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1 Clustering

1.1 CS 335 KMeans Implementation

2 Kernel design and Kernelized clustering

2.1 CS 337: Proving Kernel Validity

We are going to use the following property of kernels from Lecture slides (Lecture 11):

$$K(x,y) = \sum_{d=1}^{r} \alpha_d(x^T y)^d$$
 where $\alpha_d \ge 0$ is a kernel $(r \text{ can be } \infty)$

Another property of kernels which we are going to use is:

$$K(x,y)$$
 is a kernel $\implies K'(x,y) = f(x)f(y)K(x,y)$ is also a kernel Corresponding feature map, $\phi'(x) := f(x)\phi(x)$

An important property of exponential function which we are going to exploit is:

$$\exp(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

Using the above properties, we can conclude that $\exp(\alpha x^T y)$ where $\alpha \geq 0$ is a kernel.

Now, if take
$$\alpha = \frac{1}{\sigma^2}$$
 and $f(x) = \exp\left(-\frac{x^T x}{2\sigma^2}\right)$, we get:
$$K_{\alpha}(x,y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right) = \exp\left(-\frac{x^T x}{2\sigma^2}\right) \exp\left(-\frac{y^T y}{2\sigma^2}\right) \exp\left(\frac{x^T y}{\sigma^2}\right)$$
 is a kernel. Hence, proved.

2.2 CS 337: Simple Kernel Design

(i)

We proved in Lecture slides (Lecture 13, Part 2) that the vanilla KMeans algorithm would converge in finite number of iterations (say, N).

Without loss of generality, let $r_1 \geq r_2$.

For the sake of contradiction, let's assume that after N iterations we get μ_1, μ_2 which can correctly classify the clusters. Obviously, $\mu_1 \neq \mu_2$.

So, blue points have $Pr_1 = 1$ and $Pr_2 = 0$ while red points have $Pr_1 = 0$ and $Pr_2 = 1$.

As the algorithm has converged, the Prs for all points and μs won't change any further.

The decision boundary would be
$$f(x) = \left(x - \frac{\mu_1 + \mu_2}{2}\right) \cdot (\mu_2 - \mu_1) = \left(x \cdot (\mu_2 - \mu_1)\right) - \frac{||\mu_1 - \mu_2||^2}{2}$$
.

This decision boundary is linear in x, therefore, due to radial symmetry some of blue and red points would be on same side.

However, we know that $Pr_1 = 0$ for red points and $Pr_1 = 1$ for blue points. So in $(N+1)^{th}$ iteration, the values of Pr_1 would change for some points.

This leads to contradiction.

Thus, even after convergence, the vanilla KMeans algorithms won't be able to correctly classify the clusters for any value of r_1 and r_2 .

(ii)

We see that the two clusters differ in distance from origin.

We propose $\phi(x) = ||x||_2$. Thus, $K(x, x') = ||x||_2 ||x'||_2$.

$$\int_{x} \int_{x'} K(x, x') g(x) g(x') dx dx' = \left(\int_{x} ||x||_{2} g(x) dx \right) \left(\int_{x'} ||x'||_{2} g(x') dx' \right) = \left(\int_{x} ||x||_{2} g(x) dx \right)^{2} \ge 0$$

Therefore, chosen kernel function is a valid kernel.