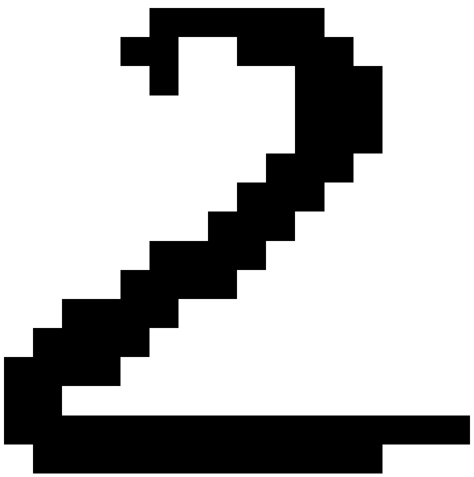
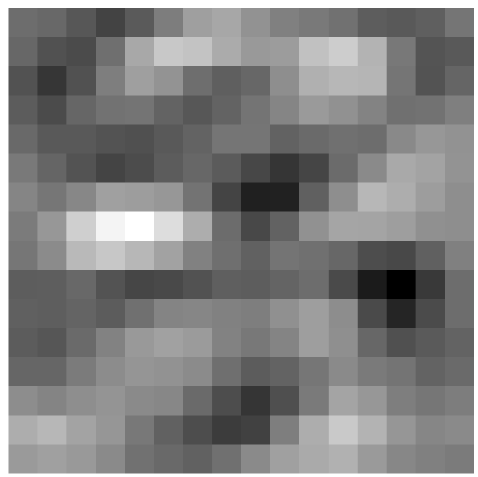
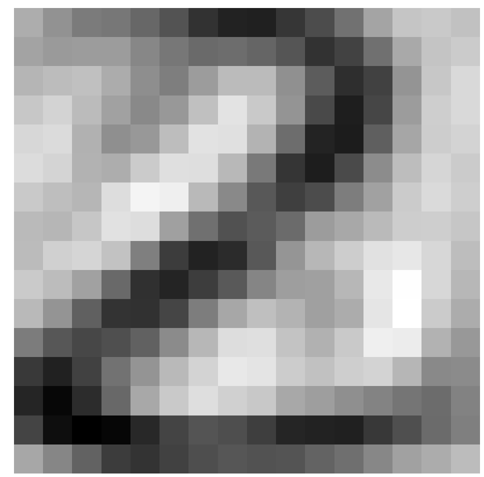
Advanced Machine Learning

Principal Component Analysis (PCA)

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1



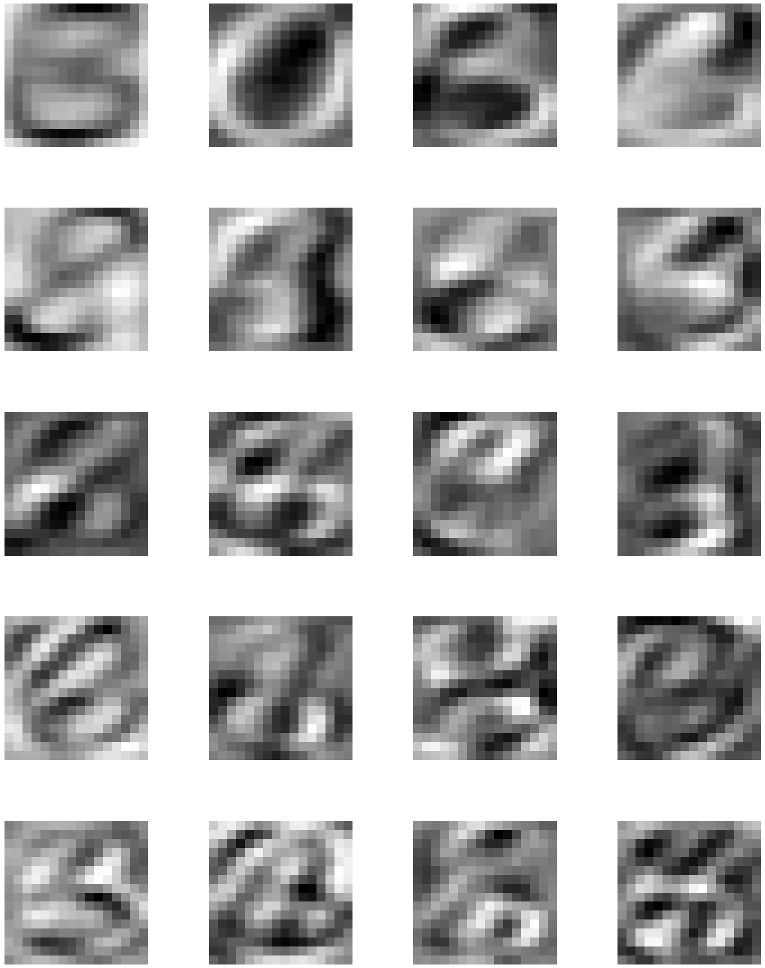




Covariance matrices, dimensionality reduction, PCA, Duality

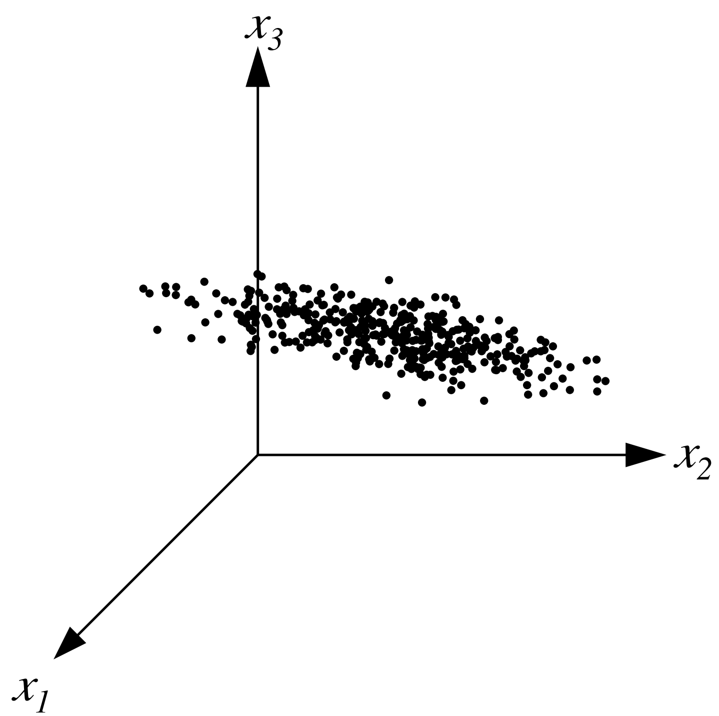
Outline

1. **Covariance Matrices**
2. Principal Component Analysis
3. Duality



Spread of Data

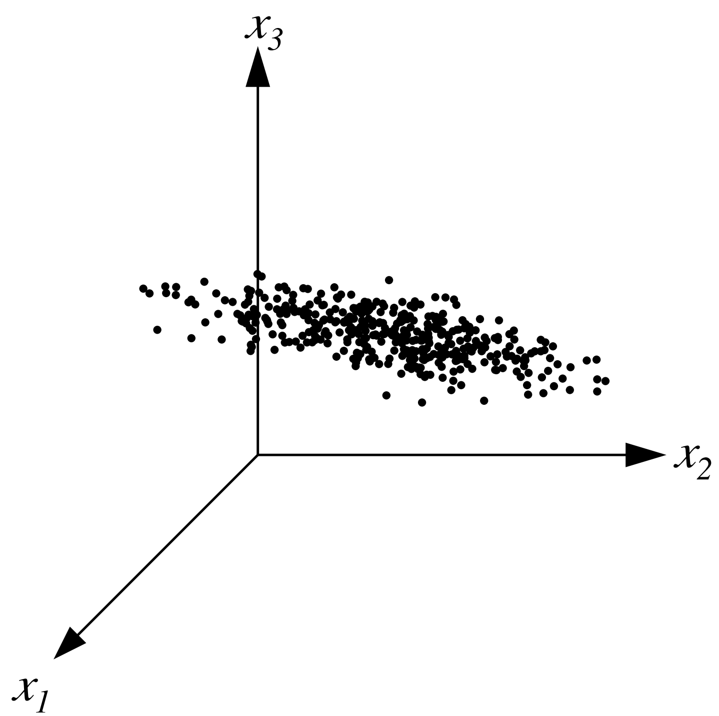
- Often data varies significantly in only some directions



- Reduce dimensions by projecting onto low dimensional subspace with maximum variation

Spread of Data

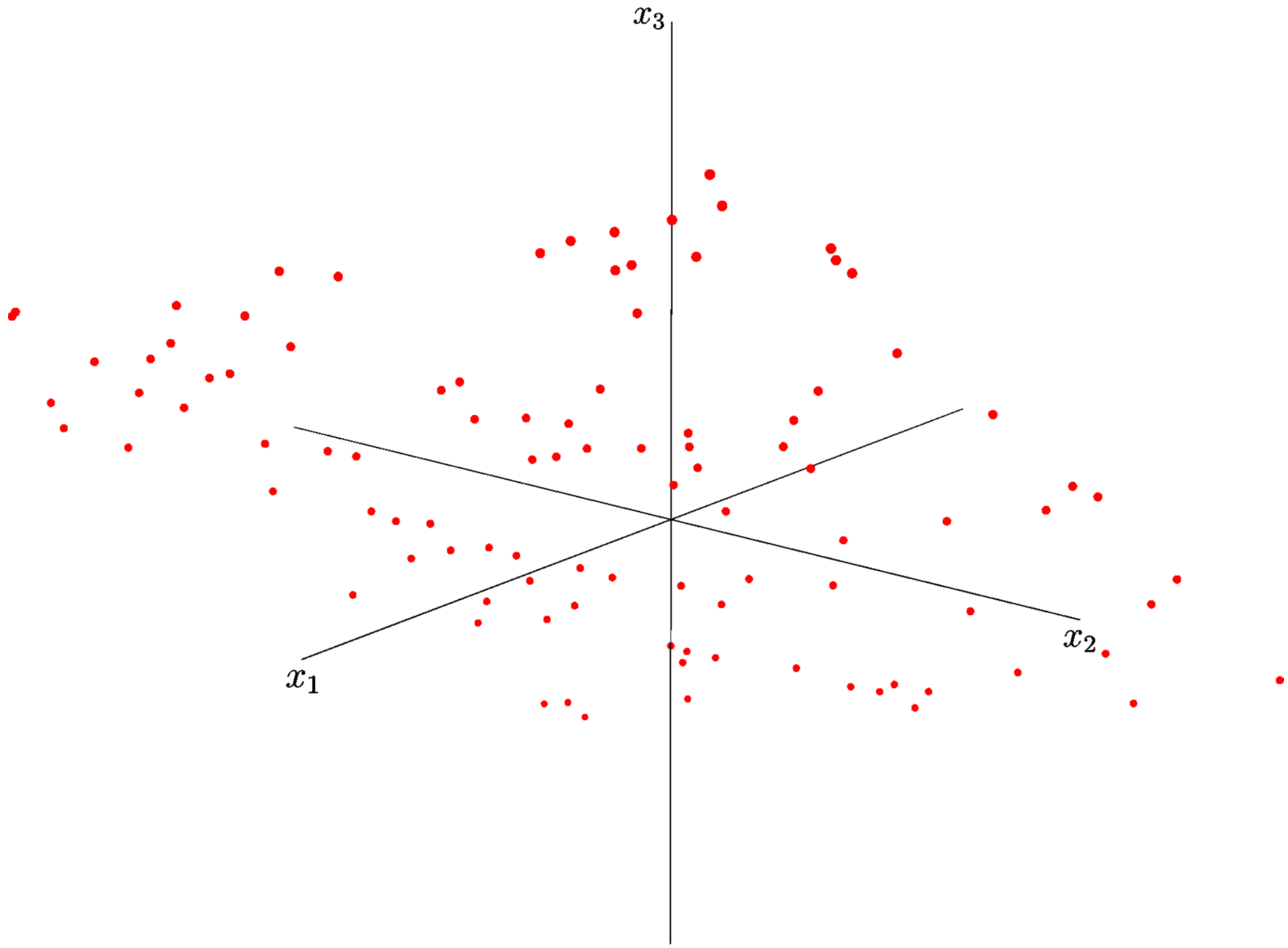
- Often data varies significantly in only some directions



- Reduce dimensions by projecting onto low dimensional subspace with maximum variation

