Fundamentals of Machine Learning

PRINCIPAL COMPONENT ANALYSIS

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Acknowledgments: Adapted from slides at https://probml.github.io/pml-book/teaching1.html by Prof. Saw Shier Nee

Outline

- EigenValue Decomposition
- Singular Value Decomposition
- Principal Components Analysis

Eigenvalue Decomposition

Given a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{R}$ is an **eigenvalue** of $\mathbf{A}$ and $u \in \mathbb{R}^n$ is the corresponding **eigenvector** if

$$\mathbf{A}u = \lambda u, \quad u \neq 0 \ .$$

$$(\lambda \mathbf{I} - \mathbf{A})u = \mathbf{0}, \quad u \neq 0$$

Characteristic Equation $\quad \det(\lambda \mathbf{I} - \mathbf{A}) = 0$

- The trace of a matrix is equal to the sum of its eigenvalues,

$$\mathrm{tr}(\mathbf{A}) = \sum_{i=1}^{n} \lambda_i \ .$$

- The determinant of $\mathbf{A}$ is equal to the product of its eigenvalues,

$$\det(\mathbf{A}) = \prod_{i=1}^{n} \lambda_i \ .$$

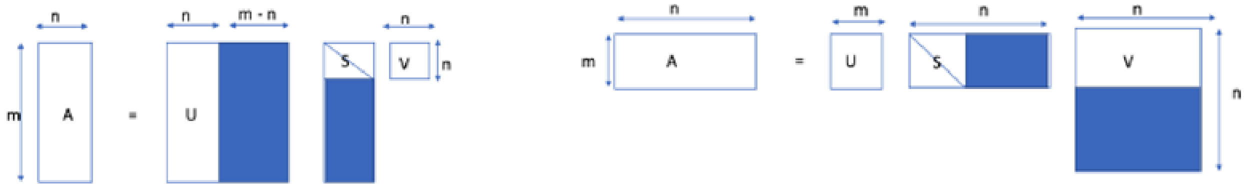
- The rank of $\mathbf{A}$ is equal to the number of non-zero eigenvalues of $\mathbf{A}$.

Singular Value Decomposition

Any (real) $m \times n$ matrix $\mathbf{A}$ can be decomposed as

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T} = \sigma_1 \begin{pmatrix} | \\ u_1 \\ | \end{pmatrix} \begin{pmatrix} - & v_1^\mathsf{T} & - \end{pmatrix} + \cdots + \sigma_r \begin{pmatrix} | \\ u_r \\ | \end{pmatrix} \begin{pmatrix} - & v_r^\mathsf{T} & - \end{pmatrix}$$

where $\mathbf{U}$ is an $m \times m$ whose columns are orthornormal (so $\mathbf{U}^\mathsf{T}\mathbf{U} = \mathbf{I}_m$), $\mathbf{V}$ is $n \times n$ matrix whose rows and columns are orthonormal (so $\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{V}\mathbf{V}^\mathsf{T} = \mathbf{I}_n$), and $\mathbf{S}$ is a $m \times n$ matrix containing the $r = \min(m, n)$ **singular values** $\sigma_i \geq 0$ on the main diagonal, with 0s filling the rest of the matrix.



Relationship between EVD and SVD

If $\mathbf{A}$ is real, symmetric and positive definite, then the singular values are equal to the eigenvalues, and the left and right singular vectors are equal to the eigenvectors (up to a sign change):

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T} = \mathbf{U}\mathbf{S}\mathbf{U}^\mathsf{T} = \mathbf{U}\mathbf{S}\mathbf{U}^{-1}$$

For an arbitrary real matrix **A**

$$\mathbf{A}^\mathsf{T}\mathbf{A} = \mathbf{V}\mathbf{S}^\mathsf{T}\mathbf{U}^\mathsf{T}\,\mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T} = \mathbf{V}(\mathbf{S}^\mathsf{T}\mathbf{S})\mathbf{V}^\mathsf{T}$$

Hence

$$(\mathbf{A}^\mathsf{T}\mathbf{A})\mathbf{V} = \mathbf{V}\mathbf{D}_n$$

eigenvectors of $\mathbf{A}^\mathsf{T}\mathbf{A}$ are equal to $\mathbf{V}$

eigenvalues $\mathbf{A}^\mathsf{T}\mathbf{A}$ are equal to $\mathbf{D}_n = \mathbf{S}^\mathsf{T}\mathbf{S}$

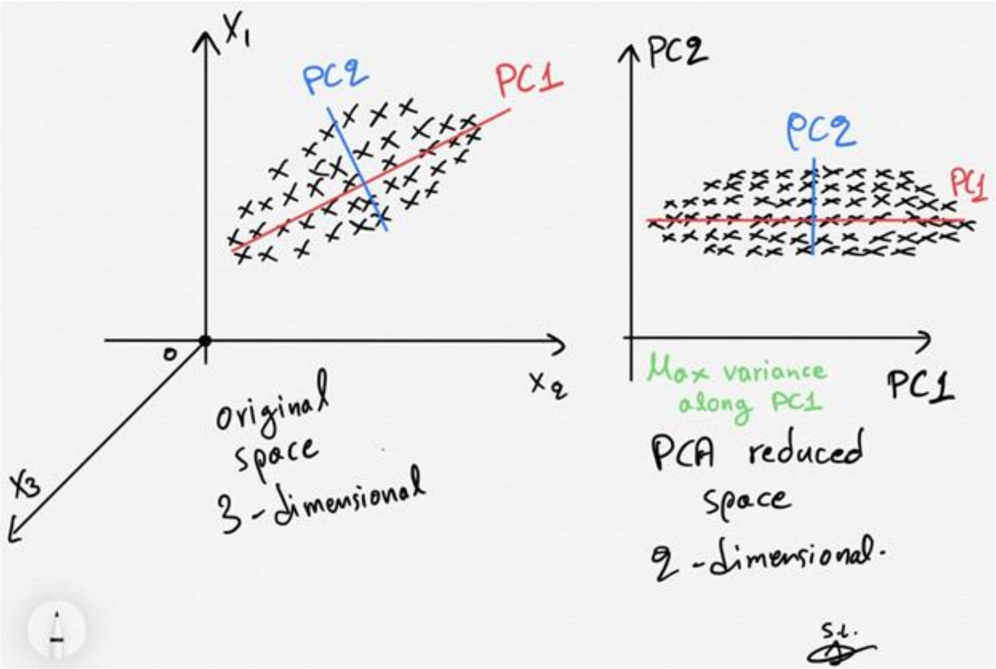
$$\mathbf{A}\mathbf{A}^\mathsf{T} = \mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T}\,\mathbf{V}\mathbf{S}^\mathsf{T}\mathbf{U}^\mathsf{T} = \mathbf{U}(\mathbf{S}\mathbf{S}^\mathsf{T})\mathbf{U}^\mathsf{T}$$

$$(\mathbf{A}\mathbf{A}^\mathsf{T})\mathbf{U} = \mathbf{U}\mathbf{D}_m$$

eigenvectors of $\mathbf{A}\mathbf{A}^\mathsf{T}$ are equal to $\mathbf{U}$

eigenvalues $\mathbf{A}\mathbf{A}^\mathsf{T}$ are equal to $\mathbf{D}_m = \mathbf{S}\mathbf{S}^\mathsf{T}$

Principal Component Analysis (PCA)

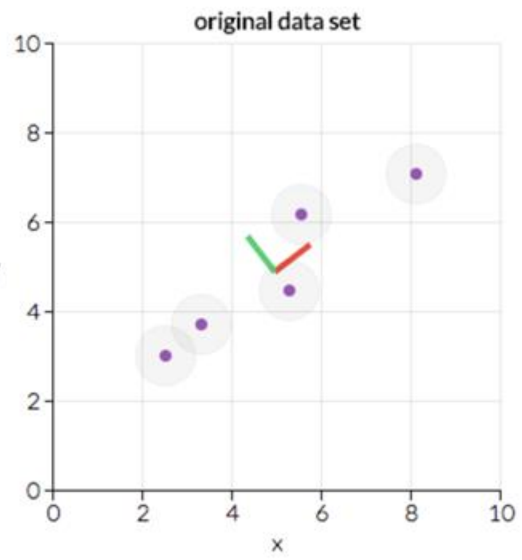


- Reduce dimension
- PC component describe the largest data variance

Image from https://towardsdatascience.com/pca-clearly-explained-how-when-why-to-use-it-and-feature-importance-a-guide-in-python-7c274582c37e

Principal Component Analysis

- Mathematically, the principal components are the eigenvectors of the covariance matrix of the original dataset.
- Because the covariance matrix is symmetric, the eigenvectors are orthogonal.
- The principal components (eigenvectors) correspond to the direction (in the original n-dimensional space) with the greatest variance in the data.



Our original data in the xy-plane. (Source.)

Principal Component Analysis

- Each eigenvector has a corresponding eigenvalue. An eigenvalue is a scalar. Recall that an eigenvector corresponds to a direction.
- The corresponding eigenvalue is a number that indicates how much variance there is in the data along that eigenvector (or principal component).
- In other words, a larger eigenvalue means that that principal component explains a large amount of the variance in the data.
- A principal component with a very small eigenvalue does not do a good job of explaining the variance in the data.
- In the extreme case, if a principal component had an eigenvalue of zero, then it would mean that it explained none of the variance in the data.

Maths behind PCA - Example

Step 1: Standardize the dataset.

Step 2: Calculate the covariance matrix for the features in the dataset.

Step 3: Calculate the eigenvalues and eigenvectors for the covariance matrix.

Step 4: Sort eigenvalues and their corresponding eigenvectors.

Step 5: Pick k eigenvalues and form a matrix of eigenvectors.

Step 6: Transform the original matrix.

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 1: Standardize the dataset.

$$x_{new} = \frac{x - \mu}{\sigma}$$

	f1	f2	f3	f4
μ =	4	3	3	3.4
σ =	3	1.58114	1.73205	2.30217

Mean and standard deviation before standardization

f1	f2	f3	f4
1	2	3	4
5	5	6	7
1	4	2	3
5	3	2	1
8	1	2	2

Dataset matrix

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

$$cov(f1, f1) = \frac{1}{n}\sum(f1 - \overline{f1})(f1 - \overline{f1})$$

$$\frac{(-1)^2 + 0.33^2 + (-1)^2 + 0.33^2 + 1.33^2}{5} = 0.8$$

$$cov\ mat = \begin{bmatrix} 0.8 & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}$$

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

$$cov(f2, f2) = \frac{1}{n}\sum(f2 - \overline{f2})(f2 - \overline{f2})$$

$$\frac{(-0.63)^2 + 1.26^2 + 0.63^2 + 0^2 + (-1.26)^2}{5} = 0.8$$

$$cov\ mat = \begin{bmatrix} 0.8 & & & \\ & 0.8 & & \\ & & & \\ & & & \end{bmatrix}$$

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Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

$$Repeat\ the\ rest\ for\ diagonal$$

$$cov\ mat = \begin{bmatrix} 0.8 & & & \\ & 0.8 & & \\ & & 0.8 & \\ & & & 0.8 \end{bmatrix}$$

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Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

$$cov(f1, f2) = \frac{1}{n}\sum(f1 - \overline{f1})(f2 - \overline{f2})$$

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

$$= \frac{(-1)(-0.63) + (0.33)(1.26) + (-1)(0.63) + 0 + (1.33)(-1.26)}{5} = -0.25$$

$$cov\ mat = \begin{bmatrix} 0.8 & -0.25 & & \\ -0.25 & 0.8 & & \\ & & 0.8 & \\ & & & 0.8 \end{bmatrix}$$

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Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

$$cov(f1, f3) = \frac{1}{n}\sum(f1 - \overline{f1})(f3 - \overline{f3})$$

$$= \frac{(-1)(0) + (0.33)(1.73) + (-1)(-0.58) + (0.33)(-0.58) + (1.33)(-0.58)}{5}$$

$$= 0.04$$

$$cov\ mat = \begin{bmatrix} 0.8 & -0.25 & 0.04 & \\ -0.25 & 0.8 & & \\ 0.04 & & 0.8 & \\ & & & 0.8 \end{bmatrix}$$

