STA 4273H: Statistical Machine Learning

Russ Salakhutdinov

Department of Computer Science
Department of Statistical Sciences
rsalakhu@cs.toronto.edu
http://www.cs.utoronto.ca/~rsalakhu/

Lecture 8

Project Reminder

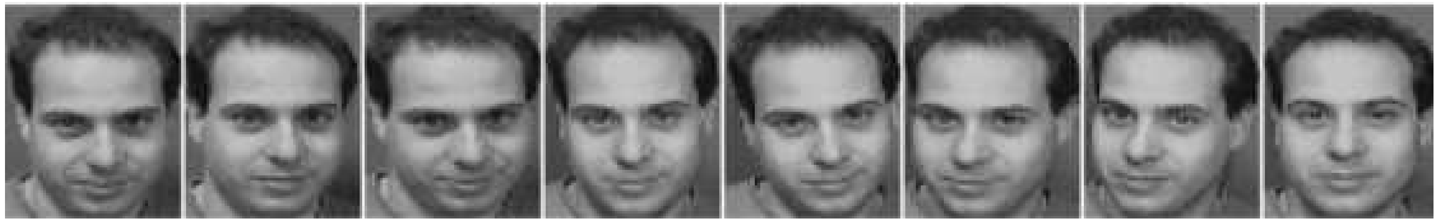
- Brief 5-minute presentations of projects will take place on Monday, March 23. You need to send me 6-7 slides in pdf formtat describing your project.
- **Deadline: Sunday March 22, 2015. Submit your slides by e-mail: rsalakhu@cs.toronto.edu**
- You should have your name, and project title on the first slide.
- You will have 5-7 mins to briefly describe your project and what you would want to accomplish in this project.
- Brief presentations will be done in an alphabetical order.

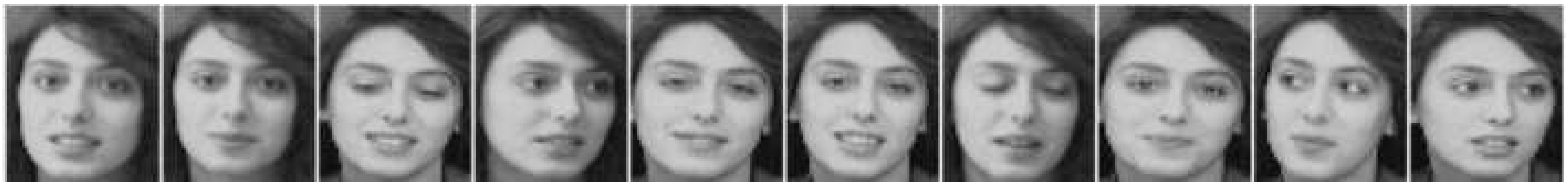
Continuous Latent Variable Models

- Often there are some unknown underlying causes of the data.
- So far we have looked at models with discrete latent variables, such as mixture of Gaussians.
- Sometimes, it is more appropriate to think in terms of continuous factors which control the data we observe.
- Motivation: for many datasets, data points lie close to a manifold of much lower dimensionality compared to that of the original data space.
- Training continuous latent variable models often called **dimensionality reduction,** since there are typically many fewer latent dimensions.
- Examples: Principal Components Analysis, Factor Analysis, Independent Components Analysis

Intrinsic Latent Dimensions

• What are the intrinsic latent dimensions in these two datasets?

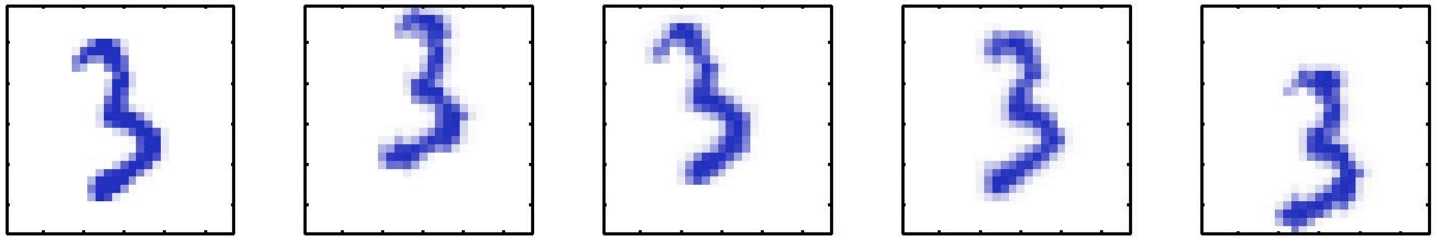




• How can we find these latent dimensions from this high-dimensional data.

Intrinsic Latent Dimensions

• In this dataset, there is only 3 degrees of freedom of variability, corresponding to the vertical and horizontal translations, and rotations.



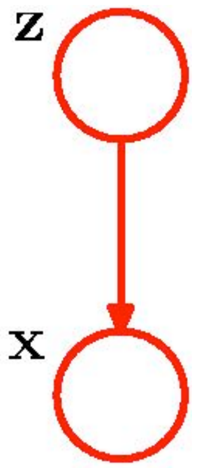
• Each image undergoes a random displacement and rotation within some larger image field.

• The resulting images have 100 $\times$ 100 = 10,000 pixels.

Generative View

• Each data example generated by first selecting a point from a distribution in the latent space, then generating a point from the conditional distribution in the input space

• Simplest latent variable models: Assume Gaussian distribution for both latent and observed variables.



• This leads to probabilistic formulation of the Principal Component Analysis and Factor Analysis.

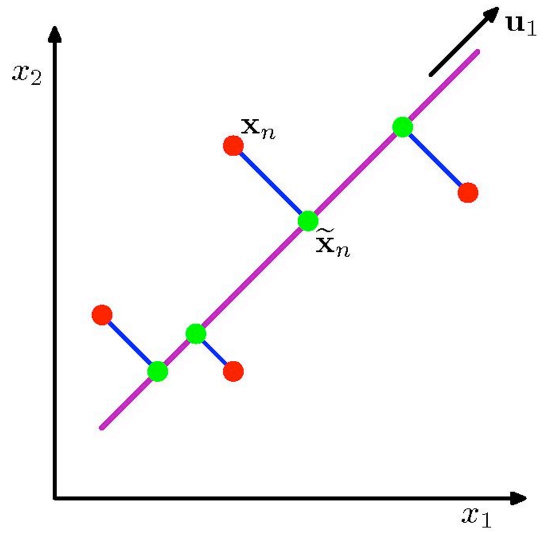
• We will first look at standard PCA, and then consider its probabilistic formation.

• Advantages of probabilistic formulation: use of EM for parameter estimation, mixture of PCAs, Bayesian PCA.

Principal Component Analysis

- Used for data compression, visualization, feature extraction, dimensionality reduction.

- The goal is find M principal components underlying D-dimensional data
  - select the top M eigenvectors of **S** (data covariance matrix): $\{\mathbf{u}_1, ..., \mathbf{u}_M\}$.
  - project each input vector **x** into this subspace, e.g. $z_{n1} = \mathbf{x}_n^T \mathbf{u}_1$.



- Full projection into M dimensions takes form:

$$\begin{bmatrix} \mathbf{u}_1^\top \\ \cdots \\ \mathbf{u}_M^\top \end{bmatrix} [\mathbf{x}_1 \cdots \mathbf{x}_N] = [\mathbf{z}_1 \cdots \mathbf{z}_N]$$

- Two views/derivations:
  - Maximize variance (scatter of green points).
  - Minimize error (red-green distance per data point).

Maximum Variance Formulation

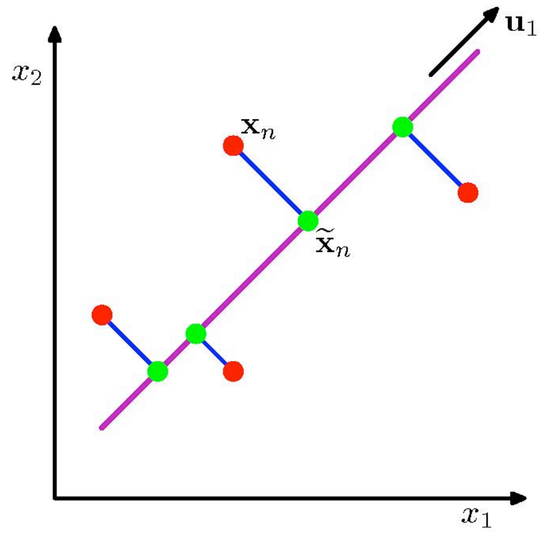
- Consider a dataset $\{x_1,\ldots,x_N\}$, $x_n \in R^D$. Our goal is to project data onto a space having dimensionality $M < D$.

- Consider the projection into M=1 dimensional space.

- Define the direction of this space using a D-dimensional unit vector u_1, so that $\mathbf{u}_1^T\mathbf{u}_1 = 1$.

- Objective: maximize the variance of the projected data with respect to u_1.

$$\frac{1}{N}\sum_{n=1}^{N}\{\mathbf{u}_1^T\mathbf{x}_n - \mathbf{u}_1^T\bar{\mathbf{x}}\}^2 = \mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$$



where sample mean and data covariance is given by:

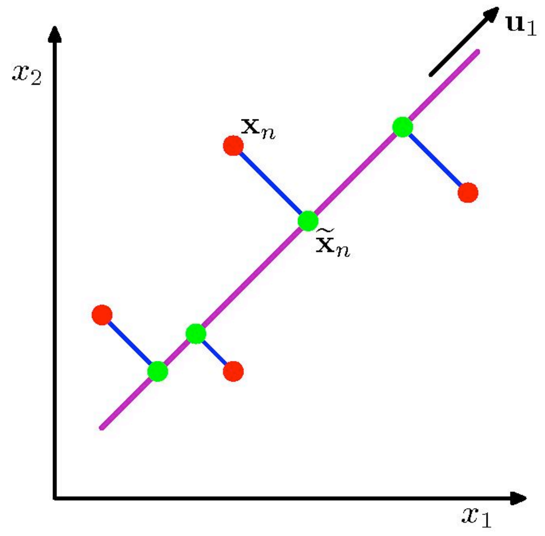
$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n$$

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^T$$

Maximum Variance Formulation

- Maximize the variance of the projected data:

$$\frac{1}{N}\sum_{n=1}^{N}\{\mathbf{u}_1^T\mathbf{x}_n - \mathbf{u}_1^T\bar{\mathbf{x}}\}^2 = \mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$$



- Must constrain $||u_1|| = 1$. Using Langrage multiplier, maximize:

$$\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1 + \lambda(1 - \mathbf{u}_1^T\mathbf{u}_1)$$

- Setting the derivative with respect to $\mathbf{u}_1$ to zero:

$$\mathbf{S}\mathbf{u}_1 = \lambda_1\mathbf{u}_1.$$

- Hence u_1 must be an eigenvector of **S**.
- The maximum variance of the projected data is given by:

$$\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1 = \lambda_1.$$

- Optimal $\mathbf{u}_1$ is principal component (eigenvector with maximal eigenvalue).

Minimum Error Formulation

- Introduce a complete orthonormal set of D-dimensional basis vectors:

$\{\mathbf{u}_1, ..., \mathbf{u}_D\}$:

$$\mathbf{u}_i^T \mathbf{u}_j = \delta_{ij}.$$

- Without loss of generality, we can write:

$$\mathbf{x}_n = \sum_{i=1}^{D} \alpha_{ni} \mathbf{u}_i, \quad \alpha_{ni} = \mathbf{x}_n^T \mathbf{u}_i.$$

Rotation of the coordinate system to a new system defined by $\mathbf{u}_i$.