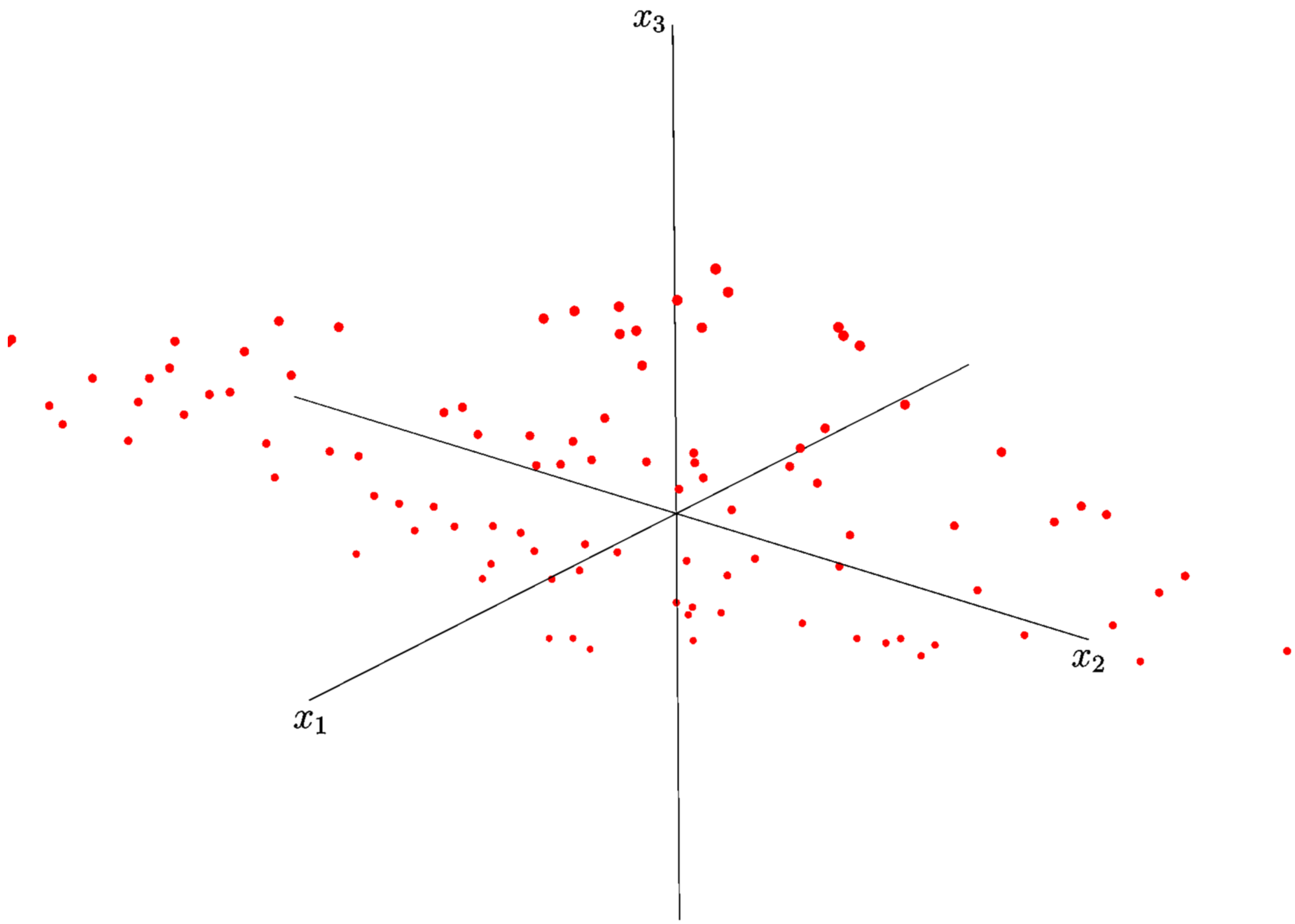
Looking is not Enough

Can't spot low dimensional data by looking at numbers



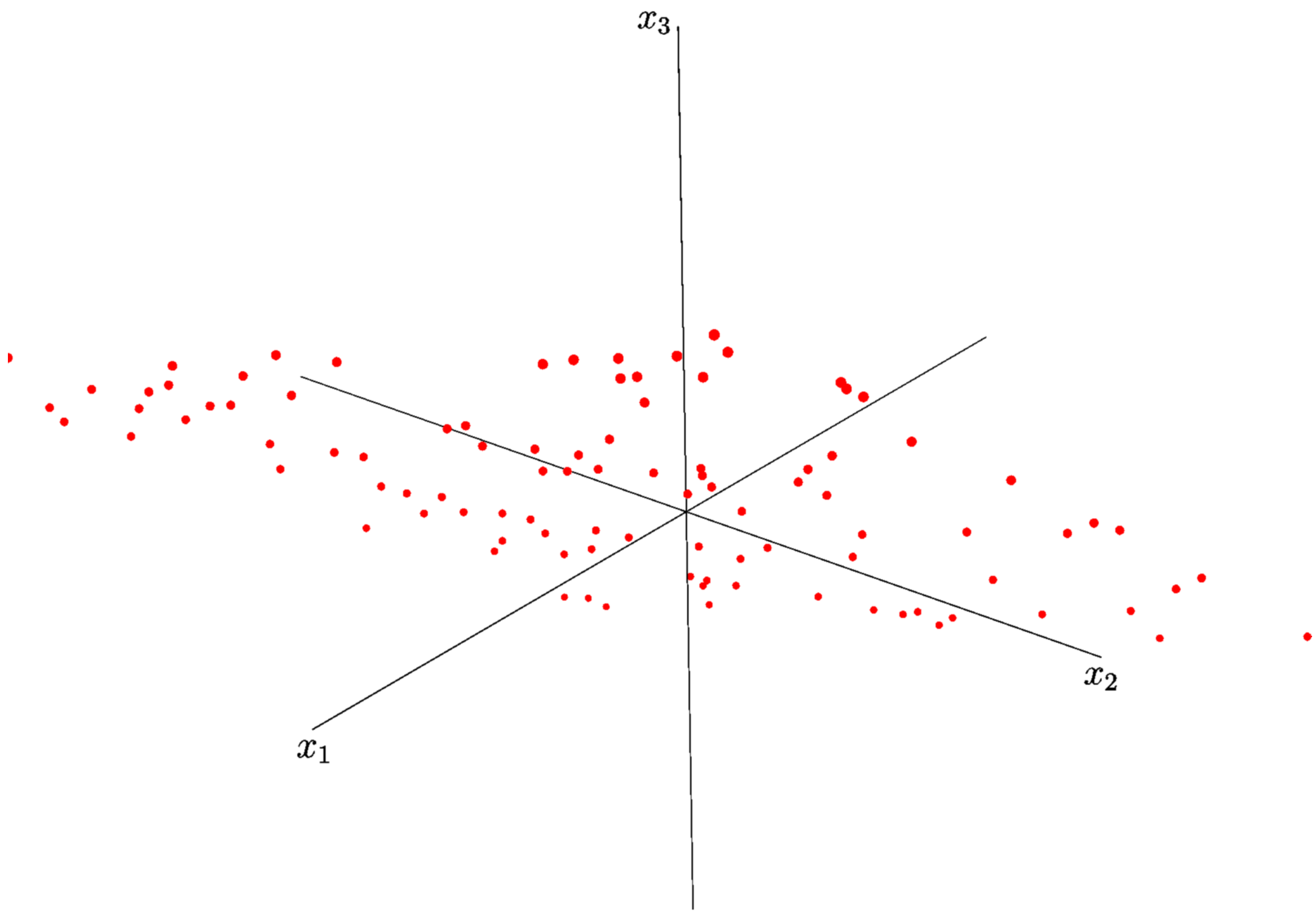
Looking is not Enough

Can't spot low dimensional data by looking at numbers



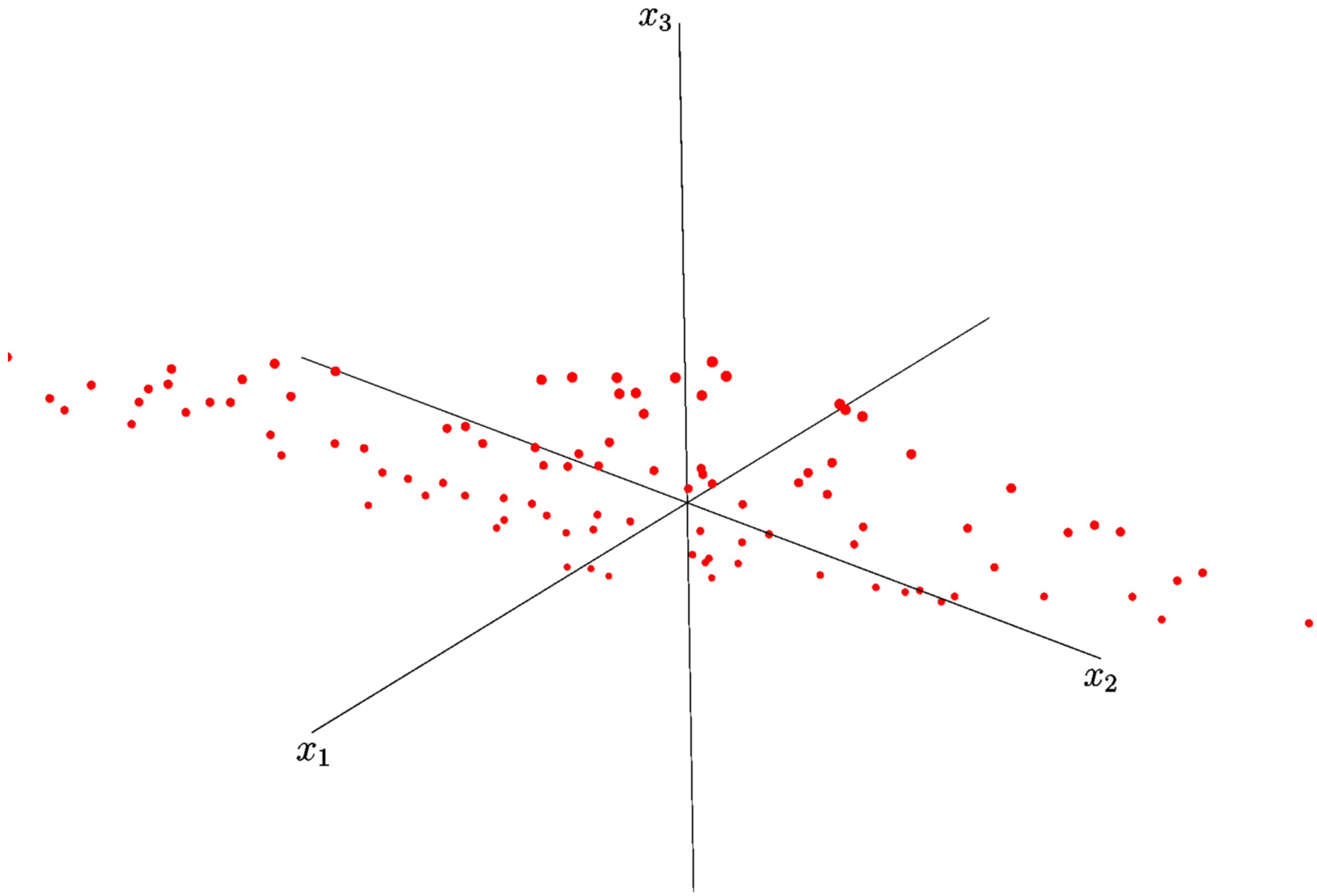
Looking is not Enough

Can't spot low dimensional data by looking at numbers



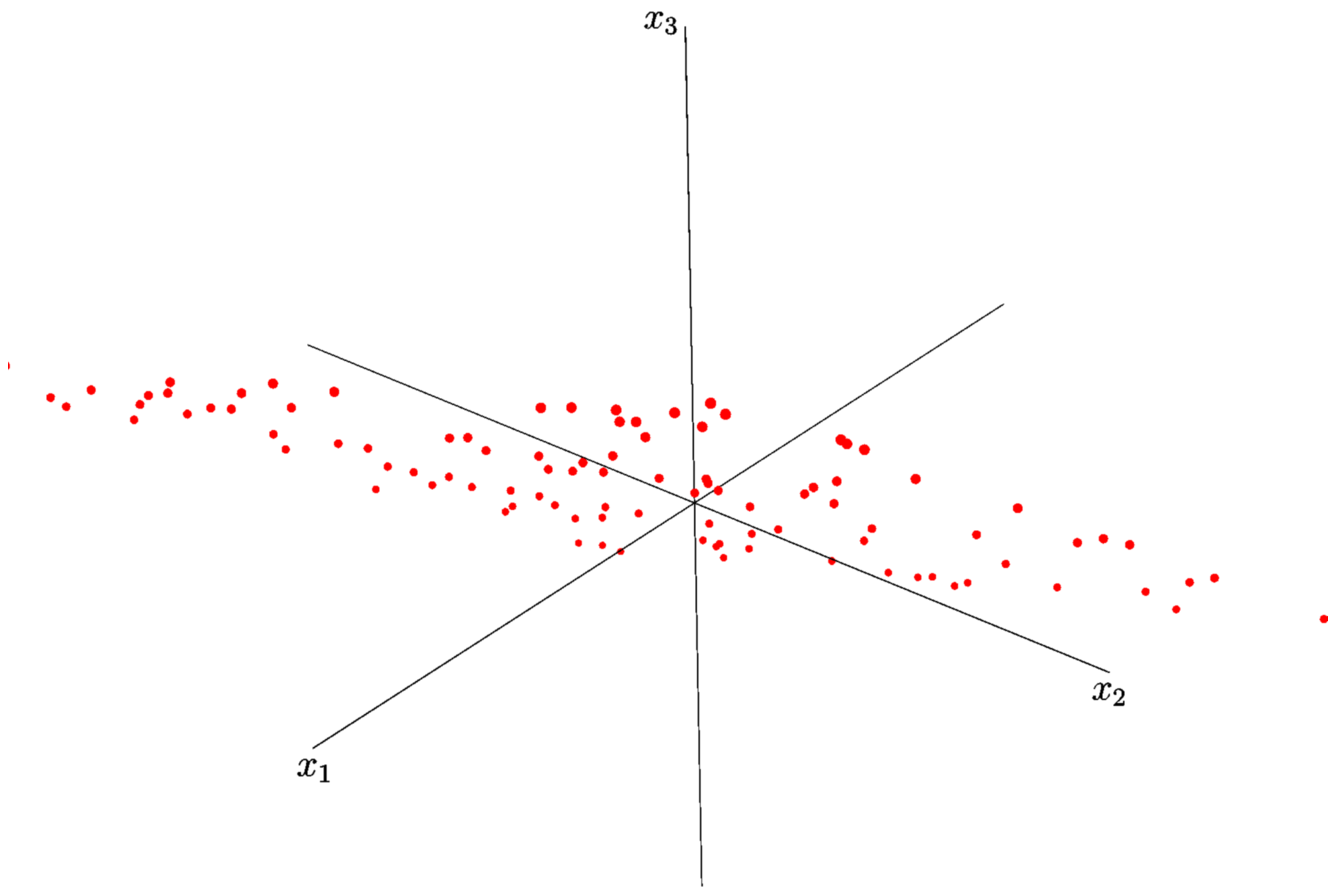
Looking is not Enough

Can't spot low dimensional data by looking at numbers



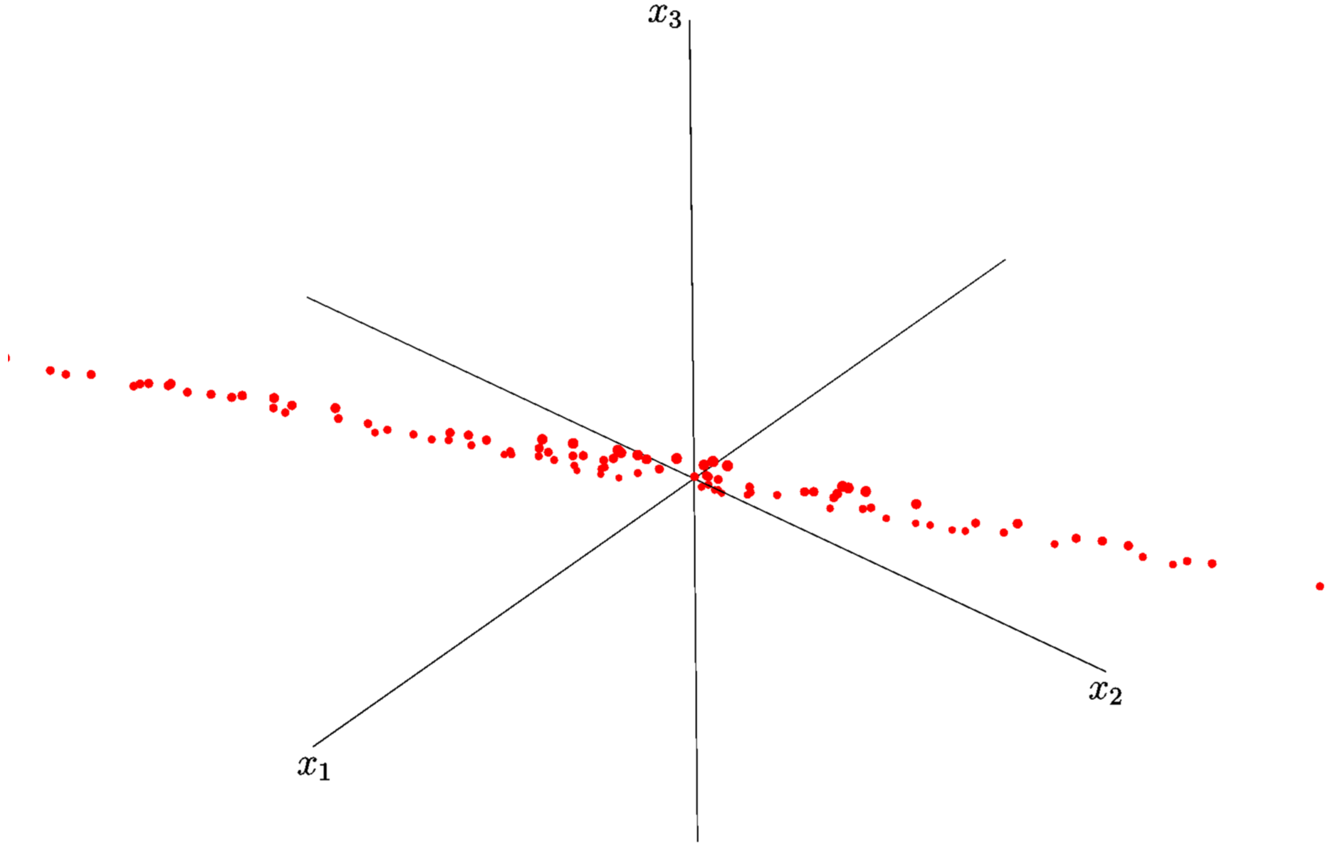
Looking is not Enough

Can't spot low dimensional data by looking at numbers



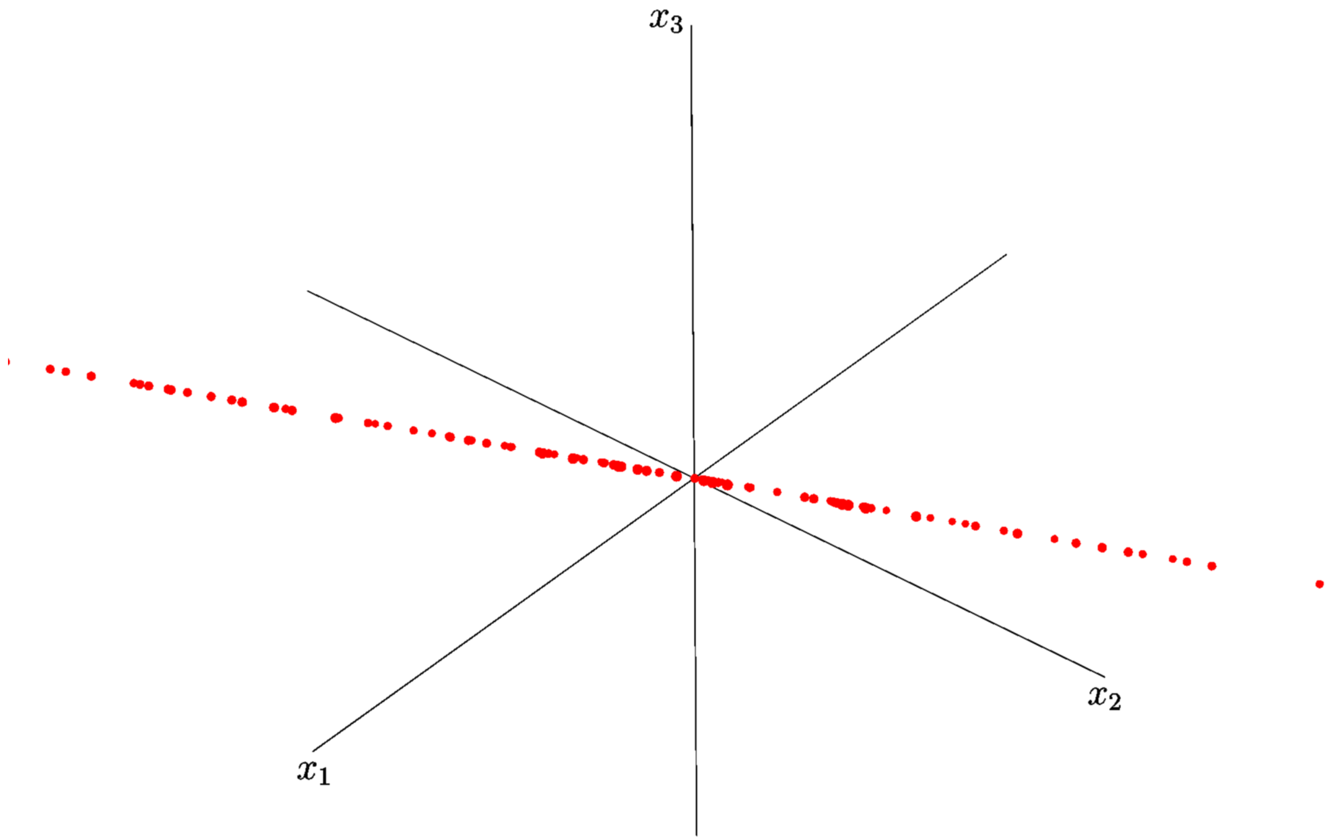
Looking is not Enough

Can't spot low dimensional data by looking at numbers



Looking is not Enough

Can't spot low dimensional data by looking at numbers



Dimensionality Reduction

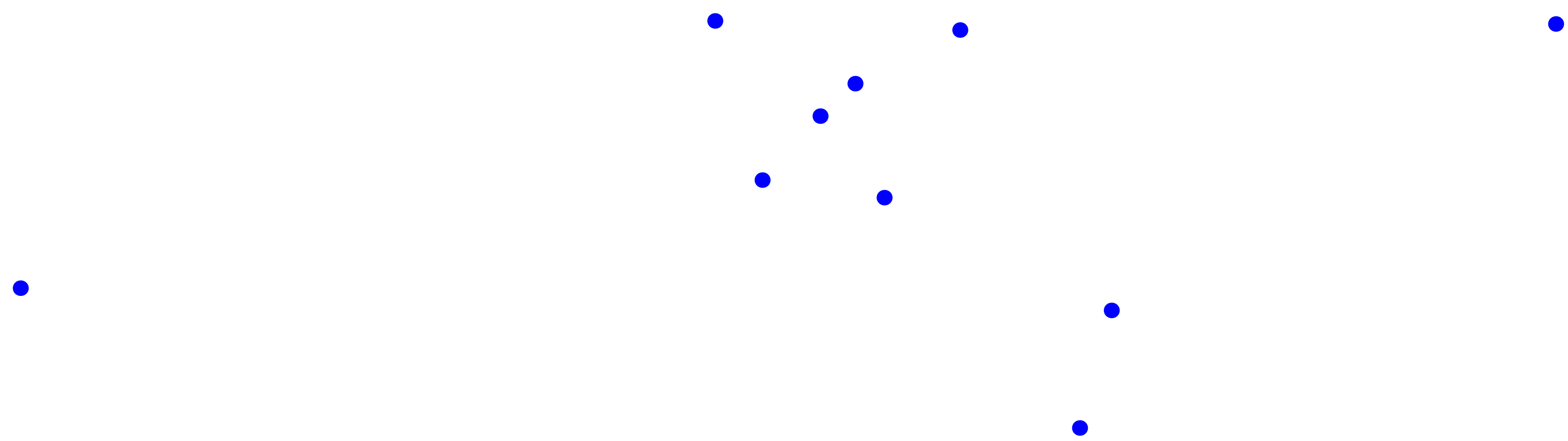
- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation

Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation

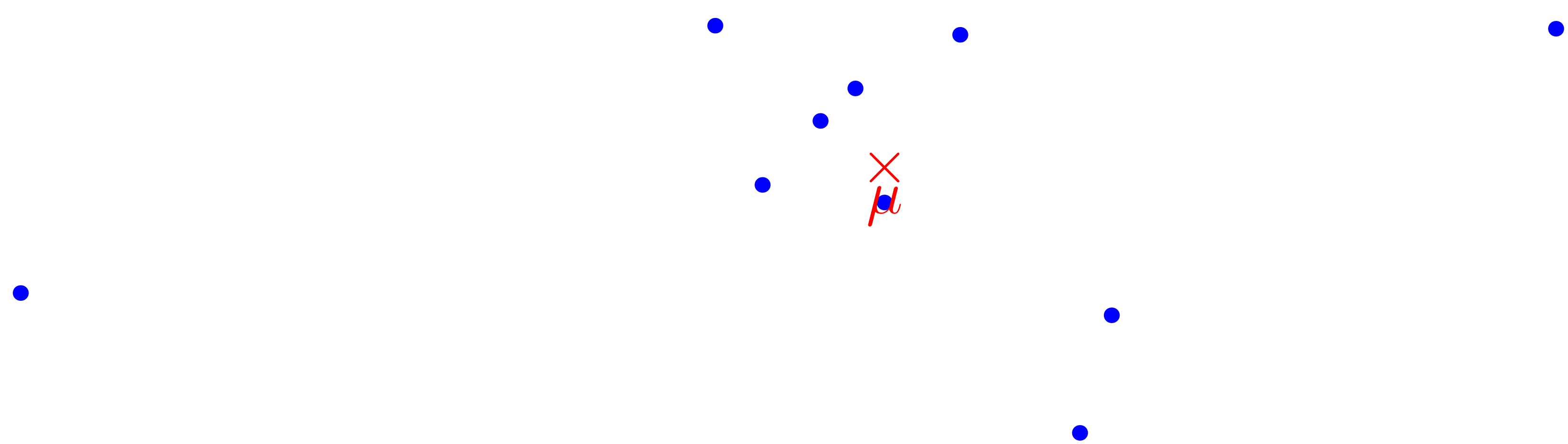
Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



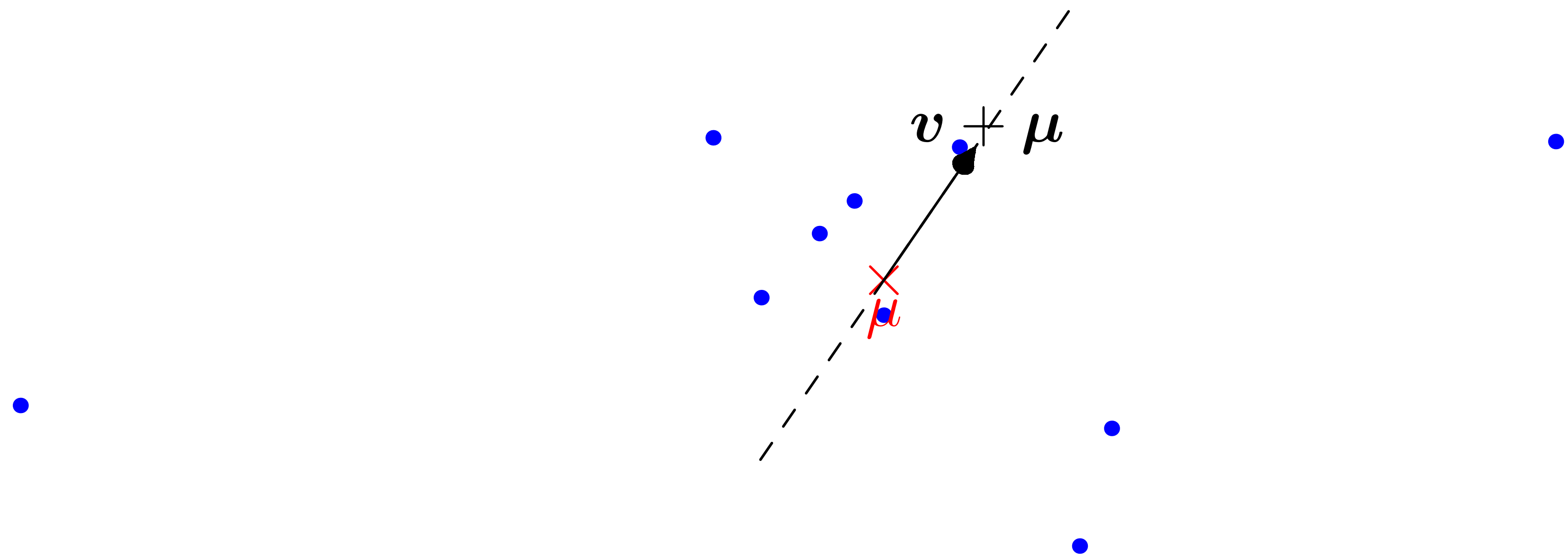
Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



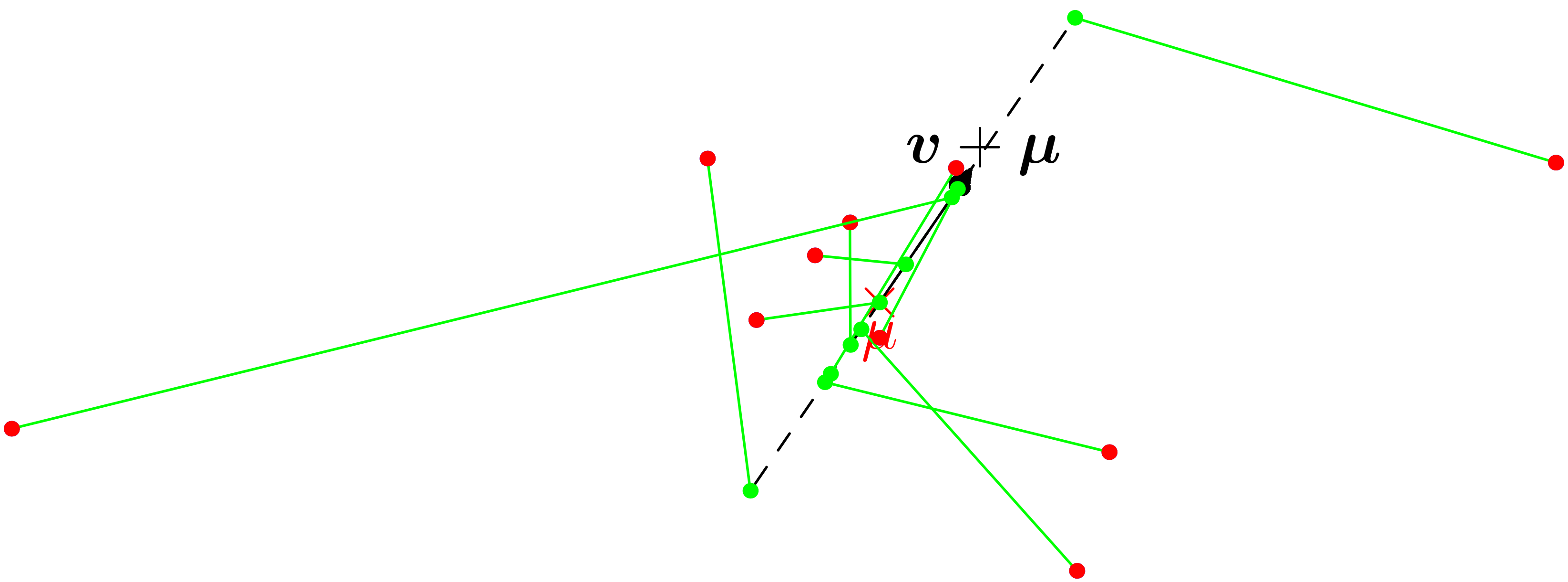
Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



