Unsupervised Learning: Dimension Reduction

Why Dimension Reduction?

For Big-Data:

- Data visualization becomes very difficult! (Cannot draw 2D scatterplots between all pairs of features).
- Big-Data often has a high degrees of redundancy. (i.e. correlation among features).
- Many features may be uninformative for the particular problem under study (noise features).
- Dimension reduction ideally allows us retain information on most important features of the data, while reducing noise and simplifying visualization & analysis.

What is Dimension Reduction?

- Map the data into a new low-dimensional space where important characteristics of the data are preserved.
- The new space often gives a (linear or non-linear) transformation of the original data.
- Visualization and analysis (clustering/prediction/...) is then performed in the new space.
- In many cases, (especially for non-linear transformations) interpretation becomes difficult.

Principal Components Analysis (PCA)

PCA

Set-up:

- Data matrix: $X_{n \times p}$, n observations and p features.

Idea:

- Not all p features are needed (much redundant info).
- Find low-dimensional linear representations that capture most of the variation in the data.

Uses:

- Ubiquitously used - Dimension reduction, data visualization, pattern recognition, exploratory analysis, etc.
- "Best" linear dimension reduction possible.

PCA - Main Idea

Question: What is a good 1D representation of the data?
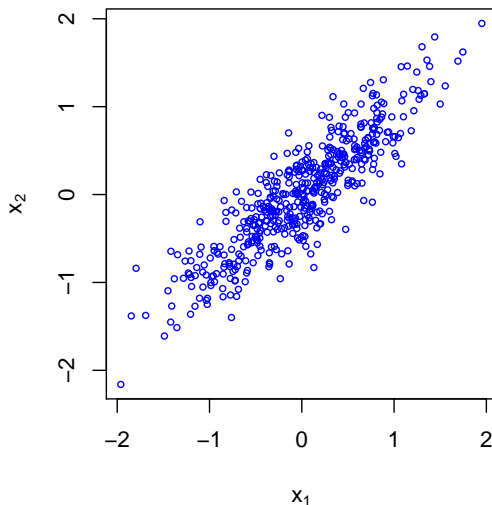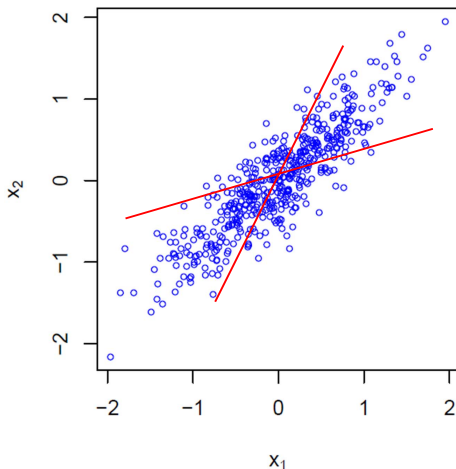
PCA - Main Idea

Some Possibilities:

- Use one of the variables (e.g. x_1).
- Better idea: use a linear combination of the variables (i.e. a weighted average).

$$z_1 = v_1 x_1 + v_2 x_2 = v^T X$$

How to choose the weights (v_1 and v_2)?
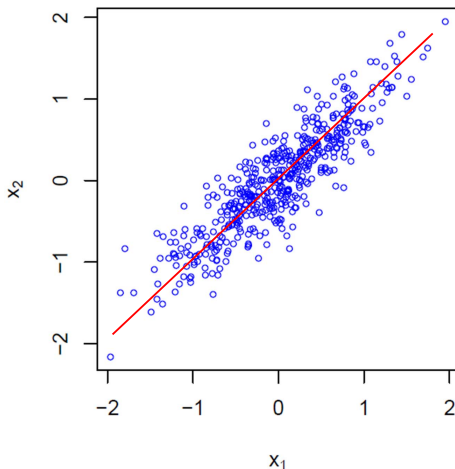
PCA - Main Idea

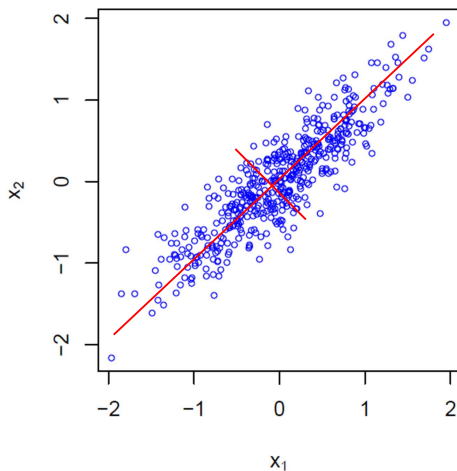Many possibilities, but which one is a good choice?

PCA - Main Idea

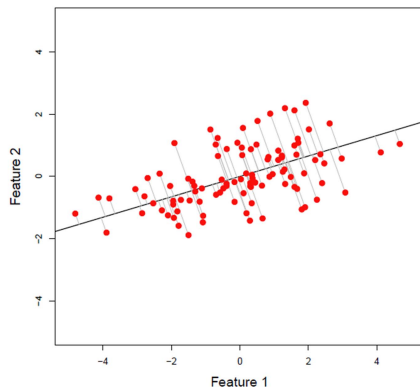Find line that maximizes the variance of the data projected onto the line:

PCA - Main Idea

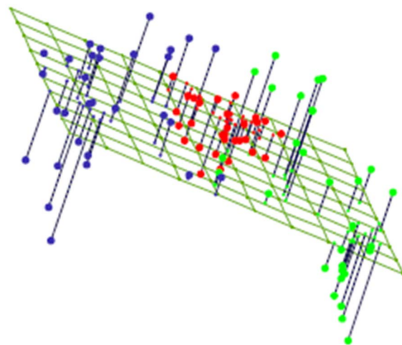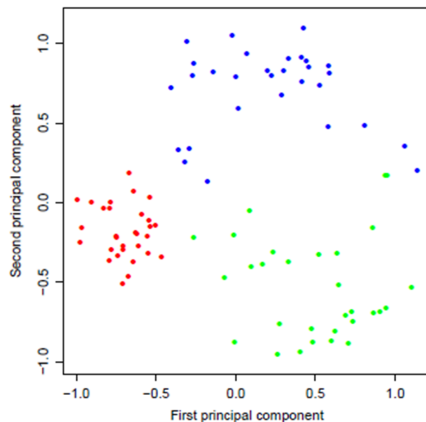Subsequent components orthogonal (perpendicular).