- Our goal is to represent data points by the projection into M-dimensional subspace (plus some distortion):
- Represent M-dim linear subspace by the first M of the basis vectors:

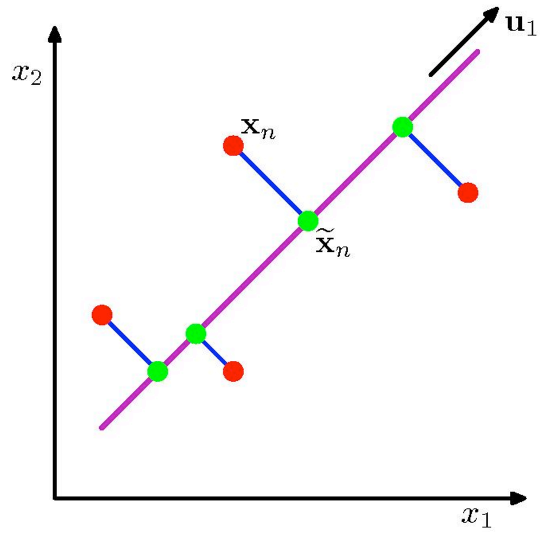
$$\tilde{\mathbf{x}}_n = \sum_{i=1}^{M} z_{ni} \mathbf{u}_i + \sum_{i=M+1}^{D} b_i \mathbf{u}_i.$$

Minimum Error Formulation

- Represent M-dim linear subspace by the first M of the basis vectors:

$$\tilde{\mathbf{x}}_n = \sum_{i=1}^{M} z_{ni}\mathbf{u}_i + \sum_{i=M+1}^{D} b_i \mathbf{u}_i.$$

where z_{ni} depend on the particular data point and b_i are constants.



- Objective: minimize distortion with respect to u_i, z_{ni}, and b_i.

$$J = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - \tilde{\mathbf{x}}_n||^2.$$

- Minimizing with respect to z_{nj}, b_j:

$$\begin{aligned} z_{nj} &= \mathbf{x}_n^T \mathbf{u}_j \\ b_j &= \bar{\mathbf{x}}^T \mathbf{u}_j \end{aligned}$$

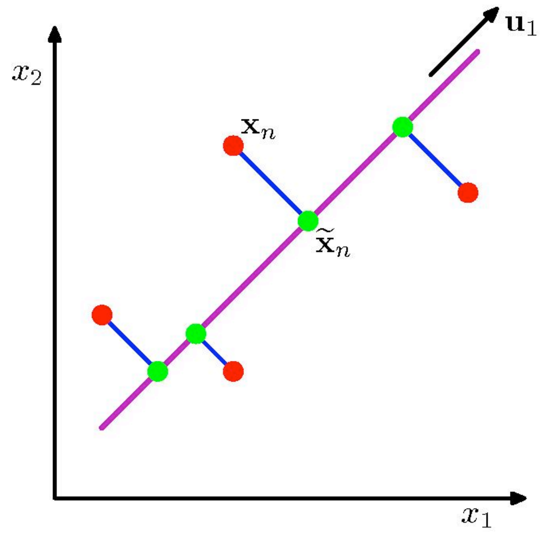
- Hence, the objective reduces to:

$$J = \frac{1}{N}\sum_{n=1}^{N}\sum_{i=M+1}^{D} (\mathbf{x}_n^T\mathbf{u}_i - \bar{\mathbf{x}}^T\mathbf{u}_i)^2 = \sum_{i=M+1}^{D} \mathbf{u}_i^T \mathbf{S}\mathbf{u}_i.$$

Minimum Error Formulation

- Minimize distortion with respect to $\mathbf{u}_i$: constraint minimization problem:

$$J = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - \tilde{\mathbf{x}}_n||^2 = \sum_{i=M+1}^{D} \mathbf{u}_i^T \mathbf{S} \mathbf{u}_i.$$



- The general solution is obtained by choosing $\mathbf{u}_i$ to be eigenvectors of the covariance matrix:

$$\mathbf{S}\mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

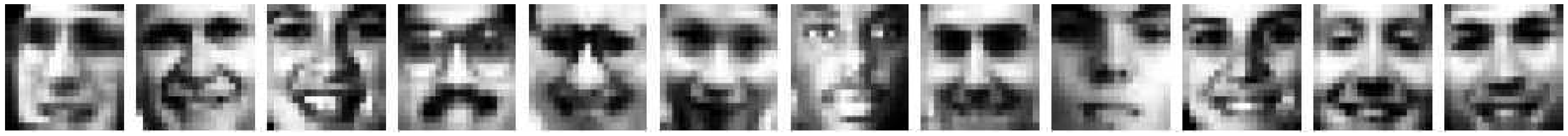
- The distortion is then given by: $J = \sum_{i=M+1}^{D} \lambda_i.$

- The objective is minimized when the remaining D-M components are the eigenvectors of **S** with ***lowest eigenvalues*** → same result.

- We will later see a generalization: deep autoencoders.

Applications of PCA

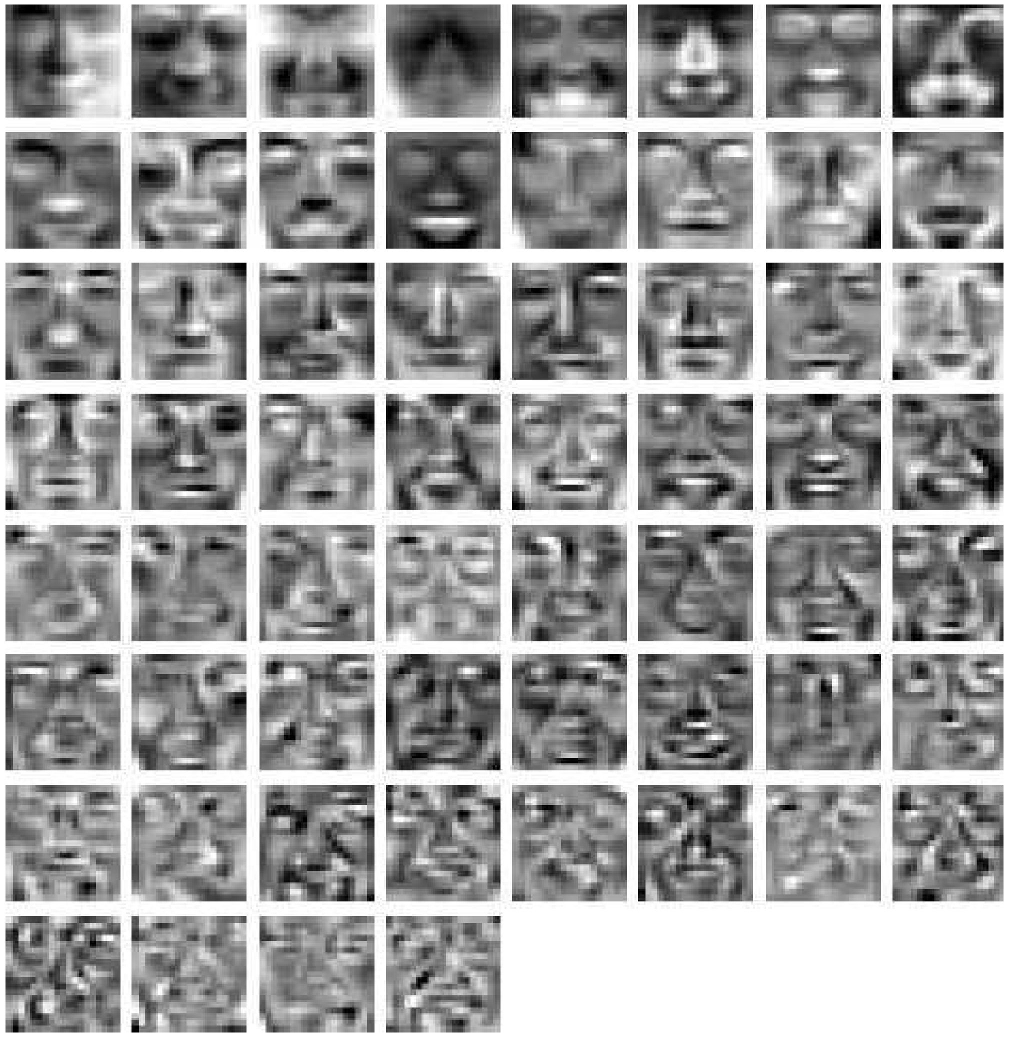
- Run PCA on 2429 19x19 grayscale images (CBCL database)



- Data compression: We can get good reconstructions with only 3 components.
- Pre-processing: We can apply a standard classifier to latent representation -- PCA with 3 components obtains 79% accuracy on face/non-face discrimination in test data vs. 76.8% for mixture of Gaussians with 84 components.
- Data visualization: by projecting the data onto the first two principal components.

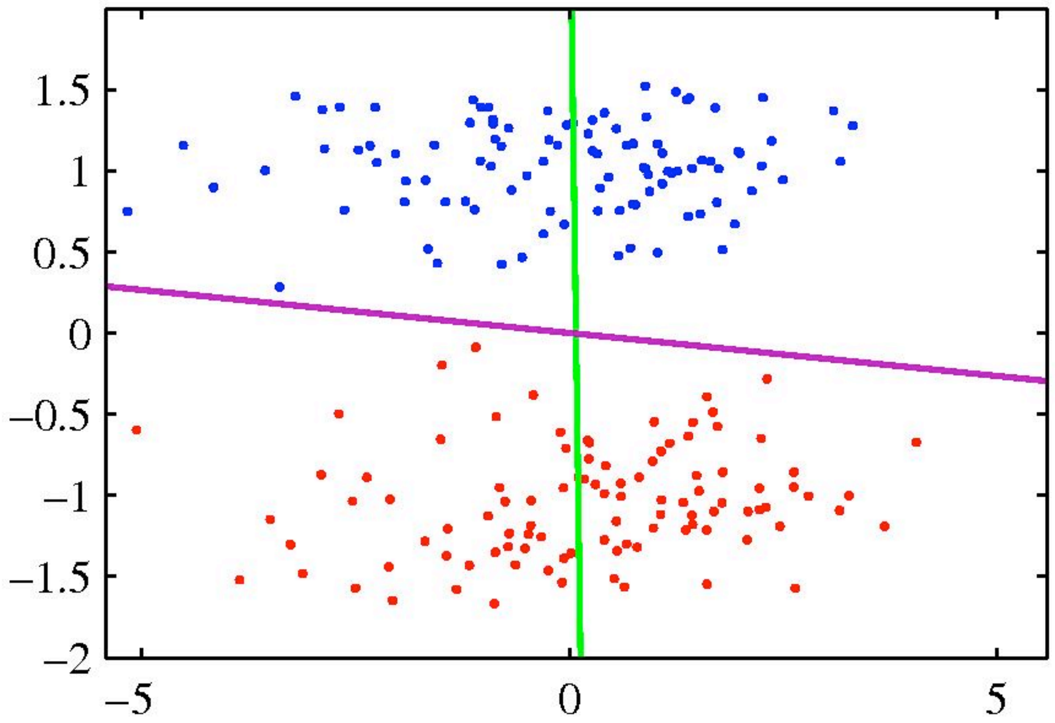
Learned Basis

- Run PCA on 2429 19x19 grayscale images (CBCL database)



PCA vs. Fisher’s LDA

• A comparison of PCA with Fisher’s LDA for linear dimensionality reduction.



