CSE 575: Statistical Machine Learning

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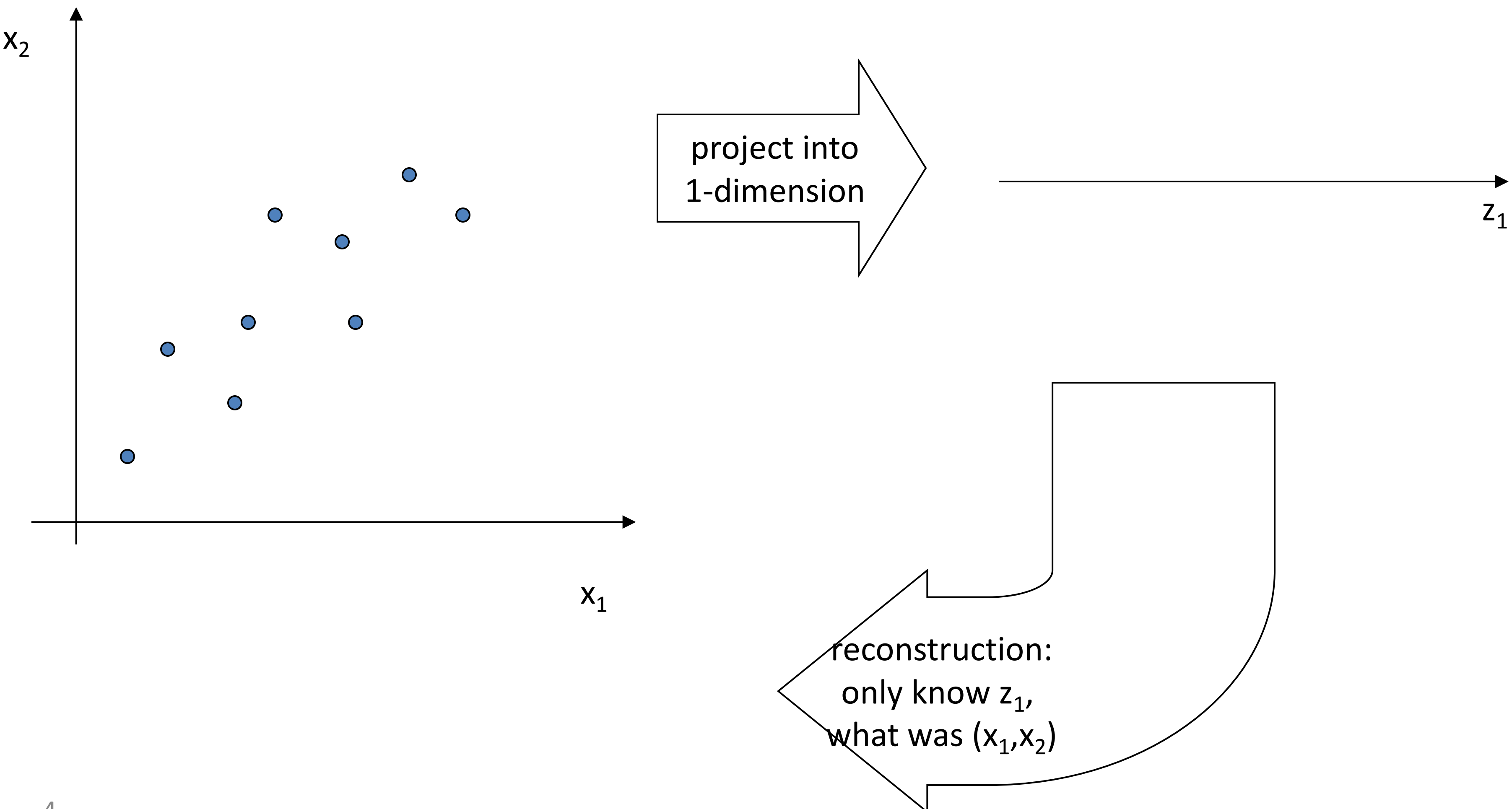
Dimensionality Reduction

Lower dimensional projections

- Rather than picking a subset of the features, we can create new features that are combinations of existing features

