Machine Learning Homework 2[*]

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1 PCA algorithm

1.1 Eigenvalue Decomposition

The original PCA adopts eigenvalue decomposition as a solution to find principal components.

Algorithm 1: PCA based on Eigenvalue Decomposition

```
Input  : Dataset $\mathbf{X} = \{\mathbf{x_1}, \cdots, \mathbf{x}_N\}$ where $\mathbf{x_i} \in \mathbb{N}^d$
Output : The first principal component $\mathbf{w}$
Normalize $\mathbf{X}$ to make sure the mean is $\mathbf{0}$
Calculate the covariance matrix of $\mathbf{X}$ as
    $\mathbf{\Sigma} = \mathbf{X}\mathbf{X}^T$
Calculate the eigenvalues and eigenvectors of $\mathbf{\Sigma}$
Choose the maximum eigenvalue $\lambda_1$ and the corresponding eigenvector $\mathbf{x}_1$
Calculate the first principal component
    $\mathbf{w} = \mathbf{x}_1^T\mathbf{X}$
return $\mathbf{w}$
```

Advantages

- Quite easy to understand and easy to implement

Disadvantages

- When $\mathbf{X}$ is of high dimension, the computation of $\mathbf{X}\mathbf{X}^T$ is expensive
- The eigenvalue decomposition is not so efficient and computation expensive in high dimensions
- It's hard to interpret the meaning of principal components found by the algorithm

1.2 Singular Value Decomposition

SVD is another approach of matrix decomposition. It can be also used to find principal components. The SVD is like

$$X_{m\times n} = U_{m\times m}\Sigma_{m\times n}V_{n\times n}^T \tag{1}$$

where U and V are orthogonal matrices and Σ contains singular values on it's diagonal. If $\mathbf{X}$ is our dataset, then $\mathbf{U}$ is actually made up of eigenvectors of $\mathbf{X}\mathbf{X}^T$, the covariance matrix.

[*] GitHub repo: https://github.com/DeanAlkene/CS420-MachineLearning/tree/master/A2

Algorithm 2: PCA based on Singular Value Decomposition

```
Input   :Dataset $\mathbf{X} = \{\mathbf{x_1}, \cdots, \mathbf{x}_N\}$ where $\mathbf{x_i} \in \mathbb{N}^d$
Output :The first principal component $\mathbf{w}$
Normalize $\mathbf{X}$ to make sure the mean is $\mathbf{0}$
Apply SVD on $\mathbf{X}$ as
    $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$
Multiply $\mathbf{U}^T$ on the both side and denote it as $\mathbf{X}'$
    $\mathbf{U}^T\mathbf{X} = \mathbf{\Sigma}\mathbf{V}^T = \mathbf{X}'$
Let the first row of $\mathbf{X}'$ be $\mathbf{w}$
return $\mathbf{w}$
```

Advantages

- There is iterative methods to solve SVD and we don't need to calculate $\mathbf{X}\mathbf{X}^T$ it will be more efficient than doing eigenvalue decomposition
- SVD can reduce dimension in both row and column directions, while eigenvalue decomposition cannot
- SVD can solve non-square matrices while eigenvalue decomposition cannot

Disadvantages

- The sparsity of data might be lost
- It's also hard to interpret the meaning of decomposed matrices found by the algorithm

2 Factor Analysis (FA)

By Bayesian formula, we know that

$$p(\mathbf{y}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{y})p(\mathbf{y})}{p(\mathbf{x})} \tag{2}$$

Here,

$$p(\mathbf{x}) = p(\mathbf{A}\mathbf{y} + \mu + \mathbf{e}) \tag{3}$$

and

$$p(\mathbf{x}|\mathbf{y}) = G(\mathbf{x}|\mathbf{A}\mathbf{y} + \mu, \Sigma_e), p(\mathbf{y}) = G(\mathbf{y}|0, \Sigma_y) \tag{4}$$

generally

$$p(\mathbf{e}) = G(\mathbf{e}|\mu_e, \Sigma_e) \tag{5}$$

Here, $\mathbf{A}\mathbf{y} + \mu$ is an affine transformation of $\mathbf{y}$, thus

$$p(\mathbf{x}) = G(\mathbf{A}\mathbf{y} + \mu|\mu, \mathbf{A}\Sigma_y\mathbf{A}^T) + G(\mathbf{e}|\mu_e, \Sigma_e) = G(\mathbf{x}|\mu + \mu_e, \mathbf{A}\Sigma_y\mathbf{A}^T + \Sigma_e) \tag{6}$$

