

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

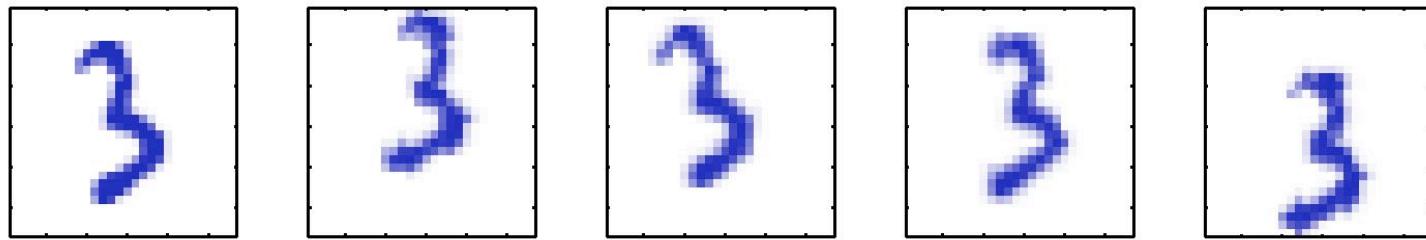
- What are the **intrinsic latent dimensions** in these two datasets?



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

Intrinsic Latent Dimensions

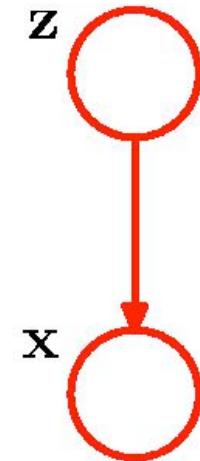
- In this dataset, there is only **3 degrees of freedom of variability**, corresponding to vertical and horizontal translations, and the rotations.



- Each image undergoes a random displacement and rotation within some larger image field.
- The resulting images have $100 \times 100 = 10,000$ pixels.

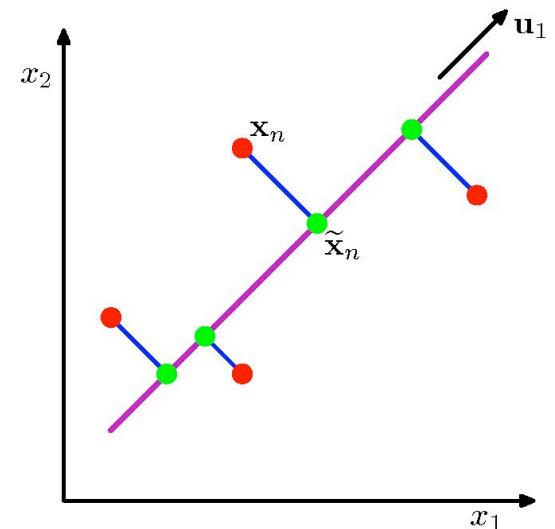
Generative View

- 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 formulation.
- 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 \mathbf{S} (data covariance matrix): $\{\mathbf{u}_1, \dots, \mathbf{u}_M\}$.
 - project each input vector \mathbf{x} into **this subspace**, e.g. $z_{n1} = \mathbf{x}_n^T \mathbf{u}_1$.



- Full projection into M dimensions takes form:

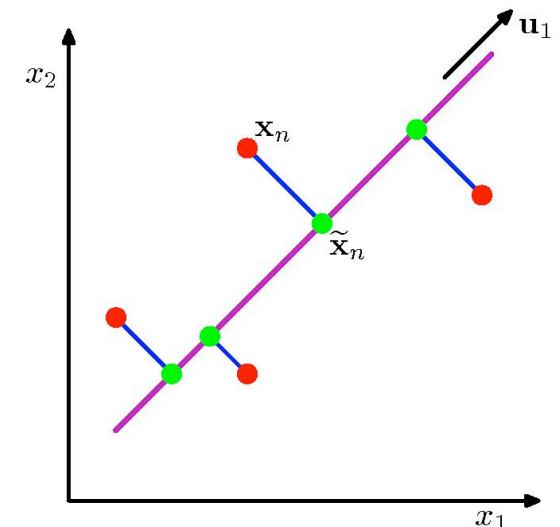
$$\begin{bmatrix} \mathbf{u}_1^\top \\ \vdots \\ \mathbf{u}_M^\top \end{bmatrix} [\mathbf{x}_1 \cdots \mathbf{x}_N] = [\mathbf{z}_1 \cdots \mathbf{z}_N]$$

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

Maximum Variance Formulation

- Consider a dataset $\{x_1, \dots, x_N\}$, $x_n \in \mathbb{R}^D$. 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 $u_1^T u_1 = 1$.
- **Objective:** maximize the variance of the projected data with respect to u_1 .

$$\frac{1}{N} \sum_{n=1}^N \{u_1^T x_n - u_1^T \bar{x}\}^2 = u_1^T S u_1$$



where sample **mean** and **data covariance** is given by:

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

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

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 $\|\mathbf{u}_1\| = 1$. Using Langrange multiplier, maximize:

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

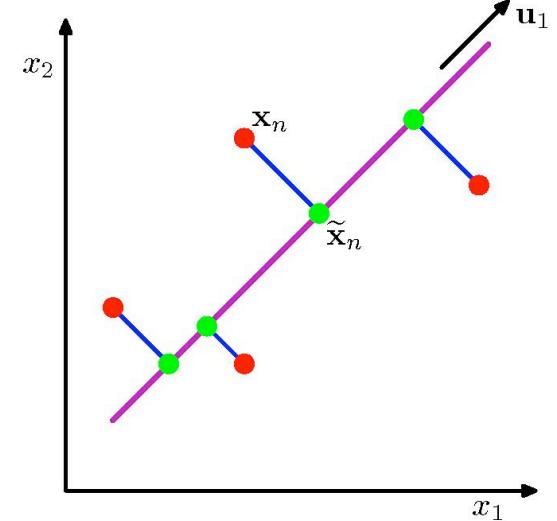
- Setting the derivative with respect to \mathbf{u}_1 to zero:

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

- Hence \mathbf{u}_1 must be an eigenvector of \mathbf{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).



用1个 2*1的向量表达
本来需要用2个 2*1的向量表达
的点x_n

对称阵求出来的特征向量彼此垂直

Minimum Error Formulation

- Introduce a complete orthonormal set of D-dimensional basis vectors:
 $\{\mathbf{u}_1, \dots, \mathbf{u}_D\}$:

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

- 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:

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

前M个就是主成分
精确表达，故系数与各自的数据点 x_n 相关

理解为 u_1

理解为 u_2

b_i 其实就是 x_n 投影到 u_2 上的均值 (scalar) , 与各自的数据点 x_n 无关。
所有的样本点在 u_2 方向上使用同一个系数 (均值) , 以消除在 u_2 方向上的残差

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 \mathbf{u}_i , z_{ni} , and b_i .

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

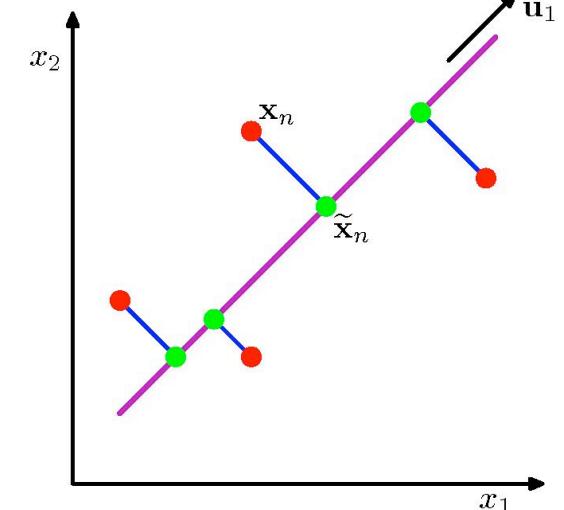
残差

- 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:

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



这些维度上，没有被精确表达，故残差只和这些维度有关

Minimum Error Formulation

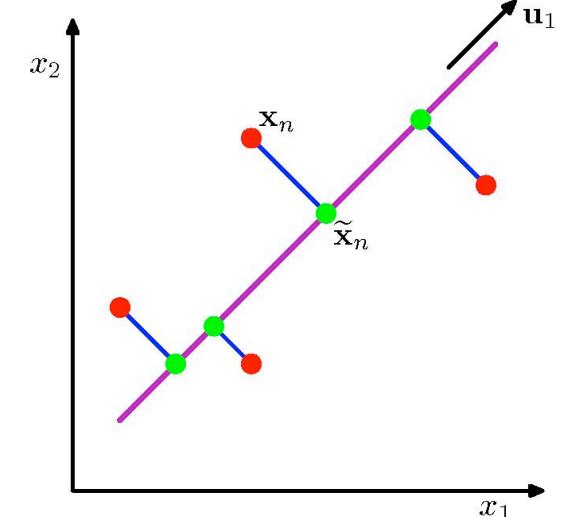
- Minimize distortion with respect to \mathbf{u}_i : constraint minimization problem:

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

- 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.

