Kernel Learning Using Neural Networks

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Outline

Training part and test part of K

$$K = \begin{bmatrix} TrainingPart_{N \times N} & [TestPart^T]_{N \times T} \\ TestPart_{T \times N} & \text{unused} \end{bmatrix}$$

T is the size of the test set and N is the size of the training set.
K is a $(N + T) \times (N + T)$ matrix.

Existing kernel learning methods

- diffusion kernels
- linear combinations of kernels based on Kernel Alignment with SDP
- hyperkernels
- convex combinations of kernels via semi-infinite linear programming

Kernel Alignment

- Kernel Alignment aligns a linear combination of kernels, $K_1, K_2, \cdots, K_m$, to an optimal kernel computed using class information of the training data.
- A column vector y contains the binary class membership of all training data points, $K_{opt} = yy^T$, where $y \in \{-1, +1\}^N$ and N is the size of the training set.
- The objective function of Kernel Alignment is

$$\ell = \frac{Tr(K_{tr}K_{opt}^T)}{\sqrt{Tr(K_{tr}K_{tr}^T)Tr(K_{opt}K_{opt}^T)}} = \frac{Tr(K_{tr}K_{opt}^T)}{N\sqrt{Tr(K_{tr}K_{tr}^T)}} \tag{1}$$

where $K = \theta_1 K_1 + \theta_2 K_2 + \cdots + \theta_m K_m$, $K \succeq 0$, and tr denotes the training part of K.

Limitations of Existing Kernel Learning Methods

- Use blackbox packages to optimize
- Computationally Expensive
- Impractical for problems with fair-size datasets

Outline

Why Neural Nets

- We want to have a powerful non-linear feature mapping
- We want to make use of the rich structure information existing in the dataset not just labels
- We want an efficient learning approach applicable to large datasets

Learn the Desired Feature Directly

$$max_K \quad \ell = \frac{Tr(K_{tr}K_{opt}^T)}{N\sqrt{Tr(K_{tr}K_{tr}^T)}}$$

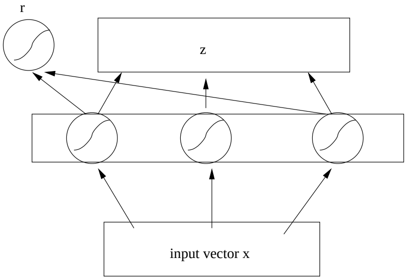
$$\text{subject to } Tr(K) = 1, K \succeq 0.$$

- $K_{tr} = F_{tr}^T F_{tr}$, F_{tr}: the feature vectors learned from neural networks for the training data.
- f, a column of F_{tr}, represents the feature vector learned for one data point.
- Learn the weights $->$ Learn the mapping $->$ Learn the kernel.

the constraint $Tr(K) = 1$

- To enforce the constraint, we make $f = \frac{z}{||z||}$, where z is the linear output vector of an encoder with one logistic hidden layer.
- All the feature vectors lie on the surface of a unit sphere.
- Relaxing this constraint so that some points can lie inside the sphere, we use a logistic unit r to represent the norm of a feature vector
- Then $f = r\frac{z}{||z||}$.

The Structure of the Encoder



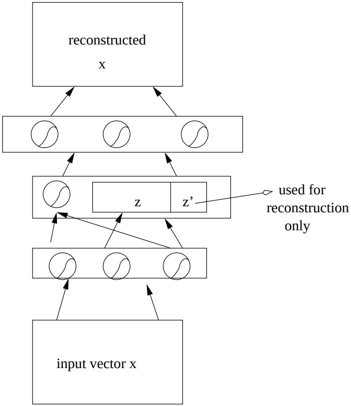
Learn the Weights in the Network

- $\frac{\partial \ell}{\partial K_{tr}} = \frac{K_{opt} Tr(K_{tr} K_{tr}^T)^{\frac{1}{2}} - K_{tr} Tr(K_{tr} K_{opt}^T) Tr(K_{tr} K_{tr}^T)^{-\frac{1}{2}}}{Tr(K_{tr} K_{tr}^T)}$
- $\frac{\partial \ell}{\partial f^{(j)}} = \sum_k \frac{\partial \ell}{\partial K_{tr,kj}} f^{(k)} + \sum_k \frac{\partial \ell}{\partial K_{tr,jk}} f^{(k)};$
- Back Propagation using Stochastic Gradient Descent with adpated learning rates invented by Geoff.

Combined with Unsupervised Learning

- The Class information is limited. Might overfit.
- The structure in the original data is rich: put a lot of constraints on the weights.
- Maximizing the Kernel Alignment objective + Reconstucting the original data vectors.
- Autoencoder!
- As in [Hinton and Salakhutdinov, 2006] and its following work, make some componets in the code (feature) vector ONLY participate in reconstruction.

The Structure of the autoencoder



Old Results on Handwritten Digit Classification

- Dataset 1: 1100 8s (600 for training, 500 for testing) and 1100 9s (600 for training, 500 for testing)
- Dataset 2: 1100 4s (600 for training, 500 for testing) and 1100 6s (600 for training, 500 for testing)
- Old Results:

Kernels	Gaussian Kernel	NN Ball Surface	NN Sphere	Auto	Auto-RBM
dataset1(1000)	11	9	4	3	3
dataset2(1000)	13	12	7	4	3

The number of errors is out of 1000. Here, in the final 50 iterations of the training, we only minimize the kernel alignment cost.

Extensions to Multi-Class Classification

- Define the optimal kernel as follows:

$$K_{opt}(i,j) = \begin{cases} +1 & \text{if } i \text{ and } j \text{ are in the same class or } i = j \\ -1 & \text{otherwise;} \end{cases} \quad (2)$$

- Still maximize the Kernel Alignment Objective.
- Use one-vs-the-rest SVM k times or use multi-class SVM.
  k: the number of classes.

Outline

Work in progress

- Train the model on MNIST to do multi-class classification (the binary classification task is too easy).
- Learn an Autoencoder with 4 hidden layers using stacked RBM stead of only using RBM to learn the first hidden layer.
- Relax the $Tr(K) = 1$ constraint by using logistic units for the feature vector.

Work in progress

- deal with the dual of SVM directly without minimizing kernel alignment cost
- coordinate optimization: iterate between optimizing the dual parameters and the weights in the neural networks

Optimization in the dual

- $min_w \quad max_\alpha \quad \sum_i \alpha_i - \sum_{ij} \frac{1}{2}\alpha_i\alpha_j f_i^T f_j$
  s.t. $0 \leq \alpha_i \leq C, i, j = 1, \ldots, n.$
- Use log-barrier method to change the constrained optimization to an unconstrained optimization
- annealing the log-barrier coefficient.
- coordinate optimization (current implementation is stochastic gradient-based. Conjugate-Gradient and SMO can be used here.).

The End

Thank you!