Machine Learning

Feature Learning

Feature Learning

- Feature representations are important for supervised learning problems as well as Reinforcement Learning problems
  - Feature representation can change the complexity of the decision boundary
  - Feature representation can change the dimensionality of the problem
- Features can be either designed or learned
  - Supervised: e.g. ANN hidden units learn features
  - Unsupervised: e.g. cluster IDs as features

Unsupervised Feature Learning

- Unsupervised features have to be built around general principles for “good” features
  - Metric for “good” features has to be built into the algorithm
- Clustering can be used to form features IDs can be used as discrete features (similar items have the same/similar features)
  - Cluster ID as discrete feature
  - Cluster probability as continuous feature
- Other criteria for “good” features can be used

Unsupervised Feature Learning

- A common criterion for “good” features are
  - How precisely they can represent the data
  - How compact the basis is
- Representation accuracy is aimed at ensuring that the unsupervised feature learning does not loose significant amounts of information
  - Information loss might make some subsequent tasks impossible to do/learn
- Compactness is aimed at simplicity
  - Reduce overfitting
  - Reduce complexity for subsequent tasks

Principal Component Analysis

- Principal component analysis (PCA) is one of the most used approaches for unsupervised learning of a compact feature space
  - Uses both accuracy of representation of data and compactness of the representation
  - Assumes linear representation of data in terms of learned, constant, unit length basis vectors

$$\hat{x}^{(i)} = \bar{x} + \sum_k \phi_k(x^{(i)})\hat{u}_k$$

    - Accuracy of representation is defined in terms of a common criterion for "good" features are

$$E_{k,\phi,\hat{u},D} = \sum_i \left\| x^{(i)} - \hat{x}^{(i)} \right\|^2 = \sum_i \left\| x^{(i)} - \left(\bar{x} + \sum_{j=1}^{k} \phi_j(x^{(i)})\hat{u}_j \right) \right\|^2$$

Principal Component Analysis

- PCA basically forms a new basis for the data in such a way that for every number of features, k, the resulting basis minimizes the square reconstruction error
  - Each feature tries to capture as much of the remaining data variation as possible, reducing the squared error as much as possible
    - Feature value that minimizes the error for all k:

$$f_k(x^{(i)}) = \hat{u}_k^T \left(x^{(i)} - \bar{x} \right)$$

    - Corresponding basis vectors have to minimize the error

$$\hat{u}^* = \arg\min_u \sum_i \left\| x^{(i)} - \left(\bar{x} + \sum_{j=1}^{k} f_j(x^{(i)}) \hat{u}_j \right) \right\|^2$$

Principal Component Analysis

- To solve for the basis it is important to note:
  - The vectors have to be orthogonal
  - The error for *k=d* is *0*
- Thus the error for a *k* is equal to the value of the higher components

$$E_{k,f,\hat{u},D} = \sum_i \left\| \sum_{j=k+1}^{d} \hat{u}_j^T \left(x^{(i)} - \bar{x}\right) \hat{u}_j \right\|^2$$

$$= \sum_i \sum_{j=k+1}^{d} \left(\hat{u}_j^T \left(x^{(i)} - \bar{x}\right)\right)^2$$

$$= \sum_{j=k+1}^{d} \sum_i \left(\hat{u}_j^T \left(x^{(i)} - \bar{x}\right)\right)^2 = \sum_{j=k+1}^{d} \sum_i \left(\left(x^{(i)} - \bar{x}\right)^T \hat{u}_j\right)^2$$

