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

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kNN Classification with Metric Learning

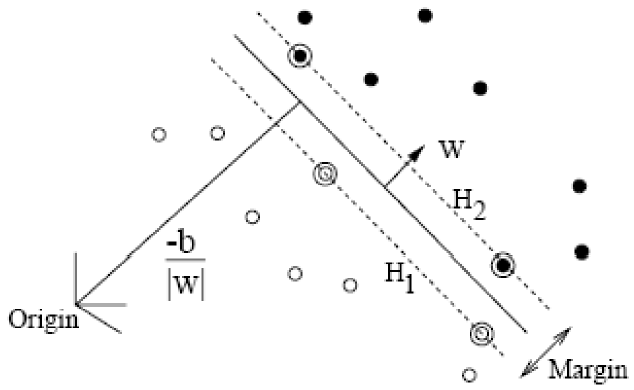
- KNN is popular in almost all fields of data analysis: simple and effective
- When kNN fails:
  - A lot of class-irrelevant features present
  - Bad distance metric adopted
- Distance Metric Learning required for good performance
  - Linear feature transformation is widely used, but it is incapable 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.

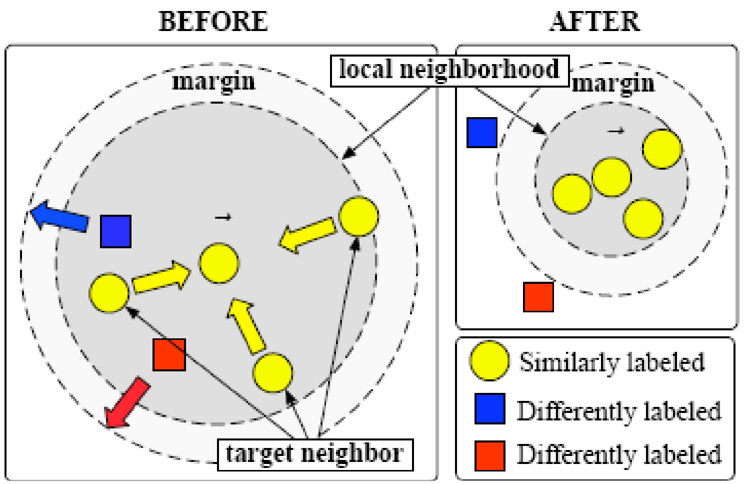
Why deep and non-linear feature mapping

- 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

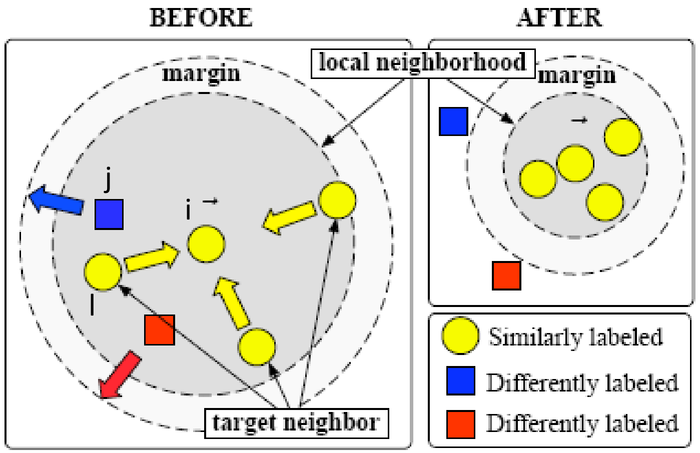
- In 1990s, many researchers abandoned neural networks and turned to use SVMs
- Maximizing margin enables robust classifiers to be learned
  - Linear SVM and Kernel SVM
  - Linear metric learning toward the goal of large-margin separation in the kNN classification framework (Weinberger, NIPS 2005)
  - 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:



$y_{ij} = 1$ to represent that i and j are in the same class

$\eta_{ij} \in \{0,1\}$ to

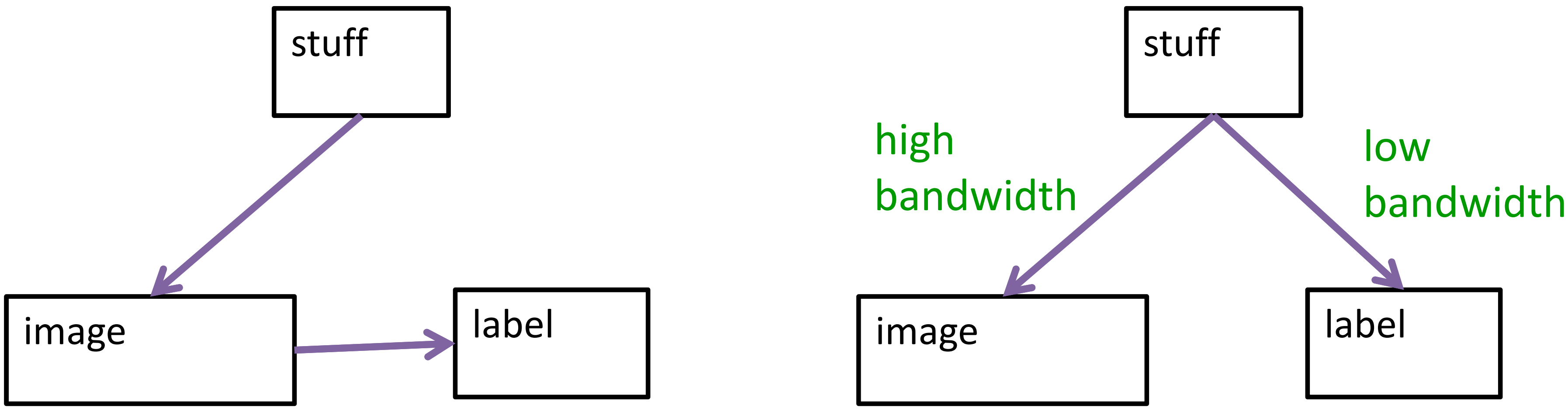
indicate whether input $\vec{x}_j$ is a target neighbor of input $\vec{x}_i$.

$\gamma_{ij} = 1$ if and only if i 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)

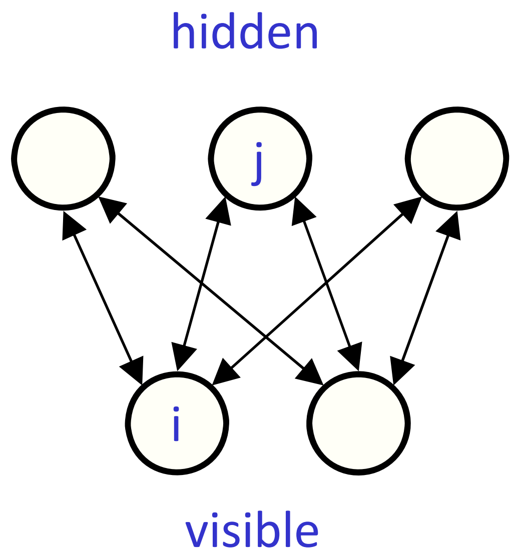
binary state of visible unit i

binary state of hidden unit j

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

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

weight between units i and j

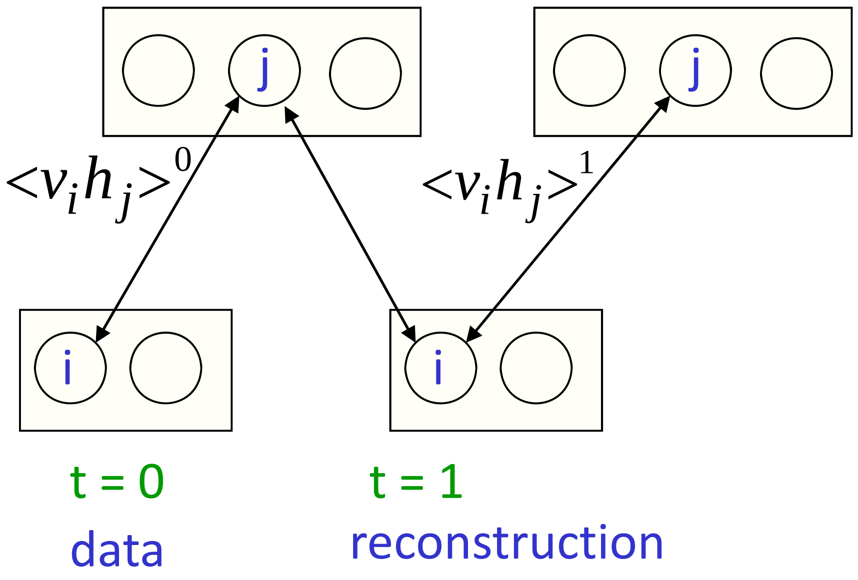


$$p(v,h) \propto e^{-E(v,h)}$$

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

$$\frac{\partial \log p(v)}{\partial w_{ij}} = \langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^\infty$$

Learn a Deep Generative Model Using Restricted Boltzmann Machines by Hinton (2)



Start with a training vector on the visible units.