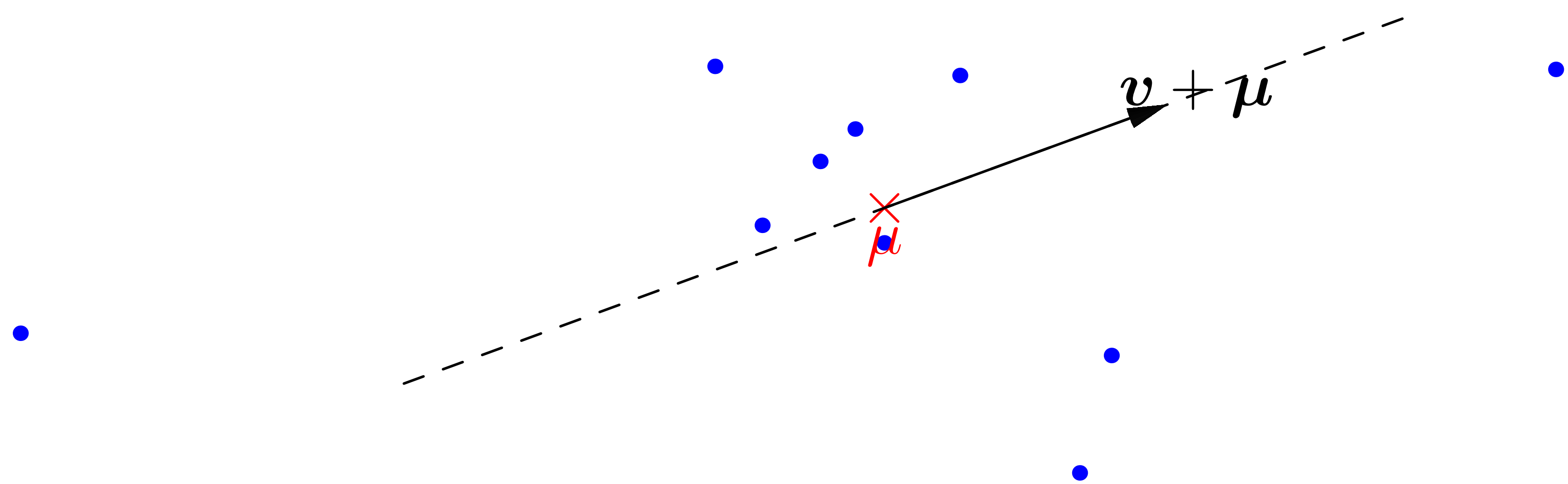
Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



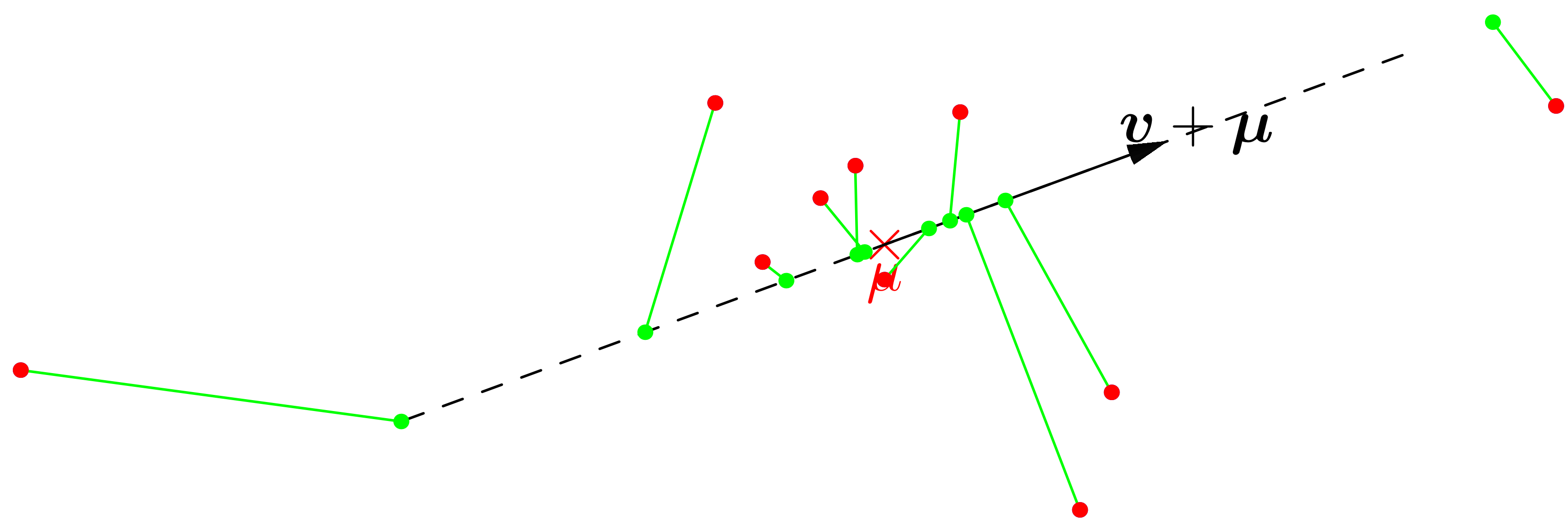
Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



Dimensionality Reduction

- Often helpful to consider only directions where data varies significantly
- Want to find directions along which data has its greatest variation



Direction of Maximum Variation

- Look for the vector $\boldsymbol{v}$ with $\|\boldsymbol{v}\|^2 = 1$ to maximise

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_i - \boldsymbol{\mu}) \right)^2$$

- This is a constrained optimisation problem

- Solve by maximising Lagrangian

$$\mathcal{L} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_k - \boldsymbol{\mu}) \right)^2 - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

- λ is a Lagrange multiplier

Direction of Maximum Variation

- Look for the vector $\boldsymbol{v}$ with $\|\boldsymbol{v}\|^2 = 1$ to maximise

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu})\right)^2$$

- This is a constrained optimisation problem

- Solve by maximising Lagrangian

$$\mathcal{L} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k - \boldsymbol{\mu})\right)^2 - \lambda \left(\|\boldsymbol{v}\|^2 - 1\right)$$

- λ is a Lagrange multiplier

Direction of Maximum Variation

- Look for the vector $\boldsymbol{v}$ with $\|\boldsymbol{v}\|^2 = 1$ to maximise

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_i - \boldsymbol{\mu}) \right)^2$$

- This is a constrained optimisation problem
- Solve by maximising Lagrangian

$$\mathcal{L} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_k - \boldsymbol{\mu}) \right)^2 - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

- λ is a Lagrange multiplier

Direction of Maximum Variation

- Look for the vector $\boldsymbol{v}$ with $\|\boldsymbol{v}\|^2 = 1$ to maximise

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_i - \boldsymbol{\mu}) \right)^2$$

- This is a constrained optimisation problem

- Solve by maximising Lagrangian

$$\mathcal{L} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_k - \boldsymbol{\mu}) \right)^2 - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

- λ is a Lagrange multiplier

Direction of Maximum Variation

- Expanding the Lagrangian

$$\begin{aligned}
\mathcal{L} &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})\right)^2-\lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{v}\right)-\lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\left(\frac{1}{m-1}\sum_{k=1}^{m}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\right)\boldsymbol{v}-\lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v}-\lambda\left(\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v}-1\right)
\end{aligned}$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla}\mathcal{L} = 2(\mathbf{C}\,\boldsymbol{v}-\lambda\,\boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

Direction of Maximum Variation

- Expanding the Lagrangian

$$\mathcal{L} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_k - \boldsymbol{\mu}) \right)^2 - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

$$= \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}} (\boldsymbol{x}_k - \boldsymbol{\mu})(\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{v} \right) - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

$$= \boldsymbol{v}^{\mathsf{T}} \left(\frac{1}{m-1} \sum_{k=1}^{m} (\boldsymbol{x}_k - \boldsymbol{\mu})(\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}} \right) \boldsymbol{v} - \lambda \left(\|\boldsymbol{v}\|^2 - 1 \right)$$

$$= \boldsymbol{v}^{\mathsf{T}} \mathbf{C} \boldsymbol{v} - \lambda \left(\boldsymbol{v}^{\mathsf{T}} \boldsymbol{v} - 1 \right)$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla} \mathcal{L} = 2(\mathbf{C}\, \boldsymbol{v} - \lambda\, \boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\, \boldsymbol{v} = \lambda\, \boldsymbol{v}$$

Direction of Maximum Variation

- Expanding the Lagrangian

$$\begin{aligned}
\mathcal{L} &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})\right)^2 - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{v}\right) - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\left(\frac{1}{m-1}\sum_{k=1}^{m}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\right)\boldsymbol{v} - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} - \lambda\left(\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v}-1\right)
\end{aligned}$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla}\mathcal{L} = 2(\mathbf{C}\,\boldsymbol{v} - \lambda\,\boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

Direction of Maximum Variation

- Expanding the Lagrangian

$$\begin{aligned}
\mathcal{L} &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})\right)^2 - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{v}\right) - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\left(\frac{1}{m-1}\sum_{k=1}^{m}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\right)\boldsymbol{v} - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\
&= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} - \lambda\left(\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v}-1\right)
\end{aligned}$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla}\mathcal{L} = 2(\mathbf{C}\,\boldsymbol{v} - \lambda\,\boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

Direction of Maximum Variation

- Expanding the Lagrangian

$$\begin{aligned}
\mathcal{L} &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})\right)^2 - \lambda\left(\|\boldsymbol{v}\|^2-1\right) \\
&= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{v}\right) - \lambda\left(\|\boldsymbol{v}\|^2-1\right) \\
&= \boldsymbol{v}^{\mathsf{T}}\left(\frac{1}{m-1}\sum_{k=1}^{m}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\right)\boldsymbol{v} - \lambda\left(\|\boldsymbol{v}\|^2-1\right) \\
&= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} - \lambda\left(\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v}-1\right)
\end{aligned}$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla}\mathcal{L} = 2(\mathbf{C}\,\boldsymbol{v} - \lambda\,\boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

Direction of Maximum Variation

- Expanding the Lagrangian

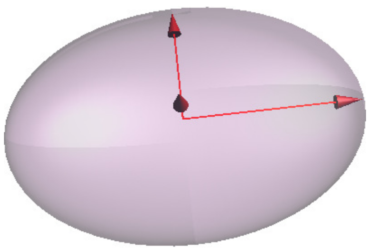
$$\begin{aligned}\mathcal{L} &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})\right)^2 - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\ &= \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{v}\right) - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\ &= \boldsymbol{v}^{\mathsf{T}}\left(\frac{1}{m-1}\sum_{k=1}^{m}(\boldsymbol{x}_k-\boldsymbol{\mu})(\boldsymbol{x}_k-\boldsymbol{\mu})^{\mathsf{T}}\right)\boldsymbol{v} - \lambda\left(\|\boldsymbol{v}\|^2-1\right)\\ &= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} - \lambda\left(\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v}-1\right)\end{aligned}$$

- Extrema of the Lagrangian

$$\boldsymbol{\nabla}\mathcal{L} = 2(\mathbf{C}\,\boldsymbol{v} - \lambda\,\boldsymbol{v}) = 0 \qquad \Rightarrow \qquad \mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

Direction of Maximum Variation

- The eigenvectors are directions that are extrema of the variance



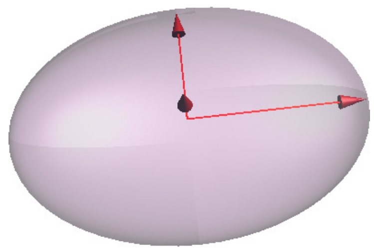
- The variance in direction $\boldsymbol{v}$ is equal to

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^\mathsf{T} (\boldsymbol{x}_i - \boldsymbol{\mu}) \right)^2$$
$$= \boldsymbol{v}^\mathsf{T} \mathbf{C} \boldsymbol{v} = \lambda \boldsymbol{v}^\mathsf{T} \boldsymbol{v} = \lambda$$

- The variance is maximised by the eigenvector with the maximum eigenvalue

Direction of Maximum Variation

- The eigenvectors are directions that are extrema of the variance



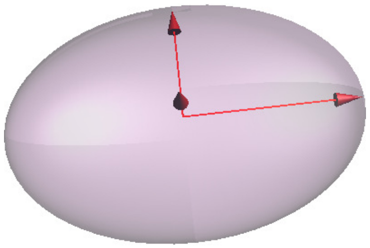
- The variance in direction $\boldsymbol{v}$ is equal to

$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^\mathsf{T} (\boldsymbol{x}_i - \boldsymbol{\mu}) \right)^2$$
$$= \boldsymbol{v}^\mathsf{T} \mathbf{C} \boldsymbol{v} = \lambda \boldsymbol{v}^\mathsf{T} \boldsymbol{v} = \lambda$$

- The variance is maximised by the eigenvector with the maximum eigenvalue

Direction of Maximum Variation

- The eigenvectors are directions that are extrema of the variance



- The variance in direction $\boldsymbol{v}$ is equal to

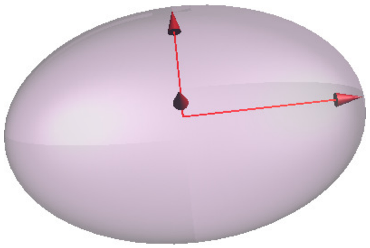
$$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu})\right)^2$$

$$= \boldsymbol{v}^{\mathsf{T}} \mathbf{C} \boldsymbol{v} = \lambda \boldsymbol{v}^{\mathsf{T}} \boldsymbol{v} = \lambda$$

- The variance is maximised by the eigenvector with the maximum eigenvalue

Direction of Maximum Variation

- The eigenvectors are directions that are extrema of the variance



- The variance in direction $\boldsymbol{v}$ is equal to

$$\sigma^2 = \frac{1}{m-1}\sum_{i=1}^{m}\left(\boldsymbol{v}^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu})\right)^2$$
$$= \boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} = \lambda \boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda$$

- The variance is maximised by the eigenvector with the maximum eigenvalue

Covariance Matrix

- The **covariance matrix** is defined as

$$\mathbf{C} = \frac{1}{m-1} \sum_{k=1}^{m} (\boldsymbol{x}_k - \boldsymbol{\mu}) (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}$$

- The components C_{ij} measure how the i^{th} and j^{th} components co-vary

$$C_{ij} = \frac{1}{m-1} \sum_{k=1}^{m} (x_{ik} - \mu_i) (x_{jk} - \mu_j)$$

- C.f. covariance of random variables

$$\mathrm{Cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X]) (Y - \mathbb{E}[Y])]$$

Covariance Matrix

- The **covariance matrix** is defined as

$$\mathbf{C} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right) \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right)^{\mathsf{T}}$$

- The components C_{ij} measure how the i^{th} and j^{th} components co-vary

$$C_{ij} = \frac{1}{m-1} \sum_{k=1}^{m} \left(x_{ik} - \mu_i\right) \left(x_{jk} - \mu_j\right)$$

- C.f. covariance of random variables

$$\mathrm{Cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])\,(Y - \mathbb{E}[Y])]$$

Covariance Matrix

- The **covariance matrix** is defined as

$$\mathbf{C} = \frac{1}{m-1}\sum_{k=1}^{m}\left(\boldsymbol{x}_k - \boldsymbol{\mu}\right)\left(\boldsymbol{x}_k - \boldsymbol{\mu}\right)^{\mathsf{T}}$$

- The components C_{ij} measure how the i^{th} and j^{th} components co-vary

$$C_{ij} = \frac{1}{m-1}\sum_{k=1}^{m}\left(x_{ik} - \mu_i\right)\left(x_{jk} - \mu_j\right)$$

- C.f. covariance of random variables

$$\mathrm{Cov}(X,Y) = \mathbb{E}[(X - \mathbb{E}[X])\,(Y - \mathbb{E}[Y])]$$

Outer Product

- Remember that the outer-product of two vectors is defined as

$$\boldsymbol{x}\,\boldsymbol{y}^{\mathsf{T}} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix} = \begin{pmatrix} x_1\,y_1 & x_1\,y_2 & \cdots & x_1\,y_n \\ x_2\,y_1 & x_2\,y_2 & \cdots & x_2\,y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n\,y_1 & x_n\,y_2 & \cdots & x_n\,y_n \end{pmatrix}$$

- C.f. Inner product

$$\boldsymbol{x}^{\mathsf{T}}\,\boldsymbol{y} = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = x_1\,y_1 + x_2\,y_2 + \cdots + x_n\,y_n$$

Outer Product

- Remember that the outer-product of two vectors is defined as

$$\boldsymbol{x}\,\boldsymbol{y}^{\mathsf{T}} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix} = \begin{pmatrix} x_1\,y_1 & x_1\,y_2 & \cdots & x_1\,y_n \\ x_2\,y_1 & x_2\,y_2 & \cdots & x_2\,y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n\,y_1 & x_n\,y_2 & \cdots & x_n\,y_n \end{pmatrix}$$

- C.f. Inner product

$$\boldsymbol{x}^{\mathsf{T}}\,\boldsymbol{y} = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = x_1\,y_1 + x_2\,y_2 + \cdots + x_n\,y_n$$

Outer Product

- Remember that the outer-product of two vectors is defined as

$$\boldsymbol{x}\,\boldsymbol{y}^{\mathsf{T}} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix} = \begin{pmatrix} x_1\,y_1 & x_1\,y_2 & \cdots & x_1\,y_n \\ x_2\,y_1 & x_2\,y_2 & \cdots & x_2\,y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n\,y_1 & x_n\,y_2 & \cdots & x_n\,y_n \end{pmatrix}$$

- C.f. Inner product

$$\boldsymbol{x}^{\mathsf{T}}\boldsymbol{y} = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = x_1\,y_1 + x_2\,y_2 + \cdots + x_n\,y_n$$

Outer Product

- Remember that the outer-product of two vectors is defined as

$$\boldsymbol{x}\,\boldsymbol{y}^{\mathsf{T}} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix} = \begin{pmatrix} x_1\,y_1 & x_1\,y_2 & \cdots & x_1\,y_n \\ x_2\,y_1 & x_2\,y_2 & \cdots & x_2\,y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n\,y_1 & x_n\,y_2 & \cdots & x_n\,y_n \end{pmatrix}$$

- C.f. Inner product

$$\boldsymbol{x}^{\mathsf{T}}\,\boldsymbol{y} = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = x_1\,y_1 + x_2\,y_2 + \cdots + x_n\,y_n$$

Matrix Form

- The covariance matrix is

$$\mathbf{C} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right) \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right)^{\mathsf{T}}$$

- Define the matrix

$$\mathbf{X} = \frac{1}{\sqrt{m-1}} \left(\boldsymbol{x}_1 - \boldsymbol{\mu}, \boldsymbol{x}_2 - \boldsymbol{\mu}, \cdots \boldsymbol{x}_m - \boldsymbol{\mu}\right)$$

- We can write the covariance matrix as

$$\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$$

Matrix Form

- The covariance matrix is

$$\mathbf{C} = \frac{1}{m-1} \sum_{k=1}^{m} (\boldsymbol{x}_k - \boldsymbol{\mu}) (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}$$

- Define the matrix

$$\mathbf{X} = \frac{1}{\sqrt{m-1}} (\boldsymbol{x}_1 - \boldsymbol{\mu}, \boldsymbol{x}_2 - \boldsymbol{\mu}, \cdots \boldsymbol{x}_m - \boldsymbol{\mu})$$

- We can write the covariance matrix as

$$\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$$

Matrix Form

- The covariance matrix is

$$\mathbf{C} = \frac{1}{m-1} \sum_{k=1}^{m} \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right) \left(\boldsymbol{x}_k - \boldsymbol{\mu}\right)^{\mathsf{T}}$$

- Define the matrix

$$\mathbf{X} = \frac{1}{\sqrt{m-1}} \left(\boldsymbol{x}_1 - \boldsymbol{\mu}, \boldsymbol{x}_2 - \boldsymbol{\mu}, \cdots \boldsymbol{x}_m - \boldsymbol{\mu}\right)$$

- We can write the covariance matrix as

$$\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$$

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^\mathsf{T}\mathbf{M}\boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^\mathsf{T}\mathbf{C}\boldsymbol{v} = \boldsymbol{v}^\mathsf{T}\mathbf{X}\mathbf{X}^\mathsf{T}\boldsymbol{v} = \boldsymbol{u}^\mathsf{T}\boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

where $\boldsymbol{u} = \mathbf{X}^\mathsf{T}\boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{M} \boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{C} \boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}} \mathbf{X} \mathbf{X}^{\mathsf{T}} \boldsymbol{v} = \boldsymbol{u}^{\mathsf{T}} \boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

  where $\boldsymbol{u} = \mathbf{X}^{\mathsf{T}} \boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{M}\boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}}\mathbf{X}\mathbf{X}^{\mathsf{T}}\boldsymbol{v} = \boldsymbol{u}^{\mathsf{T}}\boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

  where $\boldsymbol{u} = \mathbf{X}^{\mathsf{T}}\boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{M} \boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{C} \boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}} \mathbf{X} \mathbf{X}^{\mathsf{T}} \boldsymbol{v} = \boldsymbol{u}^{\mathsf{T}} \boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

  where $\boldsymbol{u} = \mathbf{X}^{\mathsf{T}} \boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{M}\boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}}\mathbf{X}\mathbf{X}^{\mathsf{T}}\boldsymbol{v} = \boldsymbol{u}^{\mathsf{T}}\boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

where $\boldsymbol{u} = \mathbf{X}^{\mathsf{T}}\boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Properties of Covariance Matrix

- The **quadratic form** of a vector and matrix is defined as

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{M} \boldsymbol{v}$$

- The quadratic form of a covariance matrix is non-negative for any vector

$$\boldsymbol{v}^{\mathsf{T}} \mathbf{C} \boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}} \mathbf{X} \mathbf{X}^{\mathsf{T}} \boldsymbol{v} = \boldsymbol{u}^{\mathsf{T}} \boldsymbol{u} = \|\boldsymbol{u}\|^2 \geq 0$$

  where $\boldsymbol{u} = \mathbf{X}^{\mathsf{T}} \boldsymbol{v}$

- Matrices with non-negative quadratic forms are known as **positive semi-definite**

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^\mathsf{T}$

$$\boldsymbol{v}^\mathsf{T}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^\mathsf{T}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^\mathsf{T}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^\mathsf{T}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Eigenvalue Decomposition

- The eigenvectors of $\mathbf{C}$ with the largest eigenvalues are known as the **principal components**
- The eigenvalues are all greater than or equal to zero
- Recall an eigenvector $\boldsymbol{v}$ satisfies the equation

$$\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- Multiplying both sides by $\boldsymbol{v}^{\mathsf{T}}$

$$\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v} = \lambda\,\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} = \lambda\|\boldsymbol{v}\|^2$$

but $\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\boldsymbol{v} \geq 0$ and $\|\boldsymbol{v}\|^2 > 0$ so

$$\lambda = \frac{\boldsymbol{v}^{\mathsf{T}}\mathbf{C}\,\boldsymbol{v}}{\|\boldsymbol{v}\|^2} \geq 0$$