• PCA chooses direction of maximum variance (magenta curve) leading to strong class overlap (unsupervised).

• LDA takes into account the class labels (supervised), leading to a projection into the green curve.

PCA for High-Dimensional Data

- In some applications of PCA, the number of data points is smaller than the dimensionality of the data space, i.e. N<D.
- In so far, we need to find the eigenvectors of the D $\times$ D data covariance matrix **S**, which scales as O(D^3).
- Direct application of PCA will often be computationally infeasible.
- Solution: Let **X** be the N $\times$ D centered data matrix. The corresponding eigenvector equation becomes:

$$\frac{1}{N}\mathbf{X}^T\mathbf{X}\mathbf{u}_i = \lambda_i\mathbf{u}_i.$$

- Pre-multiply by **X**:

$$\frac{1}{N}\mathbf{X}\mathbf{X}^T(\mathbf{X}\mathbf{u}_i) = \lambda_i(\mathbf{X}\mathbf{u}_i).$$

PCA for High-Dimensional Data

- Define $v_i = Xu_i$, and hence we have:

$$\frac{1}{N}\mathbf{X}\mathbf{X}^T\mathbf{v}_i = \lambda_i \mathbf{v}_i.$$

- This is an eigenvector equation for the N $\times$ N matrix
- It has the same N-1 eigenvalues as the original data covariance matrix **S** (which itself has an additional D-N+1 zero eigenvalues).
- Computational cost scales as $O(N^3)$ rather than $O(D^3)$.
- To determine eigenvectors, we multiply by X^T:

$$\left(\frac{1}{N}\mathbf{X}^T\mathbf{X}\right)(\mathbf{X}^T\mathbf{v}_i) = \lambda_i \mathbf{X}^T\mathbf{v}_i.$$

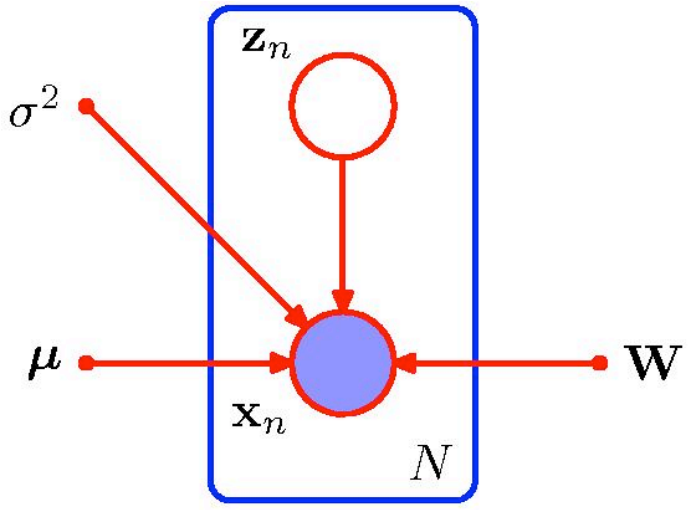
- Hence $X^T v_i$ is an eigenvector of **S** with eigenvalue λ_i.
- These eigenvectors may not be normalized.

Probabilistic PCA

- Probabilistic, generative view of data.
- Key advantages of probabilistic PCA (PPCA):
  - It represents a constrained form of the Gaussian distribution.
  - We can derive EM algorithm for PCA which is computationally efficient.
  - PPCA allows us to deal with missing values in the data set.
  - We can formulate mixture of PPCAs in a principled way.
  - PPCA forms the basis for a Bayesian PCA, in which the dimensionality of the principal subspace can be determined from the data.
  - The existence of a likelihood function allows direct comparisons with other probabilistic density models
  - PPCA can be used to model class conditional densities and hence it can be applied to classification problems.

Probabilistic PCA

- Key assumptions:
  - underlying latent M-dim variable **z** has a Gaussian distribution.
  - linear relationship between M-dim latent **z** and D-dim observed **x** variables.
  - isotropic Gaussian noise in observed dimensions

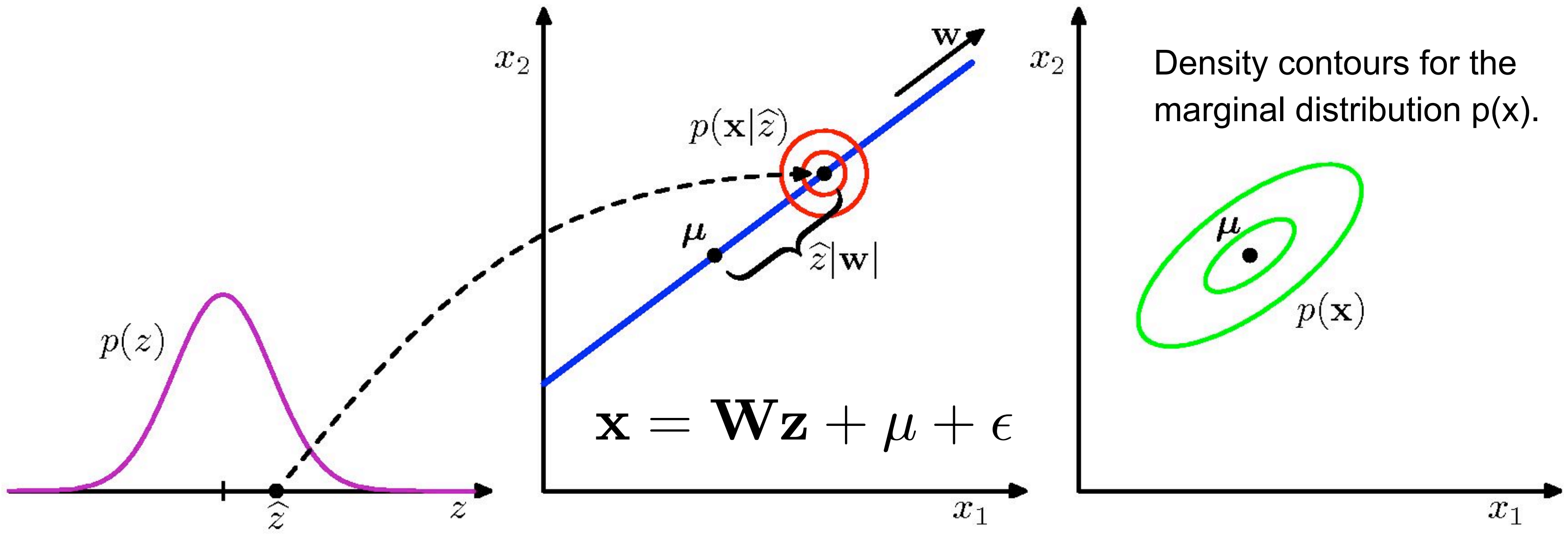


$$
\begin{aligned}
p(\mathbf{z}) &= \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}) \\
p(\mathbf{x}|\mathbf{z}) &= \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \mu, \sigma^2\mathbf{I})
\end{aligned}
$$

- Hence the mean of **x** is a linear function of **z** governed by the D $\times$ M matrix **W** and the D-dim vector μ.
- We will see that the columns of **W** span the principal subspace of the data space (Columns of **W** are the *principal components*, σ^2 is *sensor noise)*.

Generative View of PPCA

- Generative view of the PPCA for a 2-d data space and 1-d latent space:



- Draw a value of the latent variable from its prior distribution:

$$\hat{z} \sim p(z)$$

- Draw a value for x from from an isotropic Gaussian distribution:

$$\hat{x} \sim p(\mathbf{x}|\hat{z}) = \mathcal{N}(\mathbf{x}|\mathbf{w}\hat{z} + \boldsymbol{\mu}, \sigma^2 I).$$

Marginal Data Density

- The joint p(**z**,**x**), the marginal data distribution p(**x**), and the posterior distribution p(**z**|**x**) are also Gaussian.
- Marginal data density (also known as predictive distribution):

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z})d\mathbf{z} = \mathcal{N}(\mathbf{x}|\mu, \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})$$

- Can derive this result directly by computing the mean and covariance given that it is Gaussian:

$$\begin{aligned} E[\mathbf{x}] &= E[\mu + \mathbf{W}\mathbf{z} + \epsilon] = \mu + \mathbf{W}E[\mathbf{z}] + E[\epsilon] \\ &= \mu + \mathbf{W}0 + 0 = \mu \end{aligned}$$

$$\begin{aligned} \mathbf{C} &= Cov[\mathbf{x}] = \\ &= E[(\mu + \mathbf{W}\mathbf{z} + \epsilon - \mu)(\mu + \mathbf{W}\mathbf{z} + \epsilon - \mu)^T] \\ &= E[(\mathbf{W}\mathbf{z} + \epsilon)(\mathbf{W}\mathbf{z} + \epsilon)^T] \\ &= \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I} \end{aligned}$$

Redundancy in Parameterization

- The marginal distribution is governed by parameters **W**, μ, σ^2:

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z})d\mathbf{z} = \mathcal{N}(\mathbf{x}|\mu, \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})$$

- Redundancy in parameterization: rotation of the latent space coordinates.
- Let **R** be an orthogonal matrix, then define a new matrix:

$$\tilde{\mathbf{W}} = \mathbf{W}\mathbf{R}, \qquad \mathbf{R}\mathbf{R}^T = \mathbf{I}.$$

- Then

$$\tilde{\mathbf{W}}\tilde{\mathbf{W}}^T = \mathbf{W}\mathbf{R}\mathbf{R}^T\mathbf{W}^T = \mathbf{W}\mathbf{W}^T.$$

- There is a whole family of matrices all of which give rise to the same marginal distribution.

- Rotations within the latent space.