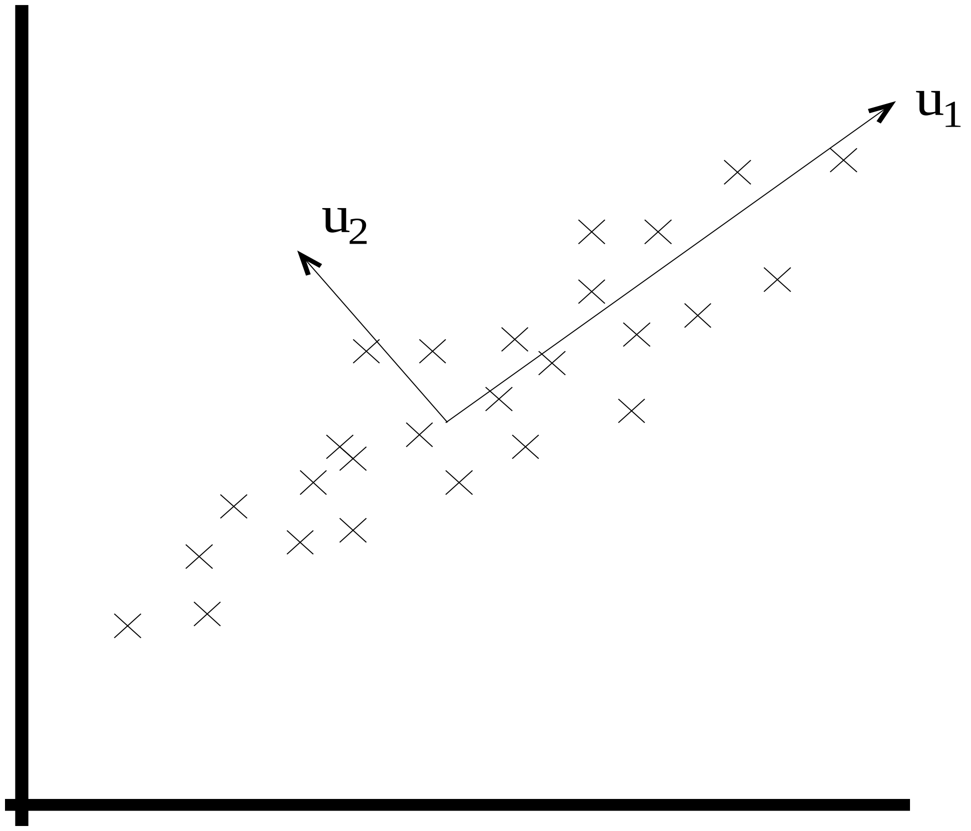
$$= \sum_{j=k+1}^{d} \sum_i \hat{u}_j^T \left(x^{(i)} - \bar{x}\right)\left(x^{(i)} - \bar{x}\right)^T \hat{u}_j = \sum_{j=k+1}^{d} \hat{u}_j^T \Sigma \hat{u}_j$$

Principal Component Analysis

- Solving from top down, starting with k=d we can notice that $\hat{u}_d = \arg\min_{\hat{u}} \hat{u}_d^T S \hat{u}_d$ has its solution for the smallest eigenvector of Σ
  - In the same way, each earlier basis vector corresponds to the next smaller eigenvector of Σ
- Principal components of a data set are the eigenvectors of normalized data's covariance matrix in order of increasing eigenvalue
  - If scales of original dimensions are incompatible, data can be normalized with standard deviation

Principal Component Analysis

- PCA example



Principal Component Analysis

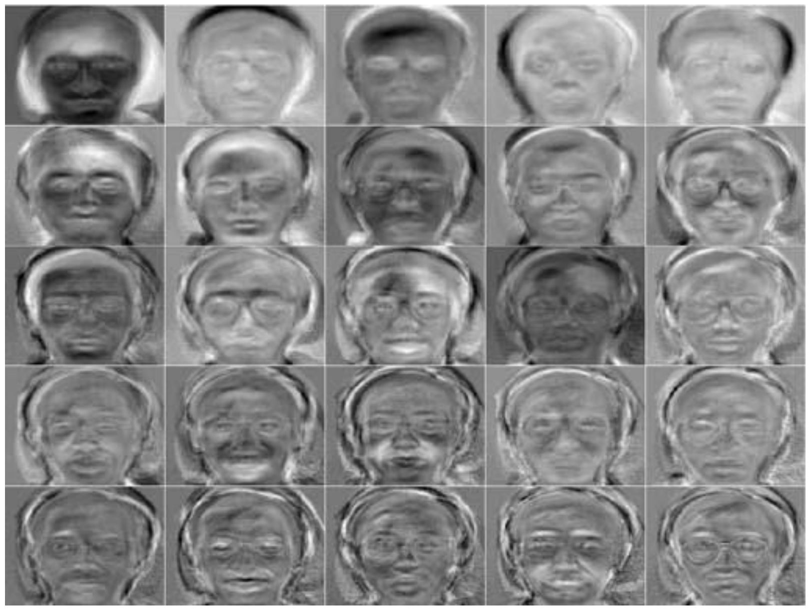
- PCA algorithm
  - Create *n x d* data matrix *D*
  - Normalize columns by subtracting column average
    - If desired, normalize columns with standard deviation
  - Compute scaled covariance matrix $\Sigma = D^T D$ of data
  - Find eigenvectors and eigenvalues of Σ
  - Sort by eigenvalue for Principal Components
- Eigenvalue indicates loss when not using the principal component
  - Shorter representation by ignoring higher components