Surface Defined by Matrix

- The set of vectors $\boldsymbol{x}$ such that

$$\boldsymbol{x}^{\mathsf{T}}\mathbf{C}^{-1}\boldsymbol{x} = 1$$

  defines a surface

- The surface is an ellipsoid, $\mathcal{E}$

- The eigenvectors point in the direction of the principal axes of the ellipsoid

- The radii of the principal axes are equal to the square root of the eigenvalues

Surface Defined by Matrix

- The set of vectors $\boldsymbol{x}$ such that

$$\boldsymbol{x}^{\mathsf{T}} \mathbf{C}^{-1} \boldsymbol{x} = 1$$

  defines a surface

- The surface is an ellipsoid, $\mathcal{E}$

- The eigenvectors point in the direction of the principal axes of the ellipsoid

- The radii of the principal axes are equal to the square root of the eigenvalues

Surface Defined by Matrix

- The set of vectors $\boldsymbol{x}$ such that

$$\boldsymbol{x}^{\mathsf{T}}\mathbf{C}^{-1}\boldsymbol{x} = 1$$

  defines a surface

- The surface is an ellipsoid, $\mathcal{E}$

- The eigenvectors point in the direction of the principal axes of the ellipsoid

- The radii of the principal axes are equal to the square root of the eigenvalues

Surface Defined by Matrix

- The set of vectors $\boldsymbol{x}$ such that

$$\boldsymbol{x}^{\mathsf{T}}\mathbf{C}^{-1}\boldsymbol{x} = 1$$

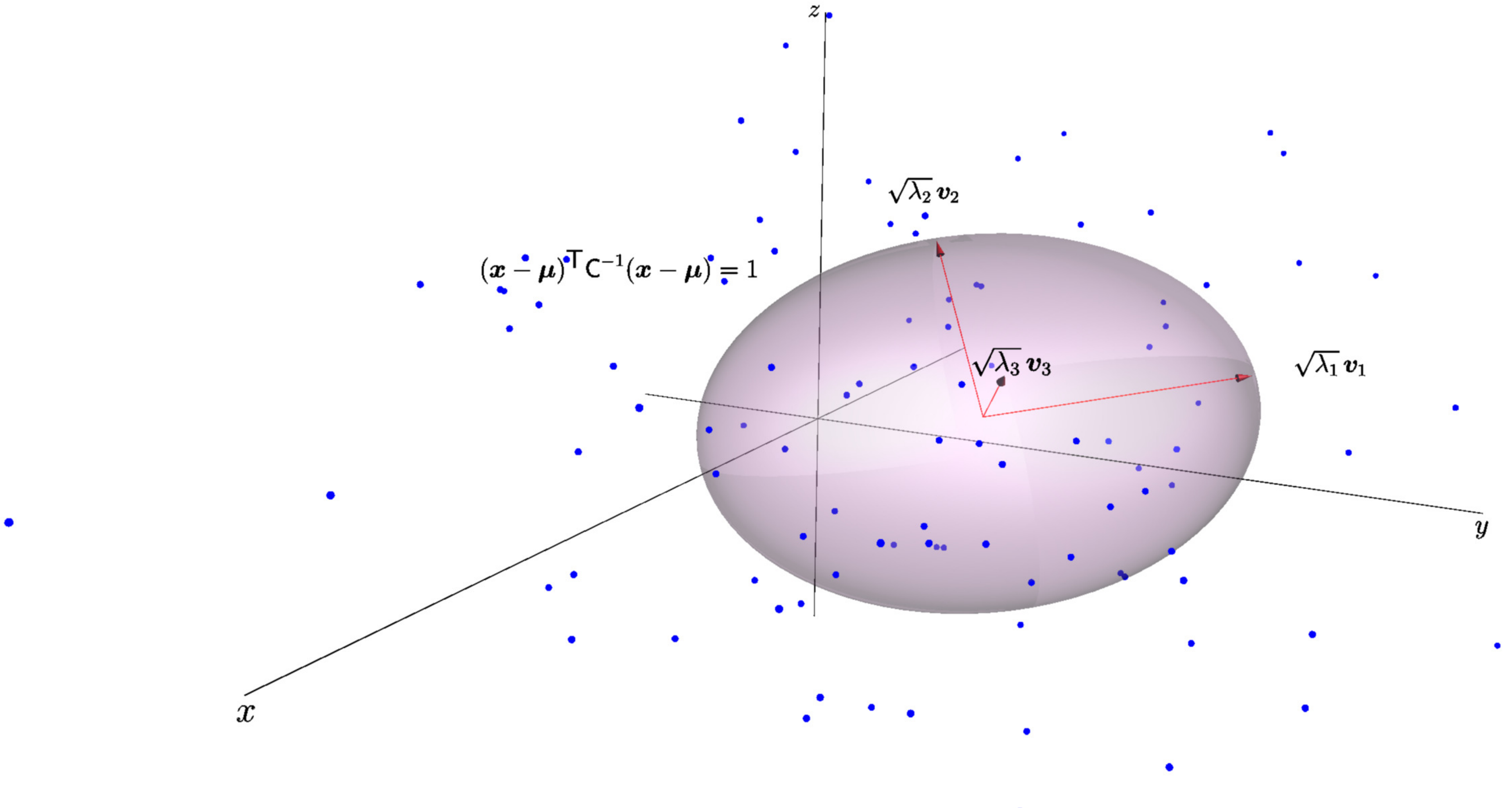
  defines a surface

- The surface is an ellipsoid, $\mathcal{E}$

- The eigenvectors point in the direction of the principal axes of the ellipsoid

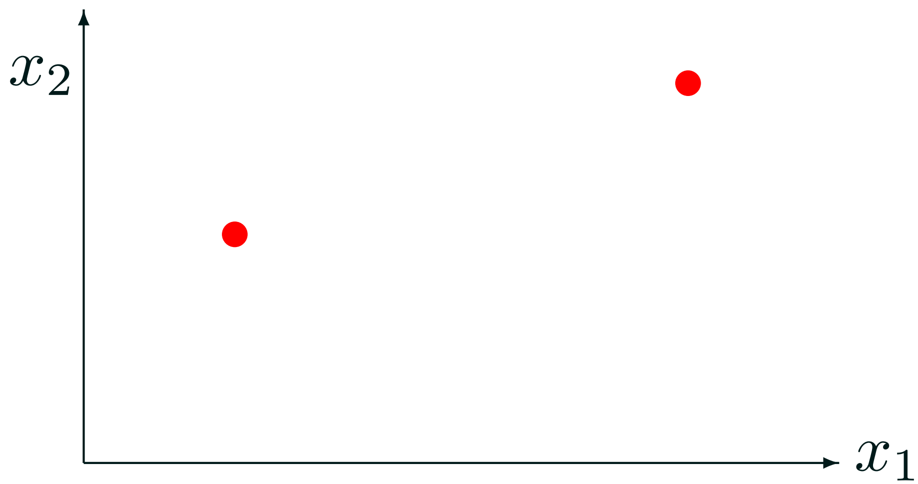
- The radii of the principal axes are equal to the square root of the eigenvalues

Ellipsoid and Eigen Space



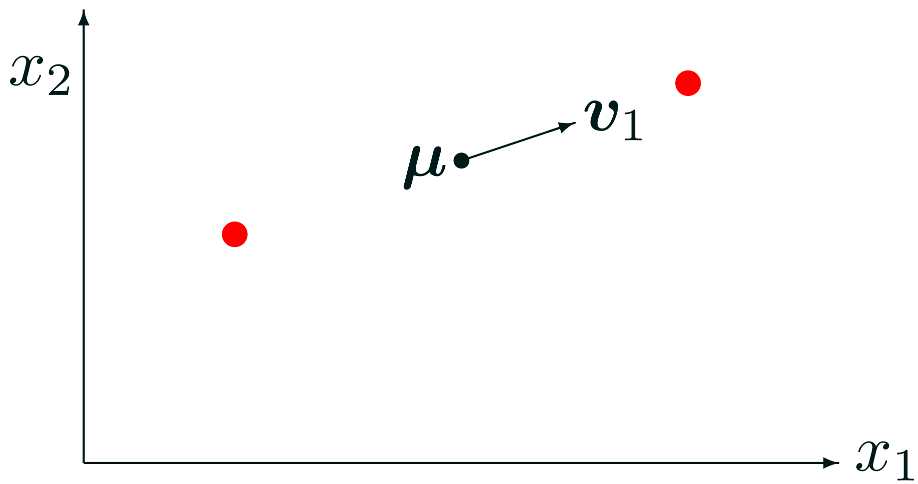
Spanning Input Space

- A covariance matrix will have a zero eigenvalue only if there is no variation in the direction of the corresponding eigenvector
- A covariance matrix will have zero eigenvalues if the number of patterns are less than or equal to the number of dimensions



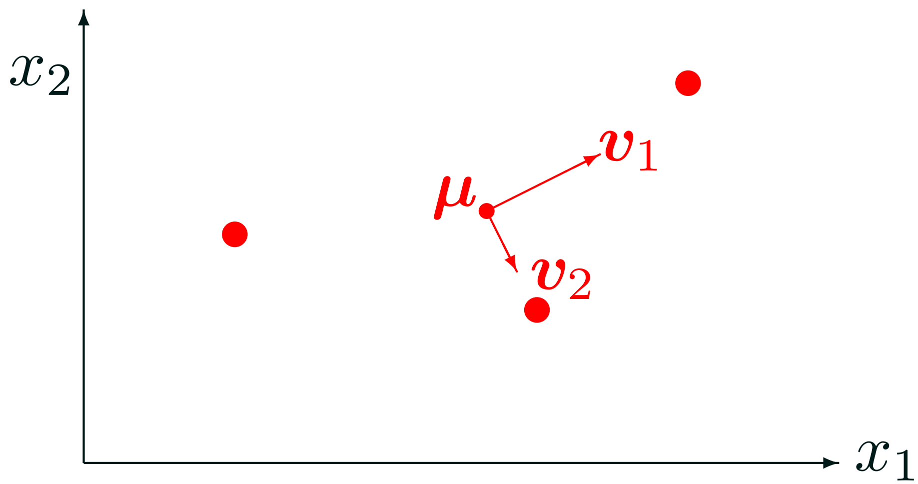
Spanning Input Space

- A covariance matrix will have a zero eigenvalue only if there is no variation in the direction of the corresponding eigenvector
- A covariance matrix will have zero eigenvalues if the number of patterns are less than or equal to the number of dimensions



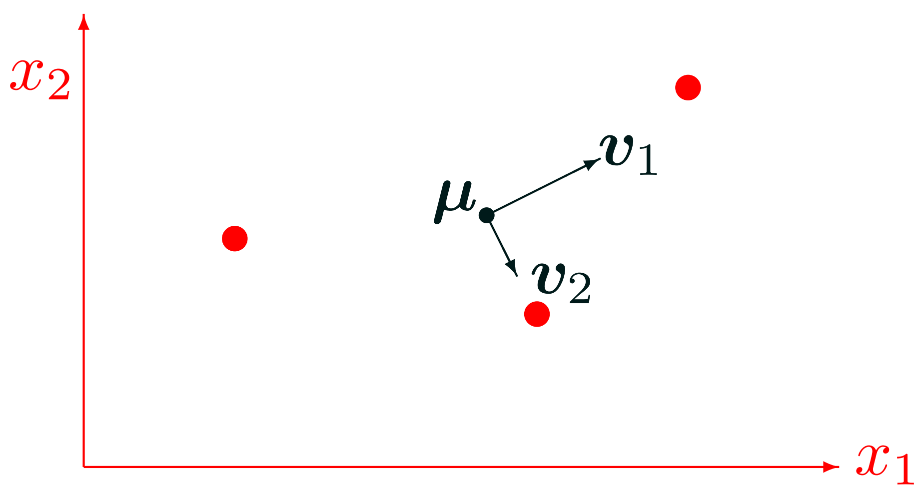
Spanning Input Space

- A covariance matrix will have a zero eigenvalue only if there is no variation in the direction of the corresponding eigenvector
- A covariance matrix will have zero eigenvalues if the number of patterns are less than or equal to the number of dimensions
- A covariance matrix formed from $m+1$ patterns that are linearly independent (i.e. you cannot form any one out of m of the other patterns) will have no zero eigenvalues



Spanning Input Space

- A covariance matrix will have a zero eigenvalue only if there is no variation in the direction of the corresponding eigenvector
- A covariance matrix will have zero eigenvalues if the number of patterns are less than or equal to the number of dimensions
- A covariance matrix formed from $m+1$ patterns that are linearly independent (i.e. you cannot form any one out of m of the other patterns) will have no zero eigenvalues



Positive Definite

- Matrices with no zero eigenvalues are called **full rank** matrices (as opposed to rank deficient)
- Full rank matrices are invertible, rank deficient matrices are singular and non-invertible
- Full rank covariance matrices have positive eigenvalues only and are said to be **positive definite**
- We would expect that when $m > p$ the covariance matrix will be positive definite (unless there are some symmetries that linearly constrain the patterns)

Positive Definite

- Matrices with no zero eigenvalues are called **full rank** matrices (as opposed to rank deficient)
- Full rank matrices are invertible, rank deficient matrices are singular and non-invertible
- Full rank covariance matrices have positive eigenvalues only and are said to be **positive definite**
- We would expect that when $m > p$ the covariance matrix will be positive definite (unless there are some symmetries that linearly constrain the patterns)

Positive Definite

- Matrices with no zero eigenvalues are called **full rank** matrices (as opposed to rank deficient)

- Full rank matrices are invertible, rank deficient matrices are singular and non-invertible

- Full rank covariance matrices have positive eigenvalues only and are said to be **positive definite**

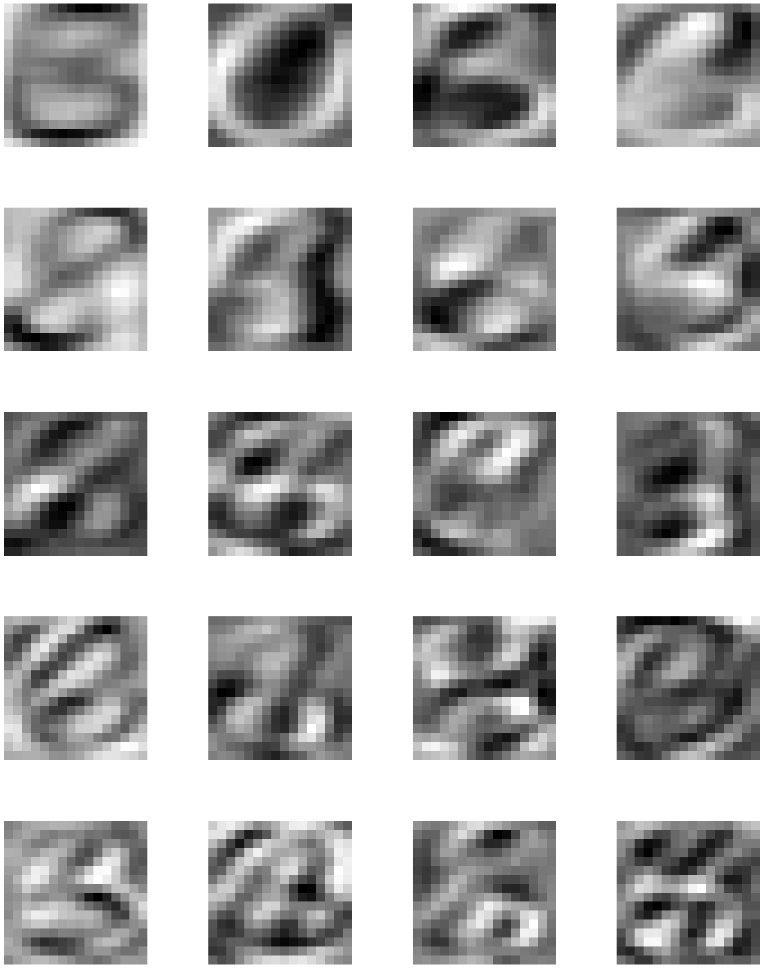
- We would expect that when $m > p$ the covariance matrix will be positive definite (unless there are some symmetries that linearly constrain the patterns)

Positive Definite

- Matrices with no zero eigenvalues are called **full rank** matrices (as opposed to rank deficient)
- Full rank matrices are invertible, rank deficient matrices are singular and non-invertible
- Full rank covariance matrices have positive eigenvalues only and are said to be **positive definite**
- We would expect that when $m > p$ the covariance matrix will be positive definite (unless there are some symmetries that linearly constrain the patterns)

Outline

1. Covariance Matrices
2. **Principal Component Analysis**
3. Duality



Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Principal Component Analysis

- PCA occurs as follows
  - ⋆ Construct the covariance matrix
  - ⋆ Find the eigenvalues and eigenvectors
  - ⋆ Keep the eigenvectors with the largest eigenvalues (principal components)
  - ⋆ Project the inputs into the space spanned by the principal components
- We then use the projected inputs as inputs to our learning machine

Projection Matrix

- To project the inputs construct the projection matrix

$$\mathbf{P} = \begin{pmatrix} \boldsymbol{v}_1^{\mathsf{T}} \\ \boldsymbol{v}_2^{\mathsf{T}} \\ \vdots \\ \boldsymbol{v}_k^{\mathsf{T}} \end{pmatrix}$$

- $k < p$ is the number of principal components we keep
- Given a p-dimensional input pattern $\boldsymbol{x}$ we can construct a k-dimensional pattern $\boldsymbol{z}$

$$\boldsymbol{z} = \mathbf{P}\left(\boldsymbol{x} - \boldsymbol{\mu}\right)$$

- Use $\boldsymbol{z}$ as our new inputs

Projection Matrix

- To project the inputs construct the projection matrix

$$\mathbf{P} = \begin{pmatrix} \boldsymbol{v}_1^\mathsf{T} \\ \boldsymbol{v}_2^\mathsf{T} \\ \vdots \\ \boldsymbol{v}_k^\mathsf{T} \end{pmatrix}$$

- $k < p$ is the number of principal components we keep
- Given a p-dimensional input pattern $\boldsymbol{x}$ we can construct a k-dimensional pattern $\boldsymbol{z}$

$$\boldsymbol{z} = \mathbf{P}\left(\boldsymbol{x} - \boldsymbol{\mu}\right)$$

- Use $\boldsymbol{z}$ as our new inputs

Projection Matrix

- To project the inputs construct the projection matrix

$$\mathbf{P} = \begin{pmatrix} \boldsymbol{v}_1^\mathsf{T} \\ \boldsymbol{v}_2^\mathsf{T} \\ \vdots \\ \boldsymbol{v}_k^\mathsf{T} \end{pmatrix}$$

- $k < p$ is the number of principal components we keep
- Given a p-dimensional input pattern $\boldsymbol{x}$ we can construct a k-dimensional pattern $\boldsymbol{z}$

$$\boldsymbol{z} = \mathbf{P}\left(\boldsymbol{x} - \boldsymbol{\mu}\right)$$

- Use $\boldsymbol{z}$ as our new inputs

Projection Matrix

- To project the inputs construct the projection matrix

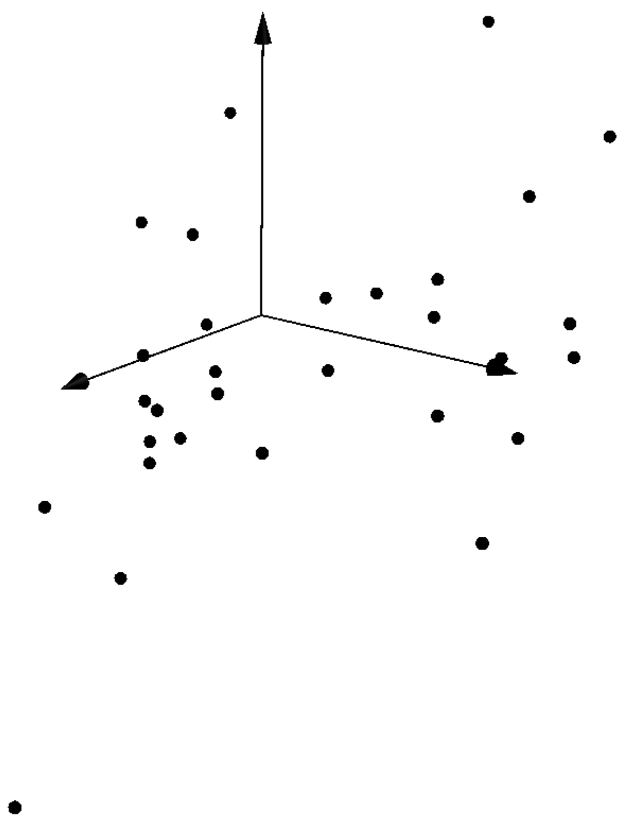
$$\mathbf{P} = \begin{pmatrix} \boldsymbol{v}_1^\mathsf{T} \\ \boldsymbol{v}_2^\mathsf{T} \\ \vdots \\ \boldsymbol{v}_k^\mathsf{T} \end{pmatrix}$$

- $k < p$ is the number of principal components we keep
- Given a p-dimensional input pattern $\boldsymbol{x}$ we can construct a k-dimensional pattern $\boldsymbol{z}$

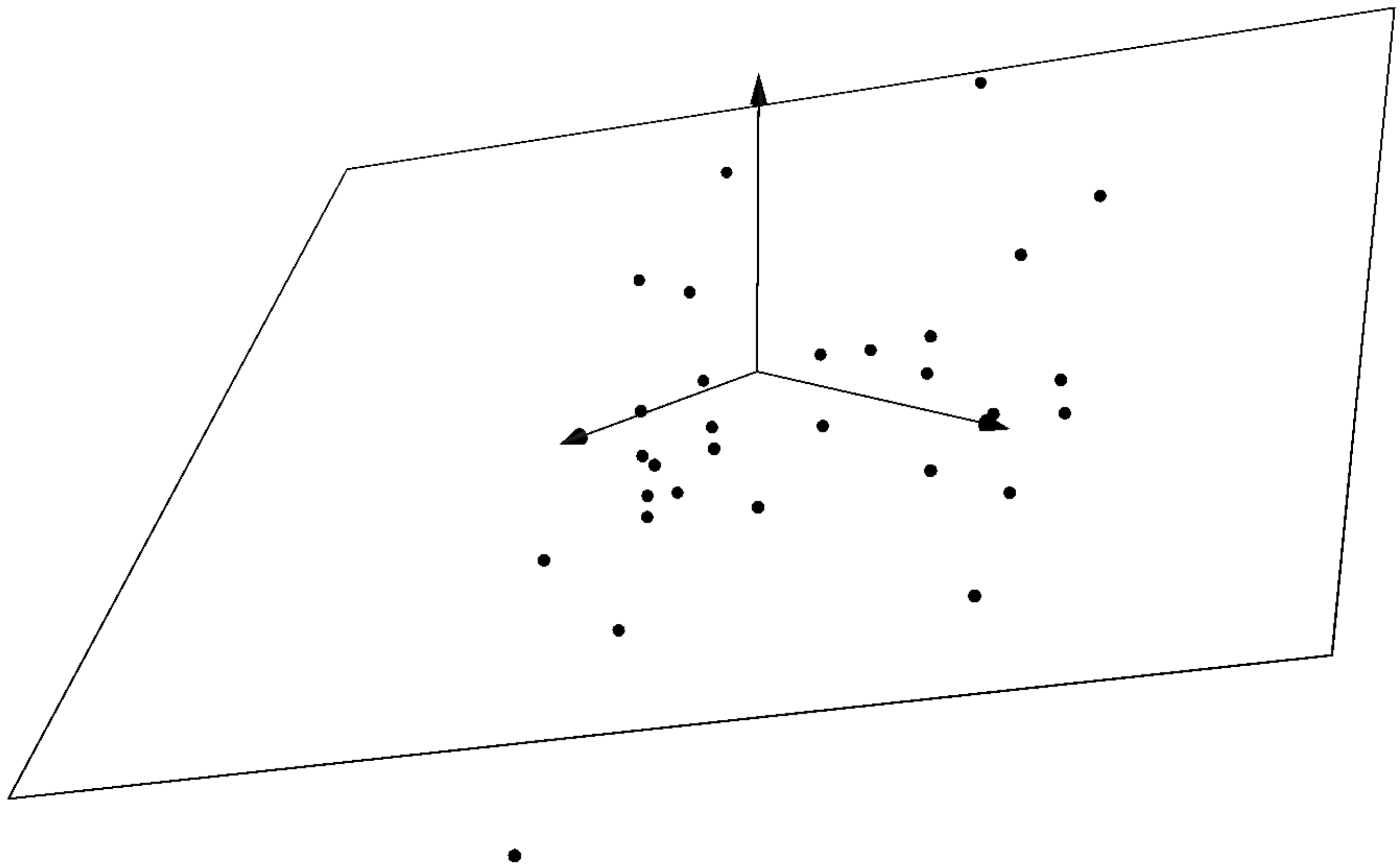
$$\boldsymbol{z} = \mathbf{P}\,(\boldsymbol{x} - \boldsymbol{\mu})$$

- Use $\boldsymbol{z}$ as our new inputs

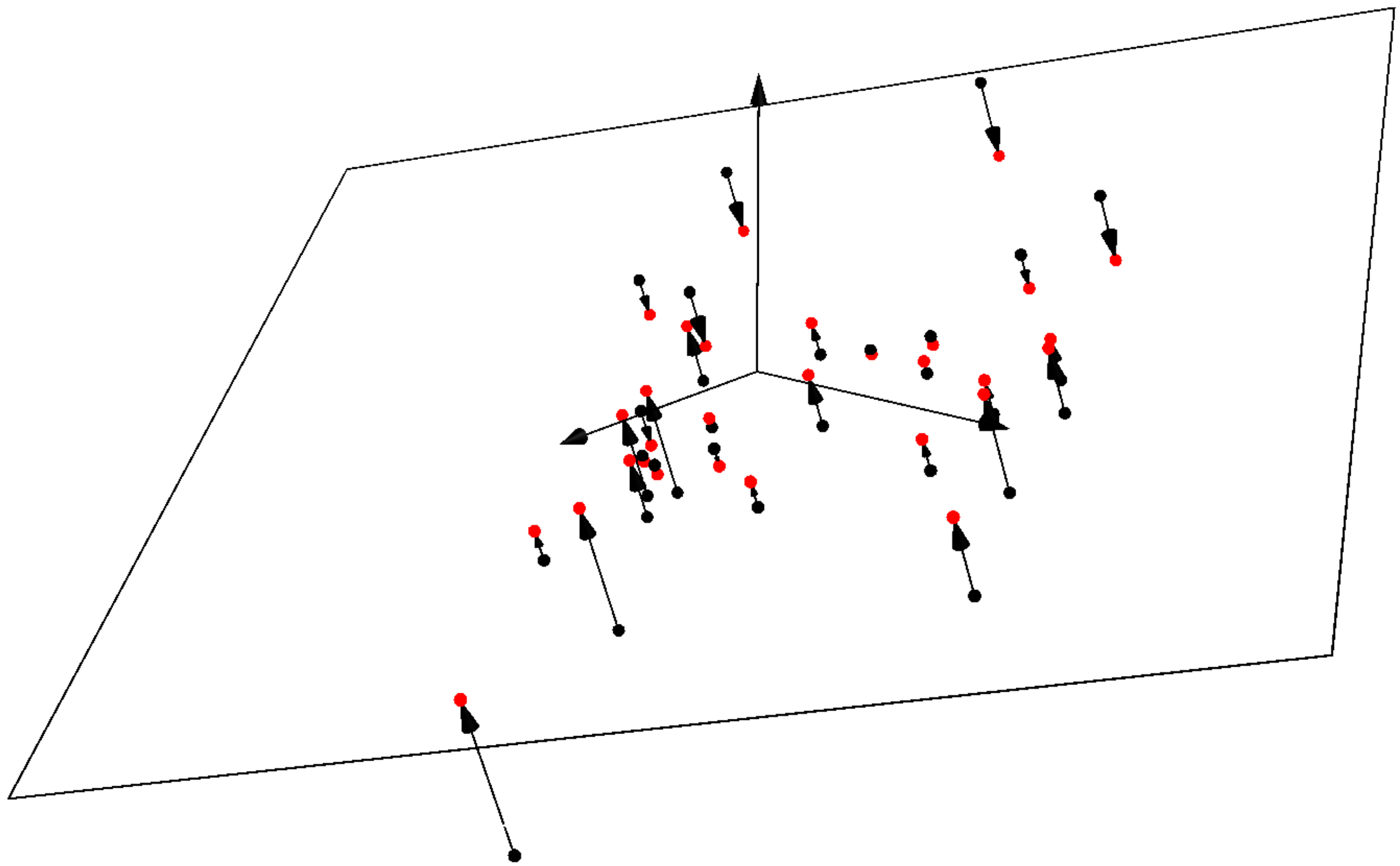
Subspace Projection



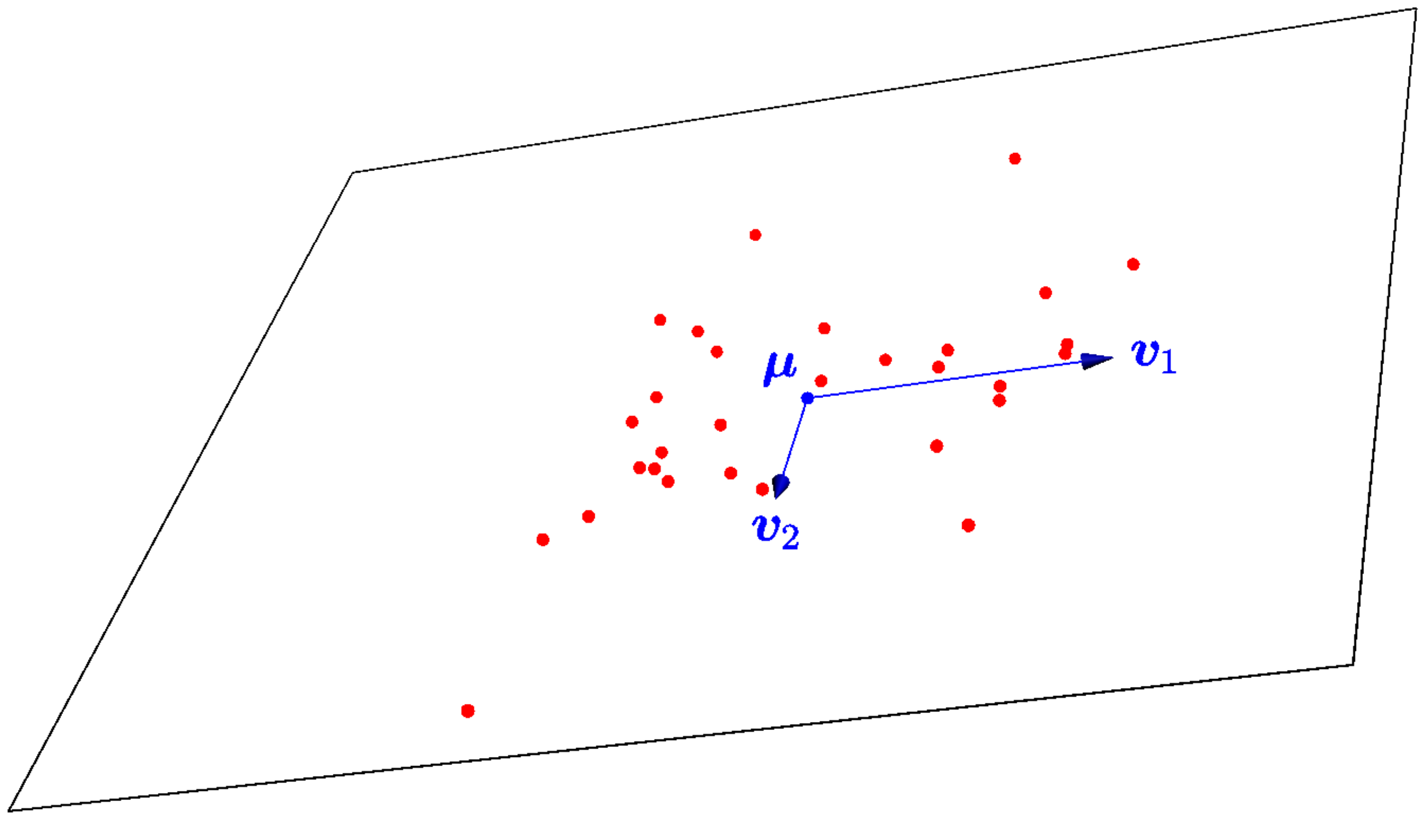
Subspace Projection



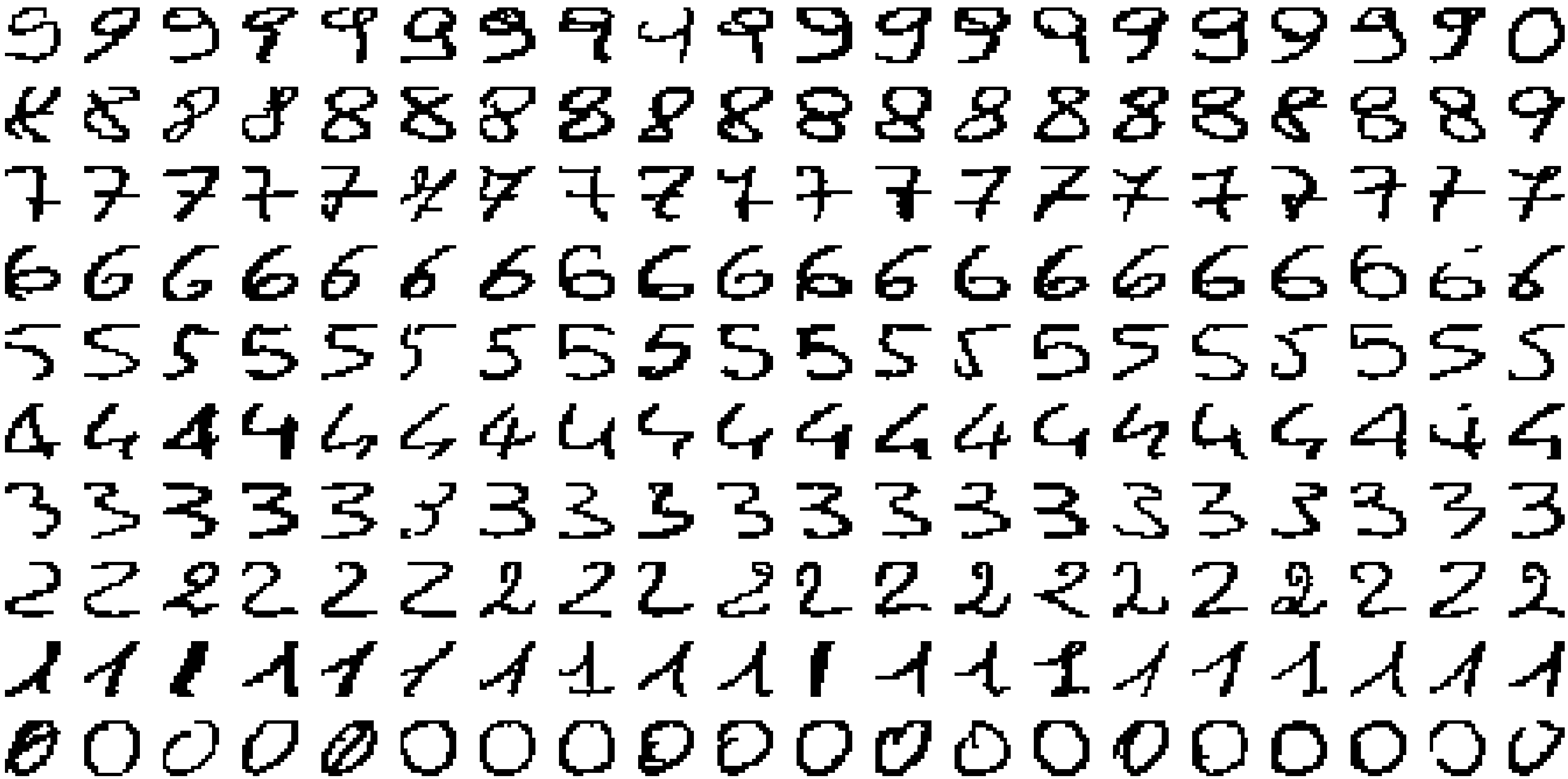
Subspace Projection



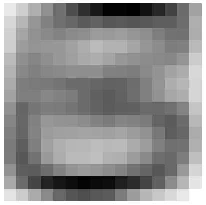
Subspace Projection

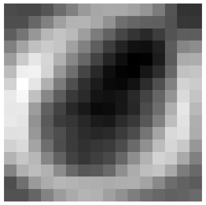


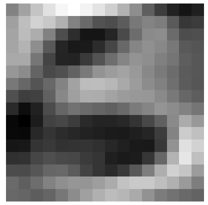
Hand Written Digits

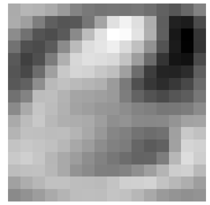


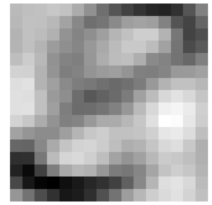
Eigenvectors

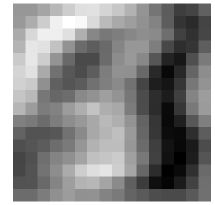

$\boldsymbol{\mu}$

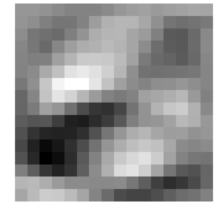

$\boldsymbol{v}_1$

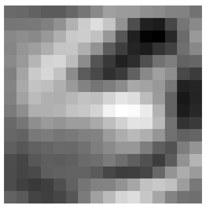

$\boldsymbol{v}_2$

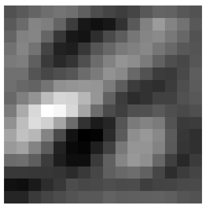

$\boldsymbol{v}_3$

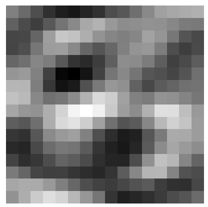

$\boldsymbol{v}_4$

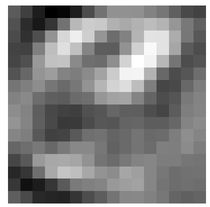

$\boldsymbol{v}_5$

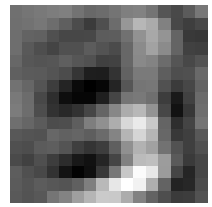

$\boldsymbol{v}_6$

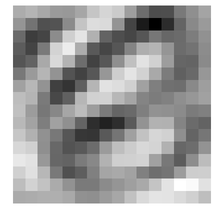

$\boldsymbol{v}_7$

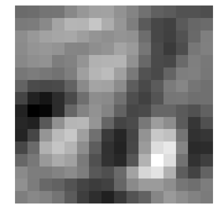

$\boldsymbol{v}_8$

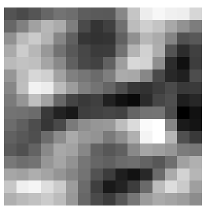

$\boldsymbol{v}_9$

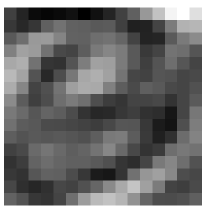

$\boldsymbol{v}_{10}$

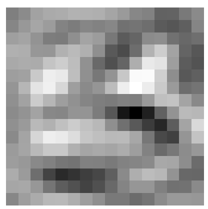

$\boldsymbol{v}_{11}$

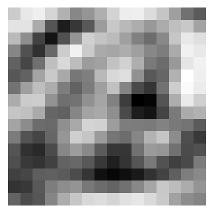

$\boldsymbol{v}_{12}$

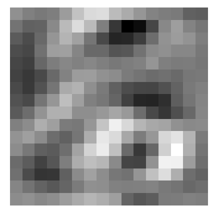

$\boldsymbol{v}_{13}$

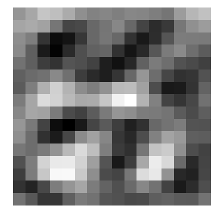

$\boldsymbol{v}_{14}$

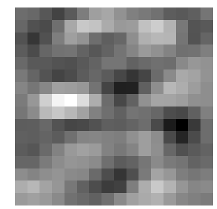

$\boldsymbol{v}_{15}$


$\boldsymbol{v}_{16}$


$\boldsymbol{v}_{17}$


$\boldsymbol{v}_{18}$


$\boldsymbol{v}_{19}$


$\boldsymbol{v}_{20}$

Reconstruction

- Projecting into a subspace of eigenvectors can be seen as approximating the inputs by

$$\hat{\boldsymbol{x}}_i = \boldsymbol{\mu} + \sum_{j=1}^{m} z_j^i \boldsymbol{v}_j, \qquad z_j^i = \boldsymbol{v}_j^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu}), \qquad \|\boldsymbol{v}_j\| = 1$$

- Principle component analysis projects the data into a subspace of size m with the minimal approximation error $\mathbb{E}\left[\|\hat{\boldsymbol{x}}_i - \boldsymbol{x}_i\|^2\right]$

- The loss of "energy" is equal to the sum of the eigenvalues in the directions that are ignored

Reconstruction

- Projecting into a subspace of eigenvectors can be seen as approximating the inputs by

$$\hat{\boldsymbol{x}}_i = \boldsymbol{\mu} + \sum_{j=1}^{m} z_j^i \boldsymbol{v}_j, \qquad z_j^i = \boldsymbol{v}_j^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu}), \qquad \|\boldsymbol{v}_j\| = 1$$

- Principle component analysis projects the data into a subspace of size m with the minimal approximation error $\mathbb{E}\left[\|\hat{\boldsymbol{x}}_i - \boldsymbol{x}_i\|^2\right]$

- The loss of "energy" is equal to the sum of the eigenvalues in the directions that are ignored

Reconstruction

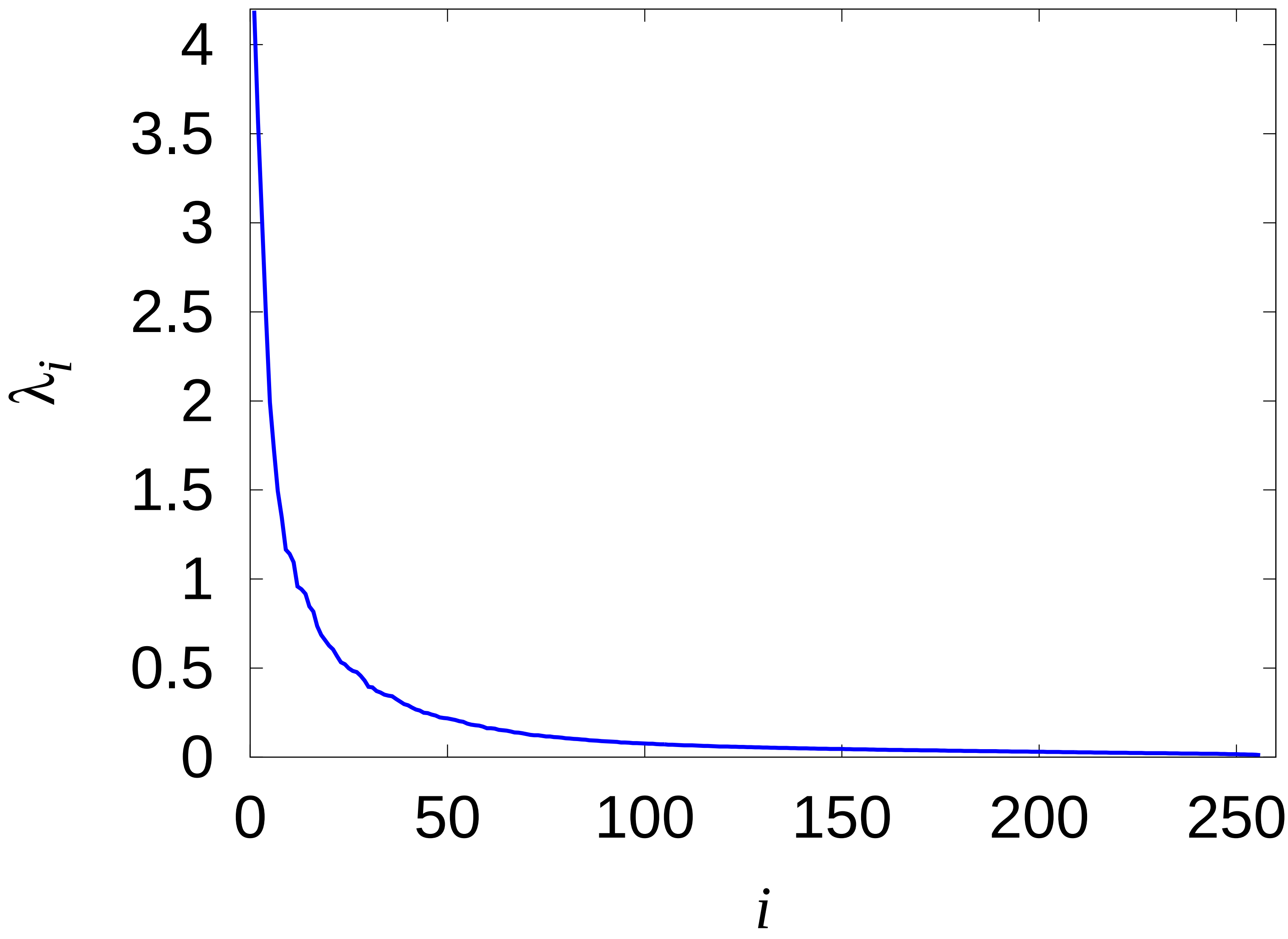
- Projecting into a subspace of eigenvectors can be seen as approximating the inputs by

$$\hat{\boldsymbol{x}}_i = \boldsymbol{\mu} + \sum_{j=1}^{m} z_j^i \boldsymbol{v}_j, \qquad z_j^i = \boldsymbol{v}_j^{\mathsf{T}}(\boldsymbol{x}_i - \boldsymbol{\mu}), \qquad \|\boldsymbol{v}_j\| = 1$$