Joint Density for PPCA

- Joint density for PPCA, where **x** is D-dim and **z** is M-dim is given:

$$p(\begin{bmatrix}\mathbf{z}\\ \mathbf{x}\end{bmatrix}) = \mathcal{N}(\begin{bmatrix}\mathbf{z}\\ \mathbf{x}\end{bmatrix} \mid \begin{bmatrix}0\\ \mu\end{bmatrix}, \begin{bmatrix} I & \mathbf{W}^\top \\ \mathbf{W} & \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}\end{bmatrix})$$

where cross covariance term forms:

$$\begin{aligned} Cov[\mathbf{z},\mathbf{x}] &= E[(\mathbf{z}-0)(\mathbf{x}-\mu)^T] = E[\mathbf{z}(\mu + \mathbf{W}\mathbf{z} + \epsilon - \mu)^T] \\ &= E[\mathbf{z}(\mathbf{W}\mathbf{z}+\epsilon)^T] = \mathbf{W}^T \end{aligned}$$

- When evaluating marginal distribution, we need to invert a D $\times$ D matrix **C**, which can be expensive.
- Reduce O(D^3) to O(M^3) by applying *matrix inversion lemma*:

$$\mathbf{C}^{-1} = \sigma^{-1}\mathbf{I} - \sigma^{-2}\mathbf{W}(\mathbf{W}^T\mathbf{W} + \sigma^2\mathbf{I})^{-1}\mathbf{W}^T$$

Posterior Distribution for PPCA

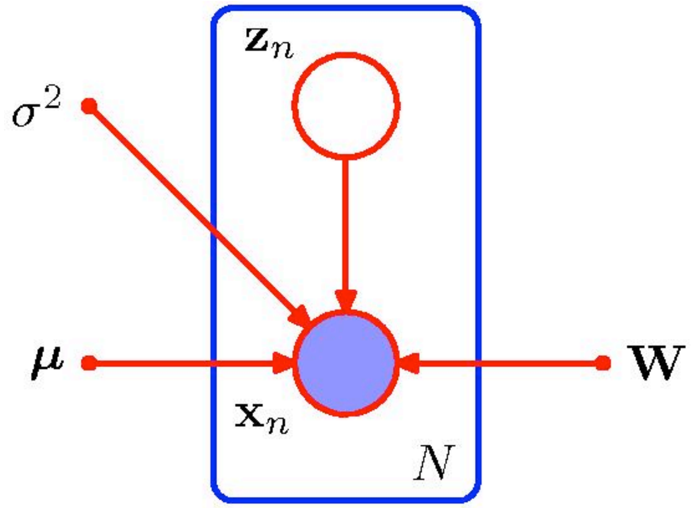
- Inference in PPCA amounts to computing posterior distribution over latent variables:

$$p(\mathbf{z}|\mathbf{x}) \;=\; \mathcal{N}(\mathbf{z}|\mathbf{m}, \mathbf{V})$$

$$\mathbf{m} = \mathbf{M}^{-1}\mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu}),$$

$$\mathbf{V} = \sigma^2\mathbf{M}^{-1},$$

$$\mathbf{M} = \mathbf{W}^T\mathbf{W} + \sigma^2\mathbf{I}.$$



- Mean of inferred **z** is the projection of centered **x**: linear operation.

- Posterior variance does not depend on the input **x** at all.

- Remember:

$$\mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}.$$

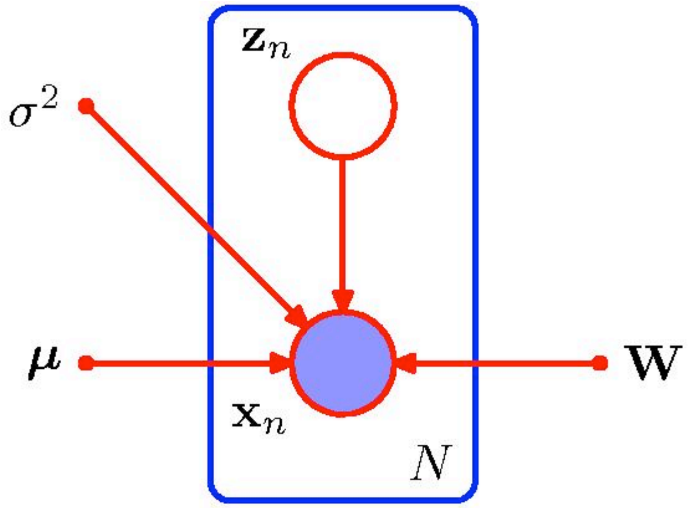
$$\mathbf{C}^{-1} = \sigma^{-1}\mathbf{I} - \sigma^{-2}\mathbf{W}\overbrace{(\mathbf{W}^T\mathbf{W} + \sigma^2\mathbf{I})}^{\text{M matrix}}{}^{-1}\mathbf{W}^T$$

Constrained Covariance

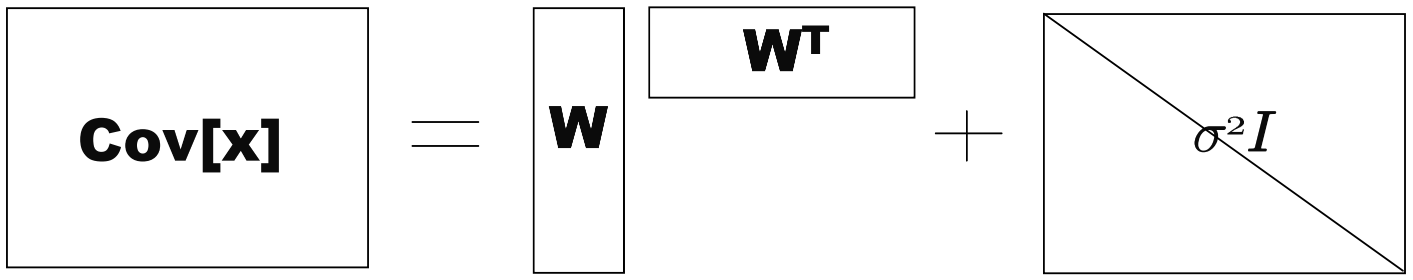
- Marginal density for PPCA has the following form:

$$p(\mathbf{x}|\theta) = \mathcal{N}(\mathbf{x}|\mu, \underbrace{\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}}_{\text{Covariance } \mathbf{C}})$$

where θ = {**W**,μ, σ^2).



- The covariance is low-rank outer product of two long skinny matrices plus a constant diagonal matrix:



- Hence PPCA is a constrained Gaussian model.
- We can fit model parameters using maximum likelihood.

Maximum Likelihood

- Model parameters can be determined using maximum likelihood (by integrating our latent variables):

$$\begin{aligned} L(\theta;\mathbf{X}) &= \log p(\mathbf{X}|\theta) = \sum_n \log p(\mathbf{x}_n|\theta) \\ &= -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}\sum_n (\mathbf{x}_n-\mu)\mathbf{C}^{-1}(\mathbf{x}_n-\mu)^T \\ &= -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}Tr[\mathbf{C}^{-1}\sum_n (\mathbf{x}_n-\mu)(\mathbf{x}_n-\mu)^T] + \text{const} \end{aligned}$$

- Maximizing with respect to the mean: $\mu_{ML} = \bar{\mathbf{x}}$.

- We then have:

$$\log p(\mathbf{X}|\theta) = -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}Tr\left[\mathbf{C}^{-1}\mathbf{S}\right] + \text{const.}$$

- Maximizing with respect to **W** and σ^2 can be solved directly.

Maximum Likelihood

- Objective:

$$\log p(\mathbf{X}|\theta) = -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}Tr\left[\mathbf{C}^{-1}\mathbf{S}\right] + \text{const.}$$

- **C** is model covariance; **S** is sample data covariance.

- In other words, we are trying to make the constrained model covariance as close as possible to the observed covariance, where "close" means the trace of the ratio.

- Sufficient statistics: mean $\bar{\mathbf{x}} = \frac{1}{N}\sum_n \mathbf{x}_n$ and sample covariance **S**.

Maximum Likelihood

- Objective:

$$\log p(\mathbf{X}|\theta) = -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}Tr\left[\mathbf{C}^{-1}\mathbf{S}\right] + \text{const.}$$

- Maximizing with respect to **W**:

$$\mathbf{W}_{ML} = \mathbf{U}_M(\mathbf{L}_M - \sigma^2\mathbf{I})^{1/2}\mathbf{R},$$

where

- U_M is a D $\times$ M matrix whose columns are given by the M principal eigenvectors of the data covariance matrix **S**.
- L_M is the M $\times$ M diagonal matrix containing M largest eigenvalues.
- **R** is an arbitrary M $\times$ M orthogonal matrix.

- If the eigenvectors have been arranged in the order of decreasing values of the corresponding eigenvalues, then the columns of **W** define the principal subspace of standard PCA.

Maximum Likelihood

- Objective:

$$\log p(\mathbf{X}|\theta) = -\frac{N}{2}\log|\mathbf{C}| - \frac{1}{2}Tr\left[\mathbf{C}^{-1}\mathbf{S}\right] + \text{const.}$$

- Maximizing with respect to σ^2:

$$\sigma^2_{ML} = \frac{1}{D-M}\sum_{i=M+1}^{D}\lambda_i,$$

which is the average variance associated with the discarded dimensions.

EM for PPCA

• Instead of solving directly, we can use EM. The EM can be scaled to very large high-dimensional datasets.

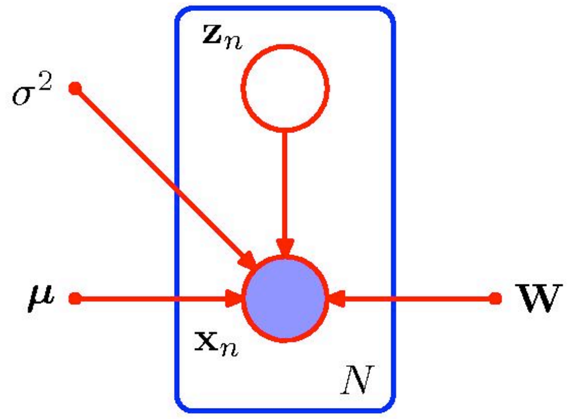
• The complete-data log-likelihood takes form:

$$\log p(\mathbf{X}, \mathbf{Z}|\mu, \mathbf{W}, \sigma^2) = \sum_n [\log p(\mathbf{x}_n|\mathbf{z}_n) + \log p(\mathbf{z}_n)]$$

• E-step: compute expectation of complete log likelihood with respect to posterior of latent variables **z**, using current parameters.

• We need to derive $\mathbb{E}[\mathbf{z}_n], \mathbb{E}[\mathbf{z}_n \mathbf{z}_n^T]$ with respect to the true posterior: p(**z** | **X**).

• M-step: maximize with respect to parameters **W** and σ^2.



• Appealing property: EM avoids direct O(ND^2) construction of covariance matrix!

• Instead EM involves sums over data cases: O(*NDM*). It can also be implemented online, without storing data.

Zero Noise Limit

• We can derive standard PCA as a limit of probabilistic PCA as the noise term goes to zero: $\sigma^2 \rightarrow 0.$

• ML parameters are the same.