Principal Component Analysis

- If d is large the eigenvector calculation becomes expensive and potentially numerically unstable
  - Can solve using Singular Value Decomposition
    $$D = USV^T$$
    - S is a diagonal matrix of the eigenvalues of $D^T D$
    - The columns of V are the eigenvectors of $D^T D$
  - SVD is more stable and often more efficient

Principal Component Analysis

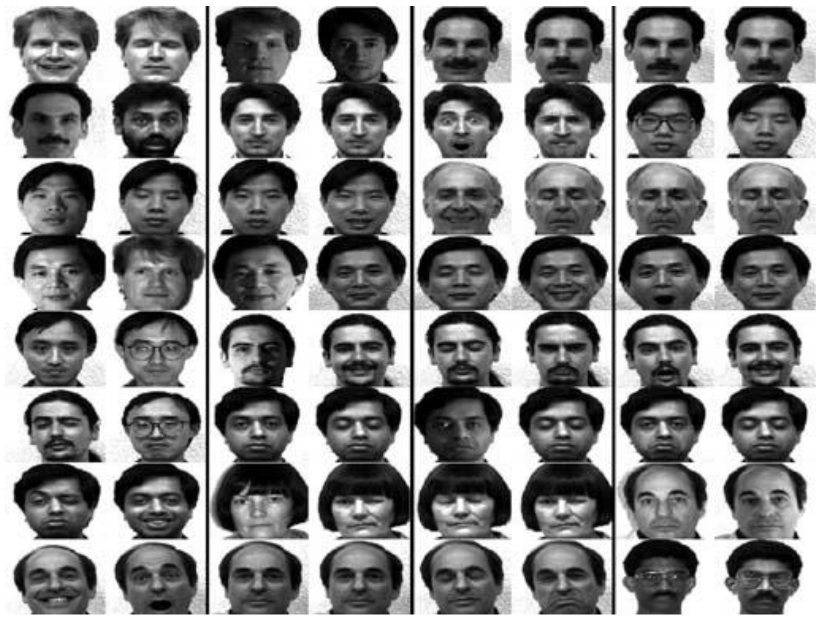
- PCA is one of the most commonly used feature learning approaches
  - E.g. Eigenfaces:
    - 25 most significant principal components of a set of face images:



C. DeCoro

Eigenfaces

- Using these 25 features we use nearest neighbor to identify the person
  - Reduction to a 25 dimensional representation
  - Recognition rate is above 80% for the test set
  - Reconstruction:



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Feature Learning

- Other techniques exist to learn a different feature representation
  - Independent component analysis (ICA)
    - Similar to PCA but finds most statistically independent components
      - Minimizes mutual information between components
      - Or: maximizes non-Gaussianity
    - Used to separate multiple sources of stochastic data
  - Sparse PCA
    - PCA where components can be in at most k dimensions
  - Sparse coding
    - PCA with a regularization term over feature values

Self-Organizing Maps

- Self-organizing maps are neural networks that are trained in an unsupervised fashion
  - Hidden units are arranged in a k-dimensional lattice with a distance function
    - Weight vectors to a unit map into the lattice
    - Neighboring unit's weight vectors are weakly linked based on the distance function
    - Training "deforms" lattice to map onto data points
      - Topological mapping
  - Units compete for Best Matching Unit (BMU)
    - Units cooperate with BMU, updating based on distance to BMU

