Principal Component Analysis

Machine Learning
CSx824/ECEx242
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	Example 1	Example 2	Example 3	Example 4	Example 5	Example 6	
Feature 1	0.3	20.1	-2.3	-6.4	0.2	-32.9	
Feature 2	200.4	108.2	428.3	352.8	722.0	50.3	
Feature 3	0.6	40.2	-4.6	-12.8	0.4	-65.8	2 (Feature 1)
Feature 4	1	1	1	1	1	1	vacuous
Feature 5	0	0	0	0	0	0	vacuous
Feature 6	-200.4	-108.2	-428.3	-352.8	-722	-50.3	- (Feature 2)
Feature 7	200.7	128.3	426.0	346.4	722.2	17.4	F1+F2

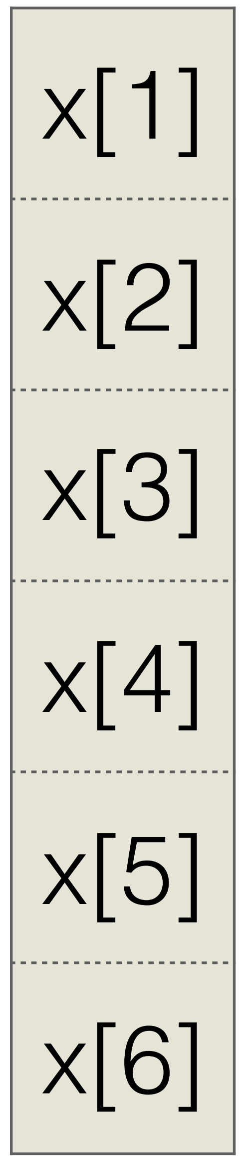
Outline

- Intuition behind principal component analysis (PCA)
- PCA recipe
- How PCA works