• Inferring the distribution over latent variables is easier: The posterior mean reduces to:

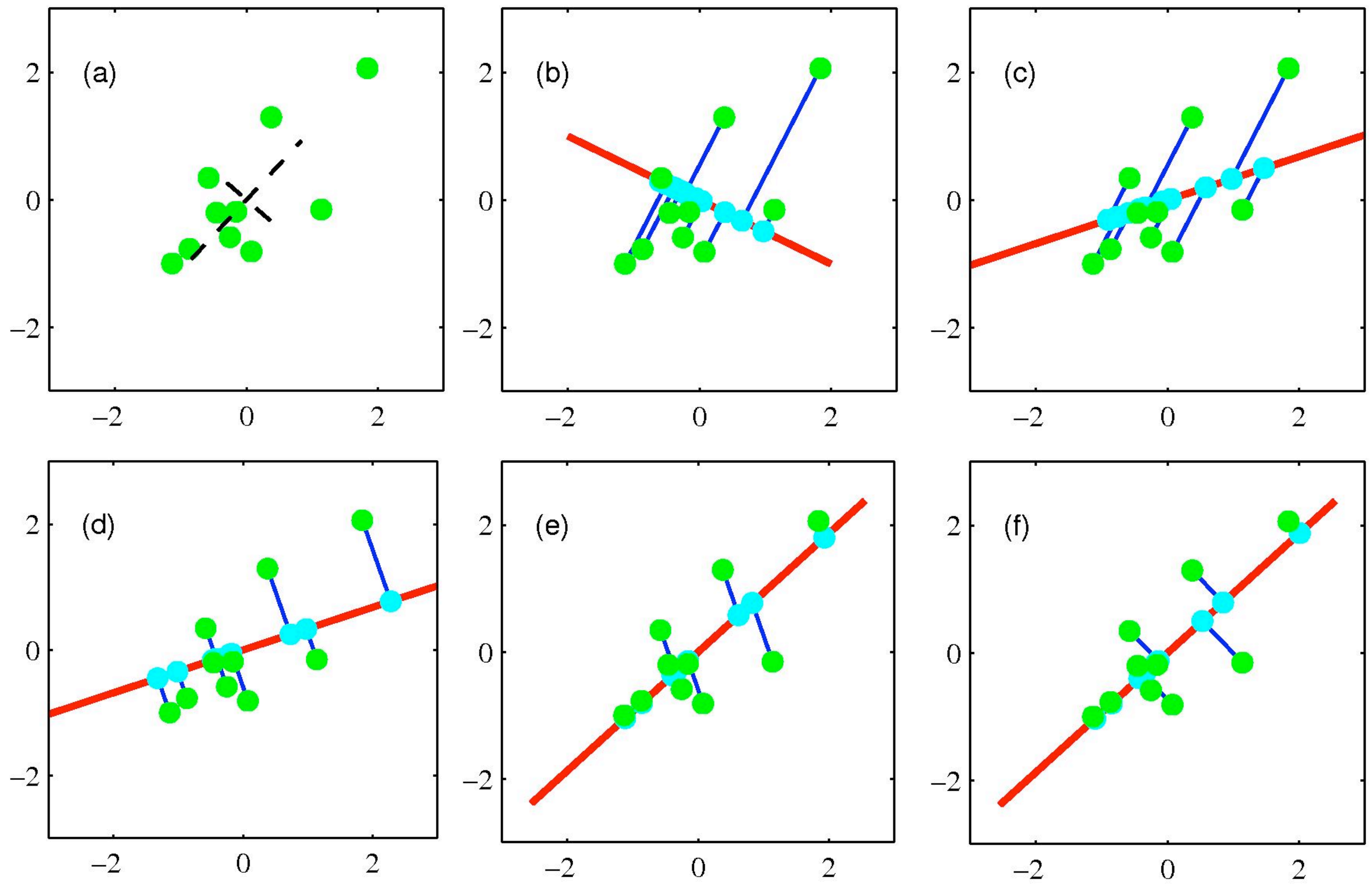
$$\lim_{\sigma^2 \rightarrow 0} (\mathbf{W}^T\mathbf{W} + \sigma\mathbf{I})^{-1}\mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{W}^T\mathbf{W})^{-1}\mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu}),$$

which represents an orthogonal projection of the data point onto the latent space – standard PCA.

• Posterior covariance goes to zero:

EM for PPCA

- EM algorithm for PCA.



Bayesian PCA

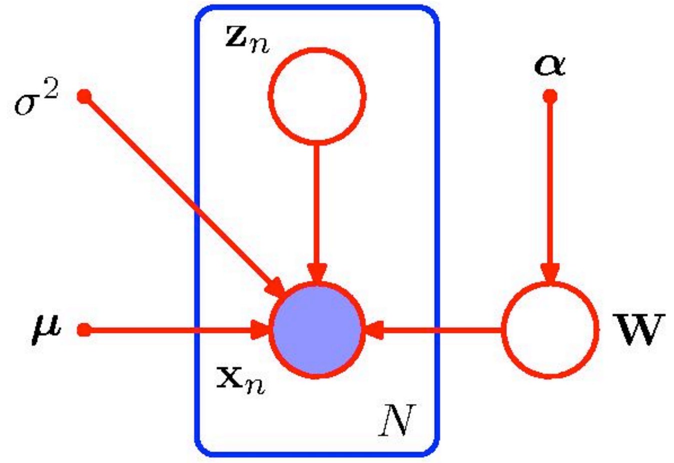
- It is easy to take a Bayesian viewpoint and place priors over model parameters.

- One option is to employ the evidence approximation (empirical Bayes) framework.

- We can define an independent Gaussian prior over each column of **W**.

- Each such Gaussian has an independent variance:

$$p(\mathbf{W}|\alpha) = \prod_{i=1}^{M} \left(\frac{\alpha_i}{2\pi}\right) \exp\left[-\frac{1}{2}\alpha_i \mathbf{w}_i^T \mathbf{w}_i\right],$$



where w_i is the ith column of **W**.

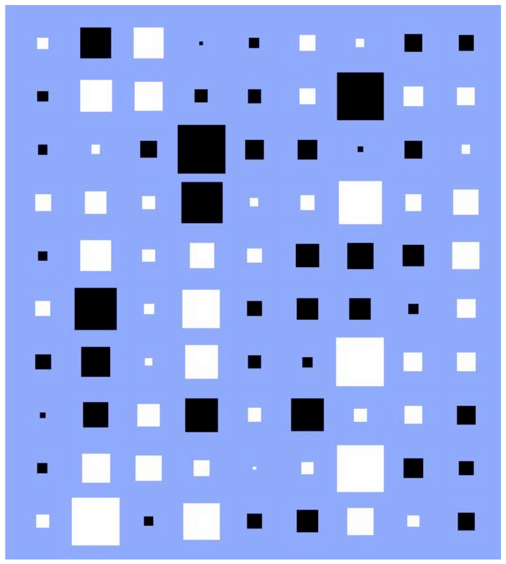
- The values of α_i are re-estimated during training by maximizing the marginal likelihood:

$$p(\mathbf{X}|\alpha, \boldsymbol{\mu}, \sigma^2) = \int p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) p(\mathbf{W}|\alpha) d\mathbf{W}.$$

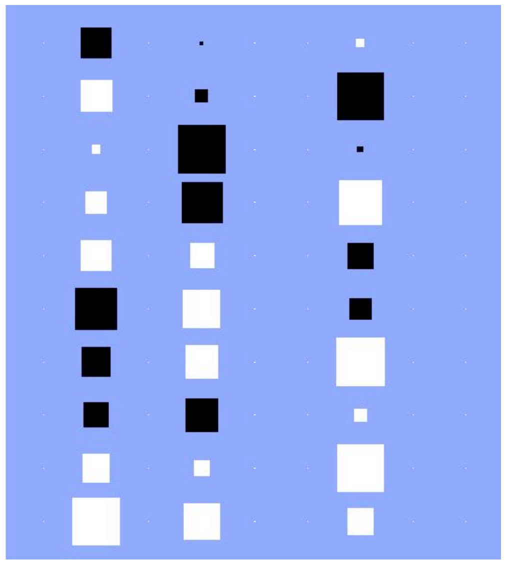
Example of Bayesian PCA

• Hinton diagram of the matrix W: each element of W is depicted as a square (white for positive and black for negative).

PPCA



Bayesian PCA



• The synthetic dataset contains 300 points in D=10 space with the intrinsic dimensionality set to D=3.

• Bayesian PCA discovers appropriate dimensionality.

Factor Analysis

- Linear Gaussian latent variable model that is closely related to PPCA.
- Key assumptions:
  - underlying latent M-dim variable **z** has a Gaussian distribution
  - linear relationship between M-dim latent **z** and D-dim observed **x** variables.
  - **diagonal** Gaussian noise in observed dimensions.

$$\begin{aligned} p(\mathbf{z}) &= \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}) \\ p(\mathbf{x}|\mathbf{z}) &= \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \mu, \mathbf{\Psi}) \end{aligned}$$

- **W** is a D $\times$ M factor loading matrix.
- Ψ is a M $\times$ M diagonal matrix (or axis-aligned).

- The only difference between PPCA and FA is that in Factor Analysis the conditional distribution of the observed variable **x** has diagonal rather than isotropic covariance.

Factor Analysis: Distributions

• As in PPCA, the joint p(**z**,**x**), the marginal data distribution p(**x**), and the posterior p(**z**|**x**) are also Gaussian.

• Marginal distribution (predictive distribution):

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z})d\mathbf{z} = \mathcal{N}(\mathbf{x}|\mu, \mathbf{W}\mathbf{W}^T + \mathbf{\Psi})$$

• The joint distribution:

$$p(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix}) = \mathcal{N}(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix} \mid \begin{bmatrix} 0 \\ \mu \end{bmatrix}, \begin{bmatrix} I & \mathbf{W}^\top \\ \mathbf{W} & \mathbf{W}\mathbf{W}^\top + \Psi \end{bmatrix})$$

Factor Analysis: Optimization

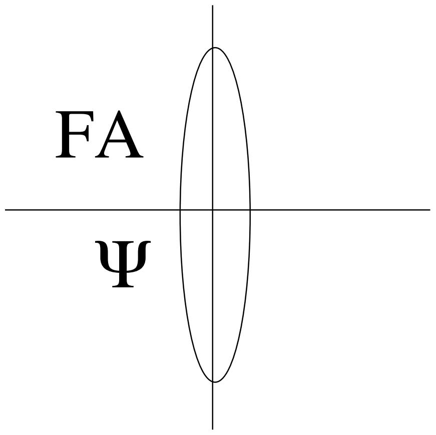
- Parameters are coupled, which makes it impossible to solve for ML parameters directly, unlike in probabilistic PCA.
- Because FA is a latent variable model, we can use EM, or other nonlinear optimization
- E-step: compute posterior $p(\mathbf{z}|\mathbf{x})$: Use matrix inversion to convert $D \times D$ matrix inversions to $M \times M$.
- M-step: take derivatives of the expected complete log likelihood with respect to parameters.
- Bayesian treatment of the factor analysis can be obtained by a straightforward extension of standard FA (as we did for PPCA).

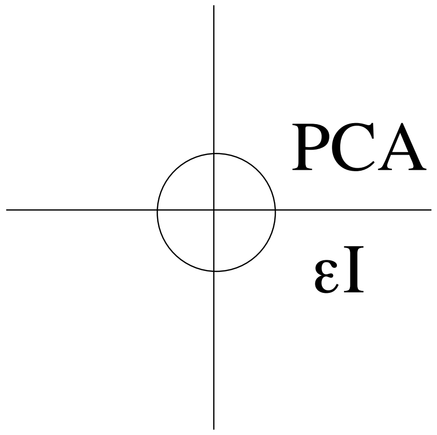
FA vs. PCA

- intuition: Gaussians are hyperellipsoids.

- Mean == center of football.
  Eigenvectors of covariance matrix == axes of football.
  Eigenvalues == lengths of axes.

- In FA our football is an axis aligned cigar.
  In PCA our football is a sphere of radius σ^2.





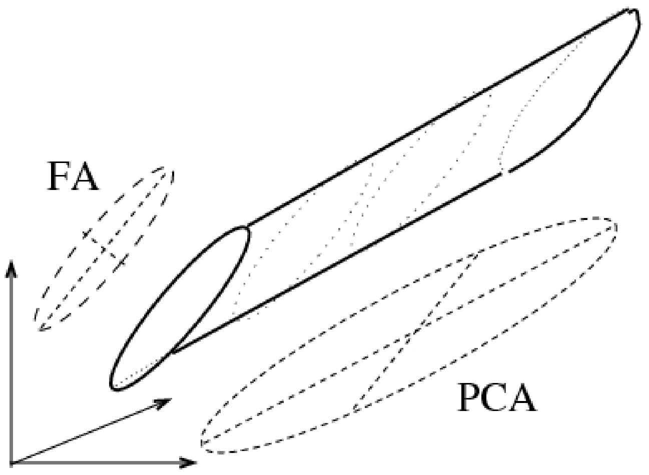
Rotation Invariance in PCA

- In PPCA the rotation of the data is unimportant: we can multiply the data **x** by a rotation matrix **Q** without changing anything:

$$\begin{aligned} \mu &\leftarrow \mathbf{Q}\mu \\ \mathbf{W} &\leftarrow \mathbf{QW} \\ \Psi &\leftarrow \Psi \end{aligned}$$

- However, the scale is important.

