Compsci 571 HW4

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1 Constructing Kernels

Let K_1 be kernels over $\mathbb{R}^n \times \mathbb{R}^n$, let $a \in \mathbb{R}$, $< a, b >$ denotes the dot product, $a^T b$. .

(a) $K(x,z) = aK_1(x,z)$

This is not a kernel. Because K_1 is a valid kernel, $K_1(x,z) \geq 0$. When $a < 0$, $K(x,z) = aK_1(x,z) \leq 0$. Because inner products $< \cdot, \cdot > \geq 0$, there won't be an inner product such that $K(x,z) =< \Phi(x), \Phi(z) >_{H_k}$.

(b) $K(x,z) =< x,z >^3 + (< x,z > -1)^2$

This is not a valid kernel.

From lecture notes we've proved $< x,z >^3$ can be expressed as inner product in a new vector space, thus a valid kernel.

For $(< x,z > -1)^2$:

$(< x,z > -1)^2 = (x^T z - 1)^2 = (\sum_{i=1}^n x^{(i)} z^{(i)} - 1)(\sum_{j=1}^n x^{(j)} z^{(j)} - 1) = \sum_{i=1}^n \sum_{j=1}^n x^{(i)} x^{(j)} z^{(i)} z^{(j)} - 2\sum_{i=1}^n x^{(i)} z^{(i)} + 1 = \sum_{i=1}^n \sum_{j=1}^n x^{(i)} x^{(j)} z^{(i)} z^{(j)} - \sum_{i=1}^n (\sqrt{2}x^{(i)})(\sqrt{2}z^{(i)}) + 1$

This equation cannot be expressed as an inner product of some $\Phi(x)$ and $\Phi(z)$. So $(< x,z > -1)^2$ is not a valid kernel.

From lecture notes we know that when $k(x,z) = k_1(x,z) + k_2(x,z)$, only if both $k_1(x,z)$ and $k_2(x,z)$ are valid kernels, will $k(x,z)$ be a valid kernel. So in this case $K(x,z)$ is not a kernel.

(c) $K(x,z) =< x,z >^2 + \exp(-\|x\|^2)\exp(-\|z\|^2)$

This is a valid kernel.

From lecture notes we've proved $< x,z >^2$ can be expressed as inner product in a new vector space, thus a valid kernel.

From lecture notes we've proved $k(x,z) = g(x)g(z)$, $g : \mathbb{R}^n \to \mathbb{R}$ is a valid kernel, so $\exp(-\|x\|^2)\exp(-\|z\|^2)$, in the same form, is a valid kernel.

So $K(x,z) =< x,z >^2 + \exp(-\|x\|^2)\exp(-\|z\|^2)$, a sum of two valid kernels, is a valid kernel.

2 Reproducing Kernel Hilbert Spaces

For $\mathscr{F}$ to be the RKHS for kernel $K(x,y) = xy$, it should satisfy:

1. $K(x,y)$ spans $\mathscr{F}$, i.e., $\mathscr{F} = span\{K(\cdot,x), x \in [0,1]\} = \{f : f(\cdot) = \sum_{i=1}^m \alpha_i K(\cdot, x_i),\}$
2. $K(x,y)$ has the reproducing kernel property: $f(x) =< f(\cdot), K(\cdot,x) >_{\mathscr{F}_K}$

If $\mathscr{F}$ satisfies condition 1, for any function $f(x) = ax$ in $\mathscr{F}$, $f(x) = \sum_{i=1}^m \alpha_i K(x,x_i) = \sum_{i=1}^m \alpha_i x x_i = (\sum_{i=1}^m \alpha_i x_i)x$, and this means the real number $a = \sum_{i=1}^m \alpha_i x_i$ for the specific m and α_i.

Under this condition, for any $f(\cdot) = a\cdot = (\sum_{i=1}^m \alpha_i x_i)\cdot$, $< f(\cdot), K(\cdot,x) >_{\mathscr{F}_K} =< \sum_{i=1}^m \alpha_i K(\cdot,x_i), K(\cdot,x) >_{\mathscr{F}_K} = \sum_{i=1}^m \alpha_i K(x,x_i) = \sum_{i=1}^m \alpha_i x x_i = (\sum_{i=1}^m \alpha_i x_i)x = ax = f(x)$. So condition 2 is also satisfied.