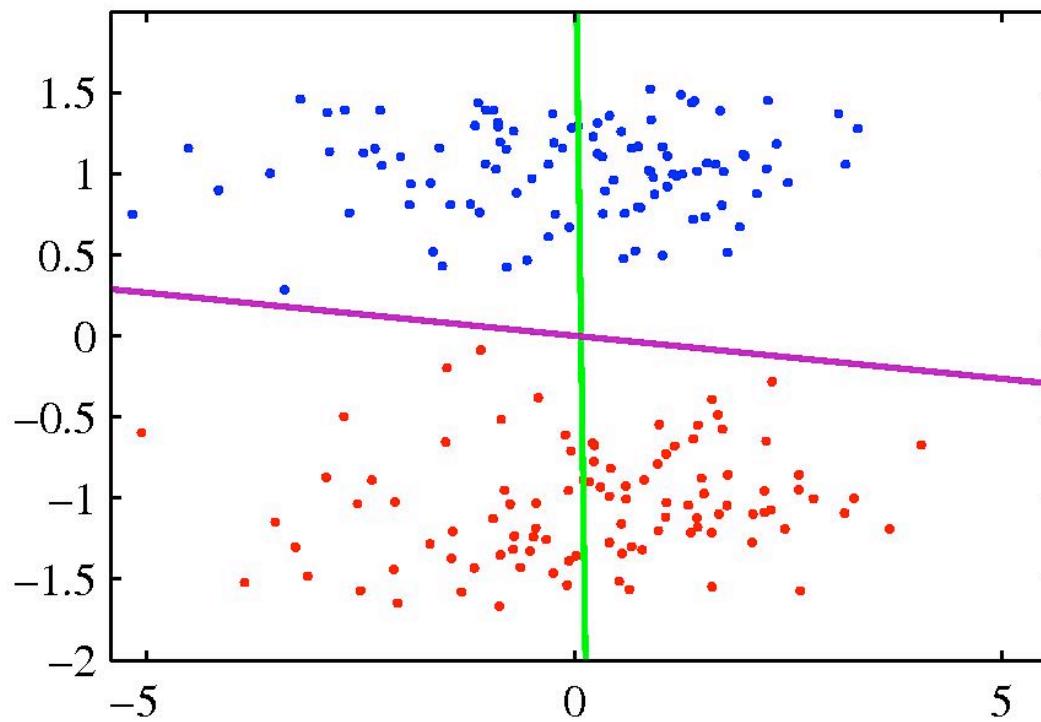
Learned Basis

- 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 \mathbf{S} , which scales as $O(D^3)$.
- Direct application of PCA will often be computationally infeasible.
- **Solution:** Let \mathbf{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 \mathbf{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 \mathbf{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 \mathbf{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 $\mathbf{X}^T v_i$ is **an eigenvector of \mathbf{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**.

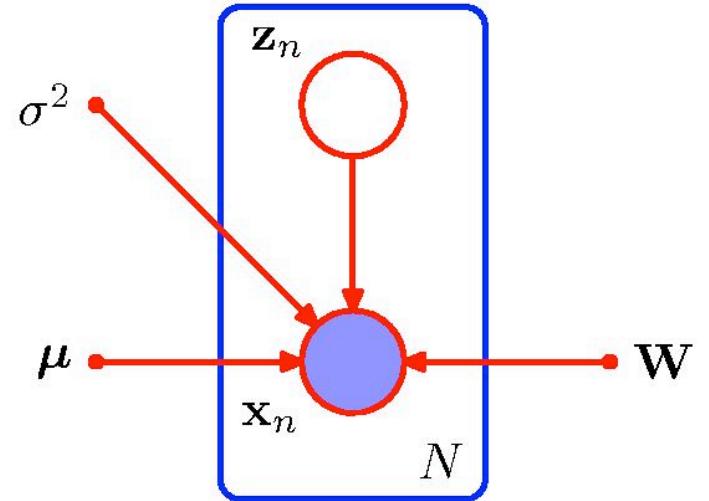
Probabilistic PCA

- Key assumptions:

- underlying latent M-dim variable \mathbf{z} has a Gaussian distribution.
- linear relationship between M-dim latent \mathbf{z} and D-dim observed \mathbf{x} variables.
- isotropic Gaussian noise in observed dimensions