- PCA looks for directions of large variance, so it will chase big noise directions.



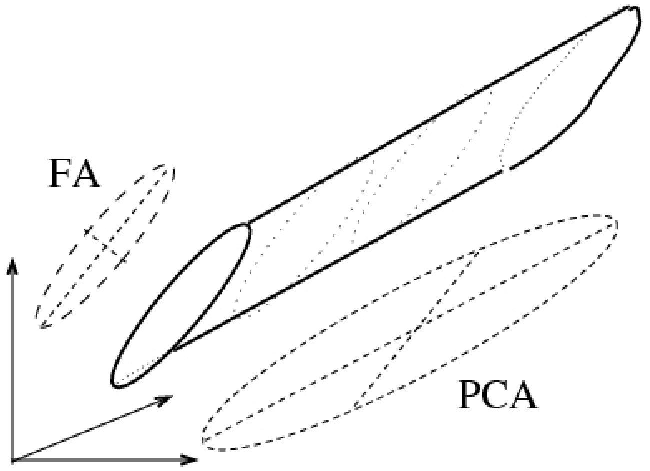
Scale Invariance in FA

- In FA, the data can be re-scaled without changing anything.
- Multiply x_i by α_i:

$$\begin{aligned} \mu_i &\leftarrow \alpha_i \mu_i \\ \mathbf{W}_{ij} &\leftarrow \alpha_i \mathbf{W}_{ij} \\ \Psi_i &\leftarrow \alpha_i^2 \Psi_i \end{aligned}$$

- However, rotation in data space is important.

- FA looks for directions of large correlation in the data, so it will not model large variance noise.



Model Identifiability

• Factors in FA are ***non-identifiable:*** not guaranteed to find the same set of parameters – not just local minimum but invariance.

• Rotate **W** by any unitary **Q** and model stays the same – **W** only appears in model as outer product $\mathbf{W}\mathbf{W}^T$

$$(\mathbf{WQ})(\mathbf{WQ})^T = \mathbf{WW}^T.$$

• This means that there is no "one best" setting of the parameters. An infinite number of parameters all give the same ML score.

• Degeneracy makes unique interpretation of learned factors impossible.

Mixture of Dimensionality Reducers

- The next logical step is to consider a model that has two kinds latent variables: one discrete cluster, and one vector of continuous causes.

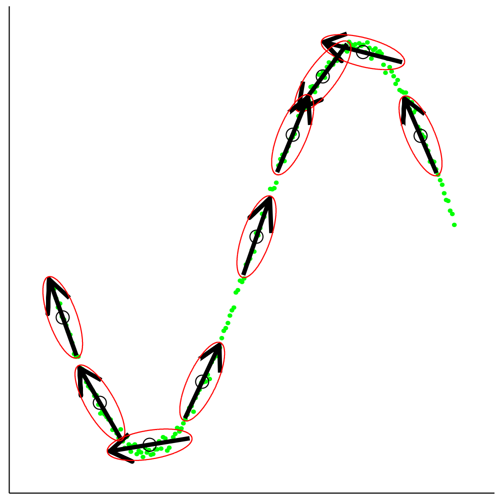
- Such models simultaneously do clustering, and within each cluster, dimensionality reduction.

- Example: Mixture of Factor Analyzers:

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}), \quad p(k) = \pi_k,$$

$$p(\mathbf{x}|\mathbf{z}, k, \theta) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k + W_k\mathbf{z}, \Psi),$$

$$\begin{aligned} p(\mathbf{x}|\theta) &= \sum_k \int_{\mathbf{z}} p(k)p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, k, \theta)d\mathbf{z} \\ &= \sum_k \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, W_k W_k^T + \Psi). \end{aligned}$$

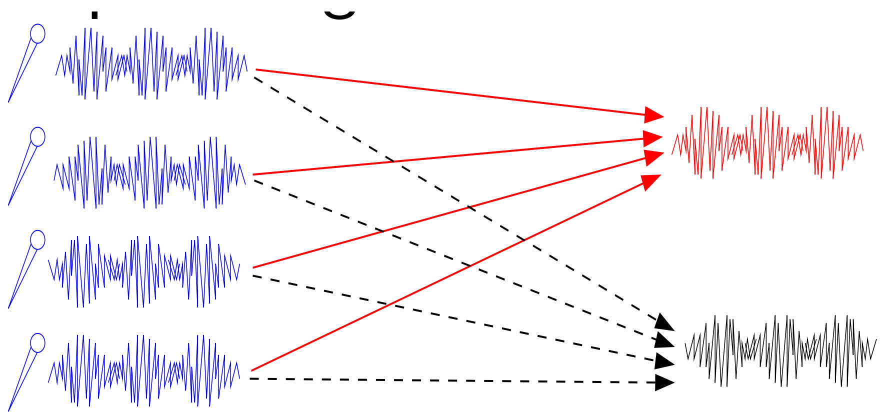


which is constrained mixture of Gaussians.

- Fitting is done via EM algorithm.

Independent Components Analysis

- ICA is another continuous latent variable model, like FA, but it has a non-Gaussian and factorized prior on the latent variables.
- This is good in situations where most of the factors are small most of the time, and do not interact with each other.
- Example: Mixture of speech signals.



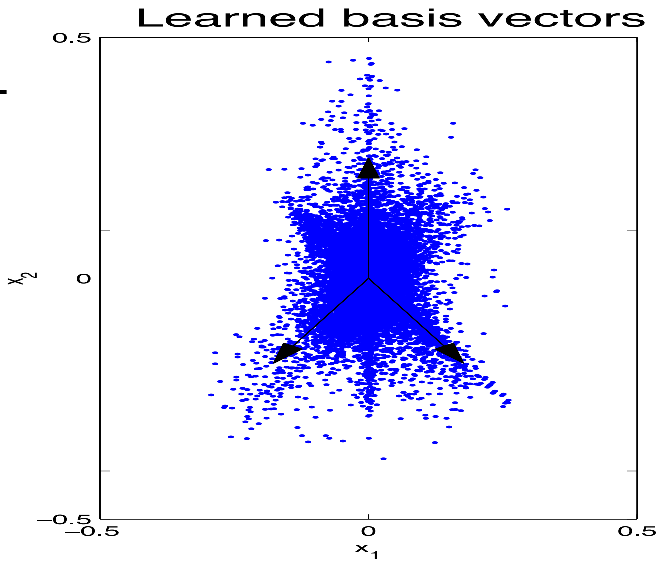
- The learning problem is the same: find the weights from the factors to the outputs and infer the unknown factor values.
- ICA: the factors are sometimes called “sources”, and the learning is sometimes called “unmixing”.

Geometric Intuition

- Since latent variables are assumed to be independent, we are trying to find linear transformation of data that recovers independent causes.
- Avoid degeneracies in Gaussian latent variable models: Assume non-Gaussian prior distribution for latent variables (sources).
- Recall that in PPCA (and FA) the model cannot distinguish between two different choices for the latent variables: These differ simply by a rotation in latent space!
- Often we use *heavy-tailed* source priors, e.g.:

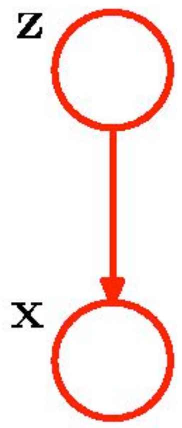
$$p(z_j) = \frac{1}{\pi \cosh(z_j)} = \frac{1}{\pi(\exp(z_j) + \exp(-z_j))}$$

- Geometric intuition: finding spikes in histograms.



ICA Model

• The simplest form of ICA has as many outputs as sources (square) and no sensor noise on the outputs:



$$
\begin{aligned}
p(\mathbf{z}) &= \prod_k p(z_k) \\
\mathbf{x} &= \mathbf{V}\mathbf{z}
\end{aligned}
$$

• Learning in this case can be done with gradient descent (plus some tricks to make the updates faster and more stable).

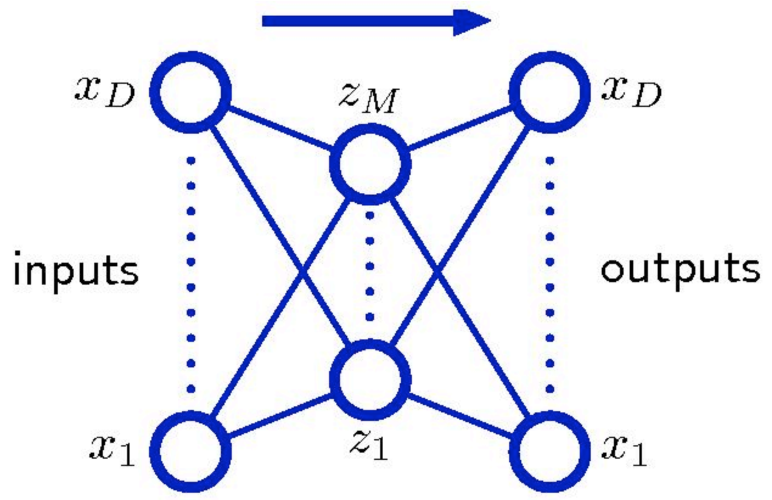
• If we keep **V** square, and assume isotropic Gaussian noise on the outputs, there is a simple EM algorithm.

• Much more complex cases have been studied also: nonsquare, convolutional, time delays in mixing, etc..

Autoencoders

- Neural networks can also be used for nonlinear dimensionality reduction.
- This is achieved by having the same number of outputs as inputs. These models are called autoencoders.
- Consider a multilayer perceptron that has D inputs, D outputs, and M hidden units, with M<D.
- It is useful if we can squeeze the information through some kind of bottleneck.

  - If we use a linear network this is very similar to Principal Components Analysis.



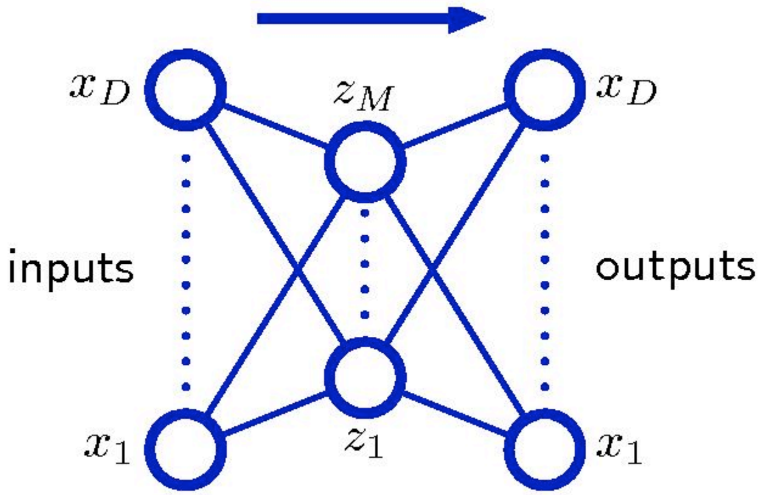
Autoencoders and PCA

- Given an input x, its corresponding reconstruction is given by:

$$y_k(\mathbf{x}, \mathbf{w}) = \sum_{j=1}^{M} w_{kj}^{(2)} \sigma \left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i \right), \quad k = 1, .., D.$$

- We can determine the network parameters **w** by minimizing the reconstruction error:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} ||y(\mathbf{x}_n, \mathbf{w}) - \mathbf{x}_n||^2.$$



- If the hidden and output layers are linear, it will learn hidden units that are a linear function of the data and minimize the squared error.

