Outlier Removal for Enhancing Kernel-Based Classifier via the Discriminant Information

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Motivation

- Kernel methods have been successful techniques in pattern recognition for a variety of applications, e.g. speech, image, and medical diagnosis.
- However, kernel based learning has at least quadratic complexity in the number of training samples, which makes their use in large scale applications problematic.





Motivation

- There are two primary approaches for efficient, large-scale kernel based learning:
 - Kernel approximation (e.g. Nyström and Random Fourier features)
 - Data sample selection or outlying data removal.
- In order to be useful for scalable learning, these methods need to be computationally efficient.
- Our work follows the sample selection approach, and we use a filtering method to remove outlying samples.
- Our method requires only linear time to assign scores to all the data samples, even in a kernel induced feature space.



Discriminant Information (DI)

• Given a supervised training dataset $\{\mathbf{X} \in \mathcal{R}^{M \times N}, \mathbf{y} \in \mathcal{R}^N\}$ with N samples and M features, the discriminant information ψ is defined as

$$\psi = \operatorname{trace} \left((\overline{\mathbf{S}} + \rho \mathbf{I})^{-1} \mathbf{S}_B \right)$$

where $\overline{\mathbf{S}}$ and \mathbf{S}_B are the scatter matrix and between-class scatter matrix, respectively.

• We can obtain an equivalent expression for DI via the kernel trick, $\psi = \text{trace}((\overline{\mathbf{K}}^2 + \rho \overline{\mathbf{K}})^{-1} \mathbf{K}_B)$

where $\overline{\mathbf{K}}$ is the centered kernel matrix and \mathbf{K}_B is the kernel between-class scatter matrix.



Discriminant Information (DI)

- DI measures the separability of the data for classification:
 - Equals to zero when the class centers overlap (no separability).
 - Close to L 1, where L is the number of data classes, when the samples are concentrated around their class centers (good separability).
- DI is indicative of a learner's classification ability, as demonstrated in earlier work.

- 1. S. Y. Kung, "Compressive privacy: From information /estimation theory to machine learning [lecture notes]," *IEEE Signal Processing Magazine*, vol. 34, no. 1, pp. 94–112, 2017.
- 2. Thee Chanyaswad, Mert Al, J. Morris Chang, and S. Y. Kung, "Differential mutual information forward search for multikernel discriminantcomponent selection with an application to privacy-preserving classification," in *Machine Learning for Signal Processing (MLSP), 2017 IEEE* 27th International Workshop on. 2017, IEEE.



Outlier Removal Discriminant Information (ORDI)

• Suppose the sample (\mathbf{x}, \mathbf{y}) has been removed from the training dataset. Let $\mathbf{\bar{S}}'$ and \mathbf{S}'_B denote the scatter matrix and between-class scatter matrix obtained from the remaining data. We define the ORDI, $\partial \psi$ of the sample (\mathbf{x}, \mathbf{y}) as

$$\partial \psi = \operatorname{trace}\left((\overline{\mathbf{S}} + \rho \mathbf{I})^{-1}\mathbf{S}_B\right) - \operatorname{trace}\left((\overline{\mathbf{S}}' + \rho \mathbf{I})^{-1}\mathbf{S}'_B\right)$$

• We can similarly define ORDI with kernel matrices as

$$\partial \psi = \operatorname{trace}\left((\overline{\mathbf{K}}^2 + \rho \overline{\mathbf{K}})^{-1} \mathbf{K}_B\right) - \operatorname{trace}\left(\left(\overline{\mathbf{K}'}^2 + \rho \overline{\mathbf{K}'}^2\right)^{-1} \mathbf{K}'_B\right)$$

• ORDI is expected to be small for outliers. Whereas it is expected to be large for samples that are easily separated from other classes.



Outlier Removal Discriminant Information (ORDI)

- Computing ORDI for a single sample can take $O(N^3)$ time and $O(N^2)$ memory.
- Need to find a criterion that is faster to compute, without compromising the predictive performance.



Bounding ORDI

• **Theorem:** Given a supervised training dataset $\{X \in \mathcal{R}^{M \times N}, y \in \mathcal{R}^{N}\}$ and a kernel function $k(x_i, x_j)$, the Outlier Removal Discriminant Information of the sample (x, y) is bounded by

$$\partial \psi(\mathbf{x}, y) = \frac{\beta \kappa_{\mathbf{x}}}{\rho(\kappa_{\mathbf{x}} - \rho)} + \frac{H_{4,1/2}(\delta_{\mathbf{x},y} + \kappa_{\mathbf{x}})}{\rho(N_{y} - 1)} + \frac{\kappa_{\mathbf{x}}(\delta_{\mathbf{x},y} + \kappa_{\mathbf{x}})}{\rho(\kappa_{\mathbf{x}} - \rho)(N_{y} - 1)}$$

where $\beta = \sum_{l=1}^{L} N_l k(\mu_l, \mu_l)$, $\kappa_x = k(\mathbf{x}, \mathbf{x})$, N_l is the number of training samples in class l, μ_l is the mean of the samples in class l, $H_{4,1/2}$ is the generalized harmonic number, and

$$\delta_{\mathbf{x},y} = N_y \left(k^2 (\boldsymbol{\mu}_y, \boldsymbol{\mu}_y) - 4k (\boldsymbol{\mu}_y, \boldsymbol{\mu}_y) k(\mathbf{x}, \boldsymbol{\mu}_y) + 2\kappa_{\mathbf{x}} k(\boldsymbol{\mu}_y, \boldsymbol{\mu}_y) + 2k^2 (\mathbf{x}, \boldsymbol{\mu}_y) \right)^{1/2}.$$

 Computing the upper bound on ORDI over the entire dataset requires only O(N) time!



Experiments (Sample Ratios)



• We compare our filtering method based on the bound on ORDI with two wrapper methods and one filtering method for outlier sample removal.



Experiments (Training Times)





Conclusion

- We proposed a filter approach for outlying data removal and sample selection in supervised learning, which only requires linear time to compute all the sample scores.
 - By removing 20% of the samples, we were able to exceed the performance of the original classifier on our two datasets, which leads to a win-win in terms of predictive performance and computational/memory cost.
 - By removing up to 80% of the samples, we were able to achieve very significant computational savings, by sacrificing relatively little accuracy.



References

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