Then,

$$p(\mathbf{y}|\mathbf{x}) = \frac{G(\mathbf{x}|\mathbf{A}\mathbf{y} + \mu, \Sigma_e)G(\mathbf{y}|0, \Sigma_y)}{G(\mathbf{x}|\mu + \mu_e, \mathbf{A}\Sigma_y\mathbf{A}^T + \Sigma_e)} \tag{7}$$

The density function of Gaussian distribution is

$$G(\mathbf{x}|\mu, \mathbf{\Sigma}) = \frac{1}{\sqrt{(2\pi)^k|\mathbf{\Sigma}|}} \exp(-\frac{1}{2}(\mathbf{x} - \mu)^T\mathbf{\Sigma}^{-1}(\mathbf{x} - \mu)) \tag{8}$$

k is the dimension of $\mathbf{x}$. Then we consider the exponential terms of $p(\mathbf{y}|\mathbf{x})$ which is

$$-\frac{1}{2}(\mathbf{x} - \mathbf{A}\mathbf{y} - \mu)^T\Sigma_e^{-1}(\mathbf{x} - \mathbf{A}\mathbf{y} - \mu) - \frac{1}{2}\mathbf{y}^T\Sigma_y^{-1}\mathbf{y} + \frac{1}{2}(\mathbf{x} - \mu + \mu_e)^T(\mathbf{A}\Sigma_y\mathbf{A}^T + \Sigma_e)^{-1}(\mathbf{x} - \mu + \mu_e) \tag{9}$$

We only consider terms containing $\mathbf{y}$, that is

$$\begin{aligned}&-\frac{1}{2}[-\mathbf{x}^T\Sigma_e^{-1}\mathbf{A}\mathbf{y}-\mathbf{y}^T\mathbf{A}^T\Sigma_e^{-1}(\mathbf{x}-\mathbf{A}\mathbf{y}-\mu)+\mu^T\Sigma_e^{-1}\mathbf{A}\mathbf{y}+\mathbf{y}^T\Sigma_y^{-1}\mathbf{y}]\\&=-\frac{1}{2}[(\mu-\mathbf{x})^T\Sigma_e^{-1}\mathbf{A}\mathbf{y}+\mathbf{y}^T\mathbf{A}^T\Sigma_e^{-1}(\mu-\mathbf{x})+\mathbf{y}^T(\mathbf{A}^T\Sigma_e^{-1}\mathbf{A}+\Sigma_y^{-1})\mathbf{y}]\end{aligned}\tag{10}$$

We know that

$$\begin{aligned}&(\mathbf{y}-\mu)^T\mathbf{\Sigma}^{-1}(\mathbf{y}-\mu)\\&=\mathbf{y}^T\Sigma^{-1}\mathbf{y}-\mathbf{y}^T\Sigma^{-1}\mu-\mu^T\Sigma^{-1}\mathbf{y}+\mu^T\Sigma^{-1}\mu\end{aligned}\tag{11}$$

Compare 10 and 11 we get,

$$\Sigma_{\mathbf{y}|\mathbf{x}}=(\mathbf{A}^T\Sigma_e^{-1}\mathbf{A}+\Sigma_y^{-1})^{-1}\tag{12}$$

and

$$\Sigma_{\mathbf{y}|\mathbf{x}}^{-1}\mu_{\mathbf{y}|\mathbf{x}}=\mathbf{A}^T\Sigma_e^{-1}(\mathbf{x}-\mu)\tag{13}$$

Hence

$$p(\mathbf{y}|\mathbf{x})=G(\mathbf{y}|(\mathbf{A}^T\Sigma_e^{-1}\mathbf{A}+\Sigma_y^{-1})^{-1}\mathbf{A}^T\Sigma_e^{-1}(\mathbf{x}-\mu),(\mathbf{A}^T\Sigma_e^{-1}\mathbf{A}+\Sigma_y^{-1})^{-1})\tag{14}$$

3 Independent Component Analysis (ICA)

In ICA, we have a linear combination of source vectors $\mathbf{x}=\mathbf{A}\mathbf{s}$ where $\mathbf{s}$ are independent sources. The goal is to find a transformation $\mathbf{W}$ to seperate each sources into $\mathbf{y}$ and make each entry in $\mathbf{y}$ as independent as possible.