- The M hidden units will span the same space as the first m principal components. The weight vectors may not be orthogonal.

Deep Autoencoders

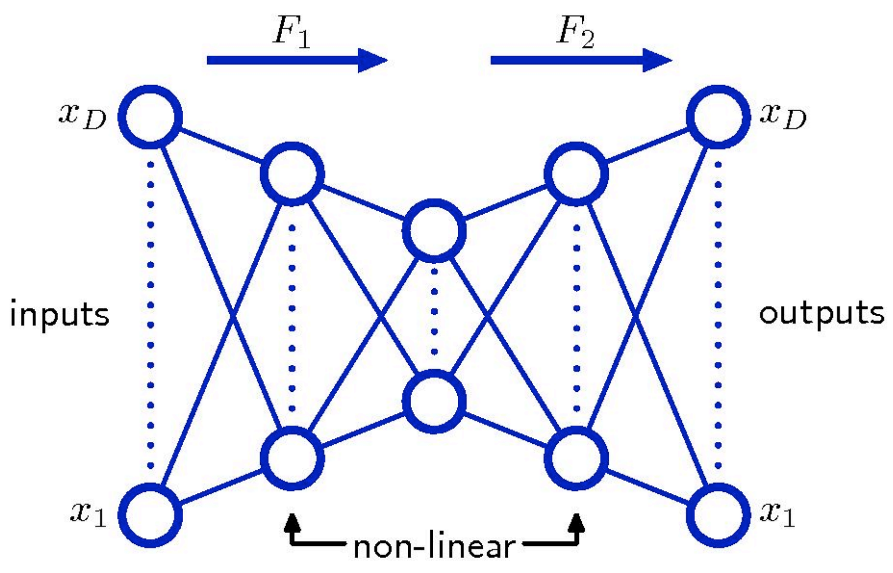
• We can put extra nonlinear hidden layers between the input and the bottleneck and between the bottleneck and the output.

• This gives nonlinear generalization of PCA.

• It should be very good for non-linear dimensionality reduction.

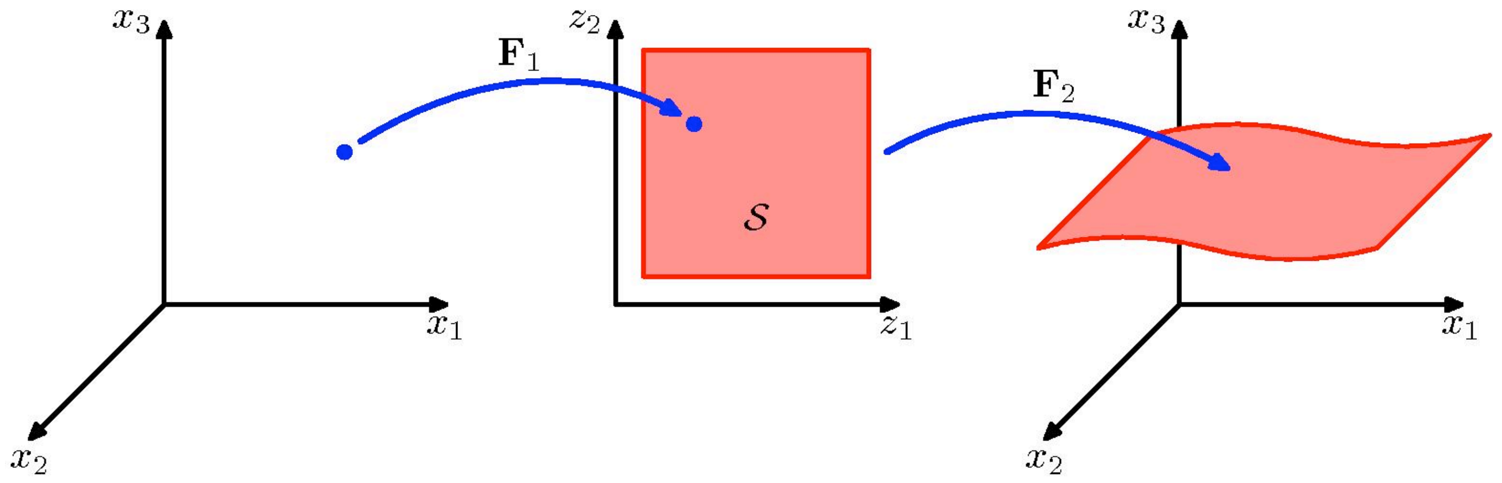
• The network can be trained by the minimization of the reconstruction error function.

• Much harder to train.



Geometrical Interpretation

• Geometrical interpretation of the mappings performed by the network with 2 hidden layers for the case of D=3 and M=2 units in the middle layer.

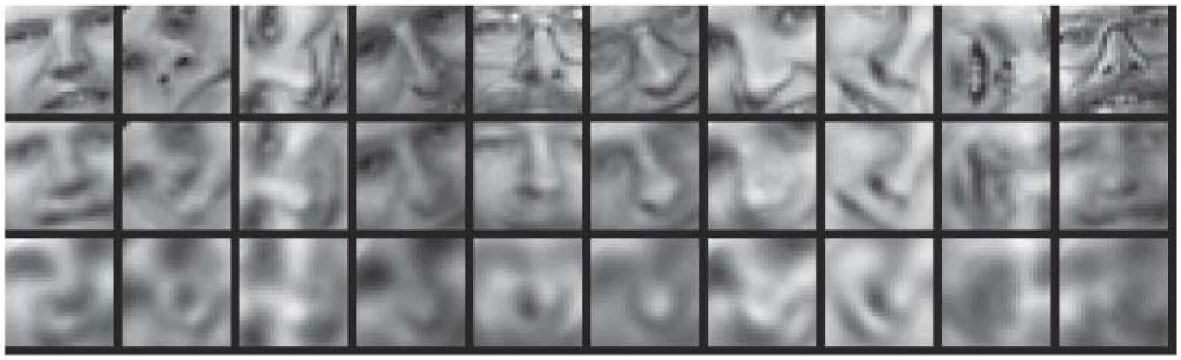


• The mapping F_1 defines a nonlinear projection of points in the original D-space into the M-dimensional subspace.

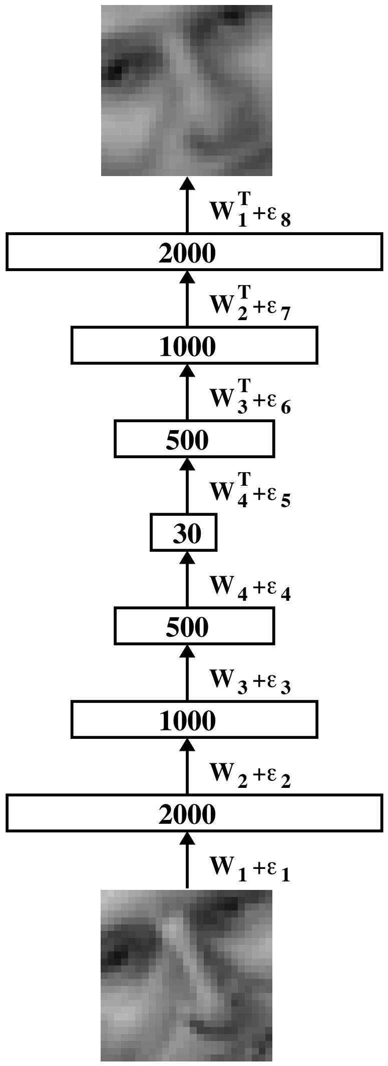
• The mapping F_2 maps from an M-dimensional space into D-dimensional space .

Deep Autoencoders

- We can consider very deep autoencoders.
- There is an efficient way to learn these deep autoencoders

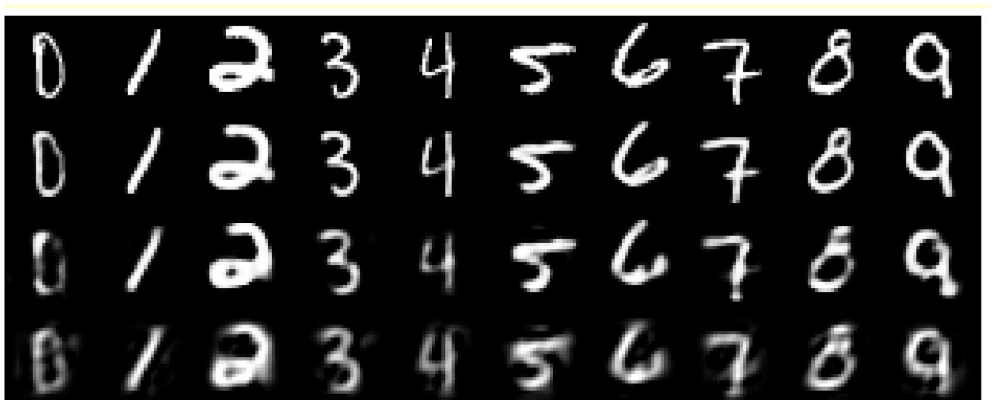


- By row: Real data, Deep autoencoder with a bottleneck of 30 linear units, and 30-d PCA.



Deep Autoencoders

- We can consider very deep autoencoders.
- Similar model for the MNIST handwritten digits:



- Deep autoencoder produces much better reconstructions.