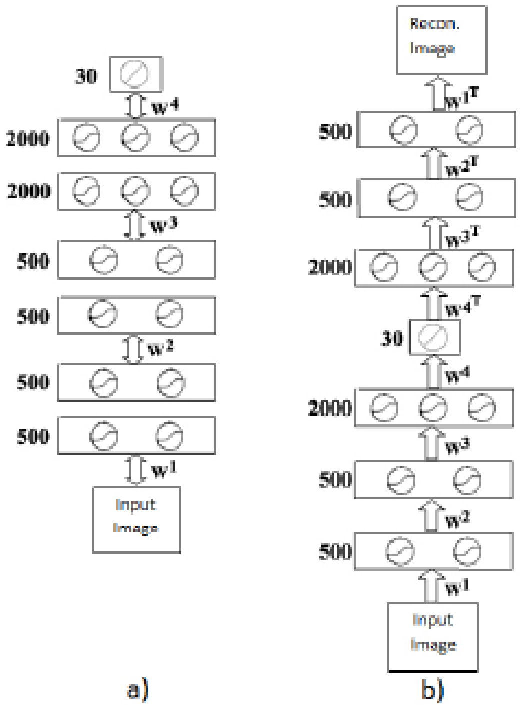
Update all the hidden units in parallel

Update the all the visible units in parallel to get a “reconstruction”.

Update the hidden units again.

$$\Delta w_{ij} = \varepsilon \, (<v_i h_j>^0 - <v_i h_j>^1)$$

Learn a Deep Generative Model Using Restricted Boltzmann Machines (3)



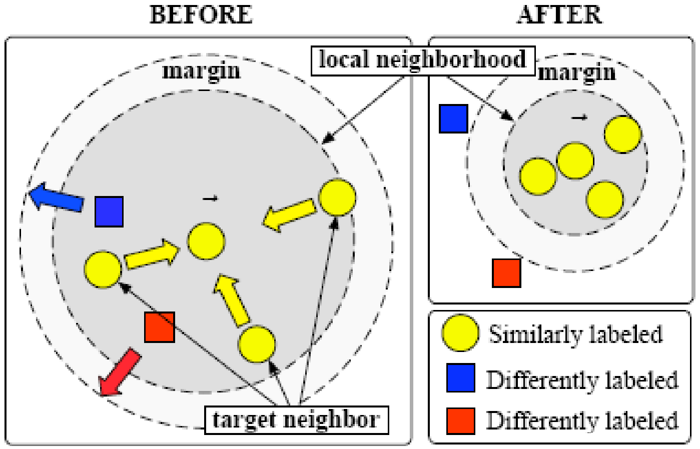
$$E(\mathbf{v},\mathbf{h}) = -\sum_{ij} W_{ij} v_i h_j - \sum_i v_i b_i - \sum_j h_j c_j$$

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

$$\Delta W_{ij} = \epsilon(< v_i h_j >_{data} - < v_i h_j >_1), \;\; binary \;\; \mathbf{h},$$

$$\Delta W_{ij} = \epsilon(< v_i \frac{h_j}{\sigma_j} >_{data} - < v_i \frac{h_j}{\sigma_j} >_1), \;\; Gaussian \;\; \mathbf{h}, \quad (8)$$

Gradient Calculations of the loss function of Dnet-kNN



$$\frac{\partial \ell_f}{\partial \mathbf{y}^{(i)}} = \begin{aligned} &-2\textstyle\sum_{jl} \eta_{il}\gamma_{ij}\theta_{ilj}(\mathbf{y}^{(l)} - \mathbf{y}^{(j)}) \\ &-2\textstyle\sum_{jk} \eta_{ki}\gamma_{kj}\theta_{kij}(\mathbf{y}^{(k)} - \mathbf{y}^{(i)}) \\ &+2\textstyle\sum_{kl} \eta_{kl}\gamma_{ki}\theta_{kli}(\mathbf{y}^{(k)} - \mathbf{y}^{(i)}) \end{aligned}$$

- 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 than the class of i, m>>k
- Searching on these triples to look for active violated margin constraints