The Central Limit Theorem tells us that a sum of independent random variables from arbitrary distributions tends towards a Gaussian distribution, under certain conditions. Let's consider ICA as

$$\mathbf{y}=\mathbf{w}^T\mathbf{x}=\mathbf{w}^T\mathbf{A}\mathbf{s}=(\mathbf{w}^T\mathbf{A})\mathbf{s}=\mathbf{z}^T\mathbf{s}\tag{15}$$

Now, $\mathbf{y}$ is a liner combination of random variables $\mathbf{s}$. According to the Central Limit Theorem, $\mathbf{y}$ should be closer to Gaussian than any s_i in $\mathbf{s}$. However, to pursue independence among each entry of $\mathbf{y}$, we ought to minimize affects of being closer to Gaussian brought by $\mathbf{z}^T$. It is equally to say, we should take $\mathbf{w}$ that maximizes the non-Gaussianity, which is a principal for ICA estimation.

In another perspective, let's prove that in ICA at most one Gaussian variable is allowed. Let's consider $\mathbf{x}=\mathbf{A}\mathbf{s}$ where $\mathbf{s}=s_1,s_2$. Without lossing of generality, let $\mathbf{s}\sim\mathcal{N}(0,I)$. Then,

$$\mathbf{x}\sim\mathcal{N}(0,\mathbf{A}\mathbf{A}^T)\tag{16}$$

Here is an orthogonal transformation matrix $\mathbf{R}$. Apply it on $\mathbf{A}$ as $\mathbf{A}'=\mathbf{A}\mathbf{R}$, we have

$$\mathbf{x}'=\mathbf{A}\mathbf{R}\mathbf{s}\sim\mathcal{N}(0,\mathbf{A}\mathbf{R}\mathbf{R}^T\mathbf{A}^T)=\mathcal{N}(0,\mathbf{A}\mathbf{A}^T)\tag{17}$$

Thus, due to the symetric property of multivariable Gaussian, we cannot tell the source $\mathbf{s}$ from the observation $\mathbf{x}$ because there're infinite much $\mathbf{s}$. In this way, we also proved that, to implement ICA we should stay away from Gaussian.

4 Dimension Reduction by FA

5 Spectral clustering

Table 1: Experiment on sample size N

N	n	m	μ	σ^2	m^*_{AIC}	m^*_{BIC}	$J_{AIC}(m^*_{AIC})$	$J_{BIC}(m^*_{BIC})$
50	10	3	0	0.1	6	4	-493.601677	-588.246816
100					6	5	-982.810455	-1111.766380
200					5	5	-1661.446367	-1824.713076
500					5	4	-4379.957981	-4588.581082
1000					6	4	-8168.984016	-8411.917903
2000					6	4	-15455.789912	-15733.034584
5000					5	4	-42272.641493	-42595.242556

Table 2: Experiment on dimension n

N	n	m	μ	σ^2	m^*_{AIC}	m^*_{BIC}	$J_{AIC}(m^*_{AIC})$	$J_{BIC}(m^*_{BIC})$
500	2	3	0	0.1	1	1	-1396.354846	-1604.977946
	3				1	1	-1718.675231	-1927.298332
	5				3	3	-2621.684229	-2830.307329
	8				5	3	-3638.028832	-3846.651933
	10				5	4	-4655.394542	-4864.017643
	15				10	8	-5445.357437	-5653.980538
	20				13	10	-6640.627083	-6849.250184
	50				40	40	-11009.236851	-11217.859952
	100				90	90	-14643.727527	-14852.350627

Table 3: Experiment on dimension m

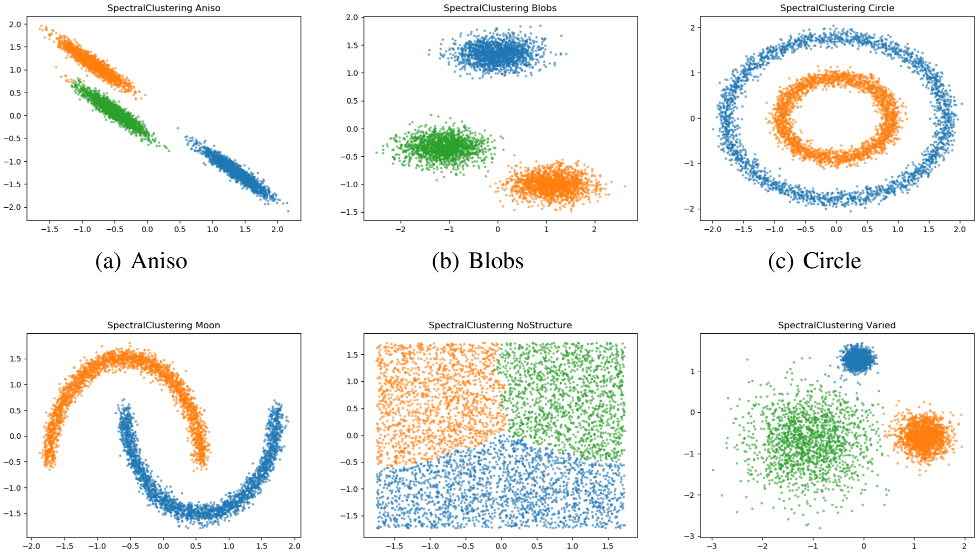
N	n	m	μ	σ^2	m^*_{AIC}	m^*_{BIC}	$J_{AIC}(m^*_{AIC})$	$J_{BIC}(m^*_{BIC})$
500	10	1	0	0.1	5	3	-2714.345491	-2922.968592
		2			6	4	-3221.695130	-3430.318231
		3			6	4	-4504.367828	-4712.990928
		5			6	5	-5266.175263	-5474.798364
		8			7	7	-6538.478659	-6747.101760
		10			7	7	-7201.846576	-7410.469677
		15			8	7	-8157.844961	-8366.468062
		20			7	7	-8959.720000	-9168.343101
		50			6	6	-11266.871473	-11475.494574

