistics, machine learning, and data mining:
  - Statistics prefer simple models to distinguish data with simple structure from noise
  - The task of machine learning and data mining, especially machine learning, is to extract a huge amount of meaningful structure from data, which can often only be represented by complicated model
- Models with shallow architectures fail to represent complex structure hidden in input data:
  - For e.g., perceptron, kernel SVM, neural network with one hidden layer
- Models with deep architectures mimic human brains to perform multi-stage information processing to extract meaningful structure from high-dimensional sensory input
  - Humans can easily recognize shapes and objects and easily extract gist information from complex scenes because human brains has a deep architecture
  - Deep non-linear mapping has many layers, each layer models the combination of patterns in the layer below
  - Researchers often use Neural Networks to construct deep non-linear mapping
Large Margin Learning

- In 1990s, many researchers abandoned neural networks and turned to use SVMs
- Maximizing margin enables robust classifiers to be learned
  - Linear SVM and Kernel SVM
  - Linear metric learning toward the goal of large-margin separation in the kNN classification framework (Weinberger, NIPS 2005)
  - Limited due to shallow architecture and linear mapping used
The Next-Generation Machine Learning Models: Large Margin Learning with Deep Architectures

- We want to learn a powerful model with deep architecture and at the same time we want it to be robust in the sense of large margin classification
- Our approach:
  - Learn a deep neural network (a deep encoder or auto-encoder)
  - Maintain large-margin classification boundaries in the learned feature (code) space
  - We chose kNN as the classification method to be used in the code space
- Objective function:

\[ y_{ij} = 1 \text{ to represent that } i \text{ and } j \text{ are in the same class} \]
\[ \eta_{ij} \in \{0, 1\} \text{ to indicate whether input } \bar{x}_j \text{ is a target neighbor of input } \bar{x}_i \]
\[ \gamma_{ij} = 1 \text{ if and only if } i \text{ is an impostor neighbor of } j \]

\[ \ell_{ilj} = h(1 + d_f(i, l) - d_f(i, j)), \]
\[ \min_f \ell_f = \sum_{ilj} \eta_{il} \gamma_{ij} \ell_{ilj}, \]
How to Learn A Deep Supervised Model by Hinton

Hypothesis by Geoff Hinton: Recognizing Objects by Generating Objects First (if you want to do computer vision, do computer graphics first)

- Perform unsupervised learning to learn a good generative model first
- Then fine-tune the model parameters by minimizing the loss function of the supervised learning model
Learn a Deep Generative Model Using Restricted Boltzmann Machines by Hinton (1)

Energy with configuration $v$ on the visible units and $h$ on the hidden units:

$$E(v, h) = - \sum_{i,j} v_i h_j w_{ij}$$

$$p(v, h) \propto e^{-E(v, h)}$$

$$- \frac{\partial E(v, h)}{\partial w_{ij}} = v_i h_j$$

$$\frac{\partial \log p(v)}{\partial w_{ij}} = \langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^\infty$$
Learn a Deep Generative Model Using Restricted Boltzmann Machines by Hinton (2)

Start with a training vector on the visible units.
Update all the hidden units in parallel
Update the all the visible units in parallel to get a “reconstruction”.
Update the hidden units again.

\[
\Delta w_{ij} = \varepsilon \left( <v_i h_j>^0 - <v_i h_j>^1 \right)
\]
Learn a Deep Generative Model Using Restricted Boltzmann Machines (3)

\[
E(v, h) = - \sum_{ij} W_{ij} v_i h_j - \sum_i v_i b_i - \sum_j h_j c_j
\]

\[
E(v, h) = - \sum_{ij} W_{ij} v_i \frac{h_j}{\sigma_j} - \sum_i v_i b_i + \sum_j \frac{(h_j - c_j)^2}{2\sigma_j^2}
\]

\[
\Delta W_{ij} = \epsilon(\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_1), \text{ binary } h,
\]

\[
\Delta W_{ij} = \epsilon(\langle v_i \frac{h_j}{\sigma_j} \rangle_{data} - \langle v_i \frac{h_j}{\sigma_j} \rangle_1), \text{ Gaussian } h, \quad (8)
\]
Gradient Calculations of the loss function of Dnet-kNN

For each data point $i$, create triples $(i, l, j)$, where $l$ is one of $i$'s top $k$ true nearest neighbors, and $j$ is one of $i$'s top $m$ imposter nearest neighbors from every other class, $m \gg k$

Searching on these triples to look for active violated margin constraints

\[
\frac{\partial \ell_f}{\partial y^{(i)}} = -2 \sum_{jl} \eta_{il} \gamma_{lj} \theta_{ilj} (y^{(l)} - y^{(j)}) + 2 \sum_{jk} \eta_{kl} \gamma_{kj} \theta_{klj} (y^{(k)} - y^{(i)}) + 2 \sum_{kl} \eta_{kl} \gamma_{ki} \theta_{kli} (y^{(k)} - y^{(i)})
\]
Learn Dnet-kNN: A Deep Non-Linear Feature Mapping for Large-Margin kNN Classification

Algorithm 1 The training procedure of DNet-kNN (the description in [] is optional).

1: **Input:** training data \( \{ x^{(i)}, y^{(i)} : i = 1, \ldots, n \} \), \( k \), \( m \), \([T]\).
2: pretrain the network in Fig. 2 with RBMs using Eq. 8 to get initial network weights \( W^{init} \).
3: [Further train a deep autoencoder for \( T \) iterations to get \( W^{init-new} \), and set \( W^{init} = W^{init-new} \).]
4: calculate each data point \( i \)'s \( k \) true nearest neighbors in its class, \( i = 1, \ldots, n \).
5: calculate each \( i \)'s \( m \times (e - 1) \) imposter nearest neighbors, \( i = 1, \ldots, n \).
6: create triples \( (i, l, j) \).
7: set \( W = W^{init} \).
8: **while** (not convergence)
9: \hspace{1em} update \( W \) using conjugate gradient based on Eq. 11-12
10: **Output:** \( W \).
Classification Results of Dnet-kNN on USPS Handwritten Digits

<table>
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<td><strong>0.00</strong></td>
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<td>4.95</td>
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<tbody>
<tr>
<td>DNet-kNN</td>
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<td>2.36</td>
<td>2.33</td>
<td>1.93</td>
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<td>1.53</td>
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Embedding Results of Dnet-kNN on USPS Handwritten Digits

Figure 5. Two-dimensional embedding of 3000 USPS-fixed test data using the Deep Neural Network kNN classifier (DNet-kNN).

Figure 6. Two-dimensional embedding of 3000 USPS-fixed test data using the Deep Autoencoder (DA).

Figure 7. Two-dimensional embedding of 3000 USPS-fixed test data using PCA.
### Classification Results of Dnet-kNN on MNIST Handwritten Digits

<table>
<thead>
<tr>
<th>Methods</th>
<th>results</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNet-kNN (dim = 30, batch size=1.0e4)</td>
<td>0.94</td>
</tr>
<tr>
<td>DNet-kNN-E (dim = 30, batch size=1.0e4)</td>
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</tr>
<tr>
<td>Deep Autoencoder (dim = 30, batch size=1.0e4)</td>
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<td>Non-linear NCA based on a Deep Autoencoder ([16])</td>
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<td>SVM: degree 9 [4]</td>
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<tr>
<td>kNN (pixel space)</td>
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<tr>
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<tr>
<td>LMNN-E</td>
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<tr>
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<tr>
<td>DNet-kNN-E (dim = 2, batch size=1.0e4)</td>
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<tr>
<td>Deep Autoencoder (dim = 2, batch size=1.0e4)</td>
<td>24.7</td>
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</table>
Embedding Results of Dnet-kNN on MNIST Handwritten Digits

Figure 8. Two-dimensional embedding of 10,000 MNIST test data using the Deep Neural Network kNN classifier (DNet-kNN).

Figure 9. Two-dimensional embedding of 10,000 MNIST test data using the Deep Autoencoder (DA).

Figure 10. Two-dimensional embedding of 10,000 MNIST test data using PCA.
Classification Results of Dnet-kNN on 20newsgroup Text Data

Table 4. Test error of different methods for 5-fold cross validation on binary 20 newsgroup text data. "-E" denotes the energy classification method (%). The lowest errors are shown in bold. DNet code dim=30

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<tr>
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<td>33.1</td>
<td>32.8</td>
<td>34.3</td>
<td>30.9</td>
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</tbody>
</table>

The released implementation of LMNN failed to work on this binary dataset.
Future Work

• We used mini-batch training for Dnet-kNN on large datasets. Instead of fixing imposter nearest neighbors, we can dynamically update imposter nearest neighbors in each dynamically changing mini-batch.

• Instead of training a general deep neural network, pre-training Dnet-kNN using a deep hand-coded convolutional neural network will possibly greatly improve the classification performance (see Lu Cun’s research)

• Learn large-margin linear classifiers in the feature space produced by deep (convolutional) neural networks

• Learn a deep network from a Bayesian perspective to constrain the weights to be learned

• Learn the weight matrices in a regularization framework for classification and discuss possible generalization bound for deep learners
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