Class Structure of the Data

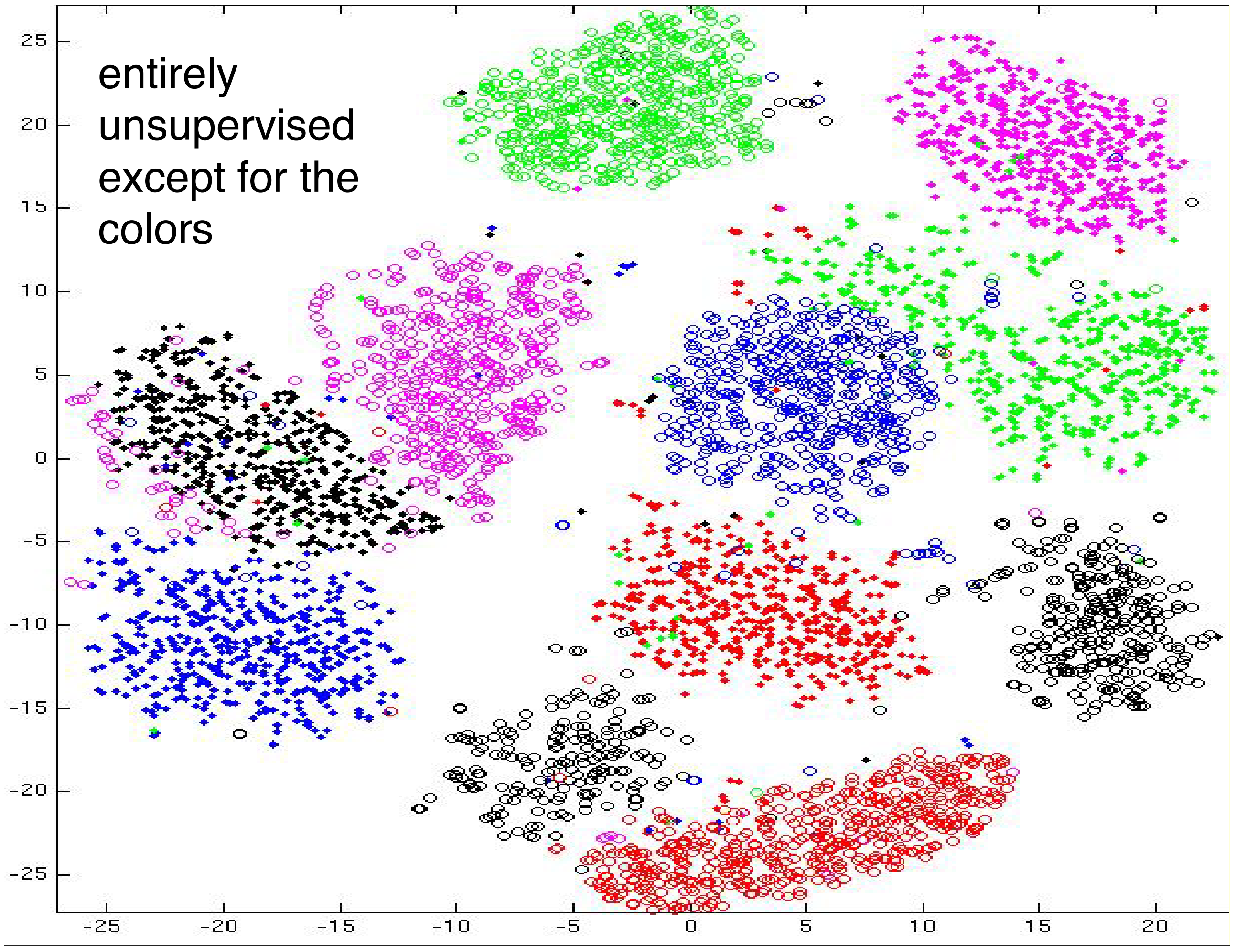
- Do the 30-D codes found by the deep autoencoder preserve the class structure of the data?

- Take the 30-D activity patterns in the code layer and display them in 2-D using a new form of non-linear multi-dimensional scaling (UNI-SNE).

- Will the learning find the natural classes?

Class Structure of the Data

- Do the 30-D codes found by the deep autoencoder preserve the class structure of the data?

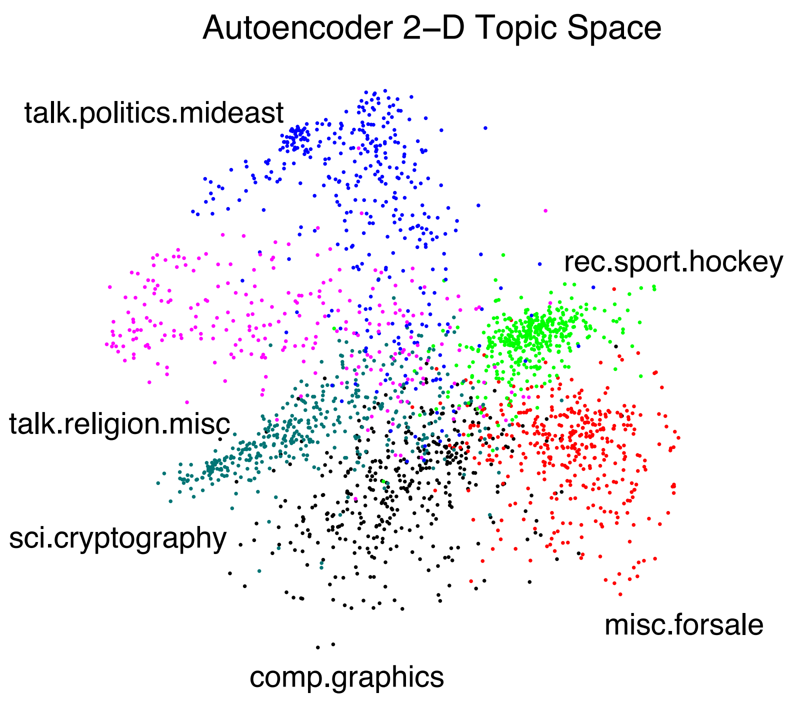


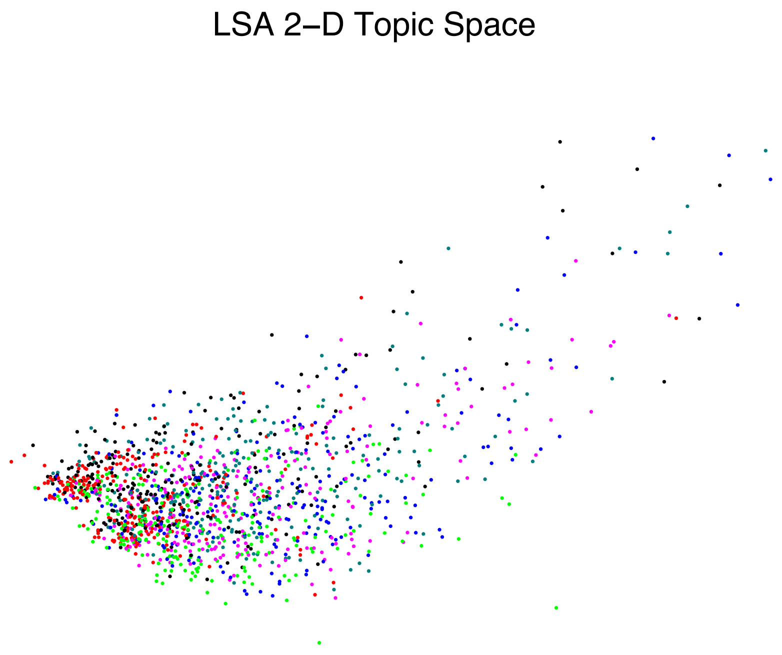
Learning 2-D topic Space

- Latent Semantics Analysis (LSA) uses SVD to get a low-rank approximation of the log of term-frequency matrix:

$$\log(1 + M(doc, w)) \sim USV$$

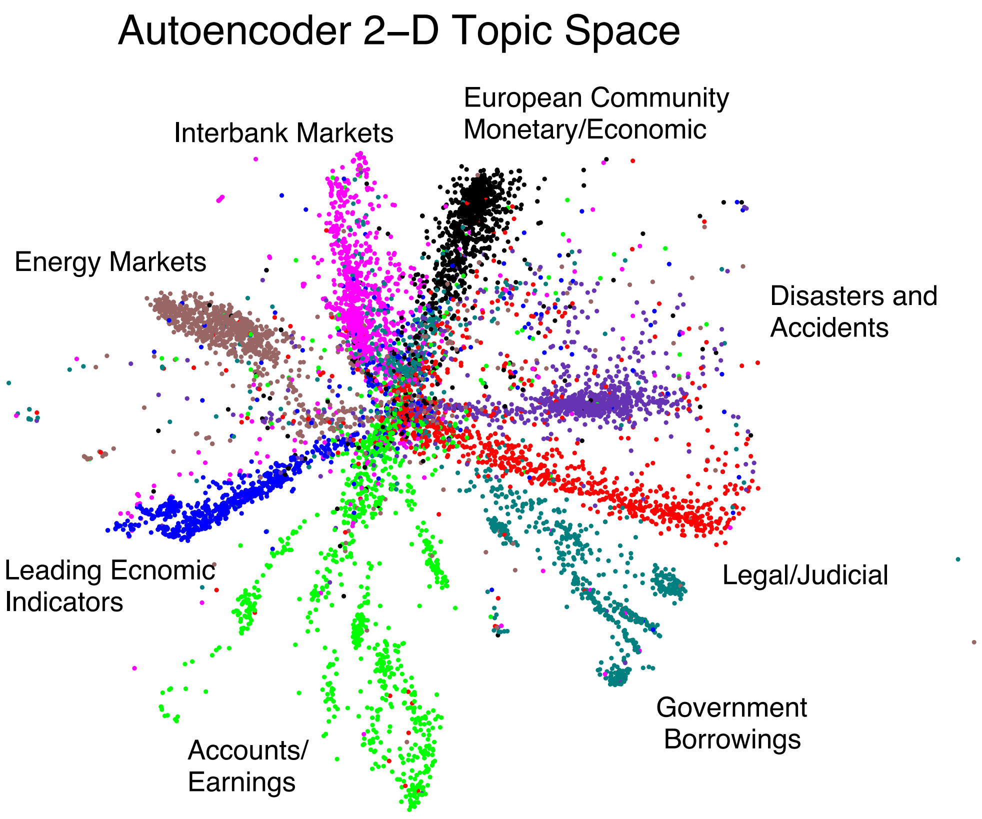
$$U = |doc| \times d, S = d \times d, V = d \times |w|.$$

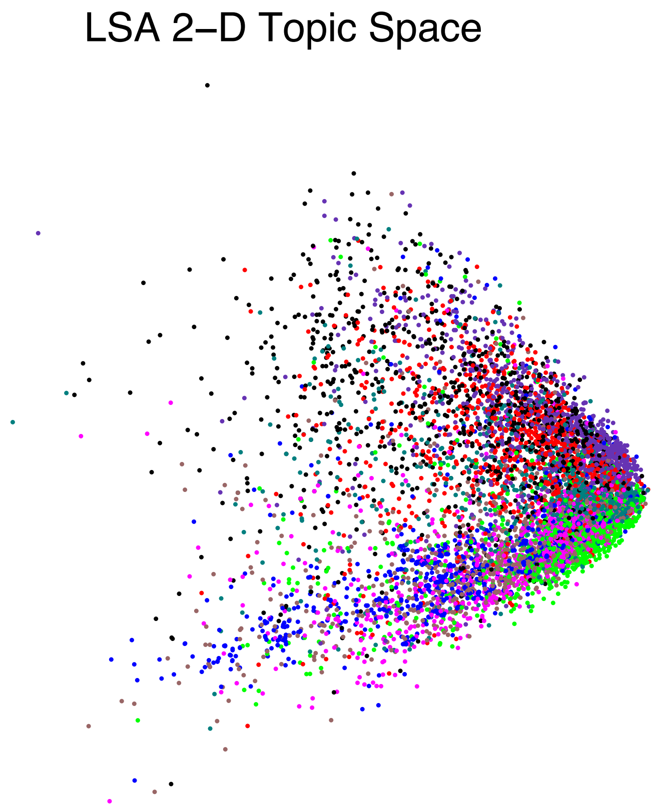




Reuters dataset

- Autoencoder: 2000-500-250-125-2


Autoencoder 2–D Topic Space
European Community Monetary/Economic
Interbank Markets
Energy Markets
Disasters and Accidents
Leading Ecnomic Indicators
Legal/Judicial
Accounts/ Earnings
Government Borrowings


LSA 2–D Topic Space