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

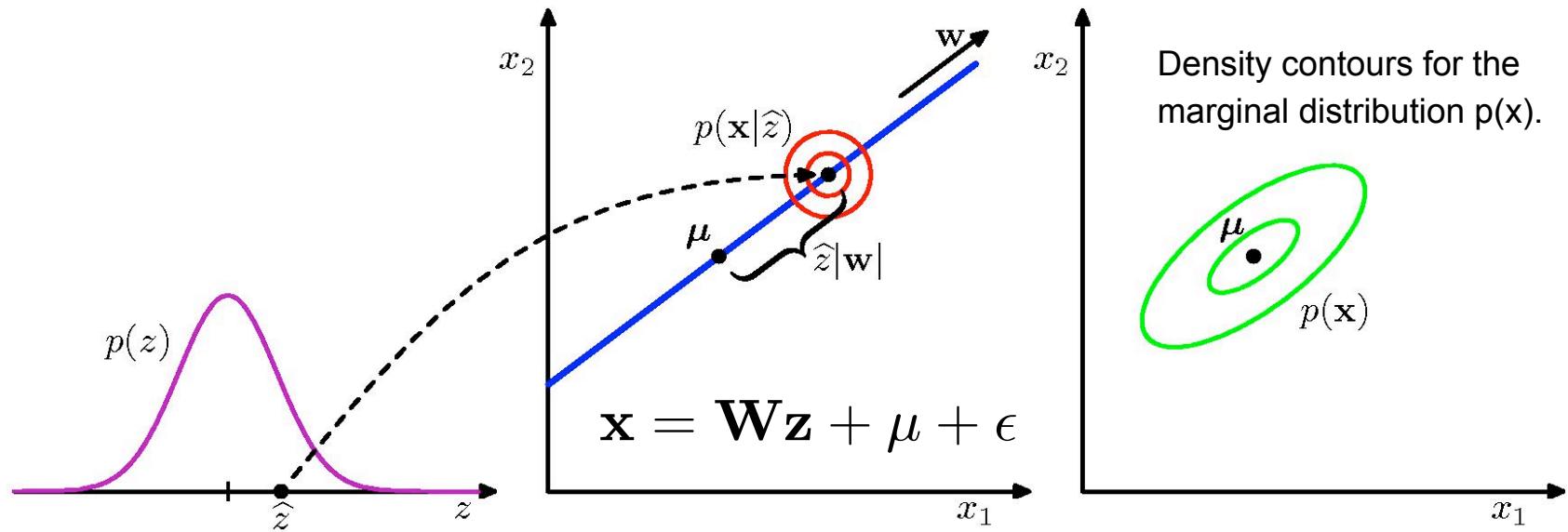
$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x} | \mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2 \mathbf{I})$$



- Hence the mean of \mathbf{x} is a linear function of \mathbf{z} governed by the $D \times M$ matrix \mathbf{W} and the D -dim vector $\boldsymbol{\mu}$.
- We will see that the columns of \mathbf{W} span the principal subspace of the data space (Columns of \mathbf{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 \mathbf{x} from an isotropic Gaussian distribution:

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

Marginal Data Density

- The joint $p(\mathbf{z}, \mathbf{x})$, the marginal data distribution $p(\mathbf{x})$ and the posterior distribution $p(\mathbf{z}|\mathbf{x})$ 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 by this result **directly by computing mean and covariance** given that it is Gaussian:

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

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

Redundancy in Parameterization

- The marginal distribution is governed by parameters \mathbf{W} , μ , σ^2 :

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

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

$$\tilde{\mathbf{W}} = \mathbf{WR}, \quad \mathbf{RR}^T = \mathbf{I}.$$

- Then

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

- 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 \mathbf{x} is D-dim and \mathbf{z} is M-dim is given:

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

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 \mathbf{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:

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

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

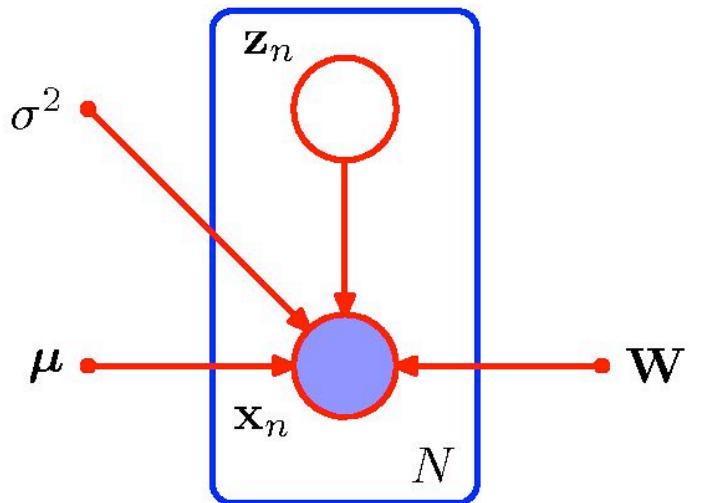
$$\mathbf{V} = \sigma^2 \mathbf{M}^{-1},$$

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

- Mean of inferred \mathbf{z} is projection of centered \mathbf{x} : linear operation.
- Posterior variance does not depend on the input \mathbf{x} at all.

- Remember:

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



Constrained Covariance

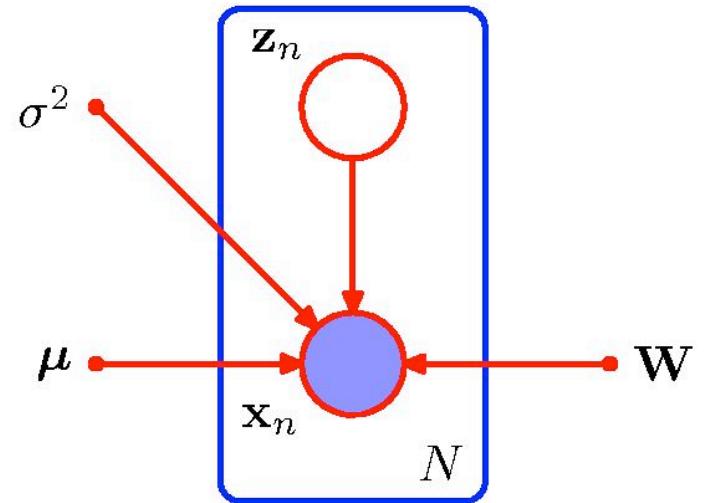
- Marginal density for PPCA has the following form:

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

where $\theta = \{\mathbf{W}, \mu, \sigma^2\}$.

