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Advanced Deep Learning and Kernel Methods

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Preface

- Kernel Methods
- Neural Tangent Kernel and Neural Networks
- Biologically inspired ANNs for Visual Cortex
- Geometric Deep Learning
- Adversarial Attacks and ANNs Implicit Bias

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Kernel Methods

1.1 Math of Kernels

1.2 Blackboard 30/09/2025

$$\alpha^* = \arg \min_{\alpha \in \mathcal{R}^n} \|y - K\alpha\|_2^2 + \lambda \alpha^T K \alpha \quad [K]_{ij} = K(x_i, x_j)$$

then:

$$\frac{\partial}{\partial \alpha} \|y - K\alpha\|_2^2 = \frac{\partial}{\partial \alpha_i} \alpha^T K \alpha \quad (1.1)$$

$$= \sum_q K_{iq} \alpha_q + \sum_{pq} \alpha_p K_{pi} \quad (1.2)$$

$$= [K\alpha]_i + [K^T]_{ip} \alpha_p \quad (1.3)$$

$$= 2[K\alpha]_i \quad (1.4)$$

$$= \frac{\partial}{\partial \alpha} (y - K\alpha)^T (y - K\alpha) \quad (1.5)$$

$$= \frac{\partial}{\partial \alpha} \left(\underbrace{-\alpha^T K^T y - y^T K \alpha}_{-2\alpha^T K^T y} + \alpha^T K^T K \alpha \right) \quad (1.6)$$

$$= 2K^T (K\alpha - y) \quad (1.7)$$

so now

$$\frac{\partial}{\partial \alpha} = \frac{K}{n} (K\alpha - y) + \lambda K \alpha = 0 \quad (1.8)$$

$$= \frac{K}{n} (K\alpha - y + n\lambda \alpha) = 0 \quad (1.9)$$

and finally

$$\alpha = (k + n\lambda I)^{-1} y \quad (1.10)$$

1.2.1 Kernel PCA demonstration

suppose to have

$$\{x_i\}_{i=1}^n \quad x_i \in \mathcal{R}^d$$

and we want to find a projection on a lower dimensional space \mathcal{R}^k with $k < d$. We calculate the covariance matrix:

$$C = \frac{1}{n} \sum_{i=1}^n x_i x_i^T = \frac{1}{n} X X^T \quad X = [x_1, \dots, x_n]$$

and we want to find the eigenvalues and eigenvectors of C :

$$Cv_i = \lambda_i v_i$$

the usual trick is to create a map $\phi : \mathcal{R}^d \rightarrow \mathcal{H}$ and then compute the covariance matrix in \mathcal{H} :

$$C_\phi = \frac{1}{n} \sum_{i=1}^n \phi(x_i) \phi(x_i)^T$$

we want to solve the eigenvalue problem:

$$C_\phi v_i = \lambda_i v_i$$

so let's now prove that v can be expressed as a linear combination of the $\phi(x_i)$:

$$C_\phi v_i = \lambda_i v_i \quad (1.11)$$

$$\frac{1}{n} \sum_{i=1}^n \phi(x_i) \phi(x_i)^T v_i = \lambda_i v_i \quad (1.12)$$

$$\frac{1}{n} \sum_{i=1}^n \phi(x_i) \underbrace{\langle \phi(x_i), v_i \rangle}_{\alpha_i} = \lambda_i v_i \quad (1.13)$$

$$v_i = \frac{1}{n\lambda_i} \sum_{i=1}^n \alpha_i \phi(x_i) \quad (1.14)$$

we can now substitute this expression in the eigenvalue problem:

$$C_\phi v_i = \lambda_i v_i \quad (1.15)$$

$$\frac{1}{n} \sum_{j=1}^n \phi(x_j) \phi(x_j)^T \left(\frac{1}{n\lambda_i} \sum_{k=1}^n \alpha_k \phi(x_k) \right) = \lambda_i \left(\frac{1}{n\lambda_i} \sum_{k=1}^n \alpha_k \phi(x_k) \right) \quad (1.16)$$

$$\frac{1}{n^2\lambda_i} \sum_{j=1}^n \sum_{k=1}^n \alpha_k \phi(x_j) \underbrace{\langle \phi(x_j), \phi(x_k) \rangle}_{K_{jk}} = \frac{1}{n} \sum_{k=1}^n \alpha_k \phi(x_k) \quad (1.17)$$

we can now multiply both sides by $\phi(x_i)$ and use the kernel trick:

$$\frac{1}{n^2\lambda_i} \sum_{j=1}^n \sum_{k=1}^n \alpha_k K_{ij} K_{jk} = \frac{1}{n} \sum_{k=1}^n \alpha_k K_{ik} \quad (1.18)$$

$$\frac{1}{n\lambda_i} \sum_{j=1}^n K_{ij} \underbrace{\left(\frac{1}{n} \sum_{k=1}^n K_{jk} \alpha_k \right)}_{(K\alpha)_j} = (K\alpha)_i \quad (1.19)$$

$$\frac{1}{n\lambda_i} (K^2 \alpha)_i = (K\alpha)_i \quad (1.20)$$

so we have to solve the eigenvalue problem:

$$K\alpha_i = n\lambda_i \alpha_i$$

and then we can find the projection of a new point x as:

$$\langle v_i, \phi(x) \rangle = \left\langle \frac{1}{n\lambda_i} \sum_{j=1}^n \alpha_j \phi(x_j), \phi(x) \right\rangle \quad (1.21)$$

$$= \frac{1}{n\lambda_i} \sum_{j=1}^n \alpha_j \underbrace{\langle \phi(x_j), \phi(x) \rangle}_{K(x_j, x)} \quad (1.22)$$

$$= \frac{1}{n\lambda_i} \sum_{j=1}^n \alpha_j K(x_j, x) \quad (1.23)$$

Bibliography

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