So $\mathscr{F}$ is the RKHS for kernel $K(x,y) = xy$. $\square$

3 Convexity and KKT Conditions

(a) The Lagrangian function for the primal form is:

$$\min L(\mathbf{w}, \eta, \eta^*, \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}(\eta_i + \eta_i^*) + \sum_{i=1}^{n} a_i[y_i - \mathbf{w}^T\mathbf{x}_i - \epsilon - \eta_i]$$

$$+\sum_{i=1}^{n} b_i[\mathbf{w}^T\mathbf{x}_i - y_i - \epsilon - \eta_i^*] - \sum_{i=1}^{n} c_i\eta_i - \sum_{i=1}^{n} d_i\eta_i^*$$

It's KKT conditions are:

- Primal feasibility:

$$\begin{gathered} y_i - \mathbf{w}^T\mathbf{x}_i - \epsilon - \eta_i \le 0, i = 1, \ldots, n \\ \mathbf{w}^T\mathbf{x}_i - y_i - \epsilon - \eta_i^* \le 0, i = 1, \ldots, n \\ \eta_i \ge 0, i = 1, \ldots, n \\ \eta_i^* \ge 0, i = 1, \ldots, n \end{gathered}$$

- Dual feasibility:

$$\begin{gathered} a_i \ge 0, i = 1, \ldots, n \\ b_i \ge 0, i = 1, \ldots, n \\ c_i \ge 0, i = 1, \ldots, n \\ d_i \ge 0, i = 1, \ldots, n \end{gathered}$$

- Complementary slackness:

$$\begin{gathered} a_i[y_i - \mathbf{w}^T\mathbf{x}_i - \epsilon - \eta_i] = 0, i = 1, \ldots, n \\ b_i[\mathbf{w}^T\mathbf{x}_i - y_i - \epsilon - \eta_i^*] = 0, i = 1, \ldots, n \\ c_i\eta_i = 0, i = 1, \ldots, n \\ d_i\eta_i^* = 0, i = 1, \ldots, n \end{gathered}$$

- Lagrangian stationary:

$$\begin{gathered} \nabla_{\mathbf{w}L} = \mathbf{w} - \sum_{i=1}^{n}(a_i - b_i)\mathbf{x}_i = 0 \\ (\nabla_{\eta L})_i = C - a_i - c_i = 0, i = 1, \ldots, n \\ (\nabla_{\eta^* L})_i = C - b_i - d_i = 0, i = 1, \ldots, n \end{gathered}$$

With these conditions, we can transform Lagrangian function into dual form:

$$\max L(\mathbf{a}, \mathbf{b}) = \sum_{i=1}^{n}(a_i - b_i)y_i - \epsilon\sum_{i=1}^{n}(a_i + b_i) - \frac{1}{2}\sum_{i,j=1}^{n}(a_i - b_i)(a_j - b_j)\mathbf{x}_i^T\mathbf{x}_j$$

subject to

$$0 \le a_i, b_i \le C, i = 1, \ldots, n$$

(b) Support vectors are the points i such that $|y_i - \mathbf{w}^T\mathbf{x}_i| \ge \epsilon$.

(c) Increasing ϵ makes the model less likely to overfit. Because the model penalizes the points that have training error larger than ϵ. If ϵ increases, the allowed/unpenalized training error increases, and the model tends to overfit less.

(d) Increasing C makes the model more likely to overfit. C is the penalty for each point that has training error larger than ϵ. If the penalty increases, the model will try to make points have smaller training error, and thus overfits.

(e) Assume we've computed the optimal dual variables as $\mathbf{a}^*$ and $\mathbf{b}^*$.

From one of the KKT conditions, we can get the optimal primal variable is $\mathbf{w}^* = \sum_{i=1}^n (a_i^* - b_i^*)\mathbf{x}_i$.