Table 4: Experiment on dimension μ

N	n	m	μ	σ^2	m^*_{AIC}	m^*_{BIC}	$J_{AIC}(m^*_{AIC})$	$J_{BIC}(m^*_{BIC})$
500	10	3	-2.0	0.1	5	4	-4495.860128	-4704.483228
			-1.0		6	5	-4469.707856	-4678.330957
			-0.8		5	4	-4264.262261	-4472.885361
			-0.5		5	4	-4042.243784	-4250.866885
			-0.2		5	3	-4303.592699	-4512.215800
			0		6	4	-4310.182025	-4518.805126
			0.2		6	3	-4213.409350	-4422.032451
			0.5		6	4	-4315.162901	-4523.786002
			0.8		6	4	-4003.357713	-4211.980814
			1.0		5	4	-4129.851244	-4338.474345
			2.0		5	4	-4769.434959	-4978.058060

Table 5: Experiment on dimension σ^2

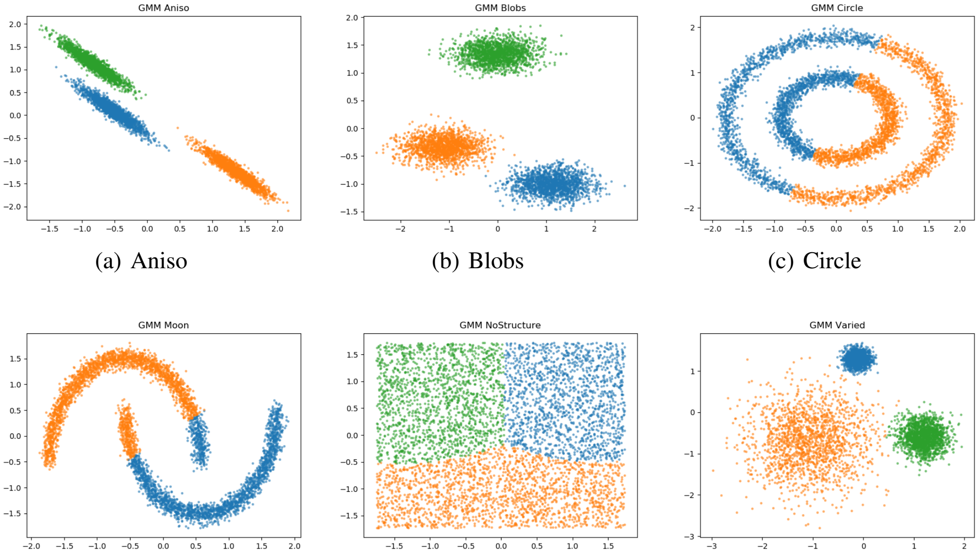
N	n	m	μ	σ^2	m^*_{AIC}	m^*_{BIC}	$J_{AIC}(m^*_{AIC})$	$J_{BIC}(m^*_{BIC})$
500	10	3	0	0.0001	5	3	-3322.894166	-3531.517267
				0.001	6	4	-2728.148545	-2936.771645
				0.01	5	4	-2287.788435	-2496.411536
				0.1	5	4	-4312.271311	-4520.894412
				1.0	6	4	-8103.451885	-8312.074986
				10.0	8	2	-13098.779997	-13307.403098
				100.0	4	4	-18672.091688	-18880.714789
				1000.0	8	3	-24448.748153	-24657.371254



(a) Aniso (b) Blobs (c) Circle

(d) Moon (e) No Structure (f) Varied

Figure 1: Spectral Clustering on Different Datasets



(a) Aniso (b) Blobs (c) Circle

(d) Moon (e) No Structure (f) Varied

Figure 2: GMM Clustering on Different Datasets