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

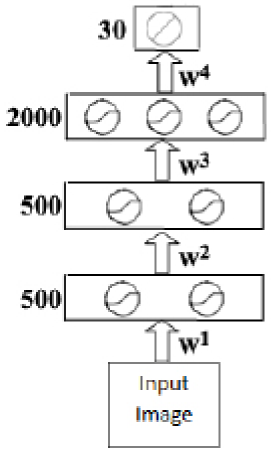
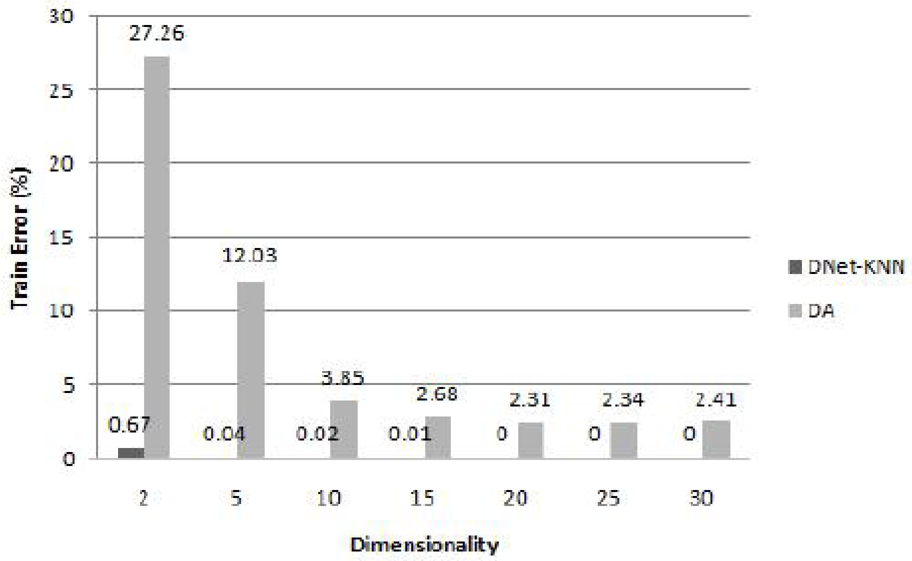


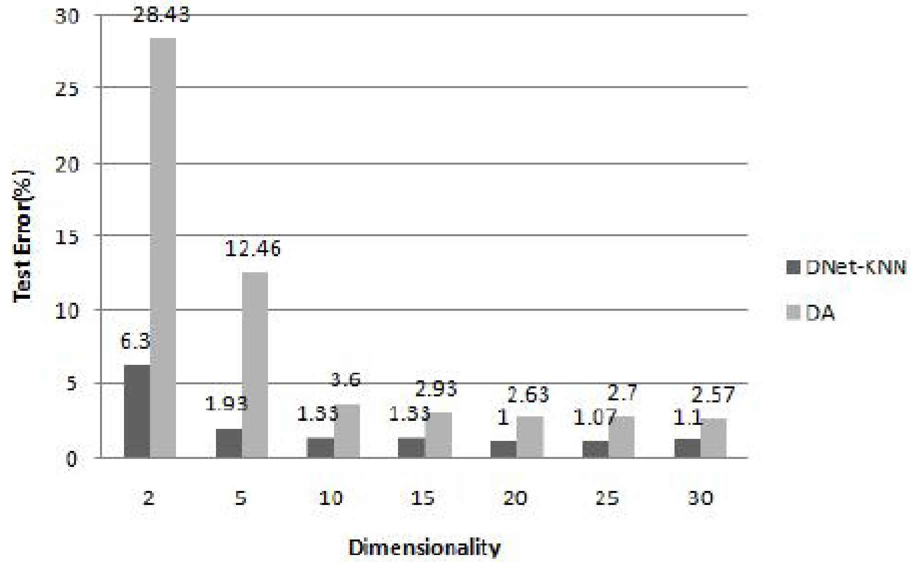
Figure 2. Deep Encoder

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

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

Classification Results of Dnet-kNN on USPS Handwritten Digits





	US1	US2	US3	US4	US5
DNet-kNN	**0.00**	**0.00**	**0.00**	**0.00**	**0.01**
LMNN	0.76	1.10	0.71	0.85	0.95
DA	2.66	2.35	2.28	2.24	2.48
kNN	5.12	5.09	4.95	5.08	4.93

	US1	US2	US3	US4	US5
DNet-kNN	**1.20**	**0.87**	**1.43**	**1.06**	1.13
DNet-kNN-E	1.43	0.97	1.50	1.20	**1.00**
LMNN	2.20	2.13	2.36	2.33	1.93
LMNN-E	1.77	1.53	1.80	1.80	1.63
DA	2.80	2.36	2.33	1.93	2.23
kNN	4.47	4.93	5.23	4.17	5.37

Embedding Results of Dnet-kNN on USPS Handwritten Digits

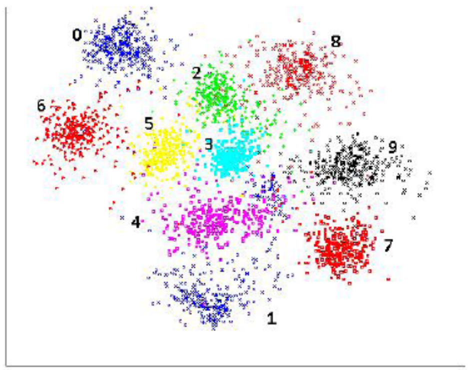


Figure 5. Two-dimensional embedding of 3000 USPS-fixed test data using the Deep Neural Network kNN classifier (DNet-kNN).