Vectors

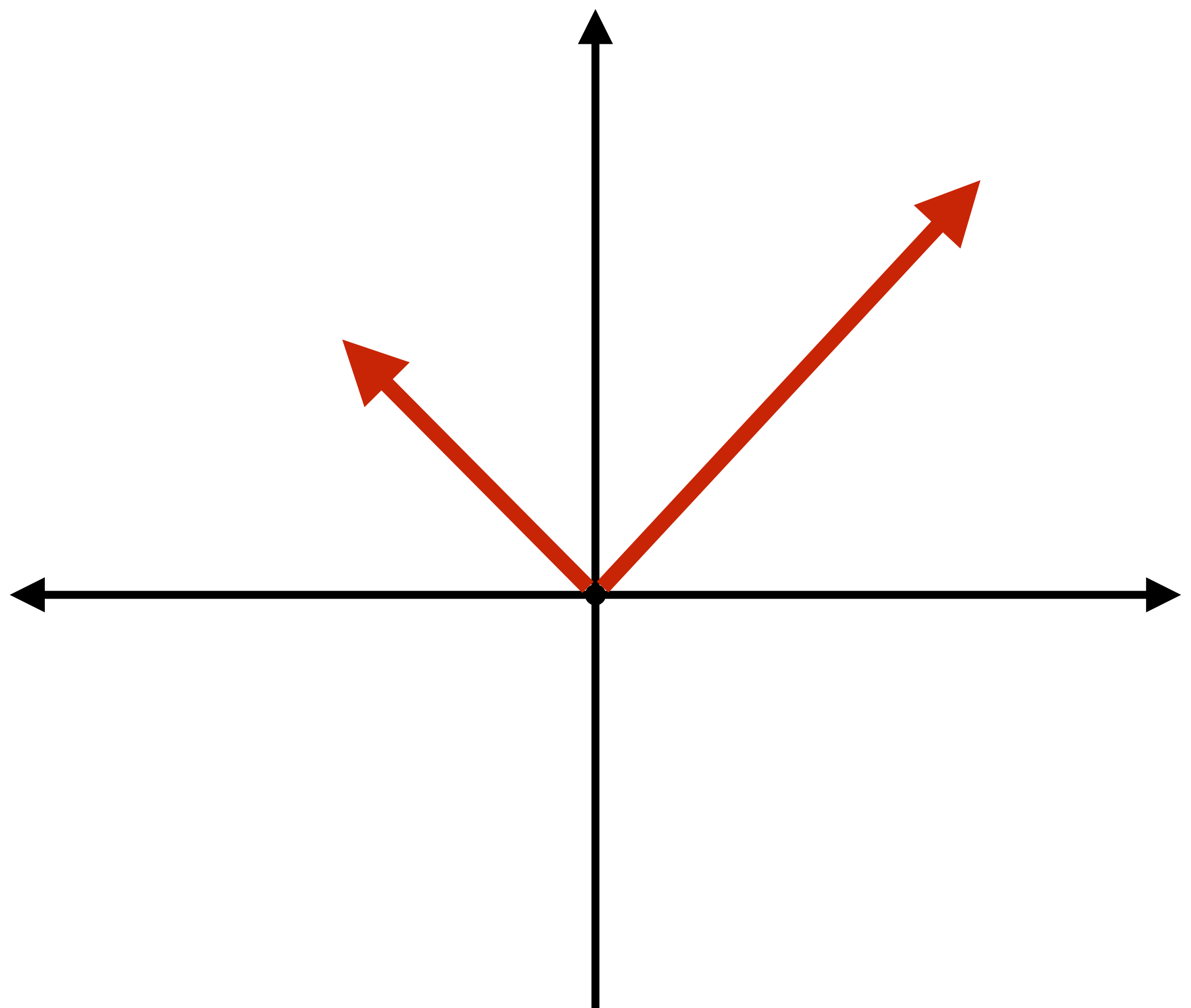
Programmers

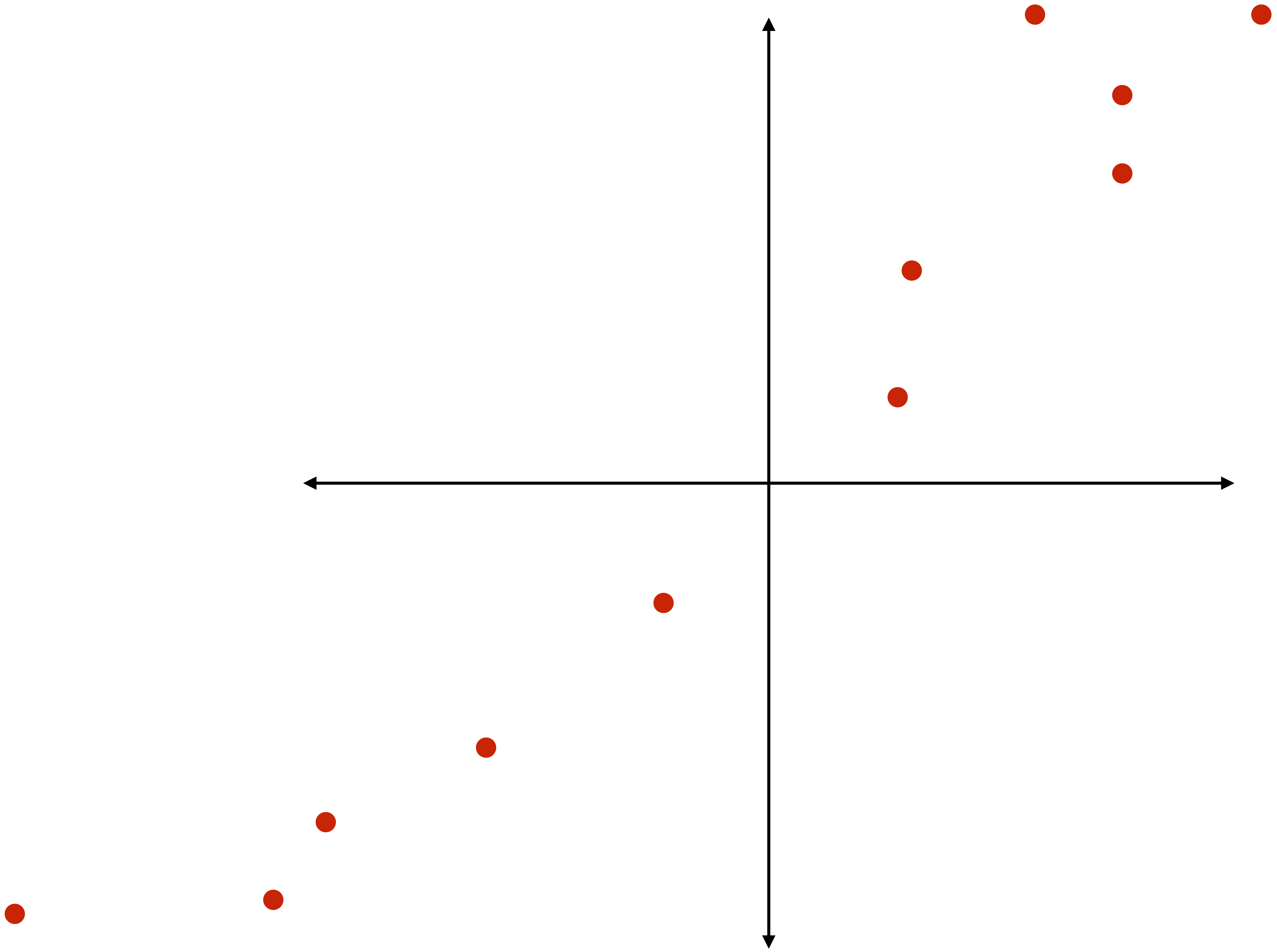
- Arrays
- Fixed basis

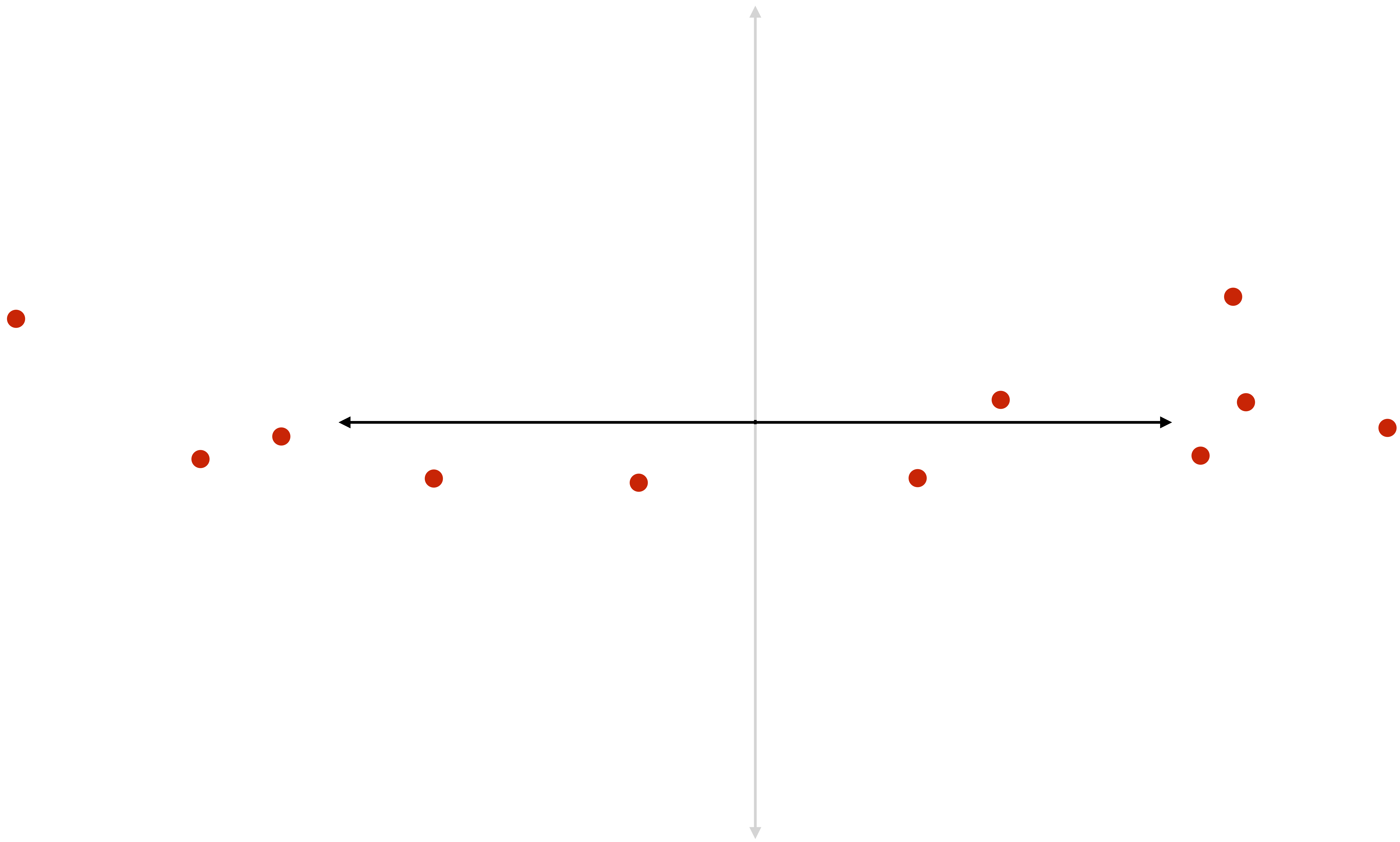


Mathematicians

- Direction in space and magnitude
- No fixed basis







PCA Intuition

- Find low-dimensional principal directions of data
  - low-dimensional representation of data that most accurately reconstructs original data

$$\frac{1}{n}||x_i - \hat{x}_i||^2$$

- Align orthogonal axis with data variance
- Use highest-variance dimensions; discard low-variance dimensions