Covariance \mathbf{C}

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



$$\mathbf{Cov}[\mathbf{x}] = \mathbf{W} \mathbf{W}^T + \sigma^2 \mathbf{I}$$

- 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):

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

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

- We then have:

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

- Maximizing with respect to \mathbf{W} and σ^2 can be solved directly.

Maximum Likelihood

- Objective:

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

- \mathbf{C} is model covariance; \mathbf{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 \mathbf{S} .

Maximum Likelihood

- Objective:

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

- Maximizing with respect to \mathbf{W} :

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

where

- \mathbf{U}_M is a $D \times M$ matrix whose columns are given by the **M principal eigenvectors** of the data covariance matrix \mathbf{S} .
 - \mathbf{L}_M is the $M \times M$ diagonal matrix containing M **largest eigenvalues**.
 - \mathbf{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 \mathbf{W} **define the principal subspace of standard PCA**.

Maximum Likelihood

- Objective:

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

- Maximizing with respect to σ^2 :

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

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:

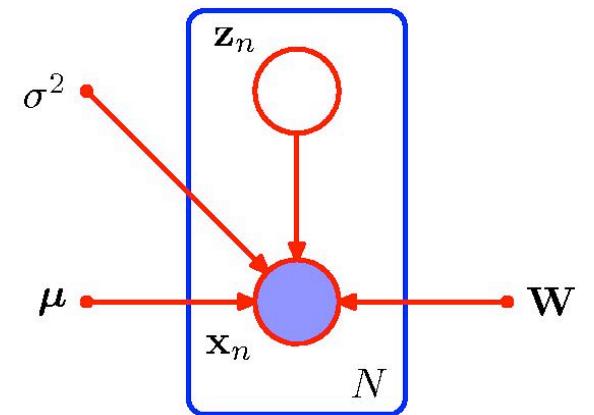
$$\log p(\mathbf{X}, \mathbf{Z} | \mu, \mathbf{W}, \sigma^2) = \sum_n [\log p(\mathbf{x}_n | \mathbf{z}_n) + \log p(\mathbf{z}_n)]$$

- E-step: compute expectation of complete log likelihood with respect to posterior of latent variables \mathbf{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: $p(\mathbf{z} | \mathbf{X})$.

- M-step: maximize with respect to parameters \mathbf{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:

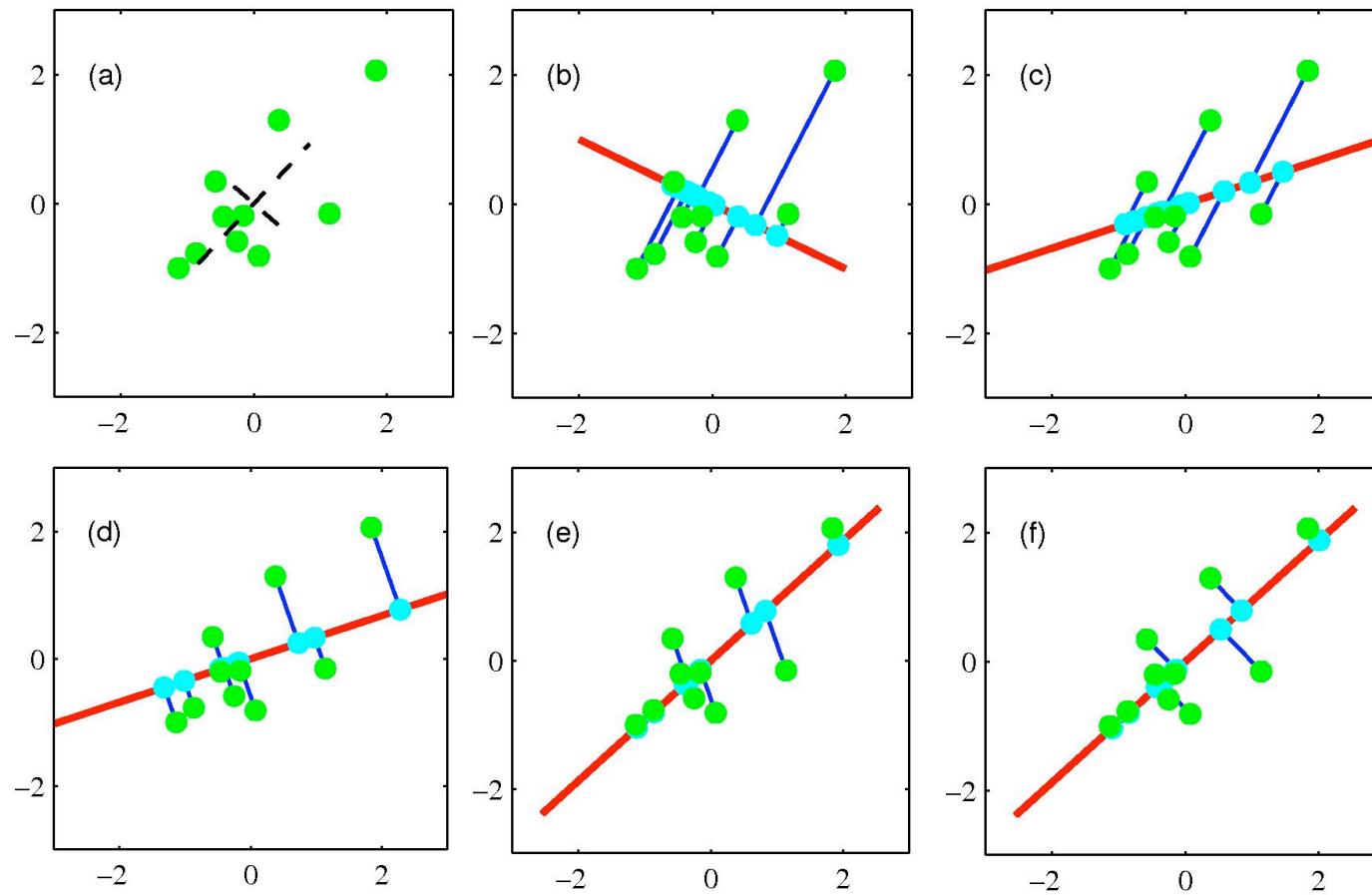
$$\lim_{\sigma^2 \rightarrow 0} (\mathbf{W}^T \mathbf{W} + \sigma \mathbf{I})^{-1} \mathbf{W}^T (\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{W}^T \mathbf{W})^{-1} \mathbf{W}^T (\mathbf{x} - \boldsymbol{\mu}),$$

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

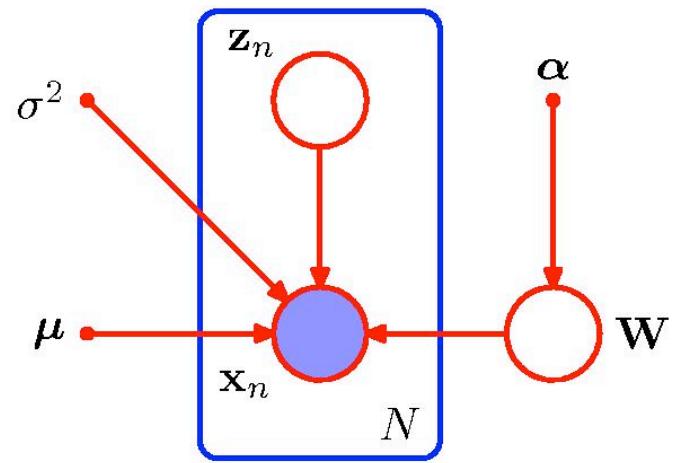
- It is easy to take a **Bayesian viewpoint** and place priors over model parameters.
- One option is to employ **the evidence approximation** (empirical Bayes) framework.
- We can define an independent Gaussian prior over each column of \mathbf{W} .
- Each such Gaussian has an **independent variance**:

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

where \mathbf{w}_i is the i^{th} column of \mathbf{W} .

