

Applied Machine Learning

Principal Component Analysis

Principal Component Analysis

- Translation and rotations
- Dimensionality reduction
- Error in low-dimensional representation of high-dimensional data

Data Transformation

- Source dataset: $\{\mathbf{x}\}$
- After translation: $\{\mathbf{m}\}$
 - $\mathbf{m}_i = \mathbf{x}_i - \text{mean}(\{\mathbf{x}\})$
- And, after rotation: $\{\mathbf{r}\}$
 - $\text{Covmat}\{\mathbf{r}\} = U^\top \Sigma U = \Lambda$
 - $\mathbf{r}_i = U^\top \mathbf{m}_i = U^\top (\mathbf{x}_i - \text{mean}(\{\mathbf{x}\}))$
 - $\text{mean}(\{\mathbf{r}\}) = \text{mean}(\{\mathbf{m}\}) = 0$
- Eigenvectors U and eigenvalues Λ of S
 - $SU = U\Lambda$
- Diagonalization
 - $U^\top SU = \Lambda$
- $A = U^\top$
- $\text{Covmat}\{\mathbf{x}\} = \Sigma = S$

Selection of Features

- Eigenvalues in Λ
 - sorted from largest to smallest
 - the larger the component, the larger the weight for the corresponding feature
- New dataset $\{\mathbf{p}\}$
 - Select s largest components in Λ and corresponding eigenvectors in U
 - Replace remaining $d - s$ components with 0

Error in New Dataset

- $\frac{1}{N} \sum_i [(\mathbf{r}_i - \mathbf{p}_i)^\top (\mathbf{r}_i - \mathbf{p}_i)]$
- $= \frac{1}{N} \sum_i \left[\sum_{j=s+1}^{j=d} (r_i^{(j)})^2 \right]$
- $= \sum_{j=s+1}^{j=d} \left[\frac{1}{N} \sum_i (r_i^{(j)})^2 \right]$
- $= \sum_{j=s+1}^{j=d} \text{var}(\{r^{(j)}\})$
- $= \sum_{j=s+1}^{j=d} \lambda_j$

- Relative error

- $\frac{\sum_{j=s+1}^{j=d} \lambda_j}{\sum_{j=1}^{j=d} \lambda_j}$ should be small

Inverse Transformation

- Lower dimensional dataset $\{\hat{\mathbf{x}}\}$

$$\hat{\mathbf{x}}_i = U\mathbf{p}_i + \text{mean}(\{\mathbf{x}\})$$

- $$= \sum_{j=1}^{j=s} r_i^{(j)} \mathbf{u}_j + \text{mean}(\{\mathbf{x}\})$$

- $$\mathbf{r}_i = U^\top (\mathbf{x}_i - \text{mean}(\{\mathbf{x}\}))$$

- $$r_i^{(j)} = \mathbf{u}_j^\top (\mathbf{x}_i - \text{mean}(\{\mathbf{x}\}))$$

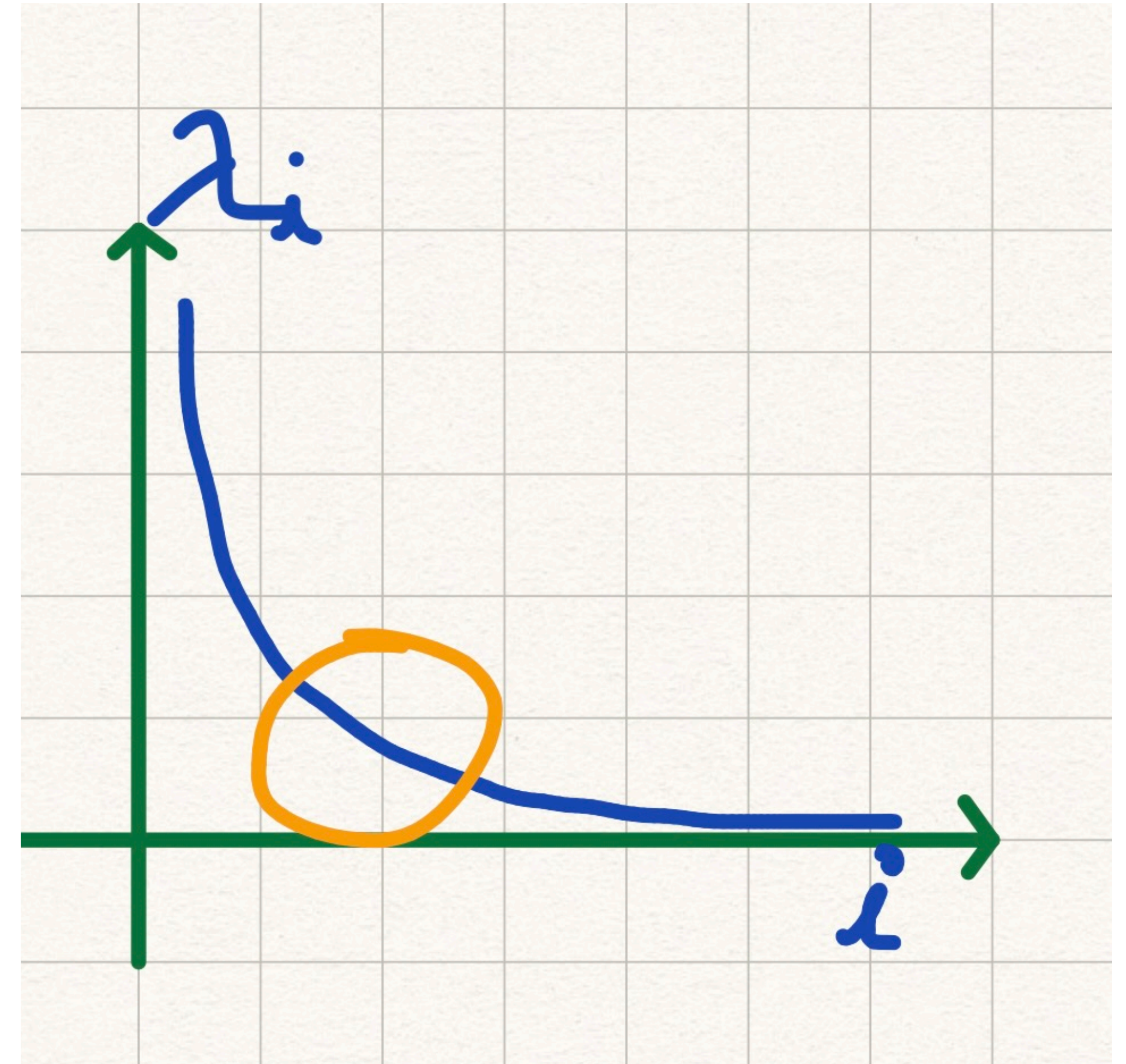
- $$\hat{\mathbf{x}}_i = \sum_{j=1}^{j=s} \left[\mathbf{u}_j^\top (\mathbf{x}_i - \text{mean}(\{\mathbf{x}\})) \mathbf{u}_j \right] + \text{mean}(\{\mathbf{x}\})$$

- Mean error

- $$\sum_{j=s+1}^{j=d} \lambda_j$$

Principal Component Analysis

- Original dataset: $\{\mathbf{x}\}$
 - d features
 - $U^T \text{Covmat}\{\mathbf{x}\} U = U^T \Sigma U = \Lambda$
- Choose s features
 - small ratio in $\frac{\sum_{j=s+1}^{j=d} \lambda_j}{\sum_{j=1}^{j=d} \lambda_j}$
 - plot relative error vs s or λ_i vs i , select s most significant
- Low-Dimensional representation $\hat{\mathbf{x}}$:
 - $\hat{\mathbf{x}}_i = \sum_{j=1}^{j=s} \left[\mathbf{u}_j^T (\mathbf{x}_i - \text{mean}(\{\mathbf{x}\})) \mathbf{u}_j \right] + \text{mean}(\{\mathbf{x}\})$



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