Maths behind PCA - Example

Step 2: Calculate the covariance matrix for the features in the dataset.

f1	f2	f3	f4
-1	-0.63246	0	0.26062
0.33333	1.26491	1.73205	1.56374
-1	0.63246	-0.57735	-0.17375
0.33333	0	-0.57735	-1.04249
1.33333	-1.26491	-0.57735	-0.60812

Standardized Dataset

Repeat the rest

$$cov\ mat = \begin{bmatrix} 0.8 & -0.25 & 0.04 & -0.14 \\ -0.25 & 0.8 & 0.51 & 0.49 \\ 0.04 & 0.51 & 0.8 & 0.75 \\ -0.14 & 0.49 & 0.75 & 0.8 \end{bmatrix}$$

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 3: Calculate the eigenvalues and eigenvectors for the covariance

	f1	f2	f3	f4
f1	0.8	-0.25298	0.03849	-0.14479
f2	-0.25298	0.8	0.51121	0.4945
f3	0.03849	0.51121	0.8	0.75236
f4	-0.14479	0.4945	0.75236	0.8

1. Solve for $\det(A - \lambda I) = 0$ to find eigenvalues.
2. Solve the system to find eigenvector

	f1	f2	f3	f4
f1	0.8 - λ	-0.25298	0.03849	-0.14479
f2	-0.25298	0.8- λ	0.51121	0.4945
f3	0.03849	0.51121	0.8 - λ	0.75236
f4	-0.14479	0.4945	0.75236	0.8 - λ

$A-\lambda I = 0$

$$\lambda = 2.01263459, 0.8522308, 0.31510964, 0.02002497$$

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 3: Calculate the eigenvalues and eigenvectors for the covariance matrix.

1. Solve for $\det(\lambda I - A) = 0$ to find eigenvalues.
2. Solve the system to find eigenvector

$\lambda = 2.01263459$

$$\begin{pmatrix} 0.800000-\lambda & -(0.252982) & 0.038490 & -(0.144791) \\ -(0.252982) & 0.800000-\lambda & 0.511208 & 0.494498 \\ 0.038490 & 0.511208 & 0.800000-\lambda & 0.752355 \\ -(0.144791) & 0.494498 & 0.752355 & 0.800000-\lambda \end{pmatrix} \times \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = 0$$

Eigenvectors for λ=2.01263459

$v1 = 0.16195986$

$v2 = -0.52404813$

$v3 = -0.58589647$

$v4 = -0.59654663$

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 3: Calculate the eigenvalues and eigenvectors for the covariance matrix.

1. Solve for $\det(\lambda I - A) = 0$ to find eigenvalues.
2. Solve the system to find eigenvector

Repeat the same for all eigenvalues, we get the following

$$\lambda = 2.01263459, 0.8522308, 0.31510964, 0.02002497$$

	e1	e2	e3	e4
v1	0.161960	-0.917059	-0.307071	0.196162
v2	-0.524048	0.206922	-0.817319	0.120610
v3	-0.585896	-0.320539	0.188250	-0.720099
v4	-0.596547	-0.115935	0.449733	0.654547

eigenvectors(4 * 4 matrix)

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Remember that: larger eigenvalue means that that principal component explains a large amount of the variance in the data.

The first principal component accounts for the largest possible variance in the dataset.

Maths behind PCA - Example

Step 4: Sort eigenvalues and their corresponding eigenvectors.

$$\lambda = 2.01263459, 0.8522308, 0.31510964, 0.02002497$$

	e1	e2	e3	e4
v1	0.161960	-0.917059	-0.307071	0.196162
v2	-0.524048	0.206922	-0.817319	0.120610
v3	-0.585896	-0.320539	0.188250	-0.720099
v4	-0.596547	-0.115935	0.449733	0.654547

eigenvectors(4 * 4 matrix)

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 5: Pick k eigenvalues and form a matrix of eigenvectors.