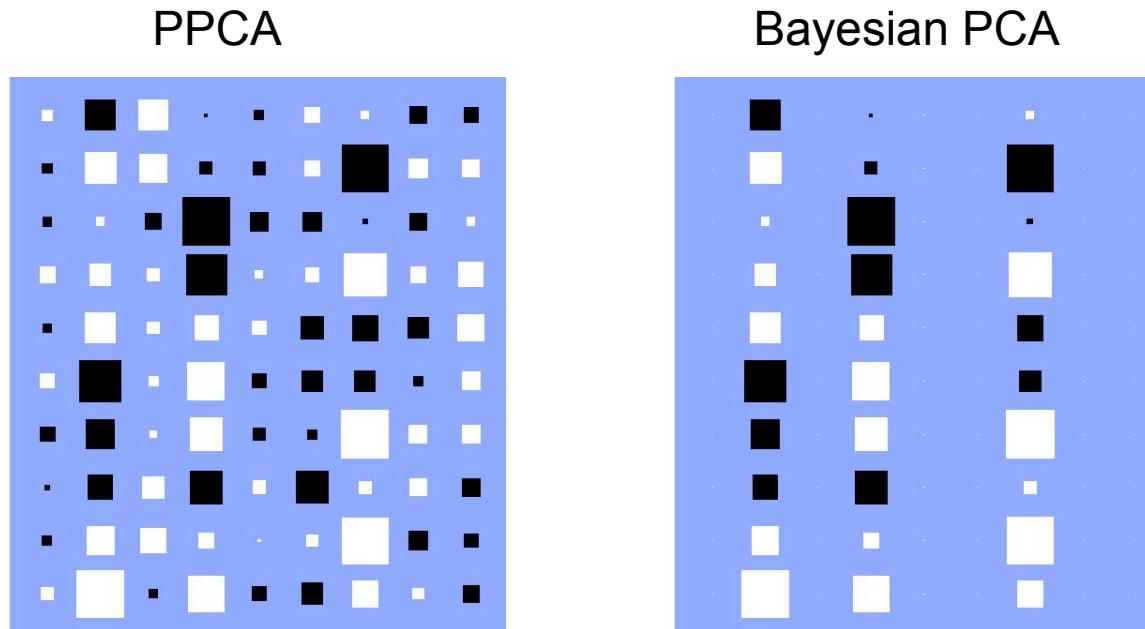
- The values of α_i are re-estimated during training by **maximizing the marginal likelihood**:

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



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).



- 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 \mathbf{z} has a Gaussian distribution
 - linear relationship between M-dim latent \mathbf{z} and D-dim observed \mathbf{x} variables.
 - **diagonal Gaussian noise** in observed dimensions.

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

- \mathbf{W} is a $D \times M$ factor loading matrix.
- $\boldsymbol{\Psi}$ 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 \mathbf{x} has diagonal rather than isotropic covariance.

Factor Analysis: Distributions

- As in PPCA, the joint $p(\mathbf{z}, \mathbf{x})$, the **marginal data distribution** $p(\mathbf{x})$ and the posterior $p(\mathbf{z}|\mathbf{x})$ are also Gaussian.
- Marginal distribution (predictive distribution):

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

- The **joint distribution**:

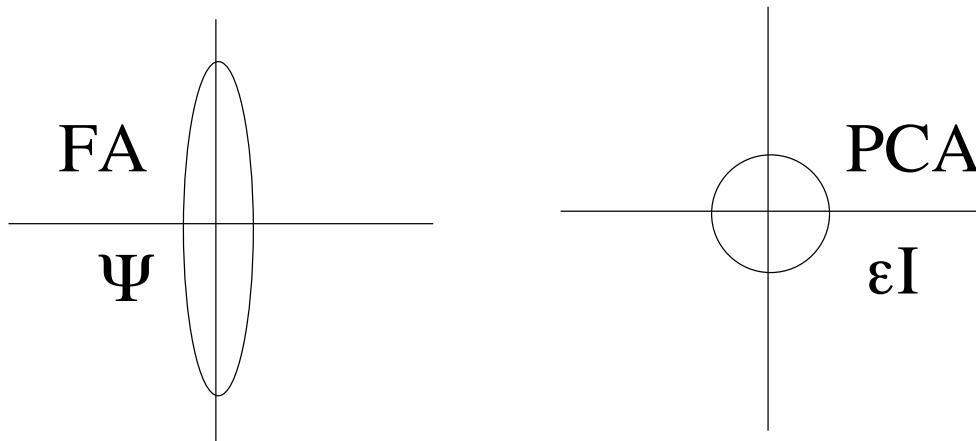
$$p\left(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix} \mid \begin{bmatrix} 0 \\ \boldsymbol{\mu} \end{bmatrix}, \begin{bmatrix} I & \mathbf{W}^\top \\ \mathbf{W} & \mathbf{W}\mathbf{W}^\top + \boldsymbol{\Psi}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

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** .

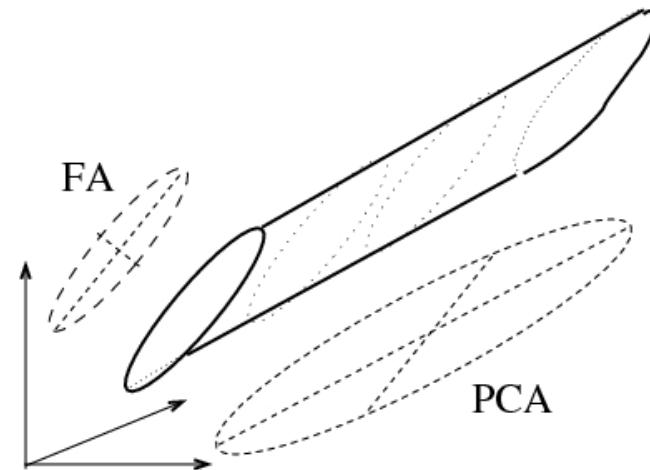


Rotation Invariance in PCA

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

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

- However, **the scale is important**.
- PCA **looks for directions of large variance**, so it will chase big noise directions.