- Let's see this in the unsupervised setting
  - just **X**, but no Y

Linear projection and reconstruction

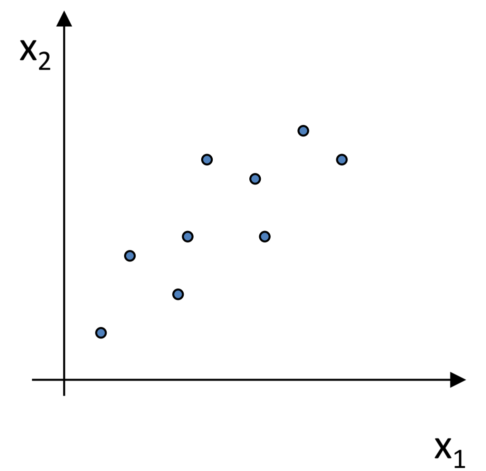


Linear projections, a review

- Project a point into a (lower dimensional) space:
  - **point**: $\mathbf{x} = (x_1,\ldots,x_n)$
  - **select a basis** – set of basis vectors – $(\mathbf{u}_1,\ldots,\mathbf{u}_k)$
    - we consider orthonormal basis:
      - $\mathbf{u}_i \bullet \mathbf{u}_i = 1$, and $\mathbf{u}_i \bullet \mathbf{u}_j = 0$ for $i \neq j$
  - **select a center** – $\bar{\mathbf{x}}$, defines offset of space
  - **best coordinates** in lower dimensional space defined by dot-products: $(z_1,\ldots,z_k)$, $z_i = (\mathbf{x}-\bar{\mathbf{x}}) \bullet \mathbf{u}_i$
    - minimum squared error

PCA finds projections that minimize reconstruction error

- Given m data points: $\mathbf{x}^i = (x_1^i,\ldots,x_n^i)$, i=1…m
- Will represent each point as a projection:
  - $\hat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^{k} z_j^i \mathbf{u}_j$ where: $\bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m} \mathbf{x}^i$ and $z_j^i = (\mathbf{x}^i - \bar{\mathbf{x}}) \cdot \mathbf{u}_j$



- PCA:
  - Given k, find $(\mathbf{u}_1,\ldots,\mathbf{u}_k)$ minimizing reconstruction error:
    $$error_k = \sum_{i=1}^{m} (\mathbf{x}^i - \hat{\mathbf{x}}^i)^2$$

Understanding reconstruction error

- Note that $\mathbf{x}^i$ can be represented exactly by n-dimensional projections:

$$\mathbf{x}^i = \bar{\mathbf{x}} + \sum_{j=1}^{n} z_j^i \mathbf{u}_j$$

$$\hat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^{k} z_j^i \mathbf{u}_j$$

$$z_j^i = (\mathbf{x}^i - \bar{\mathbf{x}}) \cdot \mathbf{u}_j$$

- Given k, find ($\mathbf{u}_1$,…,$\mathbf{u}_k$) minimizing reconstruction error:

$$error_k = \sum_{i=1}^{m} (\mathbf{x}^i - \hat{\mathbf{x}}^i)^2$$

- Rewriting error:

Reconstruction error and covariance matrix

$$error_k = \sum_{i=1}^{m} \sum_{j=k+1}^{n} [\mathbf{u}_j \cdot (\mathbf{x}^i - \bar{\mathbf{x}})]^2$$

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} (\mathbf{x}^i - \bar{\mathbf{x}})(\mathbf{x}^i - \bar{\mathbf{x}})^T$$

Minimizing reconstruction error and eigen vectors

- Minimizing reconstruction error equivalent to picking orthonormal basis ($\mathbf{u}_1,\ldots,\mathbf{u}_n$) minimizing:

$$error_k = m\sum_{j=k+1}^{n} \mathbf{u}_j^T \Sigma \mathbf{u}_j$$

- Eigen vector:

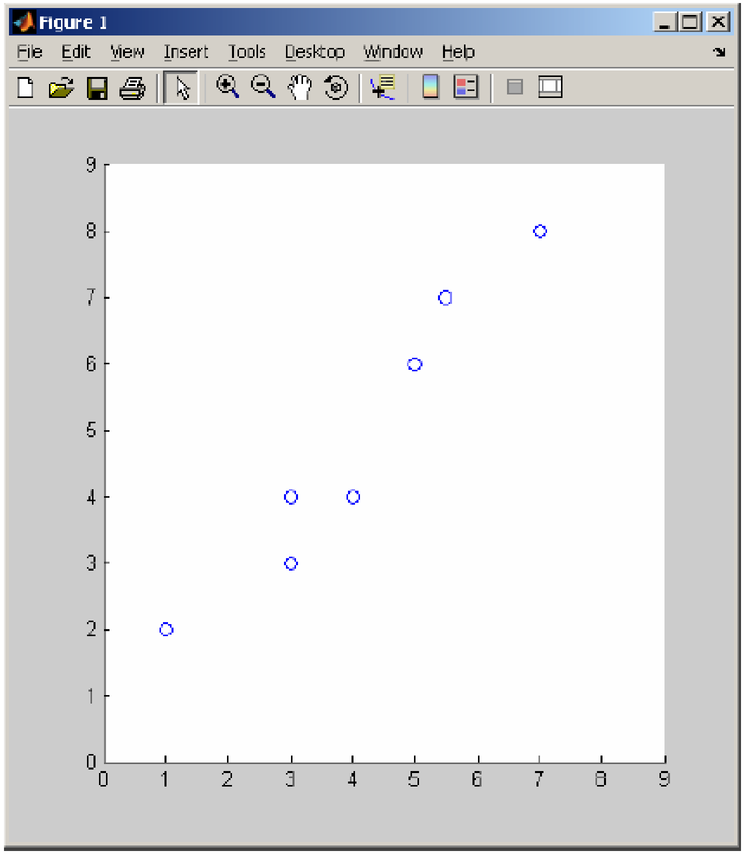
- Minimizing reconstruction error equivalent to picking ($\mathbf{u}_{k+1},\ldots,\mathbf{u}_n$) to be eigen vectors with the smallest eigen values

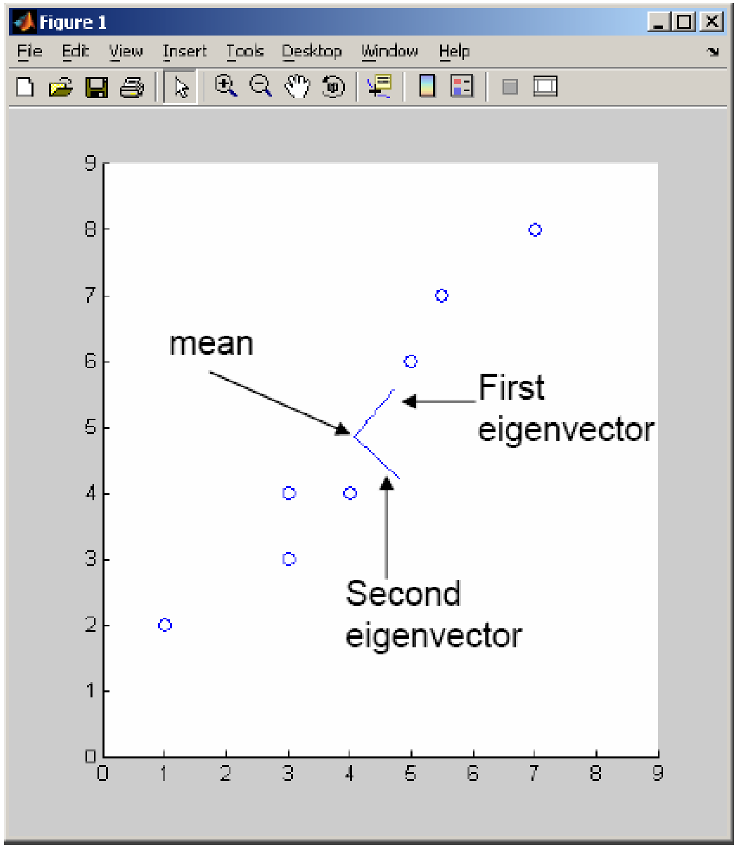
Basic PCA algorithm

- Start from m by n data matrix **X**
- **Recenter**: subtract mean from each row of **X**
  - $\mathbf{X_c} \leftarrow \mathbf{X} - \overline{\mathbf{X}}$
- **Compute covariance matrix**:
  - $\Sigma \leftarrow 1/m\ \mathbf{X_c}^{\mathbf{T}}\ \mathbf{X_c}$
- Find **eigen vectors and values** of Σ
- **Principal components:** k eigen vectors with highest eigen values