Self-Organizing Maps

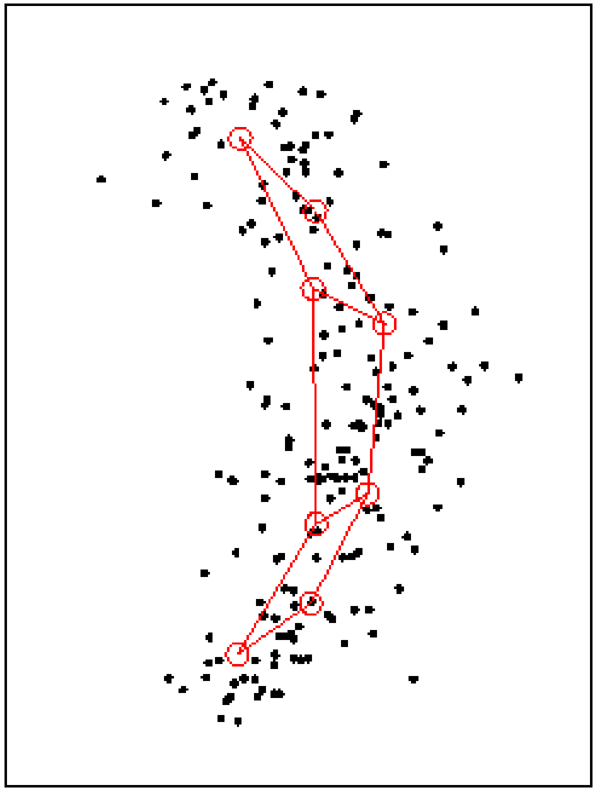
- Randomly initialize hidden unit weight vectors
- For each data point find the unit that has the weight vector most similar to the data (BMU)
  - Similarity is usually Cartesian distance
- Update the weights of all the units

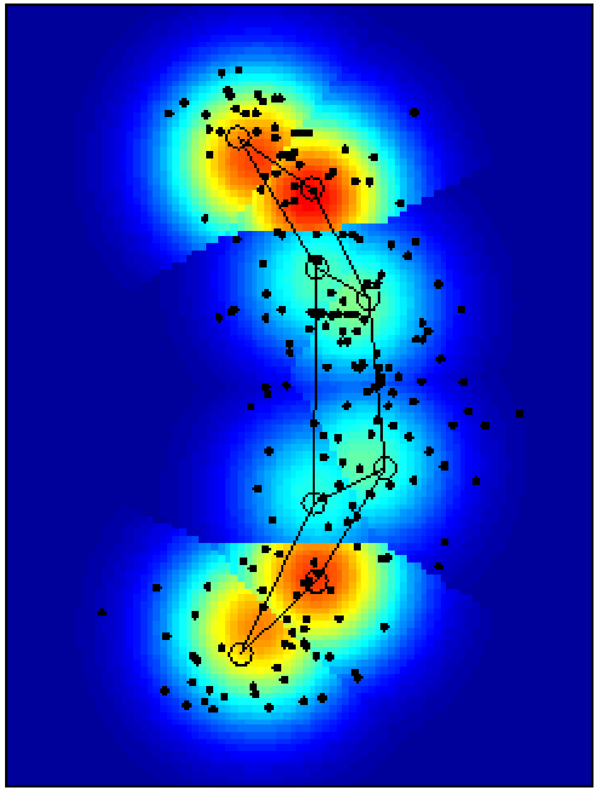
$$w_{j,k} \leftarrow w_{j,k} + \alpha(t)\Theta_t(k, BMU)\left(x_j^{(i)} - w_{j,k}\right)$$

  - $\Theta_t(k,l)$ is the similarity between the lattice location of nodes k and l
- Repeat with next data point until iteration limit

Self-Organizing Maps

- SOM example





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Unsupervised Feature Learning

- Unsupervised feature learning finds possible feature representations based on characteristics built into the algorithm
  - PCA is the most commonly used
    - PCA can always perfectly represent the original data
  - ICA and sparse methods can find more features than in the original space
    - Features can be more expressive
    - Features can be more causal
  - SOM establishes a topological mapping onto a k-dimensional lattice
    - Can be seen as a non-linear PCA