Let say, we take k = 4

e1	e2	e3	e4
0.161960	-0.917059	-0.307071	0.196162
-0.524048	0.206922	-0.817319	0.120610
-0.585896	-0.320539	0.188250	-0.720099
-0.596547	-0.115935	0.449733	0.654547

eigenvectors(4 * 4 matrix)

Credit to https://medium.com/analytics-vidhya/understanding-principle-component-analysis-pca-step-by-step-e7a4bb4031d9

Maths behind PCA - Example

Step 6: Transform the original matrix to principal component space.

Original Matrix * Top 4 eigenvector matrix = Transformed matrix

$S \cdot V = P$

f1	f2	f3	f4
-1.000000	-0.632456	0.000000	0.260623
0.333333	1.264911	1.732051	1.563740
-1.000000	0.632456	-0.577350	-0.173749
0.333333	0.000000	-0.577350	-1.042493
1.333333	-1.264911	-0.577350	-0.608121

(5,4)

*

e1	e2	e3	e4
0.161960	-0.917059	-0.307071	0.196162
-0.524048	0.206922	-0.817319	0.120610
-0.585896	-0.320539	0.188250	-0.720099
-0.596547	-0.115935	0.449733	0.654547

=

```
transform_matrix with 4 principal components
[[ 1.40033078e-02  7.55974765e-01  9.41199615e-01 -1.01852226e-01]
 [-2.55653399e+00 -7.80431775e-01 -1.06869861e-01 -5.75705265e-03]
 [-5.14801919e-02  1.25313470e+00 -3.96673397e-01  1.82141242e-01]
 [ 1.01415002e+00  2.38808310e-04 -6.79886182e-01 -2.01224649e-01]
 [ 1.57986086e+00 -1.22891650e+00  2.42229826e-01  1.26692685e-01]]
-----------------------------------------------
```

Maths behind PCA - Example

To transform back to original space

$$S = P \cdot V^{-1}$$

```
transform_matrix with 4 principal components
[[ 1.40033078e-02  7.55974765e-01  9.41199615e-01 -1.01852226e-01]
 [-2.55653399e+00 -7.80431775e-01 -1.06869861e-01 -5.75705265e-03]
 [-5.14801919e-02  1.25313470e+00 -3.96673397e-01  1.82141242e-01]
 [ 1.01415002e+00  2.38808310e-04 -6.79886182e-01 -2.01224649e-01]
 [ 1.57986086e+00 -1.22891650e+00  2.42229826e-01  1.26692685e-01]]
------------------------------------------------
```

$$\cdot \left[\begin{array}{rrrr} e1 & e2 & e3 & e4 \\ 0.161960 & -0.917059 & -0.307071 & 0.196162 \\ -0.524048 & 0.206922 & -0.817319 & 0.120610 \\ -0.585896 & -0.320539 & 0.188250 & -0.720099 \\ -0.596547 & -0.115935 & 0.449733 & 0.654547 \end{array}\right]^{-1}$$

=

f1	f2	f3	f4
-1.000000	-0.632456	0.000000	0.260623
0.333333	1.264911	1.732051	1.563740
-1.000000	0.632456	-0.577350	-0.173749
0.333333	0.000000	-0.577350	-1.042493
1.333333	-1.264911	-0.577350	-0.608121

(5,4)

Maths behind PCA - Example

Retaining only top 2 eigenvectors

f1	f2	f3	f4
-1.000000	-0.632456	0.000000	0.260623
0.333333	1.264911	1.732051	1.563740
-1.000000	0.632456	-0.577350	-0.173749
0.333333	0.000000	-0.577350	-1.042493
1.333333	-1.264911	-0.577350	-0.608121

(5,4)

*

e1	e2
0.161960	-0.917059
-0.524048	0.206922
-0.585896	-0.320539
-0.596547	-0.115935

(4,2)

=

nf1	nf2
0.014003	0.755975
-2.556534	-0.780432
-0.051480	1.253135
1.014150	0.000239
1.579861	-1.228917

(5,2)