PCA example

$$\widehat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^{k} z_j^i \mathbf{u}_j$$

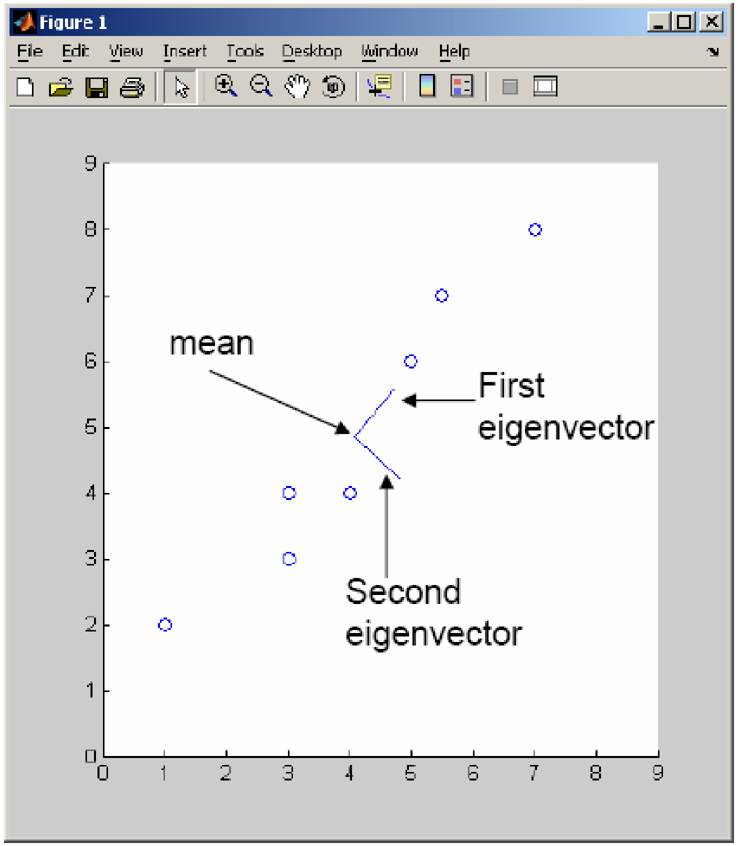


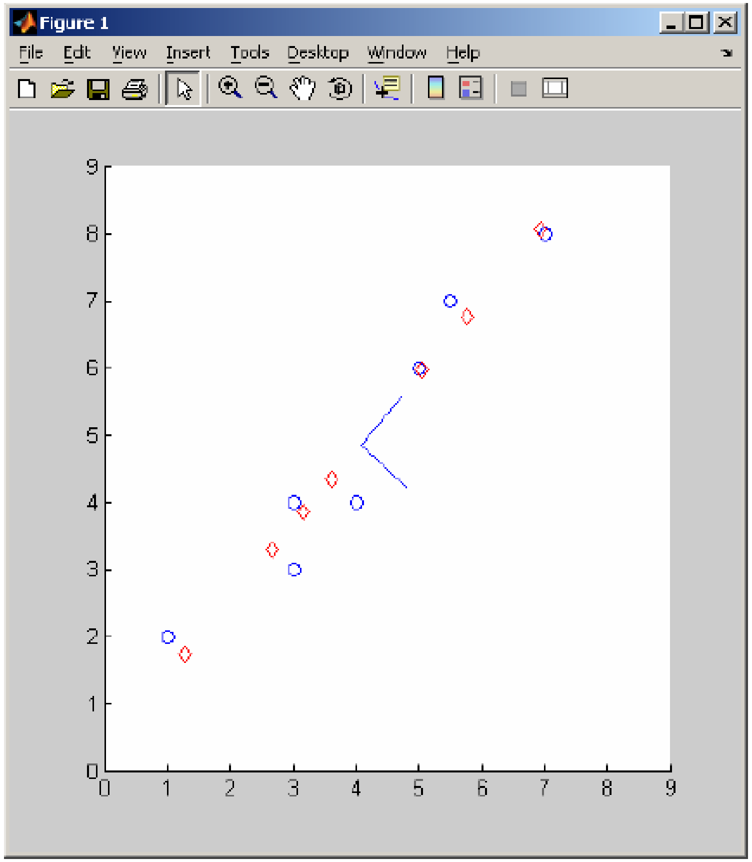


PCA example – reconstruction

$$\hat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^{k} z_j^i \mathbf{u}_j$$

only used first principal component

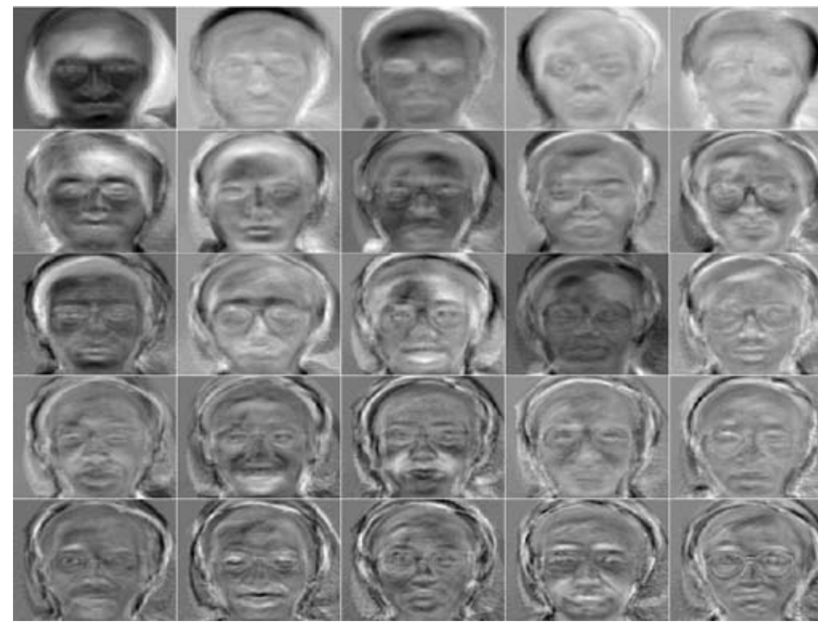




Eigenfaces [Turk, Pentland '91]

- Input images:

- Principal components:



Eigenfaces reconstruction

- Each image corresponds to adding 8 principal components:

Scaling up

- Covariance matrix can be really big!
  - Σ is n by n
  - 10000 features ! $|\Sigma|$
  - finding eigenvectors is very slow…
- Use singular value decomposition (SVD)
  - finds up to k eigenvectors
  - great implementations available, e.g., Matlab svd

SVD

- Write $\mathbf{X} = \mathbf{W}\ \mathbf{S}\ \mathbf{V}^T$
  - $\mathbf{X} \leftarrow$ data matrix, one row per data point
  - $\mathbf{W} \leftarrow$ weight matrix, one row per data point – coordinate of $\mathbf{x}^i$ in eigen space
  - $\mathbf{S} \leftarrow$ singular value matrix, diagonal matrix
    - in our setting each entry is squareroot of eigenvalue λ_j
  - $\mathbf{V}^T \leftarrow$ singular vector matrix
    - in our setting each row is eigenvector $\mathbf{v}_j$

PCA using SVD algorithm

- Start from m by n data matrix $\mathbf{X}$
- **Recenter**: subtract mean from each row of $\mathbf{X}$
  - $\mathbf{X_c} \leftarrow \mathbf{X} - \overline{\mathbf{X}}$
- Call SVD algorithm on $\mathbf{X_c}$ – ask for k singular vectors
- **Principal components:** k singular vectors with highest singular values (rows of $\mathbf{V}^T$)
  - **Coefficients** become: