Lecture 15: Dimensionality Reduction – Kernel PCA – extra slides

Textbook: Chapter 5

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Procedure

- PCA analysis: calculate covariance matrix

$$\Sigma = \frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{x}^{(i)}\right)\left(\mathbf{x}^{(i)}\right)^{T}$$

- In the $\mathcal{Z}$ space

$$\Sigma = \frac{1}{n}\sum_{i=1}^{n}\phi\left(\mathbf{x}^{(i)}\right)\phi\left(\mathbf{x}^{(i)}\right)^{T}$$

- Then, we need to obtain the eigen vector of Σ.

Procedure

- The eigenvectors of Σ can be expressed as linear combination of features

$$v = \sum_{i=1}^{n} \alpha_i \phi\left(x^{(i)}\right)$$

Procedure discussions

- λ and $\mathbf{v}$ are the eigenvalues and eigenvectors of the covariance matrix Σ respectively.
- α_i is a scalar.

$$\alpha_i = \frac{1}{n\lambda} \phi\left(\mathbf{x}^{(i)}\right)^T \mathbf{v}$$

- α_i is obtained by extracting the eigenvectors of the kernel (similarity) matrix **K**.

$$\mathbf{K}\alpha = n\lambda\alpha$$

- This is computationally very expensive.
- This is where we use the **kernel trick**. Using the kernel trick, we can compute the similarity between two high-dimension feature vectors in the original feature space.

Projecting new data points

- Training and testing data: when we apply PCA on the training data, we used the learned matrix **W** to transform the testing data.
- For Kernel PCA: eigenvector α are the samples that are already projected onto the PC components **v**.
- For new **x**′, we need to project it to the PC, $\phi(\mathbf{x}')^T\mathbf{v}$.

Projecting new data points

- However, we do not know ϕ explicitly, how can we do this calculation? We can use the kernel trick.
- Because $\mathbf{v}^j = \sum_{i=1}^{n} \alpha_i^{(j)} \phi\left(\mathbf{x}^{(i)}\right)$ where $\lambda_j \alpha^{(j)} = \mathbf{K}\alpha^{(j)}$. I.e., λ_j and $\alpha^{(j)} = (\alpha_1^{(j)}, \alpha_2^{(j)}, \dots, \alpha_n^{(j)})$) are the eigenvalues and eigenvectors of **K.**

$$\phi(\mathbf{x}')^T \mathbf{v}^j = \sum_{i=1}^{n} \alpha_i^{(j)} \phi(\mathbf{x}')^T \phi\left(\mathbf{x}^{(i)}\right) = \sum_{i=1}^{n} \alpha_i^{(j)} \cdot \kappa\left(\mathbf{x}', \mathbf{x}^{(i)}\right)$$