- Principle component analysis projects the data into a subspace of size m with the minimal approximation error $\mathbb{E}\left[\|\hat{\boldsymbol{x}}_i - \boldsymbol{x}_i\|^2\right]$

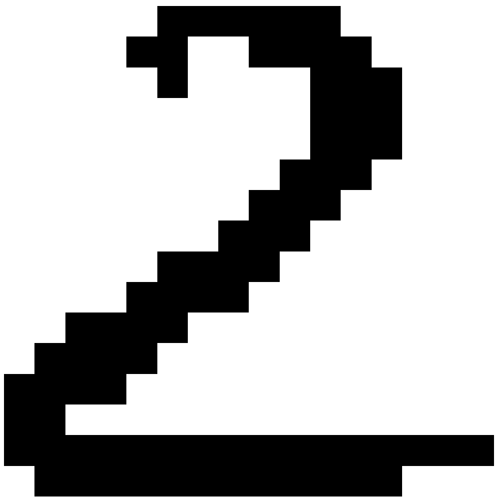
- The loss of "energy" is equal to the sum of the eigenvalues in the directions that are ignored

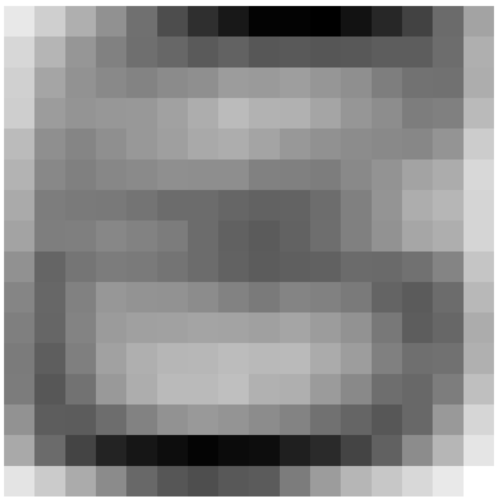
Eigenvalues for Digits



Reconstruction from Eigenvectors

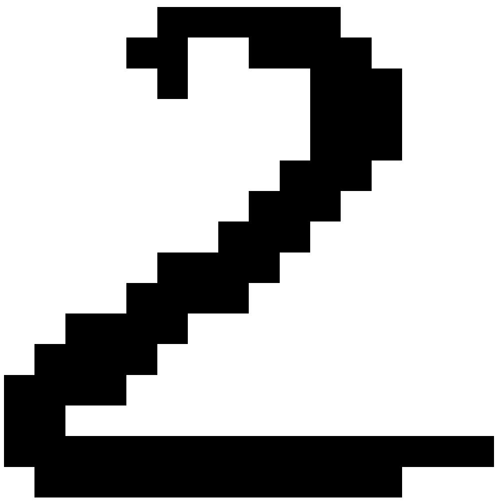
1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

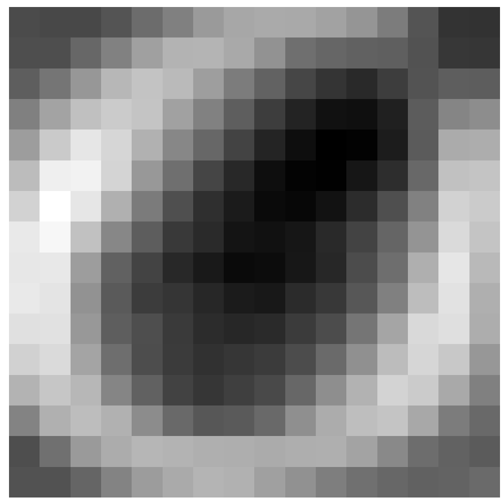


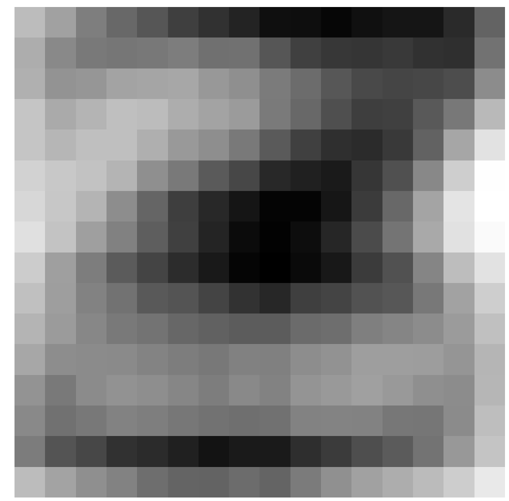


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

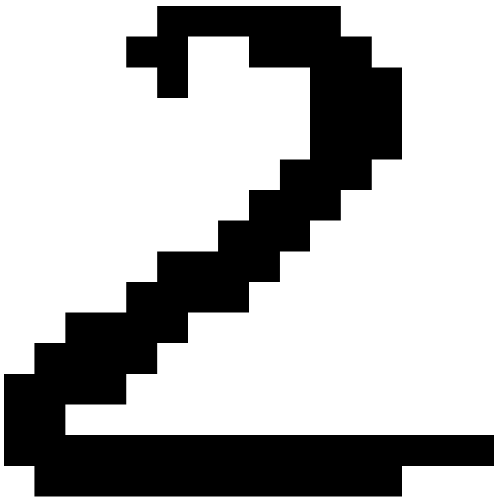
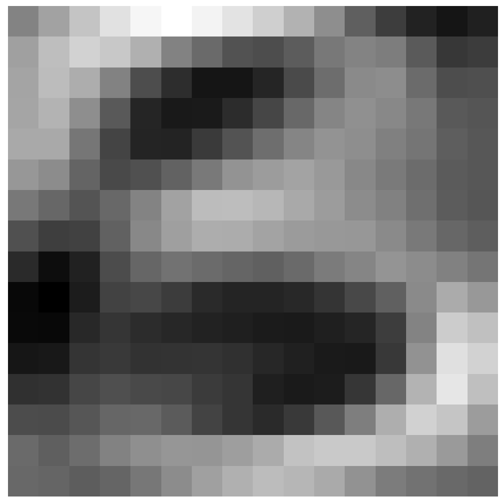
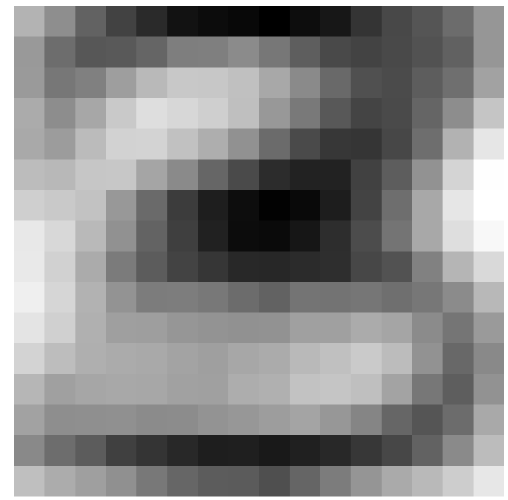






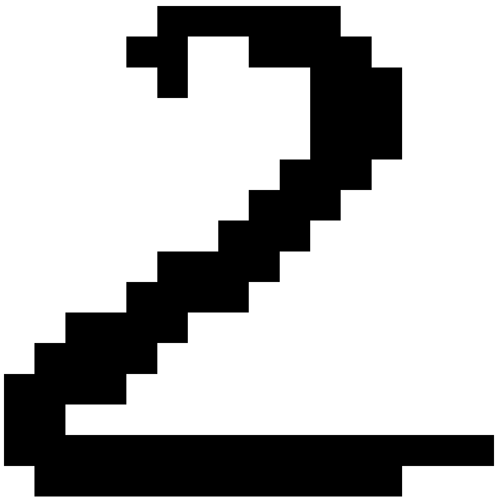
Reconstruction from Eigenvectors

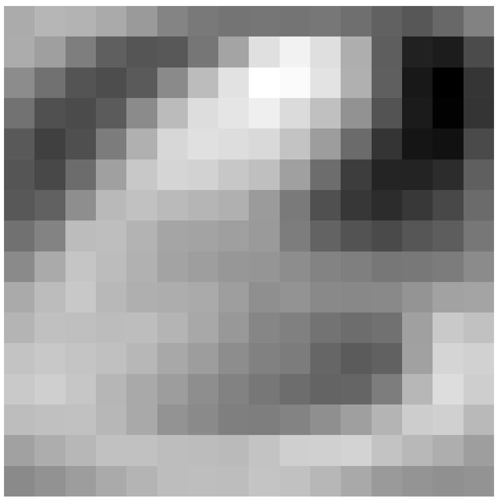
1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

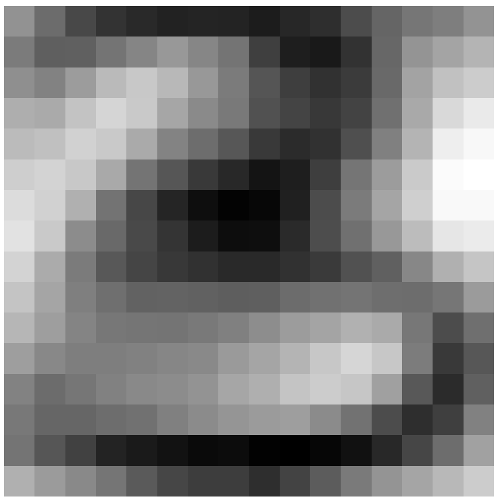




Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

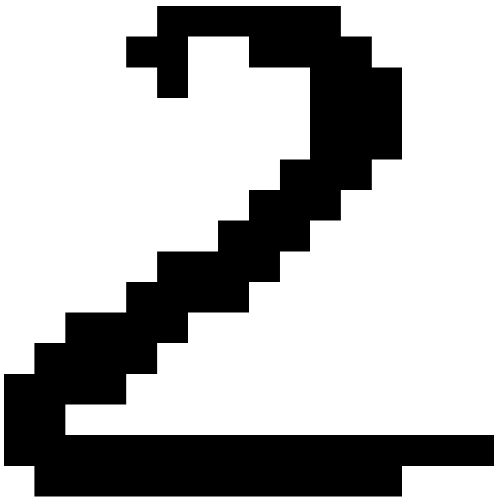


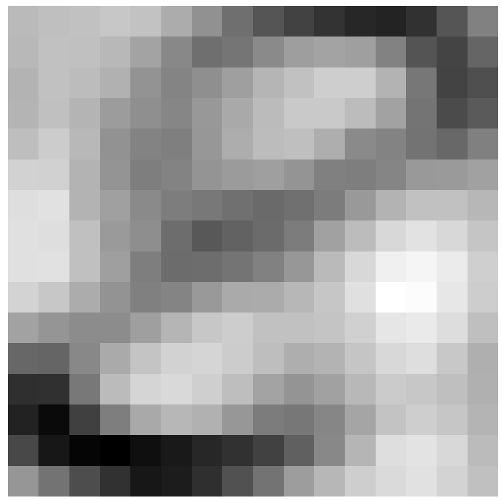


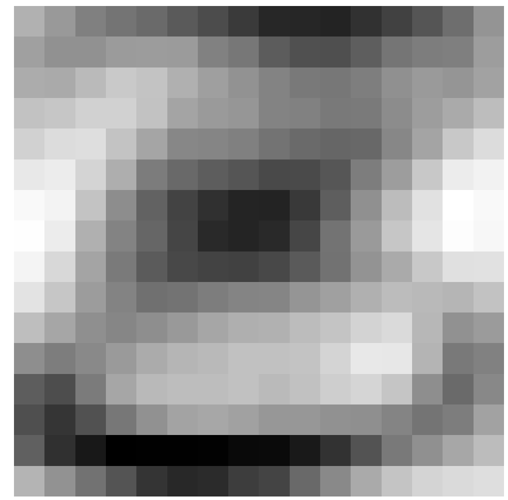


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

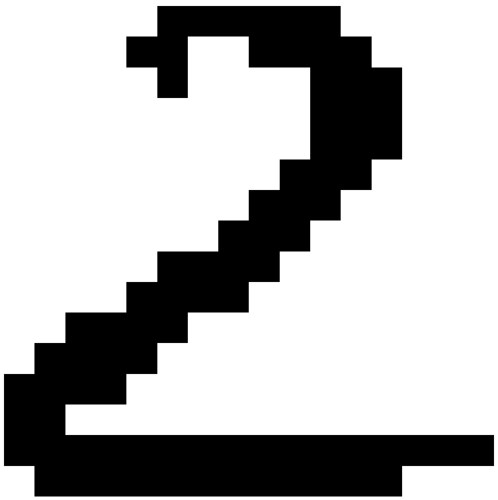


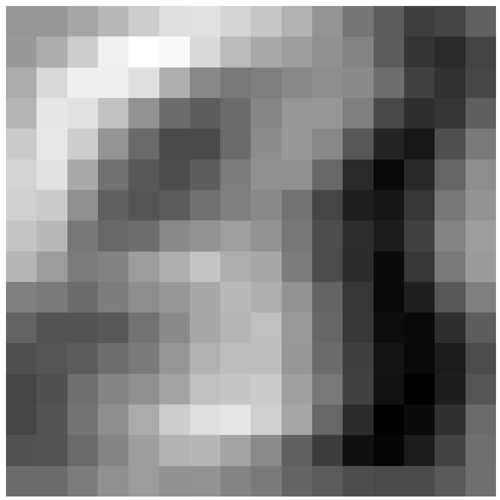


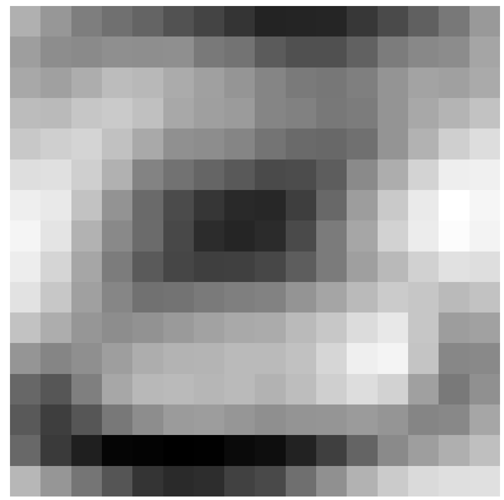


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

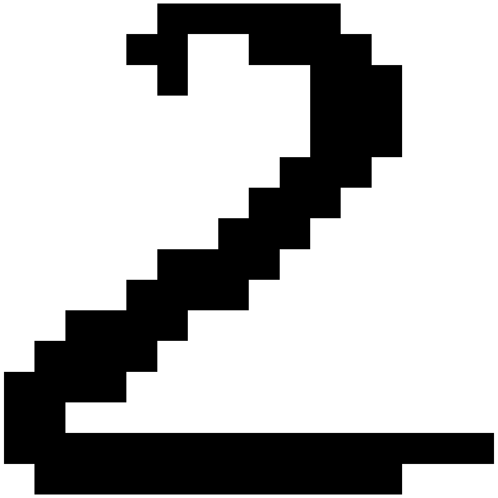


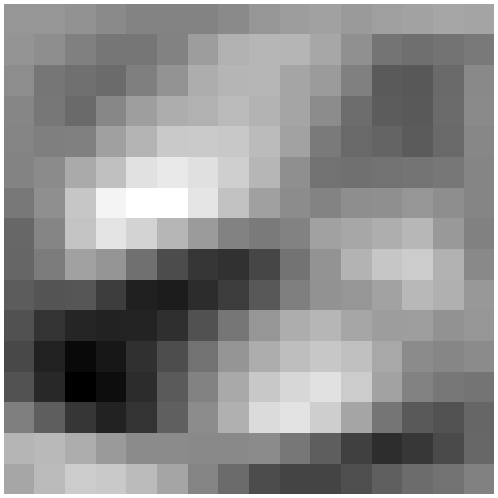


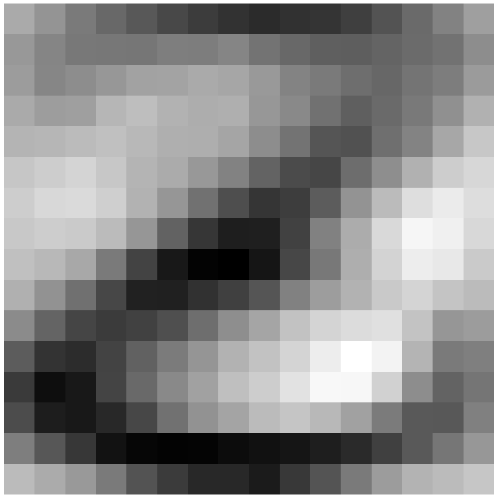


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

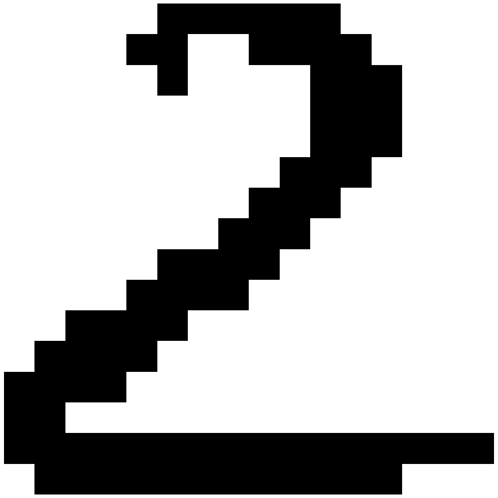


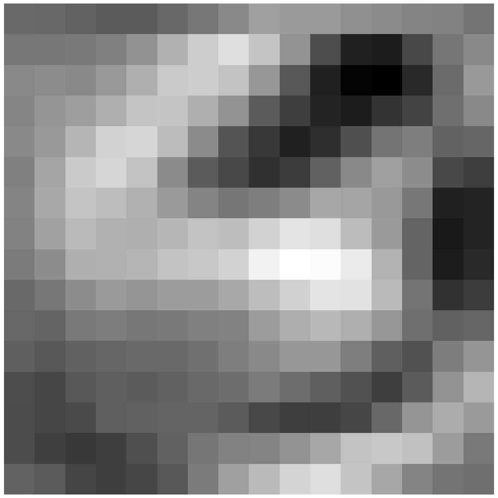


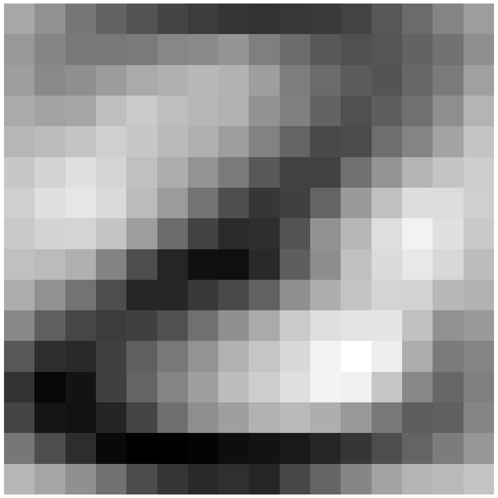


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

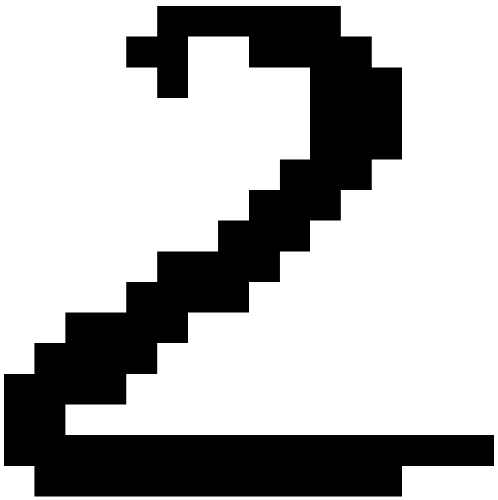


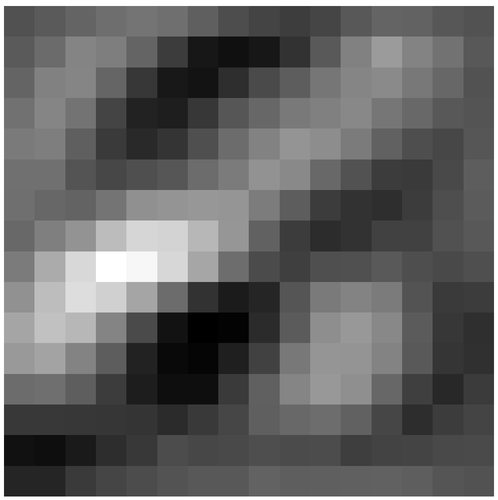


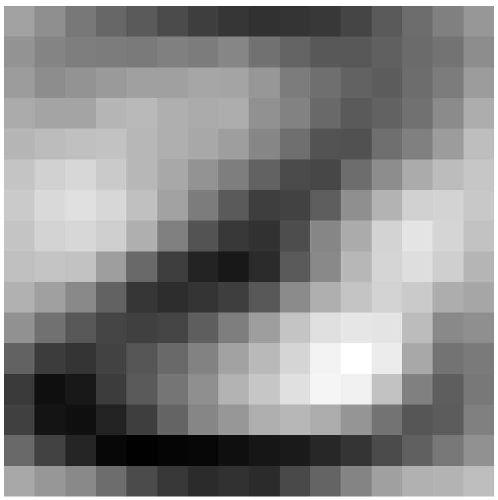


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

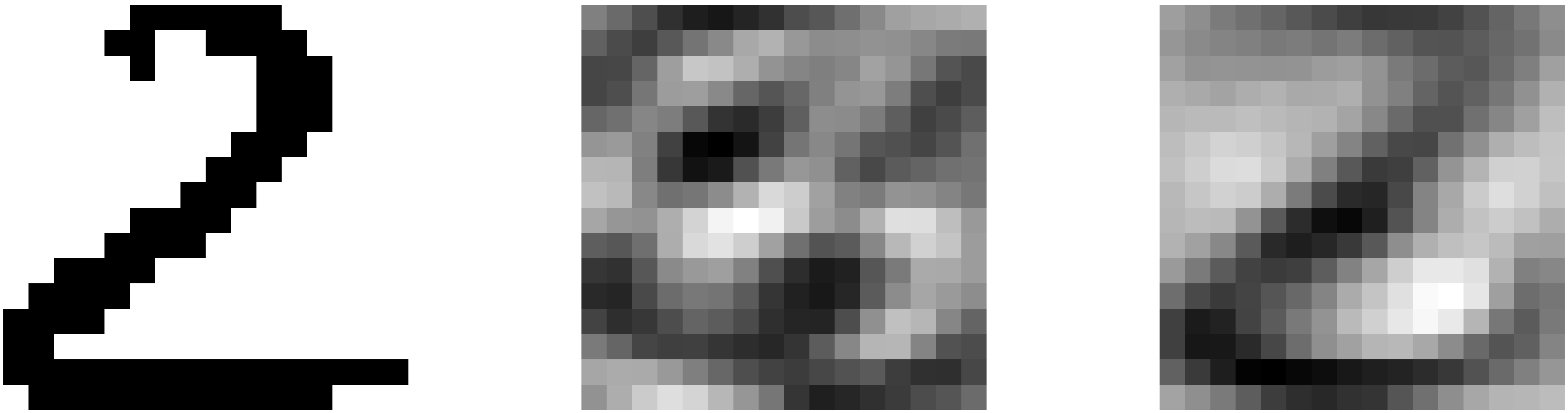






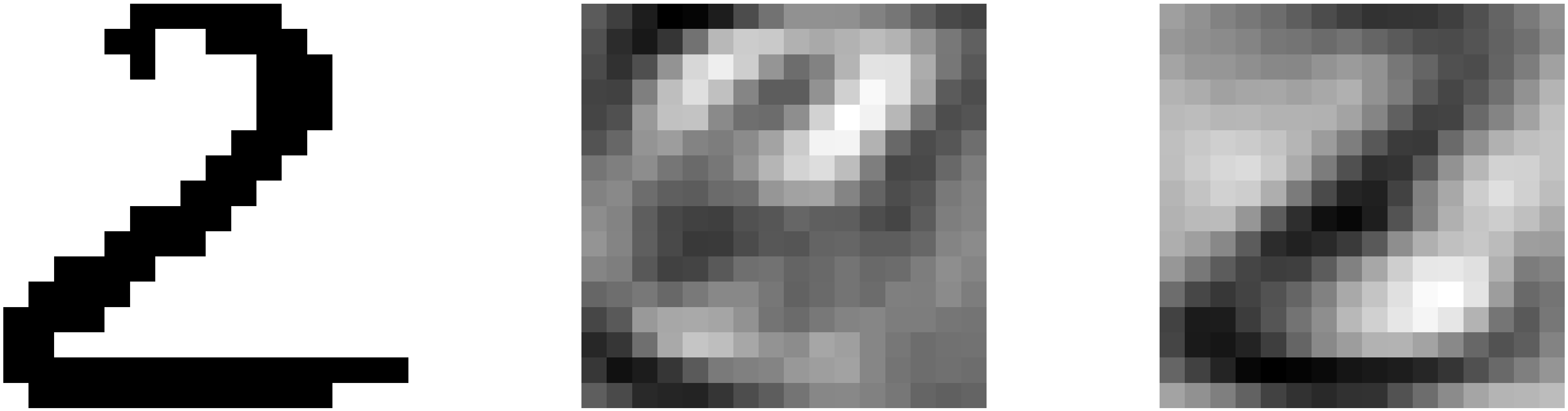
Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1



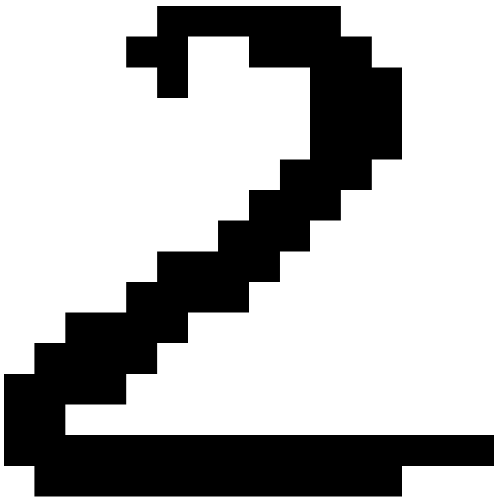
Reconstruction from Eigenvectors

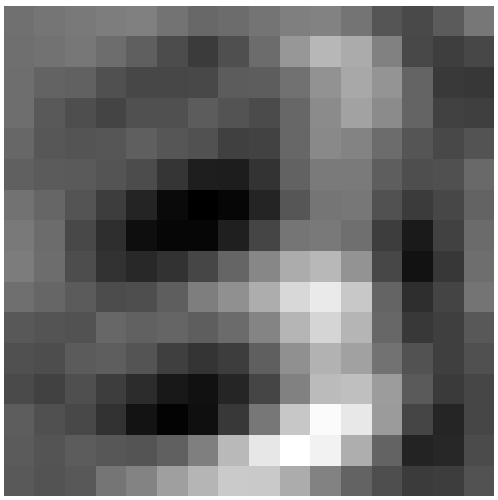
1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

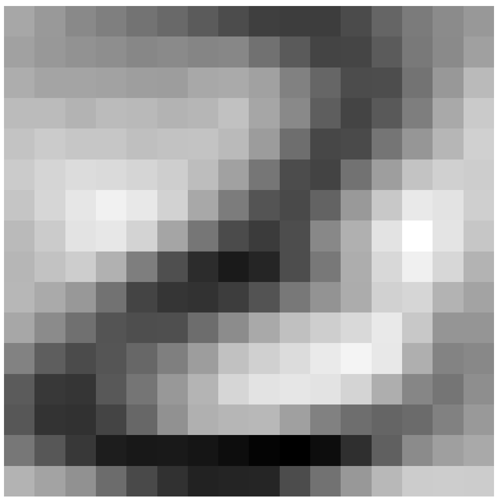


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

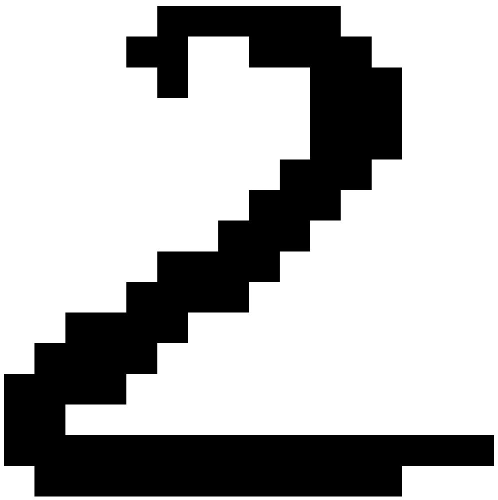


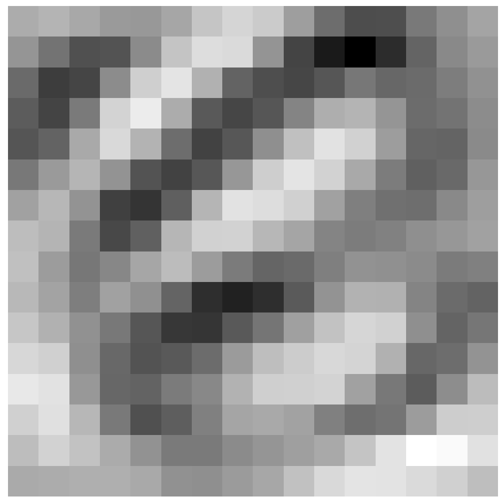


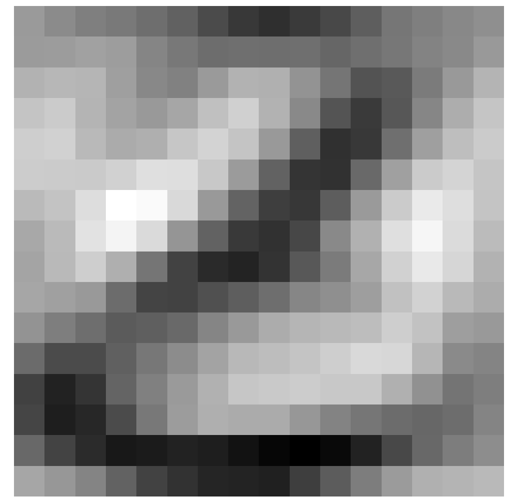


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

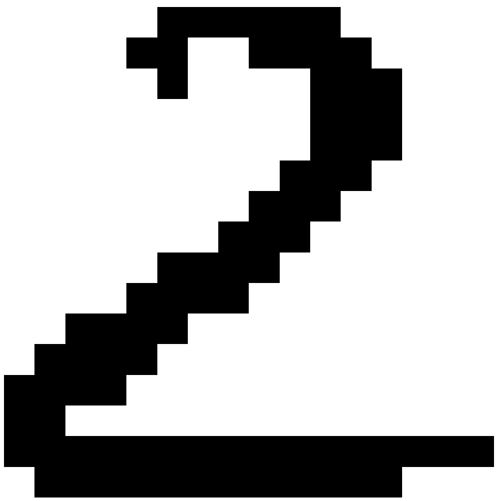


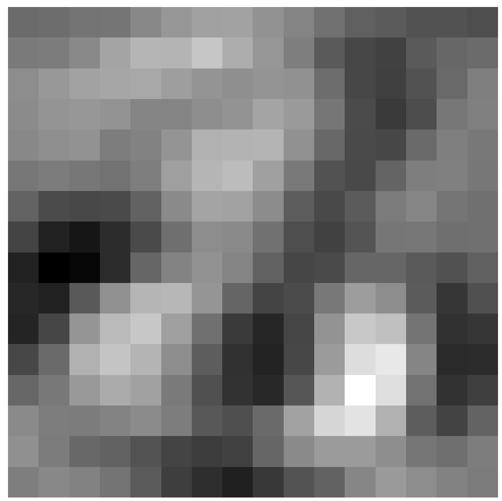


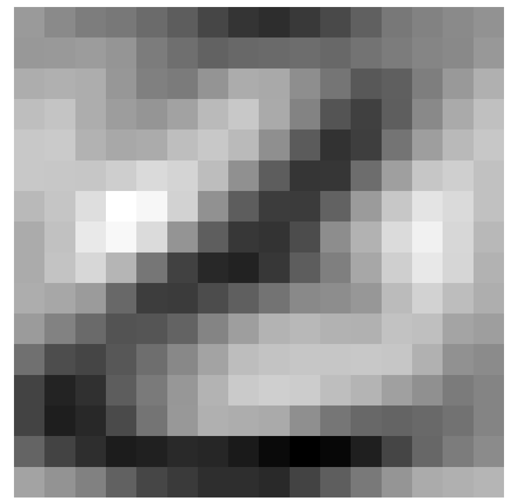


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

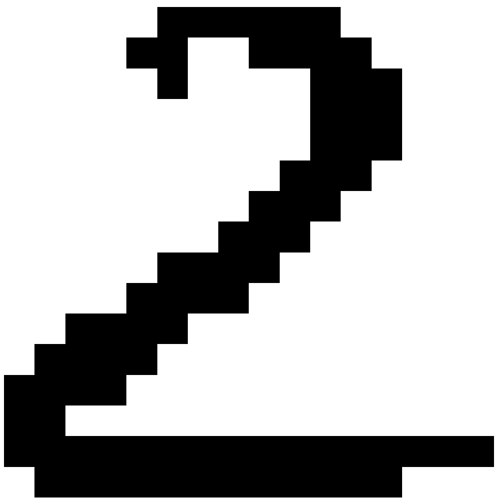


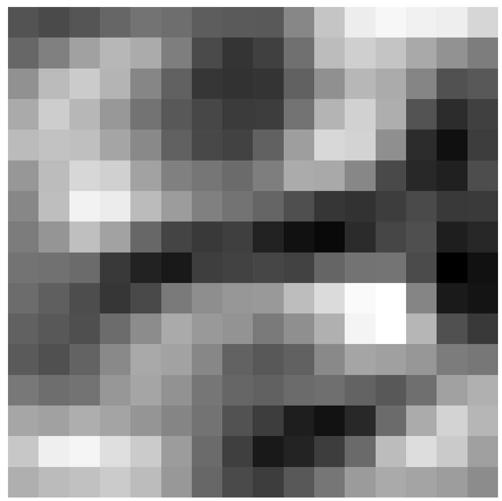


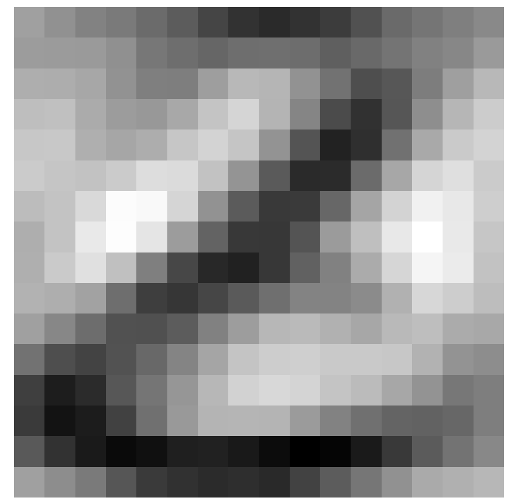


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

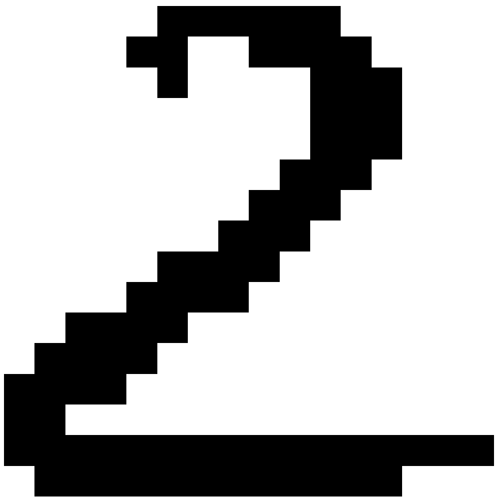


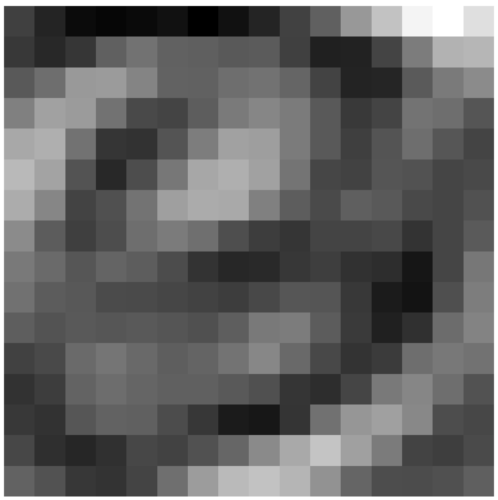


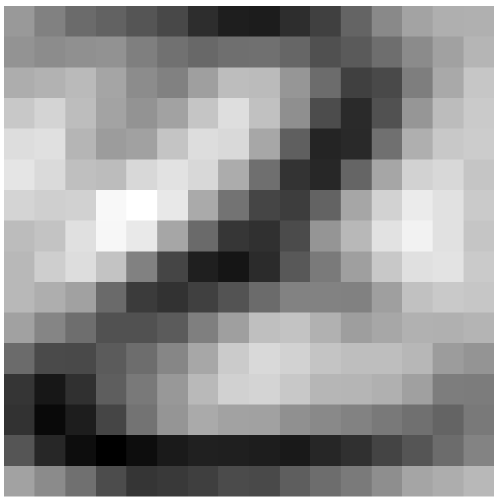


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

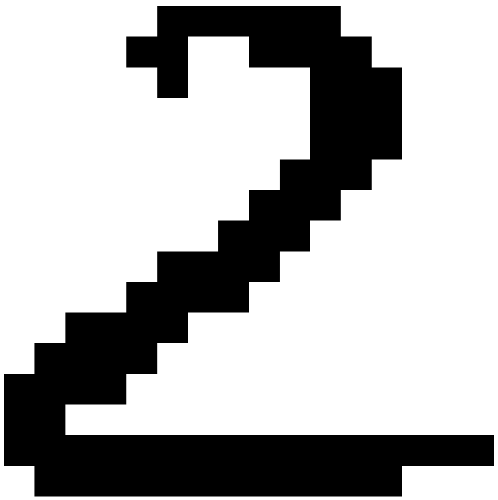


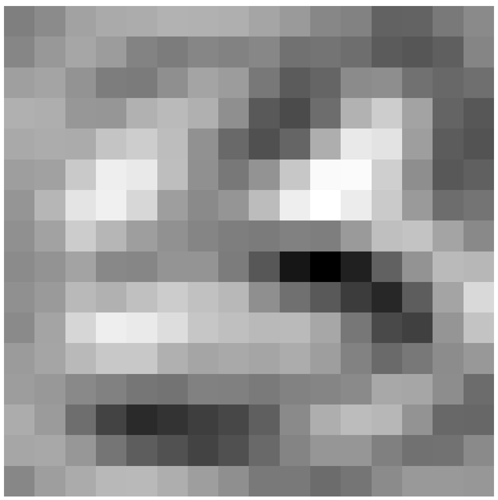


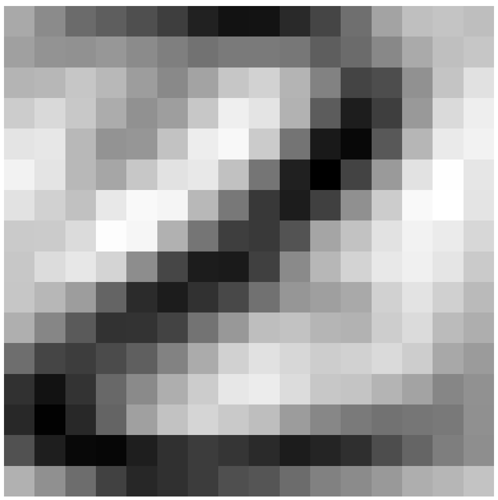


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

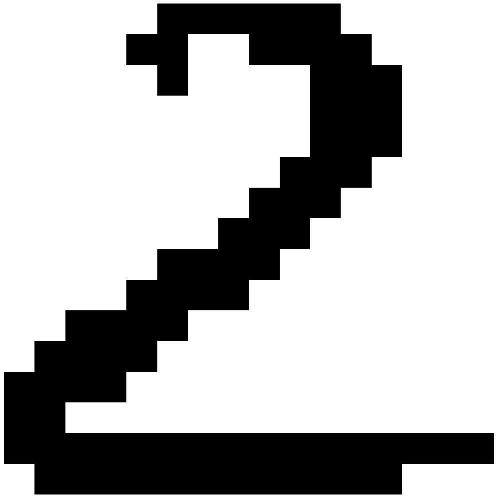


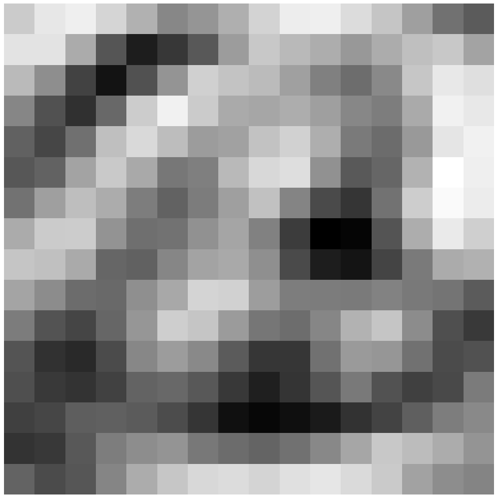


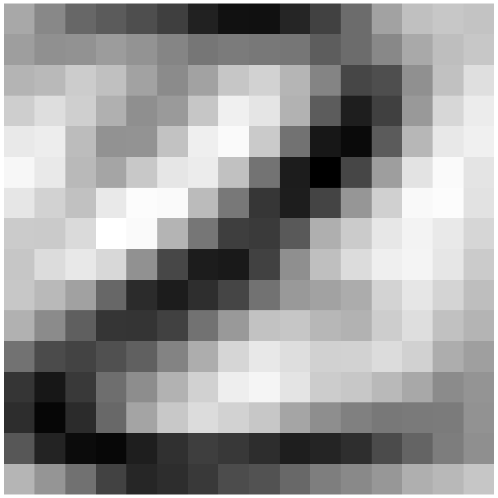


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

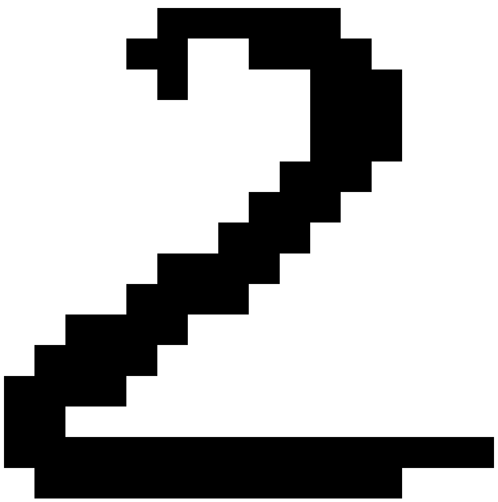


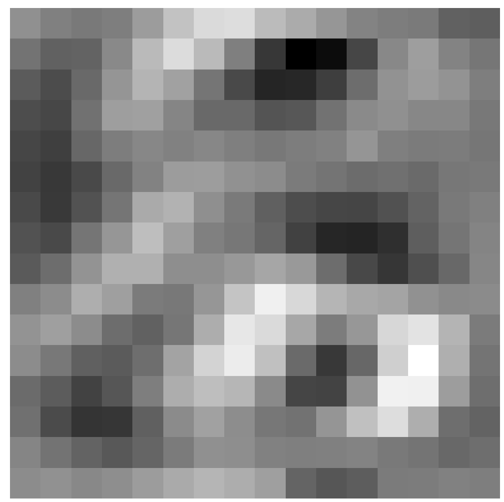


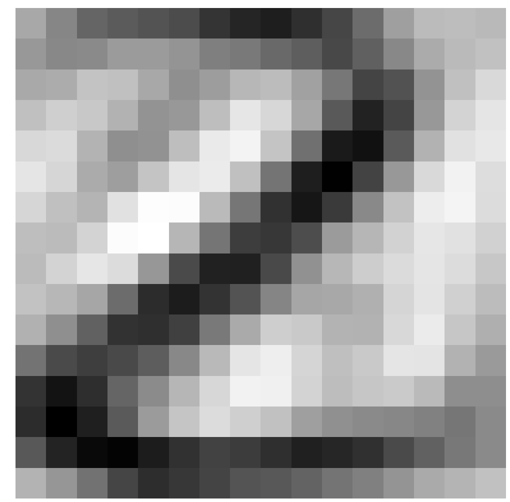


Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

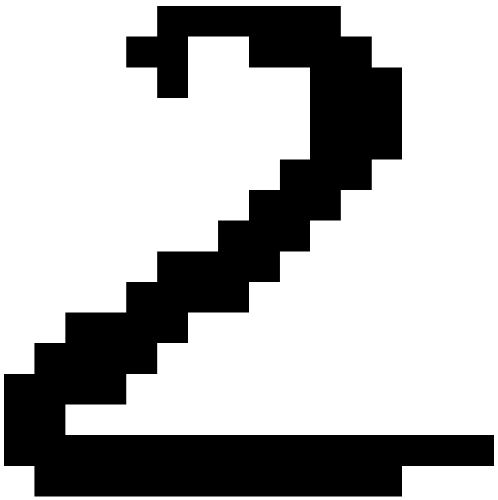
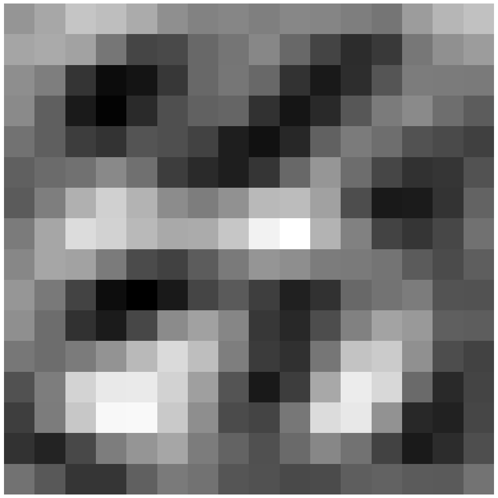
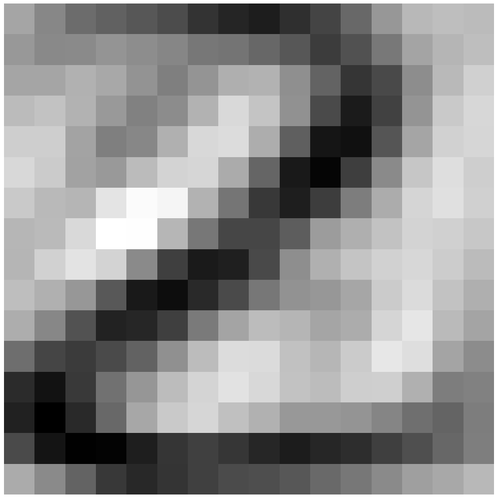