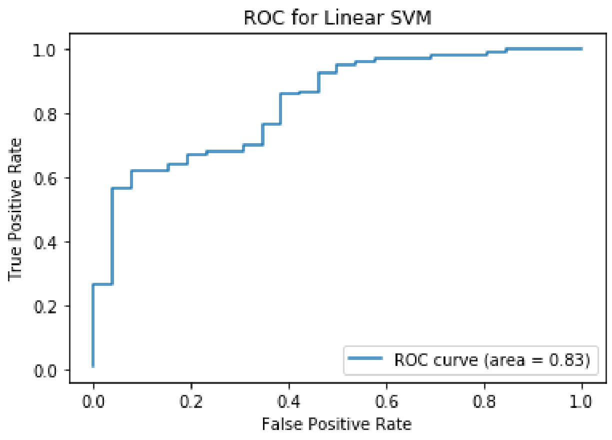
So for a new point $\mathbf{x}^{new}$, its evaluation is $f(\mathbf{x}^{new}) = \sum_{j=1}^p w_j^* x_j^{new} = \sum_{j=1}^p \sum_{i=1}^n (a_i^* - b_i^*) x_{ij} x_j^{new} = \sum_{i=1}^n (a_i^* - b_i^*)\mathbf{x}_i \cdot \mathbf{x}^{new}$.

4 SVM Implementation

(a) See `svm_classifier.py`. You could run it by typing command `python3 svm_classifier.py` in the terminal, and see a simple demo with separable data and linear kernel.

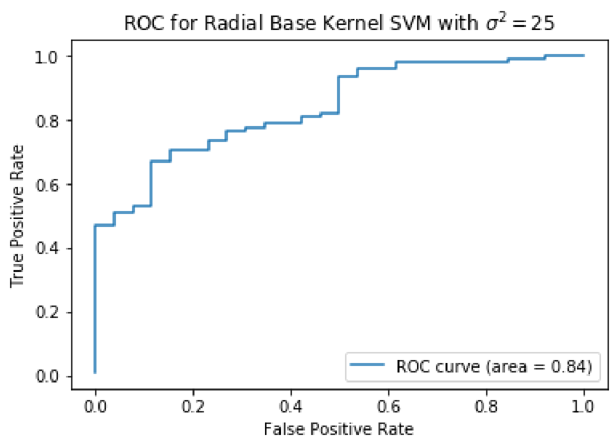
(b) **Note: for questions (b) and (c), I use `sklearn.mode_selection.train_test_split` to split the training and testing set with 2018 as the random seed. And if I use `numpy` with 2018 as the random seed to generate indices for training and testing data and then split, the split is different.** Code for these 2 questions are in `q4.ipynb`.

The accuracy of the classifier on testing data is 0.8636363636363636. The ROC curve is like following:



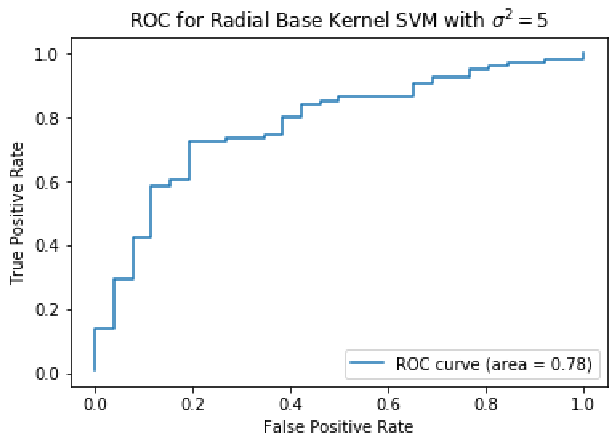
The AUC on testing data is 0.8316400580551523.

(c) For $\sigma^2 = 25$, the accuracy of the classifier on testing data is 0.8484848484848485. The ROC curve is like:



The AUC on testing data is 0.8388969521044993.

For $\sigma^2 = 5$, the accuracy for the classifier on testing data is 0.7954545454545454. The ROC curve is like:



The AUC on testing data is 0.7790275761973875.

The comparison between 2 σ^2 values suggests that for Gaussian kernel if we set σ^2 too small we may overfit.