PCA Recipe v.1

Input: centered data $X \in \mathbb{R}^{d \times n}$ $x_i \in \mathbb{R}^d$ $X\vec{1} = \vec{0}$

Covariance matrix $$\Sigma = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^\top = \frac{1}{n} X X^\top$$

Eigendecomposition $\Sigma = VDV^\top$ $V = [v_1, \dots, v_d]$ $D = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_d \end{bmatrix}$

Truncate eigenvectors $V_r = [v_1, \dots, v_r]$ $\lambda_k \geq \lambda_{k+1}$

Project onto truncated eigenvectors $z_i = V_r^\top x_i$ $Z = V_r^\top X$

$\hat{x}_i = V_r z_i$

Reconstruction

PCA Recipe v.2

Input: centered data $X \in \mathbb{R}^{d \times n}$ $x_i \in \mathbb{R}^d$ $X\vec{1} = \vec{0}$

Singular-value decomposition (SVD) of **transpose** $X^\top = USV^\top$

Truncate right singular vectors $V_r = [v_1, \ldots, v_r]$

Project onto truncated right singular vectors $z_i = V_r^\top x_i$ $Z = V_r^\top X$

$$XX^\top = (VS^\top U^\top)(USV^\top) = V(S^\top S)V^\top = VDV^\top$$

$$U^\top U = I \qquad S^\top S = D$$

right singular vectors of (n x d) data matrix = eigenvectors of covariance matrix

How PCA Reduces Reconstruction Error

$$\min_{W,Z} \frac{1}{n}\sum_{i=1}^{n} ||x_i - Wz_i||^2 \qquad W \in \mathbb{R}^{d\times r}$$

$$\text{s.t. } W^\top W = I \qquad Z \in \mathbb{R}^{r\times n}$$

$$(x_i - Wz_i)^\top (x_i - Wz_i) = x_i^\top x_i - 2x_i^\top W z_i + z_i^\top W^\top W z_i$$

$$= x_i^\top x_i - 2x_i^\top W z_i + z_i^\top z_i$$

$$\nabla_{z_i} = 2z_i - 2W^\top x_i \qquad z_i = W^\top x_i$$

$$x_i^\top x_i - 2z_i^\top z_i + z_i^\top z_i = x_i^\top x_i - z_i^\top z_i$$

$$\max_{W,Z} \frac{1}{n}\sum_{i=1}^{n} x_i^\top W W^\top x_i \text{ s.t. } W^\top W = I$$

$$\max_{W,Z} \frac{1}{n}\sum_{i=1}^{n} x_i^\top W W^\top x_i \text{ s.t. } W^\top W = I$$

$$\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{r} x_i^\top w_k w_k^\top x_i$$ explicitly write out dimensions

$$\frac{1}{n}\sum_{k=1}^{r}\sum_{i=1}^{n} x_i^\top w_k w_k^\top x_i$$ flip nested summations

$$\sum_{i=1}^{n} w_k^\top x_i x_i^\top w_k \quad = w_k^\top \Sigma w_k$$ covariance

$$L(w_k, \lambda_k) = w_k^\top \Sigma w_k + \lambda_k (w_k^\top w_k - 1)$$ Lagrangian for unitary constraint

$$\nabla_{w_k} L = 2\Sigma w_k - 2\lambda_k w_k$$ gradient wrt $\boldsymbol{w_k}$

$$\Sigma w_k = \lambda_k w_k$$ each $\boldsymbol{w_k}$ must be an eigenvector

$$w_k^\top \Sigma w_k = \lambda_k$$ variance is the eigenvalue; choose greatest eigenvalue

Summary

- PCA is a few lines in MATLAB
  - roughly the same amount of code as configuring and using built-in PCA
- Eigen-decomposition or SVD equivalent
- Showed proof for 1-D PCA.

Bonus: Pedantic Comments

- Princip**al** component analysis
- **e**igenvalue, **e**igenvector lowercase