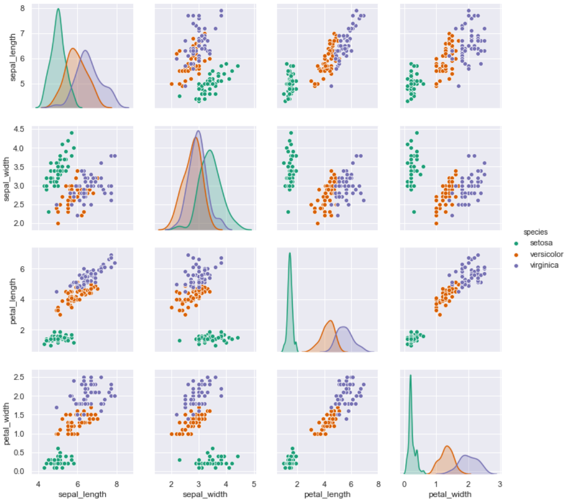
Principal Component Analysis (PCA)

Foundations of Data Analysis

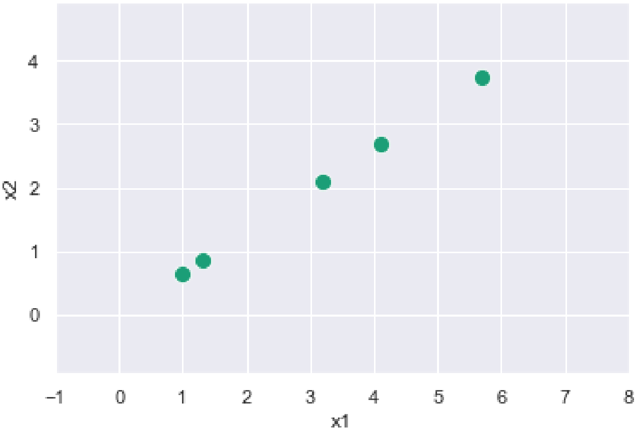
April 1, 2021

Example: Iris Data

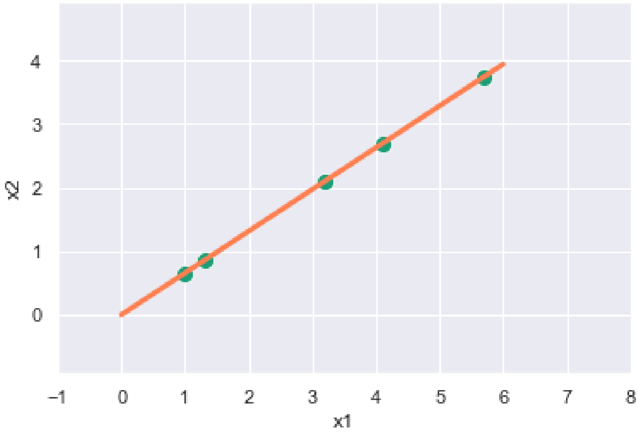


Do we need all 4 dimensions?

How Many Dimensions Are In Your Data?



How Many Dimensions Are In Your Data?



Covariance

Covariance between two random samples: $x_i, y_i \in \mathbb{R}$

$$\operatorname{cov}(x, y) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

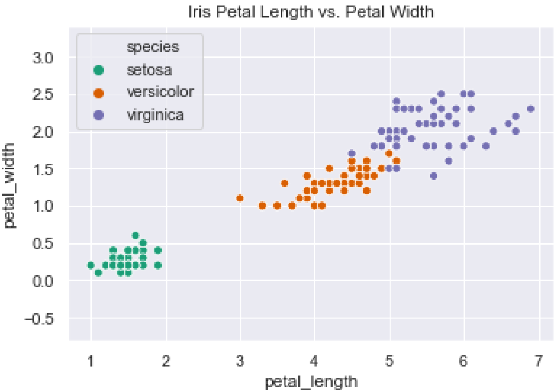
Measures how x “covaries” with y

Proportional to correlation:

$$\operatorname{cov}(x, y) = \operatorname{corr}(x, y)\operatorname{sd}(x)\operatorname{sd}(y)$$

Symmetric: $\operatorname{cov}(x, y) = \operatorname{cov}(y, x)$

Example: Iris Data




```
Covariance = 1.2869720000000002
Correlation = 0.9628654314027962
```

Centering a Data Matrix

Data matrix X: $n \times d$

n rows (data points)
d columns (dimensions, or features)

Mean of data (rows):

$$\mu = \frac{1}{n} \sum_{i=1}^{n} X_{i\bullet}$$

Centered data (subtract mean from each row):

$$\tilde{X}_{i\bullet} = X_{i\bullet} - \mu$$

Covariance Matrix

Sample covariance matrix:

$$\Sigma = \frac{1}{n-1}\tilde{X}^T\tilde{X}$$

Σ_{ij} is the covariance between the ith and jth dimension (feature)

$$\Sigma_{ij} = \frac{1}{n-1}\sum_{k=1}^{n}(X_{ki} - \mu_i)(X_{kj} - \mu_j) = \mathrm{cov}(X_{\bullet i}, X_{\bullet j})$$

Properties

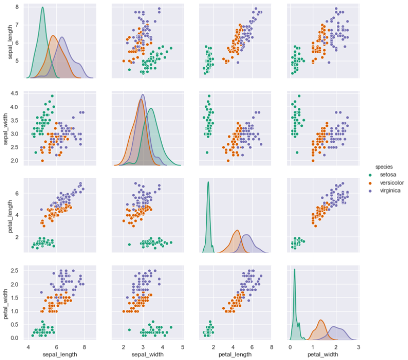
Covariance is **symmetric**: $\Sigma = \Sigma^T$

$$\Sigma_{ij} = \mathrm{cov}(X_{\bullet i}, X_{\bullet j}) = \mathrm{cov}(X_{\bullet j}, X_{\bullet i}) = \Sigma_{ji}$$

Covariance is **positive-semidefinite**:

$$v^T \Sigma v \geq 0$$

Example: Iris Data



Covariance matrix:

$$\Sigma = \begin{pmatrix} 0.6857 & -0.04243 & 1.274 & 0.5163 \\ -0.04243 & 0.1900 & -0.3297 & -0.1216 \\ 1.274 & -0.3297 & 3.116 & 1.296 \\ 0.5163 & -0.1216 & 1.296 & 0.5810 \end{pmatrix}$$

Eigenvectors, Eigenvalues

Square matrix A: $d \times d$
Eigenvector $v \in \mathbb{R}^d$ and eigenvalue $\lambda \in \mathbb{R}$:

$$Av = \lambda v$$

Meaning: The transformation A is a scaling when applied to v

Eigenanalysis of a Symmetric Matrix

Fact: If A is a $d \times d$ symmetric matrix, it has *exactly* d real eigenvalues $\lambda_k \in \mathbb{R}$ (possibly with repeats).

Each eigenvalue λ_k has a corresponding eigenvector $v_k \in \mathbb{R}^d$.

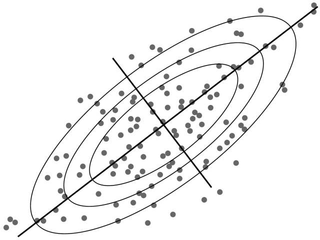
Eigenanalysis of a Symmetric Matrix

The SVD of a symmetric, positive-semidefinite matrix looks like this:

$$A = VSV^T$$

- The singular values are the eigenvalues: $s_k = \lambda_k$.
- The left and right singular vectors are the *same* and are the eigenvectors, v_k.

Principal Component Analysis



PCA is an eigenanalysis of the covariance matrix:

$$\Sigma = V \Lambda V^T$$

- Eigenvectors: $v_k = V_{\bullet k}$ are **principal components**
- Eigenvalues: λ_k are the **variance** of the data in the v_k direction

PCA Algorithm Summary

Input: Data matrix X: $n \times d$

1. Compute centered data $\tilde{X}$
2. Compute covariance matrix:

$$\Sigma = \frac{1}{n-1}\tilde{X}^T\tilde{X}$$

3. Eigenanalysis of covariance:

$$\Sigma = V\Lambda V^T$$

Hint: `numpy.linalg.eigh` computes an eigenanalysis of a symmetric matrix!

Dimensionality Reduction

Goal: Find a k-dimensional subspace, V_k, that best fits our data

Least-squares fit:

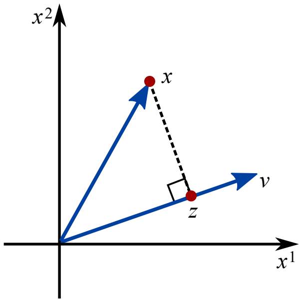
$$\arg\min_{V_k} \sum_{i=1}^{n} \mathrm{distance}(V_k, x_i)^2$$

Solution: Use first k principal components:

$$V_k = \mathrm{span}(v_1, v_2, \ldots, v_k)$$

Maximizing Variance of Projected Data

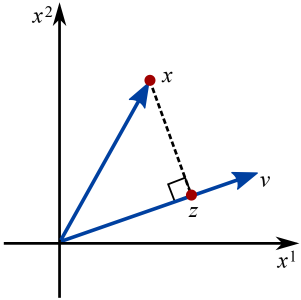
Fact: PCA finds dimensions that maximize variance



Given direction $v \in \mathbb{R}^d$, with $\|v\| = 1$,
project data point $x \in \mathbb{R}^d$ onto v:

$$z = \langle v, x \rangle$$

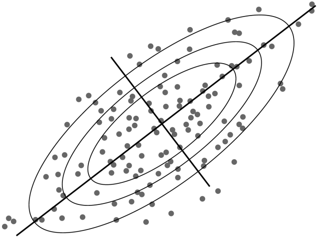
Maximizing Variance of Projected Data



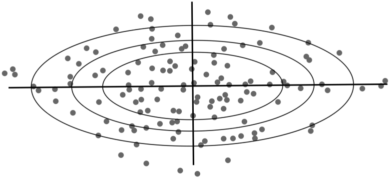
Given mean-centered data, x_i,
first principal component, v_1 maximizes variance:

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{n} \langle v, x_i \rangle^2$$

PC's as Rotation



X



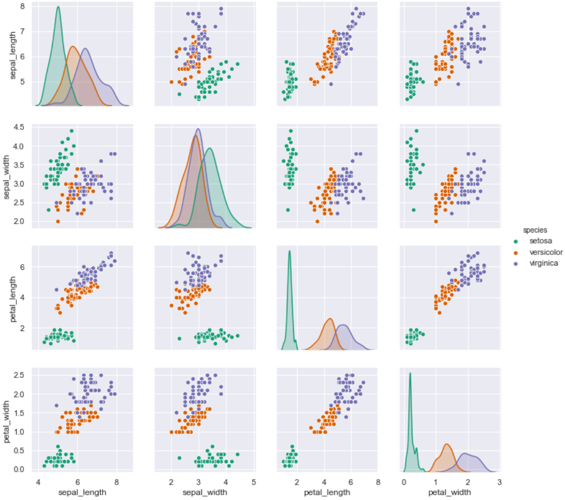
Z

The principal components matrix, V, acts as a rotation:

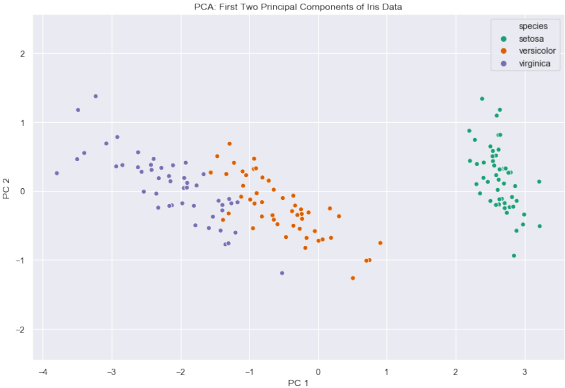
$$Z = XV$$

Columns of Z are new coordinates, called **loadings**

Example: Iris Data



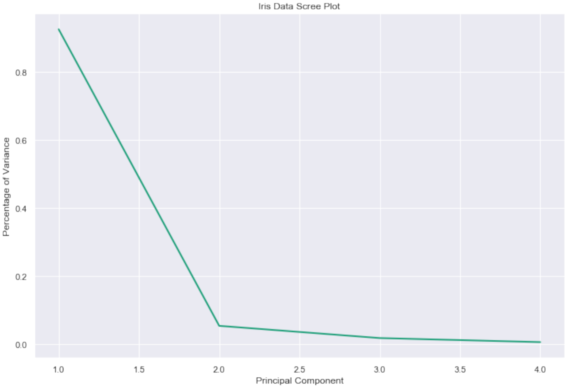
Example: Iris Data PCA



Eigenvectors: $$V = \begin{pmatrix} 0.685694 & -0.042434 & 1.274315 & 0.516271 \\ -0.042434 & 0.189979 & -0.329656 & -0.121639 \\ 1.274315 & -0.329656 & 3.116278 & 1.295609 \\ 0.516271 & -0.121639 & 1.295609 & 0.581006 \end{pmatrix}$$

Eigenvalues: $$\lambda = \begin{pmatrix} 4.22824171 & 0.24267075 & 0.0782095 & 0.02383509 \end{pmatrix}$$

Scree Plot: Eigenvalues (Variance)



Horizontal axis: which principal component (index k)

Vertical axis: proportion of variance: $\frac{\lambda_k}{\sum_{j=1}^{d} \lambda_j}$