PCA - Main Idea

- PCA minimizes orthogonal projection onto line: $Z = v_1 x_1 + v_2 x_2$.
- Slope of line $= v_2/v_1$ (if features centered).
- Note: Not same as OLS which minimizes projection of y onto x!

PCA - Main Idea

3D Projection onto a Hyperplane:

PCA - Criterion

PCA Criterion - PC 1 (Population):

$$\underset{v}{\text{maximize}} \quad \text{Var}(X v) \quad \text{subject to } ||v||_2 = 1$$

$$\underset{v}{\text{maximize}} \quad v^T \text{Var}(X) v \quad \text{subject to } ||v||_2 = 1$$

$$\underset{v}{\text{maximize}} \quad v^T \Sigma v \quad \text{subject to } ||v||_2 = 1$$

where $\Sigma = \text{Cov}(X)$.

- Finds linear combination of features that maximizes the variance.

PCA - Criterion

PCA Criterion - PC k (Population):

$$\underset{\mathsf{v}_k}{\text{maximize}} \quad \mathsf{v}_k^T \Sigma \mathsf{v}_k \quad \text{subject to } ||\mathsf{v}_k||_2 = 1 \ \& \ \mathsf{v}_k^T \mathsf{v}_j = 0 \ \forall \ j < k.$$

- Subsequent linear combinations are orthogonal to previous combinations.
- Uncorrelated.

PCA - Criterion

PCA Criterion - Sample Version:

$$\underset{v_1,\ldots v_K}{\text{maximize}} \quad v_k^T X^T X v_k \quad \text{subject to } ||v_k||_2 = 1 \ \& \ v_k^T v_j = 0 \ \forall \ j < k.$$

Replaces Σ with estimate $X^T X / n$.

Solution: Eigenvalue decomposition of $X^T X$. (`eigen()` in `R`)

PCA - Criterion

Equivalent PCA Criterion:

$$\underset{u_1,\ldots u_K, v_1,\ldots v_K}{\text{maximize}} \quad u_k^T X v_k \quad \text{subject to } \| v_k \|_2 = 1 \ \& \ v_k^T v_j = 0 \ \forall \ j < k.$$

$$\| u_k \|_2 = 1 \ \& \ u_k^T u_j = 0 \ \forall \ j < k.$$

- Finds left and right projection that maximize variance.

Solution: Singular Value Decomposition (SVD) of X. (svd() in R)

PCA - Parts of the Solution

SVD: $X_{n \times p} = U_{n \times n} D_{n \times p} V_{p \times p}^T$

- Singular vectors: (left) U and (right) V.
  - Orthonormal - $U^T U = I$ and $V^T V = I$.
- Singular values: Diagonals of D.
  - $d_1 \geq d_2 \geq \ldots \geq d_r$ where $r = \text{rank}(X)$.

SVD Solution to PCA:

- PCs: $Z = X V$ or $Z = U D$. (U are un-scaled PCs).
  - $z_k = X v_k$ - k^{th} PC.
  - $z_1 \ldots z_K$ gives best K-dimensional projection of the data.
- PC Loadings: V.
 - v_k - k^{th} PC loading (feature weights).

PCA - Properties

- Unique.
  - U and V unique up to a sign change.
  - D unique.

- Nested, Ordered components.
  - $d_1 > d_2 > \ldots d_p$.

- Orthogonal.
  - U and V orthogonal.

- Global Solution.

PCA - Pattern Recognition

- u_1 - first column of U encodes first major pattern in observation space.
- v_1 - first column of V encodes the associated first pattern in feature space.
- d_1 gives strength of first pattern.

- Subsequent patterns are uncorrelated to first pattern (i.e. orthogonal).
- $X \approx \sum_{k=1}^{K} d_k u_k v_k^T$ - data is comprised of a series of patterns.
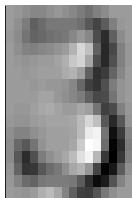
PCA - Pattern Recognition

Patterns in observation space:
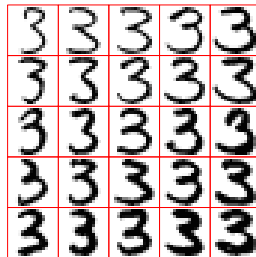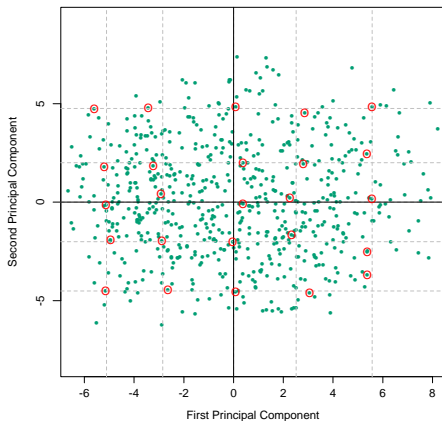
PCA - Pattern Recognition

Patterns in feature space:
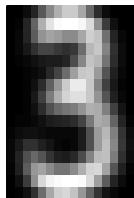
Breakout Discussion

- What pattern does the first PC find?

- What pattern does the second PC find?

- Questions?

PCA - Data Visualization

PC Scatterplots:

- Problem: Can't visualize all the features.
- Solution: Plot u_1 vs. u_2 and so forth.
- Advantages:
  - Dramatically reduces number of 2D scatterplots to visualize.
  - Focuses on patterns with most variance.

PC Loadings Plots:

- Scatterplots of v_1 vs. v_2.
- Visualizations of v_k.

Biplot:

- Scatterplot of PC 1 vs. PC 2 with loadings of v_1 vs. v_2 overlaid.

PCA - Data Visualization

Scatterplots:
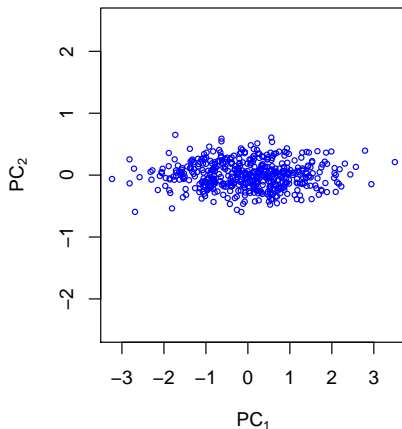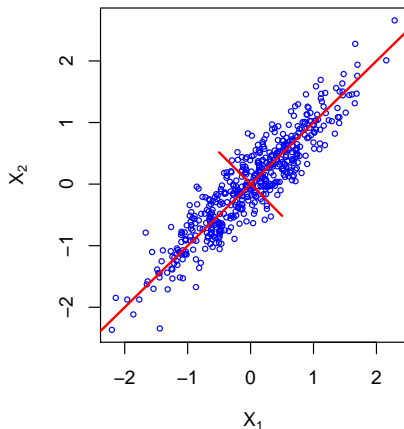
- Plotting Scatterplot PCs roughly equivalent to rotating axes of original plot.

PCA - Dimension Reduction

Best low-rank approximation to the data:

$$\underset{\tilde{X}}{\text{minimize}} \quad ||X - \tilde{X}||_F^2 \text{ subject to } \text{rank}(\tilde{X}) = K$$

Solution: $\tilde{X} = \sum_{k=1}^{K} d_k u_k v_k^T$ - SVD / PCA solution!

- PCA also finds best data compression to minimize reconstruction error.
- PCA yields "best" linear dimension reduction possible!

PCA - Dimension Reduction

How much variance is explained? (i.e. extent of dimension reduction)

- Variance explained by k^{th} PC:

$$d_k^2 = \mathsf{v}_k^T \, \mathsf{X}^T \, \mathsf{X} \, \mathsf{v}_k \, .$$

- Total variance of data:

$$\sum_{k=1}^{p} d_k^2.$$

- Proportion of variance explained by k^{th} PC:

$$d_k^2 / \sum_{k=1}^{p} d_k^2.$$

- Cumulative variance explained by first r PCs:

$$\sum_{k=1}^{r} d_k^2 / \sum_{k=1}^{p} d_k^2.$$

(Extent of dimension reduction achieve by first r PC projections.)

PCA - Dimension Reduction

Screeplot:
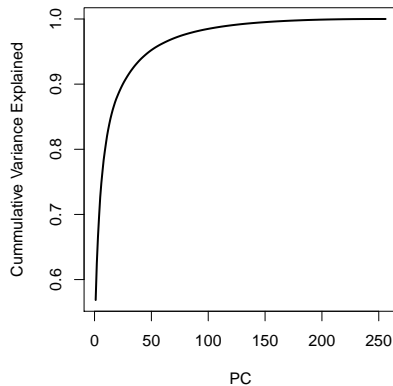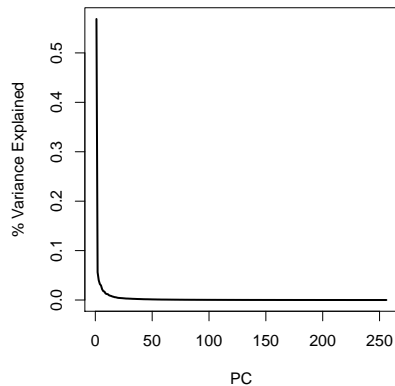
PCA - Dimension Reduction

How to choose K?

- Elbow in screeplot.
- Take K that explains at least 90% (95%, 99%, etc.) variance.

- More sophisticated:
  - ▶ Cross-Validation done internally.
  - ▶ Validation via matrix completion.
  - ▶ Nuclear norm penalties.

PCA - Center and Scale?

- Typically, one should center features (i.e. columns of X).
  - Maximizing variance interpretation (assumes multivariate Gaussian model).
- Scaling changes PCA solution.
  - Features with large scale contribute more to variance, have large PC loadings.

General Suggestions:

- Scale if features measured differently. (Example - US college data).
- Don't scale if features measured in same way & scale has meaning. (Example - gene expression data).

PCA - Applications

"EigenImages" or "EigenFaces"
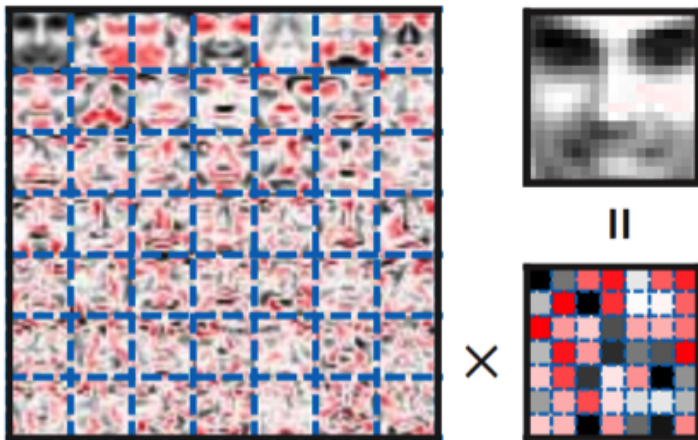
PCA - Applications
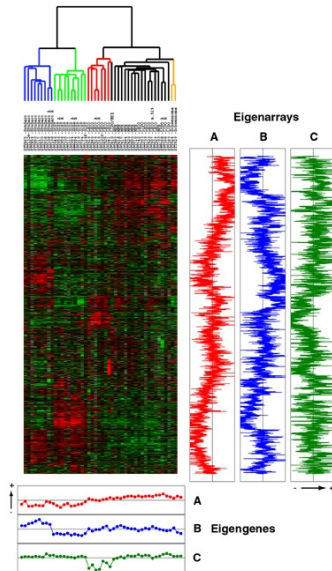
PCA - Summary

Strengths:

- "Best" linear dimension reduction.
- Interpretation:
  - Ordered / orthogonal components.
  - Unique, global solution.
- Data visualization.
- Pattern recognition.
- Others?

Weaknesses:

- Non-linear patterns.
- Others?

PCA - Best Practices

When someone gives you a data matrix . . .

Apply PCA first!

Breakout Discussion

Quick Quiz (T/F):

- You should always center and scale before applying PCA.
- PCA will perform poorly if your data doesn't lie on a line.
- You can only visualize the first two PCs.
- PCA only finds patterns amongst the observations.
- PC i always contains a more important pattern than PC $i+1$.

Discussion:

- How will you use PCA for your work?
- Questions?

PCA Extensions

Sparse PCA

Motivation:

- When $p >> n$, many features irrelevant.
- PCA can perform poorly.

Idea:

- Sparsity in V: zero out irrelevant features from PC loadings.
- Advantage: Find important features that contribute to major patterns in the data.

How?

- Typically, optimize PCA criterion with sparsity-encouraging penalty of V.
- Many methods - active area of research!

In R: SPC in PMA package.

Functional PCA

Motivation:

- Times series, ordered data, spatial data.

Idea:

- Want PC loadings to be smooth (vary continuously) over time or space.
- Advantage: Improve interpretation.

How?

- Typically, optimize PCA criterion with a penalty that encourages smoothness of V over time or space.
- Many methods for both functional data (data in the from of curves) and discretely-sampled functional data (e.g. discrete time points or specific locations).

In R: package fpca.

Kernel PCA

Motivation:

- Non-linear patterns.

Idea:

- Embed inner product distances ($x_i^T x_{i'}$) in a higher-dimensional "kernel" space, $k(x_i, x_{i'})$.
- Kernel examples:
  - Radial: $k(x_i, x_{i'}) = e^{||x_i - x_{i'}||_2^2 / 2\sigma^2}$.
  - Polynomial: $k(x_i, x_{i'}) = (c x_i^T x_{i'} + 1)^d$.
- Kernel Matrix: $K_{n \times n} : K_{ii'} = k(x_i, x_{i'})$.
  - Idea: K a non-linear distance matrix.
- Find major non-linear patterns by performing PCA on K:

$$K = U D^2 U^T$$

Supervised Dimension Reduction

Partial Least Squares:

- Best dimension reduction of cross-covariance between X and Y such that factors are orthogonal to X.

Canonical Correlations Analysis:

- Best dimension reduction of cross-covariance between X and Y such that bi-projection is orthogonal to X or Y.

Linear Discriminant Analysis (classification):

- Best dimension reduction of between class covariance matrix relative to within class covariance.

Non-Negative Matrix Factorization (NMF)

NMF

Idea: $X_{n \times p} \approx W_{n \times K} H_{K \times p} = \sum_{k=1}^{K} W_{:,k} H_{k,:}$ with $K << p$.

- $X \geq 0$ - non-negative data matrix.

- $W \geq 0$ - non-negative observation factors; often sparse (Basis Factors).
    - $W_{:,k} \geq 0$ - k^{th} observation factor.

- $H_{kj} \geq 0$ - non-negative feature factors; often sparse (Mixture Factors).
    - $H_{k,:} \geq 0$ - mixture of features that comprise the kth factor.

Like PCA except finds patterns with same direction of correlation.

NMF
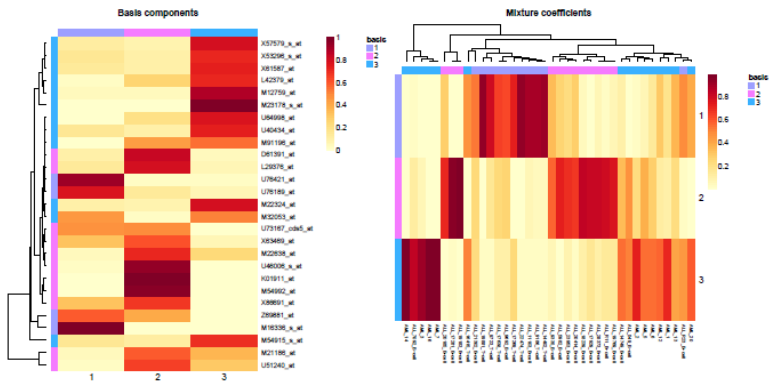
NMF Interpretation

Topic Modeling:

- X a matrix of news articles (rows) by words (columns) whose entries are word counts.
  - $X \approx \sum_{k=1}^{K} W_{:,k} H_{k,:}$ - sum of topics.
  - $X_{ij} = W_{i,:}^{T} H_{:,j}^{T} = \sum_{k=1}^{K} W_{ik} H_{kj}$.

- Topic k: Outer-product of kth column of W ($W_{:,k}$) and k^{th} row of H ($H_{k,:}$).
  - E.g. Covid-19.

- $H_{k,:}$ non-zeros- words contributing to topic k.
  - E.g. virus, hospitalizations, cases, deaths, masks, testing etc.

- $W_{:,k}$ non-zeros - news articles belonging to topic k.
  - E.g. "Virus surge visible across Texas: The tsunami is here" (*Washington Post*).

NMF Criterion - Continuous Data

$$\underset{\mathsf{W},\mathsf{H}}{\text{minimize}} \quad ||\mathsf{X} - \mathsf{W}\,\mathsf{H}||_F^2$$

$$\text{subject to} \quad \mathsf{W}_{ik} \geq 0 \ \& \ \mathsf{H}_{kj} \geq 0$$

(PCA criterion except with non-negativity constraints.)
Algorithm Updates: (Alternating Non-negative Least Squares)

$$\hat{\mathsf{W}} = \left(\mathsf{X}\,\mathsf{H}^T(\mathsf{H}^T\,\mathsf{H})^{-1}\right)_+$$

$$\hat{\mathsf{H}} = \left((\mathsf{W}^T\,\mathsf{W})^{-1}\,\mathsf{W}^T\,\mathsf{X}\right)_+$$

Local Solution.

NMF Criterion - Count Data

$$\underset{W,H}{\text{minimize}} \quad \sum_{i=1}^{n} \sum_{j=1}^{p} [X_{ij} \log(W_i H_j) - W_i H_j]$$

$$\text{subject to} \quad W_{ik} \geq 0 \ \& \ H_{kj} \geq 0$$

Algorithm Updates:

$$\hat{W}_{ik} = \hat{W}_{ik} \left(\frac{\sum_{j=1}^{p} \hat{H}_{kj} X_{ij} / \hat{W}_i^T \hat{H}_j}{\sum_{j=1}^{p} \hat{H}_{kj}} \right)$$

$$\hat{H}_{kj} = \hat{H}_{kj} \left(\frac{\sum_{i=1}^{n} \hat{W}_{ik} X_{ij} / \hat{W}_i^T \hat{H}_j}{\sum_{i=1}^{n} \hat{W}_{ik}} \right)$$
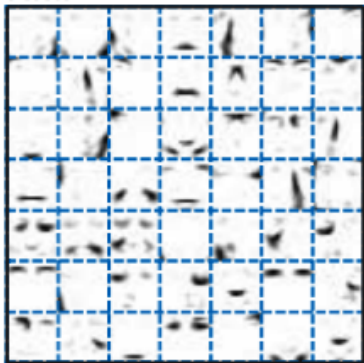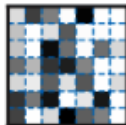
Local solution.

NMF - Uses

1. Dimension Reduction / Pattern Recognition.
   - Similar to PCA (e.g. component scatterplots) except that patterns of correlation found in the same direction.

2. Archetypal Analysis.
   - Caricatures (segments; contrastive categorization) vs. Prototypes (averages).

3. Soft-clustering.
   - Discussed Next Lecture!

NMF - Archetypal Analysis
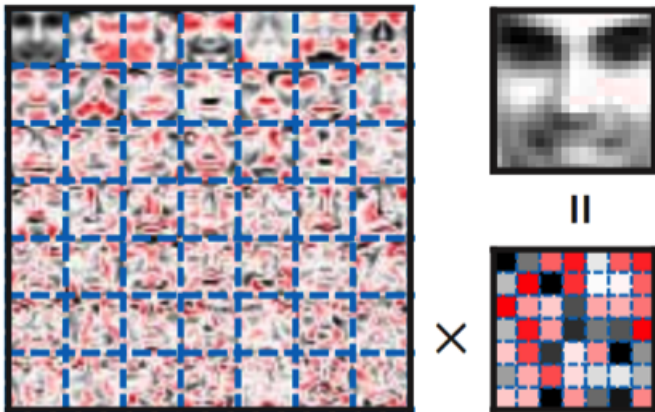
NMF - Archetypal Analysis

PCA vs. NMF

Similarities:

- Linear Dimension Reduction.
- Interpretation.

Differences:

- Factors are unordered.
- Factors NOT orthogonal.
- Changing K can fundamentally change factors.
- Non-unique, non-global solution.
- Depends on initialization. (Run several times and take the best).

Choosing K

Choice depends on goal:

- Dimension Reduction:
  - Residual sums of squares (or dispersion) - Screeplot.
- Clustering:
  - Consensus, silhouette, etc. (Discussed next lecture!).
- Archetypal Analysis:
  - Sparsity, factor purity, etc.

NMF - Summary

Strengths:

- Interpretation (often more appealing than PCA!).
- Applications - Clustering & Archetypal Analysis.
- Pattern Recognition.
- Others?

Weaknesses:

- Local solutions that depend strongly on K.
- Others?

In R: NMF package.

Independent Components Analysis (ICA)

ICA

Pre-processing Step: Reduce $X_{n \times p}$ to $\tilde{X}_{K \times p}$ with $K < n$ # independent sources. (Typically via PCA!)

Idea: $\tilde{X}_{K \times p} \approx A_{K \times K} S_{K \times p}$.

- Assumption: $\tilde{X}$ a matrix of K scrambled independent signals.

- $A_{K \times K}$ *Mixing Matrix* - denotes how signals are scrambled to form sources in data.

- $S_{K \times p}$ *Signal Matrix* - each row of S is an independent signal.

PCA finds uncorrelated, but not independent signals.

ICA Uses

1. Blind Source Separation.
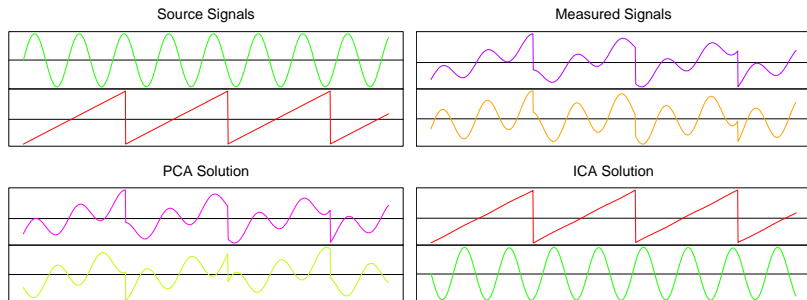   - Assume K independent signals got scrambled, but record K scrambled versions of the signal.
   - Cocktail Party Problem.
2. Denoising.
   - Noise - independent from true signals.

ICA vs. PCA

Blind Source Separation:

ICA Algorithms

Fast ICA:

- Finds projections of X that are "non-Gaussian".
- Uses non-Gaussian contrast functions:
  - $g(x) = x^4$.
  - $g(x) = tanh(x)$.
- Generalization of projection pursuit.

Others:

- Infomax (entropy).

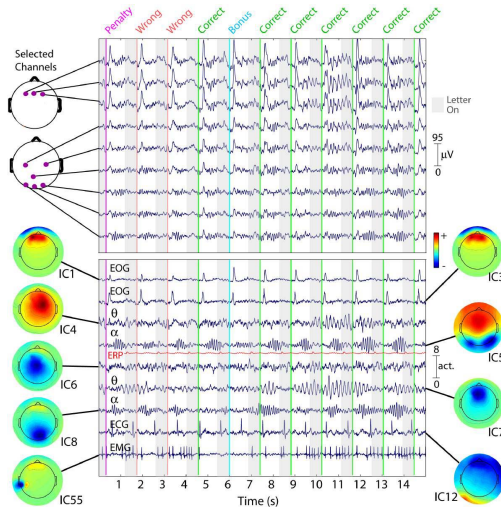Not Statistically Independent!

PCA vs. ICA

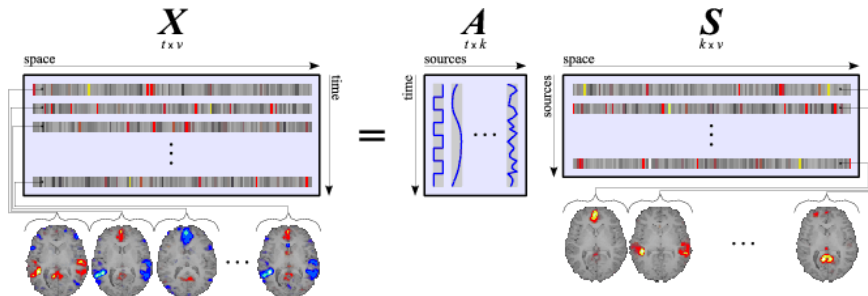Similarities:

- Linear Dimension Reduction.
- Interpretation.

Differences:

- Factors are unordered.
- Factors NOT invariant - same solution by applying a permutation.
- Factors NOT orthogonal.
- Changing K can fundamentally change factors.
- Non-unique.
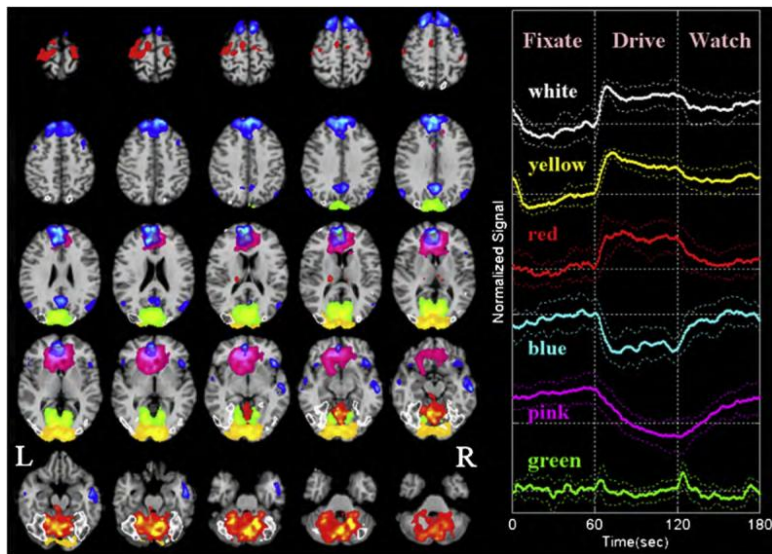- No optimization criterion to evaluate solution.

ICA Applications - EEG

ICA Applications - fMRI

ICA Applications - fMRI

ICA Summary

Strengths:

- Interpretation.
- Applications - Blind Source Separation & Denoising.
- Others?

Weaknesses:

- Solutions that depend strongly on K.
- Solutions can be rotated.
- Others?

In R: fastICA package.

Multidimensional Scaling (MDS)

Multidimensional Scaling (MDS)

Idea:

- Visually represent proximities (similarities or distances) between objects in a lower dimensional space.
- Input: Matrix of similarities or dissimilarities, $D_{n \times n}$ (don't need the data itself!).
- Goal: Find projections ($z_1, \ldots z_K$ where $z \in \mathbb{R}^n$) that preserve original distances in D in a lower dimensional space ($K << n$).
- 2 Types: Classical (Metric) MDS and Non-metric MDS.
- Non-linear dimension reduction.

MDS - Example

Consider the distances between nine American cities:

	BOS	CHI	DC	DEN	LA	MIA	NY	SEA	SF
BOS	0	963	429	1949	2979	1504	206	2976	3095
CHI	963	0	671	996	2054	1329	802	2013	2142
DC	429	671	0	1616	2631	1075	233	2684	2799
DEN	1949	996	1616	0	1059	2037	1771	1307	1235
LA	2979	2054	2631	1059	0	2687	2786	1131	379
MIA	1504	1329	1075	2037	2687	0	1308	3273	3053
NY	206	802	233	1771	2786	1308	0	2815	2934
SEA	2976	2013	2684	1307	1131	3273	2815	0	808
SF	3095	2142	2799	1235	379	3053	2934	808	0

Can we represent these cities in a 2D space like a map?

MDS - Example

cmdscale(cities)

MDS - Example

cmdscale(cities)
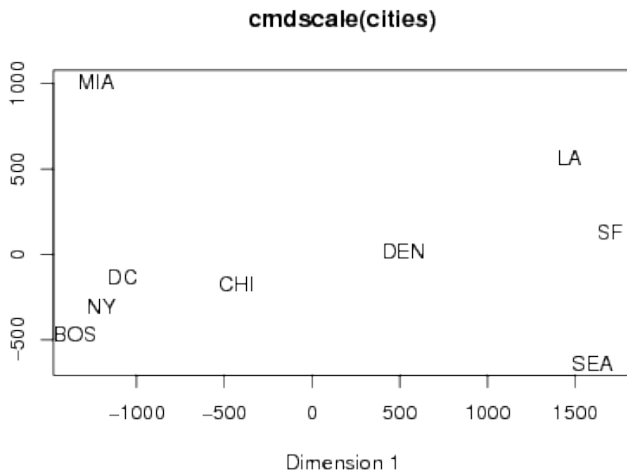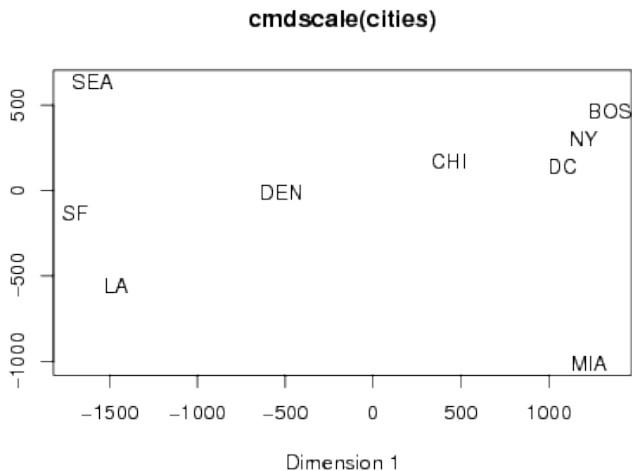
MDS - Example

Classical (Metric) MDS

- Idea: Perform PCA (eigenvalue decomposition) on the doubly centered distance matrix, D.
  - $H = I - \frac{1}{n} 11^T$ is the centering matrix.
  - $z_1, \ldots z_K$ are the top K PCs of $H D H$.

- Fact: When D is the matrix of Euclidean distances, classical MDS is equivalent to PCA.
  - Differences for other distance metrics.

In R: `cmdscale`.

Non-Metric MDS

- Idea: Optimize stress function that keeps distances in Z close to that of D.

Stress Functions:

- Least squares or Kruskal-Shephard Scaling:

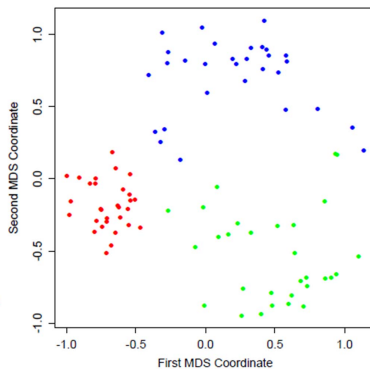$$S_D(z_1, z_2, \ldots, z_K) = \sqrt{\sum_{i \neq i'} (d_{ii'} - ||z_i - z_{i'}||)^2}.$$
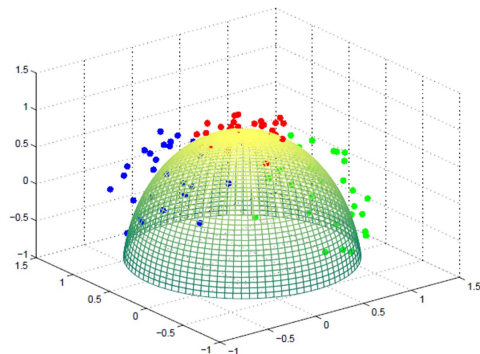
- Sammon mapping: preserve smaller pairwise distances

$$\sum_{i \neq i'} \frac{(d_{ii'} - ||z_i - z_{i'}||^2)}{d_{ii'}}.$$

- Shepard-Kruskal nonmetric scaling ($\theta(\cdot)$: an increasing function):

$$\frac{\sum_{ii'} [\theta(||z_i - z_{i'}||) - d_{ii'}]^2}{\sum_{ii'} d_{ii'}^2}.$$

MDS - Example

MDS Properties

- Data not needed - only dissimilarities.

- Choosing K:
  - Scree plot (like PCA).
  - Shepard Diagram - plot proximities against distances in Z.

- Interpreting MDS maps:
  - Axes and orientation arbitrary.
  - Can be rotated.
  - Only relative locations important.
  - Typically looks for objects close in the MDS map.
  - Can be distortions.

MDS vs. PCA

Similarities:

- Dimension reduction for visualization.

Differences:

- Non-linear vs. Linear.
- Local solution & arbitrary map.
- Non-unique & local solution.
- Only yields visualization / patterns among n objects.

MDS - Summary

Strengths:

- Visualizing proximities.
- Only need dissimilarities.
- Non-linear dimension reduction.
- Others?

Weaknesses:

- Arbitrary maps.
- High-dimensional settings? ($p >> n$ - more features than objects)
- Others?

In R: `dist`; `cmdscale` - classical MDS; `isoMDS` - Kruskals's MDS and `sammon` in `MASS` package.

Neighbor Embeddings: tSNE & UMAP

Neighbor Embeddings

Idea:

- Find lower dimensional embedding that preserves relationships between "close neighbors".
- Non-linear dimension reduction (manifold learning).
- Useful for visualizations and clustering.
- Works well for high-dimensional data ($p >> n$).

t-Stochastic Neighbor Embedding (tSNE)

- Set up: Represent data, $x_1, \ldots x_n \in \mathbb{R}^p$, in a lower dimensional space, $z_1, \ldots z_n \in \mathbb{R}^k$ where $k << p$ (usually $k = 2$).

- Data Similarity (normalized Gaussian kernel; σ related to perplexity):

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2}, \quad p_{j|i} = \frac{\exp\left(-(x_i - x_j)^2/2\sigma^2\right)}{\sum_{k \neq i} \exp\left(-(x_i - x_k)^2/2\sigma^2\right)}$$

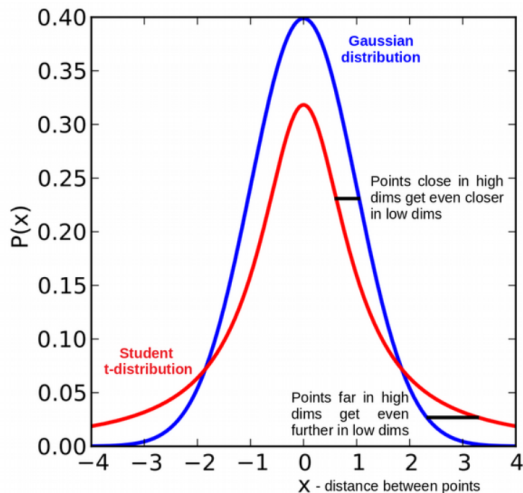- Lower-Dimensional Similarity (normalized t/Cauchy kernel):

$$q(z_i, z_j) = \frac{g(|z_i - z_j|)}{\sum_{k \neq i} g(|z_i - z_k|)}, \quad g(z) = \frac{1}{1 + z^2}.$$

- Minimize Kullback-Leibler divergence:

$$\underset{z_1, z_2, \ldots z_n}{\text{minimize}} \quad \sum_{i,j} p_{ij} \log\left(\frac{p_{ij}}{q(z_i, z_j)}\right)$$

- Gradient descent (with random initialization).

t-Stochastic Neighbor Embedding (tSNE)

UMAP

Similar to tSNE, but with a few differences:

- Data Similarity (Gaussian kernel, general distances, K-Nearest Neighbors, no normalization):

$$p_{ij} = p_{i|j} + p_{j|i} - p_{i|j}p_{j|i}, \quad p_{i|j} = \exp\left(-d(x_i, x_j)/\sigma_i\right).$$

- Lower-Dimensional Similarity (generalized Cauchy kernel):

$$q(z_i, z_j) = \frac{1}{1 + a(z_i - z_j)^{2b}}, \quad a > 1, b < 1 \text{ (thicker tails)}.$$
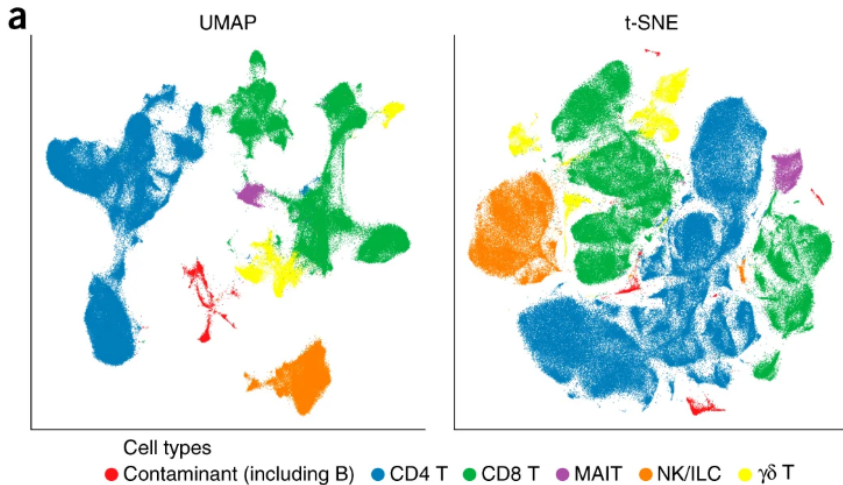
- Minimize cross-entropy:

$$\underset{z_1, z_2, \dots z_n}{\text{minimize}} \quad \sum_{i,j} p_{ij} \log\left(\frac{p_{ij}}{q(z_i, z_j)}\right) + (1 - p_{ij})\log\left(\frac{1 - p_{ij}}{1 - q(z_i, z_j)}\right)$$

- Stochastic gradient descent with spectral clustering initialization.

Overall: UMAP better preserves global structures & more tightly packs close neighbors.

tSNE & UMAP - Applications

Clustering Cell Types in Single Cell RNA-seq.

tSNE & UMAP - Summary

Strengths:

- Data visualization.
- Clustering.
- Non-linear dimension reduction.
- Preserves relationships between close neighbors.

Weaknesses:

- Local, non-unique solutions.
- Patterns only amongst observations.
- Sensitive to hyperparamters.
- Can have distortions.
- Others?

Dimension Reduction & Visualization Wrap-Up

Techniques Covered:

- PCA.
- NMF.
- ICA.
- MDS.
- SNE - tSNE & UMAP.

Breakout Discussion

Questions:

- Which techniques are useful for finding patterns amongst observations AND features? Just observations?
- List some advantages of PCA over MDS / tSNE / UMAP. List some disadvantages.
- When would you want use each of the techniques?
- Why do we need so many dimension reduction and visualization techniques?
- If you had new (test) data, how would you use this to validate the patterns you discovered?

Research Highlight
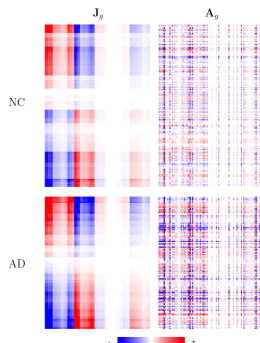
Integrated PCA

Multi-View Data:
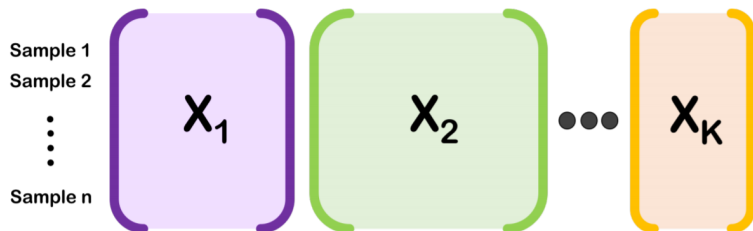
Goal: How do you find joint patterns across the shared subjects?

Solution: iPCA! (Tang and Allen, 2021)

- Generalization of PCA using matrix-variate normal.

Research Highlight

Multi-Group PCA and beyond

Solution: Joint and Individual Component Regression (JICO) (Wang et al., 2022)

- Generalization of PCA for multi-group data using continuum regression framework; covers JIVE (Lock et al., 13) as a special case.