# Principal Component Analysis (PCA) Refresher

Geometry of Data

October 1, 2024

# Centering a Data Matrix

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$d$ columns (dimensions, or features)

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Centered data (subtract mean from each row):

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

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$\Sigma_{ij}$ is the covariance between the $i$th and $j$th dimension (feature)

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

# Properties

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

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

Covariance is **positive-semidefinite**:

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

# Eigenvectors, Eigenvalues

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**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 $\lambda_k$ has a corresponding eigenvector $v_k \in \mathbb{R}^d$.

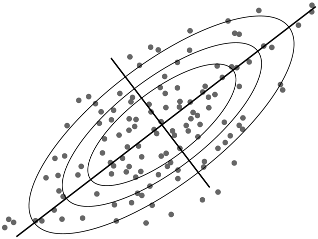
# Eigenanalysis of a Symmetric Matrix

The SVD of a symmetric 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



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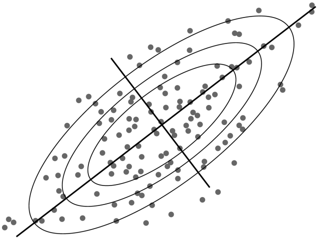

PCA is an eigenanalysis of the covariance matrix:

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- Eigenvectors: $v_k = V_{\bullet k}$ are **principal components**
- Eigenvalues: $\lambda_k$ 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:

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

3. Eigenanalysis of covariance:

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**Hint:** `numpy.linalg.eig` computes an eigenanalysis!

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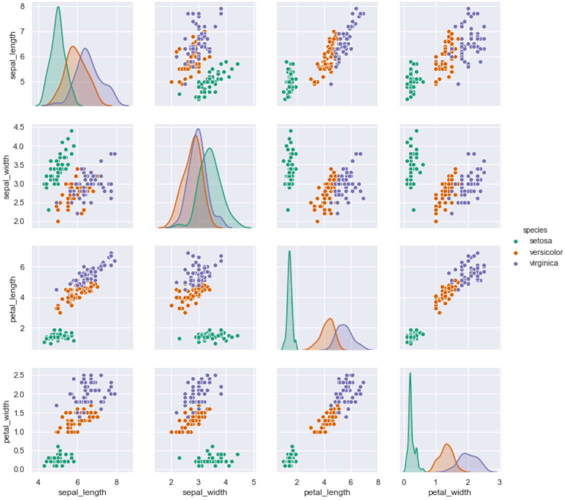
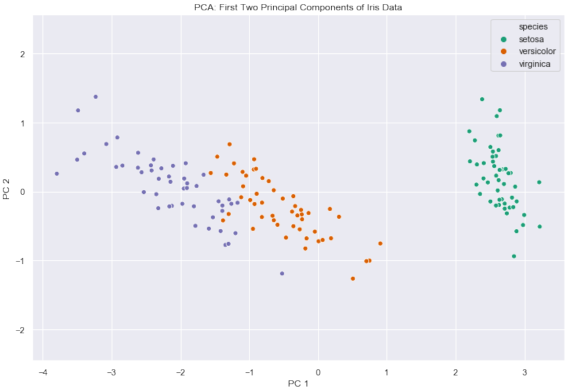
**Solution:** Use first $k$ principal components:

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

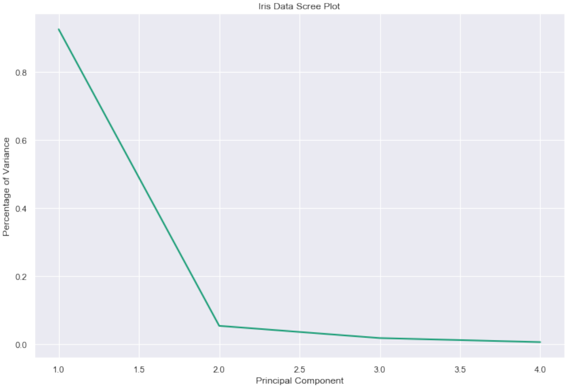
# Example: Iris Data



# Example: Iris Data PCA



# Scree Plot: Eigenvalues (Variance)




Horizontal axis: index $k$

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