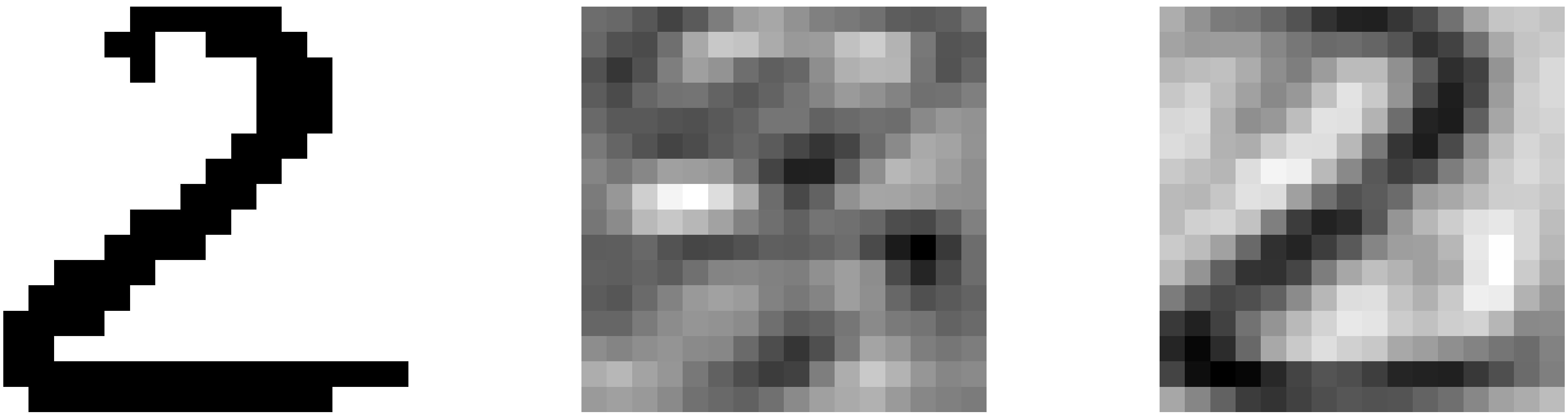
Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1

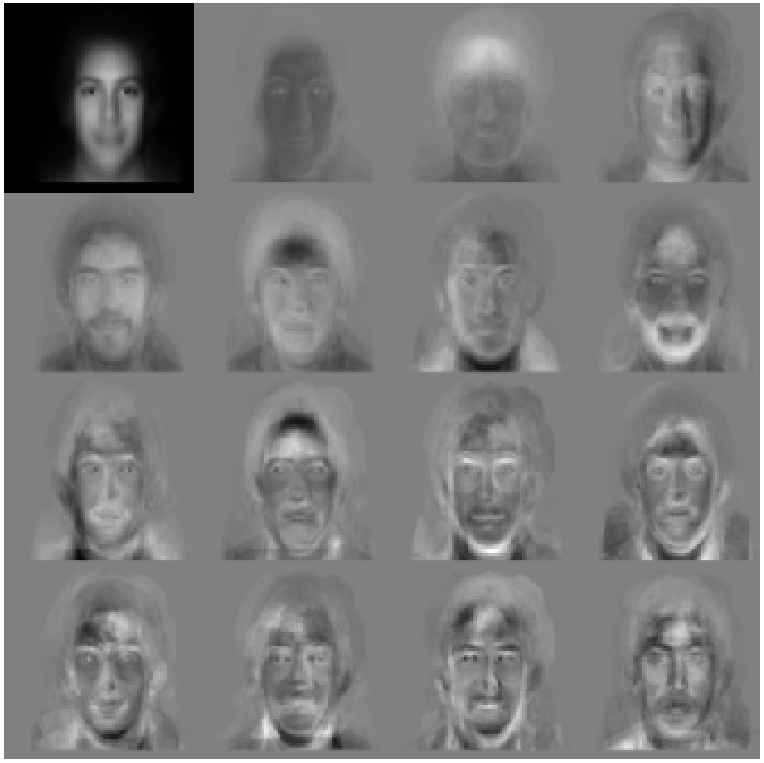
Reconstruction from Eigenvectors

1.6 -1.1 -1.6 2.1 -0.52 2.8 0.72 0.7 -0.68 -0.41 -1.4 -1.5 -0.54 -0.62 1.3 -1.4 -0.27 0.74 0.77 -1



Outline

1. Covariance Matrices
2. Principal Component Analysis
3. **Duality**



PCA for Images

- An image often contains around $p = 256 \times 256 = 64k$ pixels
- In standard PCA we would create an $p \times p$ matrix with over 4×10^9 elements
- This is intractable
- m images span at most a $m - 1$ dimensional subspace
- Usually this subspace will be much smaller than the space of all images $m \ll p$

PCA for Images

- An image often contains around $p = 256 \times 256 = 64k$ pixels
- In standard PCA we would create an $p \times p$ matrix with over 4×10^9 elements
- This is intractable
- m images span at most a $m - 1$ dimensional subspace
- Usually this subspace will be much smaller than the space of all images $m \ll p$

PCA for Images

- An image often contains around $p = 256 \times 256 = 64k$ pixels
- In standard PCA we would create an $p \times p$ matrix with over 4×10^9 elements
- This is intractable
- m images span at most a $m - 1$ dimensional subspace
- Usually this subspace will be much smaller than the space of all images $m \ll p$

PCA for Images

- An image often contains around $p = 256 \times 256 = 64k$ pixels
- In standard PCA we would create an $p \times p$ matrix with over 4×10^9 elements
- This is intractable
- m images span at most a $m - 1$ dimensional subspace
- Usually this subspace will be much smaller than the space of all images $m \ll p$

PCA for Images

- An image often contains around $p = 256 \times 256 = 64k$ pixels
- In standard PCA we would create an $p \times p$ matrix with over 4×10^9 elements
- This is intractable
- m images span at most a $m-1$ dimensional subspace
- Usually this subspace will be much smaller than the space of all images $m \ll p$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^\mathsf{T}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^\mathsf{T}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^\mathsf{T}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^\mathsf{T}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^{\mathsf{T}}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^{\mathsf{T}}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$
\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}
$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^{\mathsf{T}}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^{\mathsf{T}}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$
\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}
$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^{\mathsf{T}}$ is a $p \times p$ matrix
- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\,\mathbf{X}$
- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$\begin{aligned} \mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\ \mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\ \mathbf{X}\,\mathbf{X}^{\mathsf{T}}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\ \mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u} \end{aligned}$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- The covariance $\mathbf{C} = \mathbf{X}\,\mathbf{X}^\mathsf{T}$ is a $p \times p$ matrix

- Consider the $m \times m$ matrix $\mathbf{D} = \mathbf{X}^\mathsf{T}\,\mathbf{X}$

- Suppose $\boldsymbol{v}$ is an eigenvector of $\mathbf{D}$

$$
\begin{aligned}
\mathbf{D}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}^\mathsf{T}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\boldsymbol{v} \\
\mathbf{X}\,\mathbf{X}^\mathsf{T}\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\boldsymbol{v} \\
\mathbf{C}\,\mathbf{X}\,\boldsymbol{v} &= \lambda\,\mathbf{X}\,\boldsymbol{v} \quad \Rightarrow \quad \mathbf{C}\,\boldsymbol{u} = \lambda\,\boldsymbol{u}
\end{aligned}
$$

- $\boldsymbol{u} = \mathbf{X}\,\boldsymbol{v}$

Dual Matrix

- Matrices $\mathbf{C} = \mathbf{X}\mathbf{X}^\mathsf{T}$ and $\mathbf{D} = \mathbf{X}^\mathsf{T}\mathbf{X}$ have the same eigenvalues
- Can use the dual $m \times m$ matrix $\mathbf{D}$ to find eigenvalues and eigenvectors of $\mathbf{C}$
- Note that $\mathbf{D} = \mathbf{X}^\mathsf{T}\mathbf{X}$ has components $D_{kl} \propto (\boldsymbol{x}_k - \boldsymbol{\mu})^\mathsf{T}(\boldsymbol{x}_l - \boldsymbol{\mu})$
- Takes $O(p \times m \times m)$ time to construct $\mathbf{D}$
- We work in a "dual space" which is the space spanned by the examples

Dual Matrix

- Matrices $\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$ and $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ have the same eigenvalues
- Can use the dual $m \times m$ matrix $\mathbf{D}$ to find eigenvalues and eigenvectors of $\mathbf{C}$
- Note that $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ has components $D_{kl} \propto (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}(\boldsymbol{x}_l - \boldsymbol{\mu})$
- Takes $O(p \times m \times m)$ time to construct $\mathbf{D}$
- We work in a "dual space" which is the space spanned by the examples

Dual Matrix

- Matrices $\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$ and $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ have the same eigenvalues
- Can use the dual $m \times m$ matrix $\mathbf{D}$ to find eigenvalues and eigenvectors of $\mathbf{C}$
- Note that $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ has components $D_{kl} \propto (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}(\boldsymbol{x}_l - \boldsymbol{\mu})$
- Takes $O(p \times m \times m)$ time to construct $\mathbf{D}$
- We work in a "dual space" which is the space spanned by the examples

Dual Matrix

- Matrices $\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$ and $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ have the same eigenvalues
- Can use the dual $m \times m$ matrix $\mathbf{D}$ to find eigenvalues and eigenvectors of $\mathbf{C}$
- Note that $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ has components $D_{kl} \propto (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}(\boldsymbol{x}_l - \boldsymbol{\mu})$
- Takes $O(p \times m \times m)$ time to construct $\mathbf{D}$
- We work in a “dual space” which is the space spanned by the examples

Dual Matrix

- Matrices $\mathbf{C} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$ and $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ have the same eigenvalues
- Can use the dual $m \times m$ matrix $\mathbf{D}$ to find eigenvalues and eigenvectors of $\mathbf{C}$
- Note that $\mathbf{D} = \mathbf{X}^{\mathsf{T}}\mathbf{X}$ has components $D_{kl} \propto (\boldsymbol{x}_k - \boldsymbol{\mu})^{\mathsf{T}}(\boldsymbol{x}_l - \boldsymbol{\mu})$
- Takes $O(p \times m \times m)$ time to construct $\mathbf{D}$
- We work in a "dual space" which is the space spanned by the examples

What Does a Subspace Look Like?

- Consider $\boldsymbol{y}^1 = \begin{pmatrix} 2 \\ 4 \\ 4 \end{pmatrix}$, $\boldsymbol{y}^2 = \begin{pmatrix} 8 \\ 6 \\ 2 \end{pmatrix}$ with mean $\boldsymbol{\mu} = \begin{pmatrix} 5 \\ 5 \\ 3 \end{pmatrix}$
- Subtracting the mean $\boldsymbol{x}^i = \boldsymbol{y}^i - \boldsymbol{\mu}$ we can construct matrix

$$\mathbf{X} = \begin{pmatrix} x_1^1 & x_1^2 \\ x_2^1 & x_2^2 \\ x_3^1 & x_3^2 \end{pmatrix} = \begin{pmatrix} -3 & 3 \\ -1 & 1 \\ 2 & -2 \end{pmatrix}$$

What Does a Subspace Look Like?

- Consider $\boldsymbol{y}^1 = \begin{pmatrix} 2 \\ 4 \\ 4 \end{pmatrix}$, $\boldsymbol{y}^2 = \begin{pmatrix} 8 \\ 6 \\ 2 \end{pmatrix}$ with mean $\boldsymbol{\mu} = \begin{pmatrix} 5 \\ 5 \\ 3 \end{pmatrix}$

- Subtracting the mean $\boldsymbol{x}^i = \boldsymbol{y}^i - \boldsymbol{\mu}$ we can construct matrix

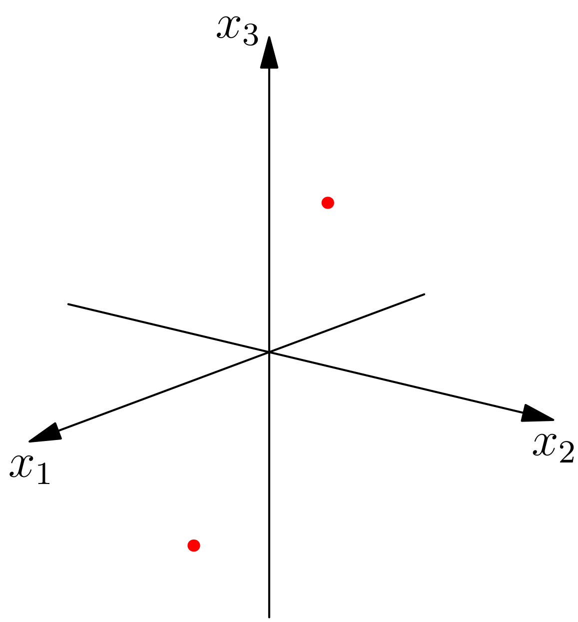
$$\mathbf{X} = \begin{pmatrix} x_1^1 & x_1^2 \\ x_2^1 & x_2^2 \\ x_3^1 & x_3^2 \end{pmatrix} = \begin{pmatrix} -3 & 3 \\ -1 & 1 \\ 2 & -2 \end{pmatrix}$$

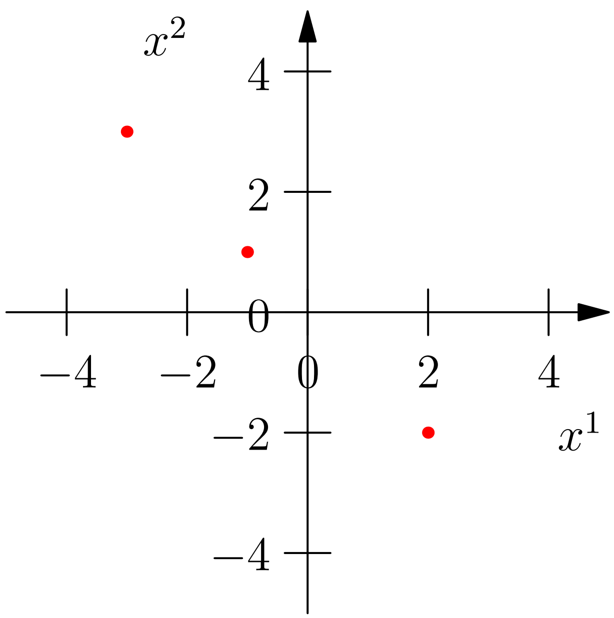
What Does a Subspace Look Like?

- Consider $\boldsymbol{y}^1 = \begin{pmatrix} 2 \\ 4 \\ 4 \end{pmatrix}$, $\boldsymbol{y}^2 = \begin{pmatrix} 8 \\ 6 \\ 2 \end{pmatrix}$ with mean $\boldsymbol{\mu} = \begin{pmatrix} 5 \\ 5 \\ 3 \end{pmatrix}$

- Subtracting the mean $\boldsymbol{x}^i = \boldsymbol{y}^i - \boldsymbol{\mu}$ we can construct matrix

$$\mathbf{X} = \begin{pmatrix} x_1^1 & x_1^2 \\ x_2^1 & x_2^2 \\ x_3^1 & x_3^2 \end{pmatrix} = \begin{pmatrix} -3 & 3 \\ -1 & 1 \\ 2 & -2 \end{pmatrix}$$



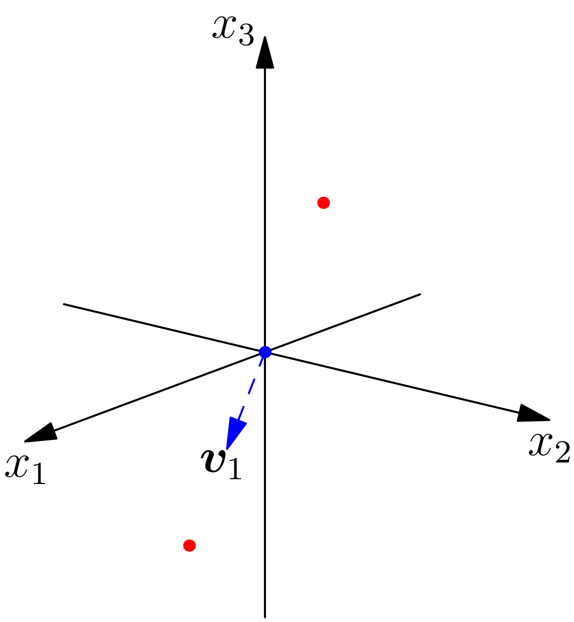


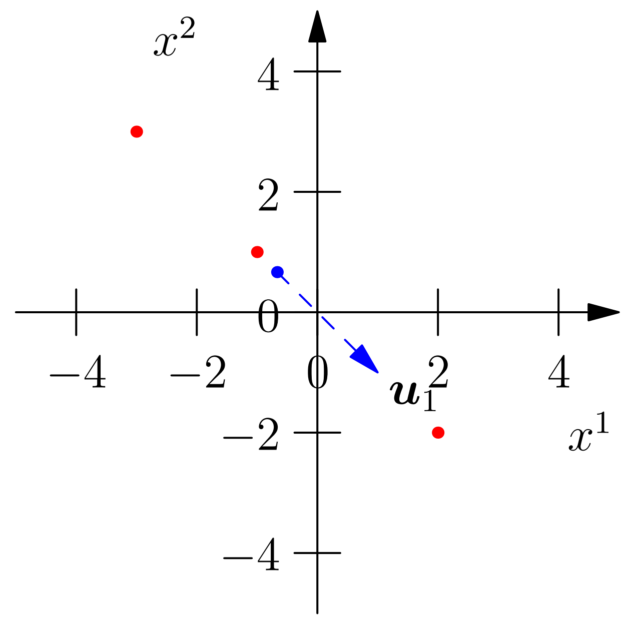
What Does a Subspace Look Like?

- Consider $\boldsymbol{y}^1 = \begin{pmatrix} 2 \\ 4 \\ 4 \end{pmatrix}$, $\boldsymbol{y}^2 = \begin{pmatrix} 8 \\ 6 \\ 2 \end{pmatrix}$ with mean $\boldsymbol{\mu} = \begin{pmatrix} 5 \\ 5 \\ 3 \end{pmatrix}$

- Subtracting the mean $\boldsymbol{x}^i = \boldsymbol{y}^i - \boldsymbol{\mu}$ we can construct matrix

$$\mathbf{X} = \begin{pmatrix} x_1^1 & x_1^2 \\ x_2^1 & x_2^2 \\ x_3^1 & x_3^2 \end{pmatrix} = \begin{pmatrix} -3 & 3 \\ -1 & 1 \\ 2 & -2 \end{pmatrix}$$





Summary

- PCA allows us to reduce the dimensionality of the inputs
- We project the inputs into a sub-space where the data varies the most
- We can work in either the original space ($\mathbf{X}\mathbf{X}^{\mathsf{T}}$) or the dual space ($\mathbf{X}^{\mathsf{T}}\mathbf{X}$)
- When we have many more features than examples (i.e. $p \gg m$) then it is more efficient working in the dual space

Summary

- PCA allows us to reduce the dimensionality of the inputs
- We project the inputs into a sub-space where the data varies the most
- We can work in either the original space ($\mathbf{X}\mathbf{X}^\mathsf{T}$) or the dual space ($\mathbf{X}^\mathsf{T}\mathbf{X}$)
- When we have many more features than examples (i.e. $p \gg m$) then it is more efficient working in the dual space

Summary

- PCA allows us to reduce the dimensionality of the inputs
- We project the inputs into a sub-space where the data varies the most
- We can work in either the original space ($\mathbf{X}\mathbf{X}^{\mathsf{T}}$) or the dual space ($\mathbf{X}^{\mathsf{T}}\mathbf{X}$)
- When we have many more features than examples (i.e. $p \gg m$) then it is more efficient working in the dual space

Summary

- PCA allows us to reduce the dimensionality of the inputs
- We project the inputs into a sub-space where the data varies the most
- We can work in either the original space ($\mathbf{X}\mathbf{X}^{\mathsf{T}}$) or the dual space ($\mathbf{X}^{\mathsf{T}}\mathbf{X}$)
- When we have many more features than examples (i.e. $p \gg m$) then it is more efficient working in the dual space

Summary

- PCA allows us to reduce the dimensionality of the inputs
- We project the inputs into a sub-space where the data varies the most
- We can work in either the original space ($\mathbf{X}\mathbf{X}^{\mathsf{T}}$) or the dual space ($\mathbf{X}^{\mathsf{T}}\mathbf{X}$)
- When we have many more features than examples (i.e. $p \gg m$) then it is more efficient working in the dual space
- We will see examples of dual spaces again when we look at SVMs