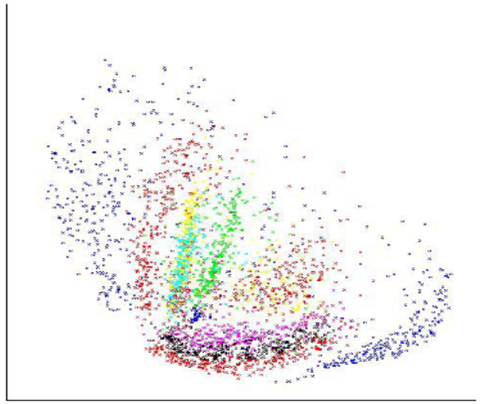


Figure 6. Two-dimensional embedding of 3000 USPS-fixed test data using the Deep Autoencoder (DA).

Figure 7. Two-dimensional embedding of 3000 USPS-fixed test data using PCA.

Classification Results of Dnet-kNN on MNIST Handwritten Digits

Methods	results
DNet-kNN (dim = 30, batch size=1.0e4)	**0.94**
DNet-kNN-E (dim = 30, batch size=1.0e4)	0.95
Deep Autoencoder (dim = 30, batch size=1.0e4)	2.13
Non-linear NCA based on a Deep Autoencoder ([16]	1.03
Deep Belief Net [11]	1.25
SVM: degree 9 [4]	1.4
kNN (pixel space)	3.05
LMNN	2.62
LMNN-E	1.58
DNet-kNN (dim = 2, batch size=1.0e4)	2.65
DNet-kNN-E (dim = 2, batch size=1.0e4)	2.65
Deep Autoencoder (dim = 2, batch size=1.0e4)	24.7

Embedding Results of Dnet-kNN on MNIST Handwritten Digits

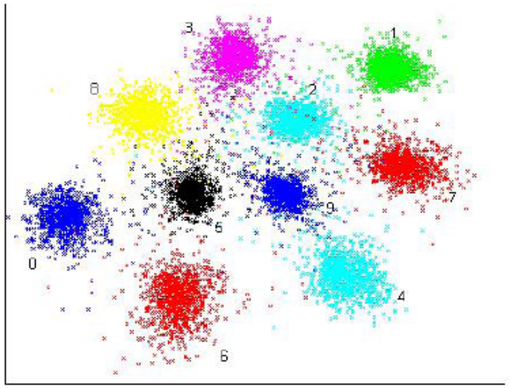


Figure 8. Two-dimensional embedding of 10,000 MNIST test data using the Deep Neural Network kNN classifier (DNet-kNN).

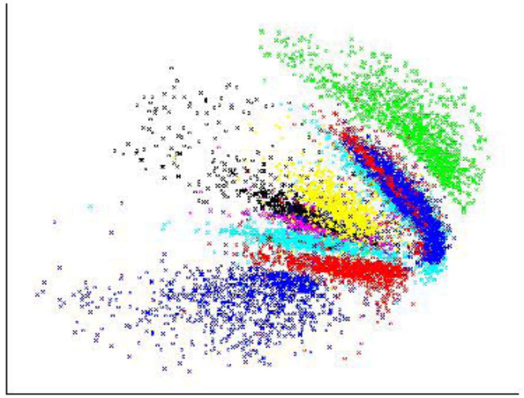


Figure 9. Two-dimensional embedding of 10,000 MNIST test data using the Deep Autoencoder (DA).

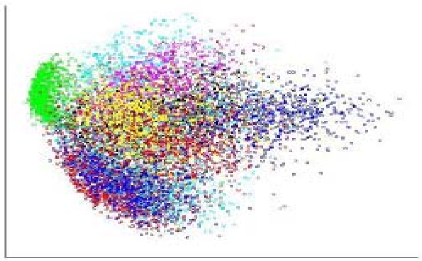


Figure 10. Two-dimensional embedding of 10,000 MNIST test data using PCA.

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

	1	2	3	4	5
DNet-kNN	23.8	22.9	23.1	24.0	22.1
DNet-kNN-E	**19.1**	**18.8**	**18.9**	**19.6**	**17.9**
DA	27.0	25.0	27.0	28.4	27.0
kNN	32.6	33.1	32.8	34.3	30.9

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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