Dimensionality Reduction by Minimum Margin Sandwich

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Abstract

The nonlinear dimensionality reduction problem is posed as finding two parallel hyperplanes in a feature space that sandwiches the mapped data points with the minimum possible thickness. The mapping to the feature space is obtained implicitly through a kernel function. The formulation is noise resistant and encourages sparsity in the sense only a few "supporting" data points participate in defining the hyperplane, the cost function leads to a quadratic program optimizing a convex function over an union of convex sets. Two alternative formulations are investigated, one where certain 0,1 "selection" variables select the constraining convex sets. With the selection variables held fixed the problem reduces to a convex Quadratic Program with closed form updates. The selection variables are optimized by mean field annealing and soft-assign. In the alternative formulation the problem is posed as a Quadratically constrained QP. The optimization problem is reduced to a sequence of one class svm problems using Legendre transformation and solving for the saddle point. Simple generalization error bounds on the probability that a future point drawn iid lands outside of the sandwich is also provided using compression bounds.

given a set of points $\mathbf{x}_i \in \mathbf{R}^n$, we seek projections with low reconstruction error, where the error is defined in a minimax sense. We invoke the margin paradigm of Large Margin methods and define the margin for this *unsupervised* learning task to be the normal distance between two hyperplanes parallel to a subspace, such that all the data points are sandwiched between them. We search for a solution where the margin is the least, or in other words search for a supspace such that the maximum projection distance is minimized.

For an arbitrary lower dimensional subspace given by the matrix W formed by the basis vectors $\mathbf{w_i}$ the cost function can be formulated as:

$$\operatorname{Min}_{W} \operatorname{Max}_{i} ||\mathbf{x}_{i} - \hat{\mathbf{x}}_{i}||^{2} \quad s.t. \quad \hat{\mathbf{x}}_{i} = WW^{\dagger} \mathbf{x}_{i} \quad \text{and} \quad$$

$$\sum_{i}^{\kappa} ||\mathbf{w}_{i}|| = 1 \quad \text{or} \quad \left| \left| W^{\dagger} W \right| \right|_{tr} = 1. \quad (1)$$