Scale Invariance in FA

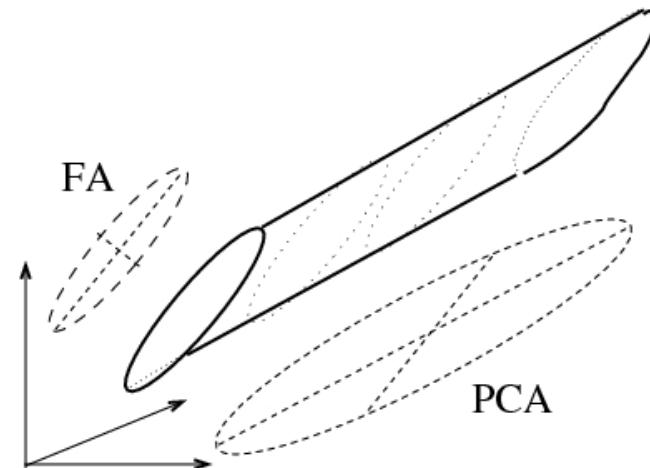
- In FA, the data can be re-scaled without changing anything.
- Multiply x_i by α_i :

$$\mu_i \leftarrow \alpha_i \mu_i$$

$$\mathbf{W}_{ij} \leftarrow \alpha_i \mathbf{W}_{ij}$$

$$\Psi_i \leftarrow \alpha_i^2 \Psi_i$$

- 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 same set of parameters – **not just local minimum but invariance**.
- Rotate \mathbf{W} by any unitary \mathbf{Q} and model stays the same – \mathbf{W} only appears in model as outer product \mathbf{WW}^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 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:

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

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

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

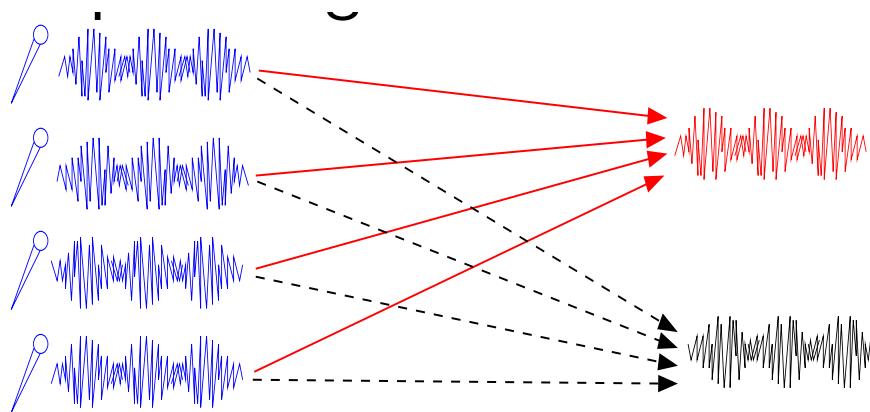


which is **constrained mixture of Gaussians**.

- 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**.



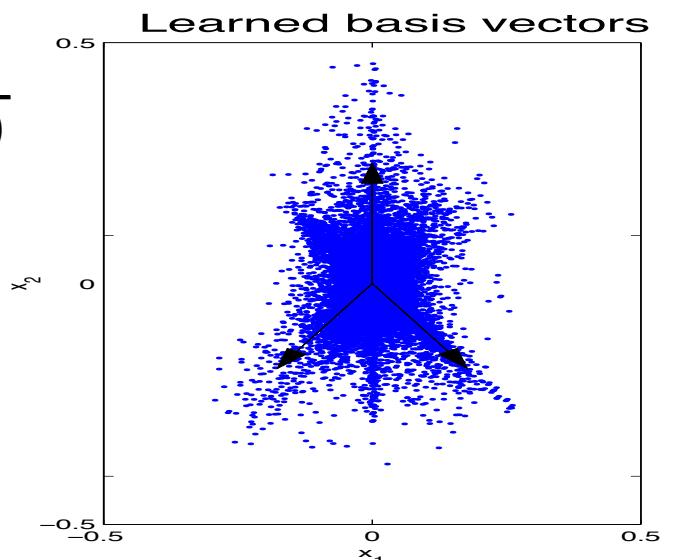
- The learning problem is the same: **find the weights from the factors to the outputs and infer the unknown factor values**.
- ICA: the factors are sometimes called “**sources**”, and the learning is sometimes called “**unmixing**”.

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.:

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

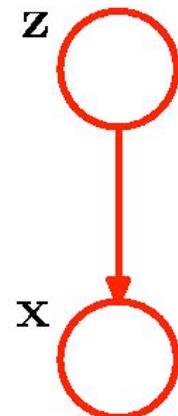
- Geometric intuition: **finding spikes in histograms.**



ICA Model

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

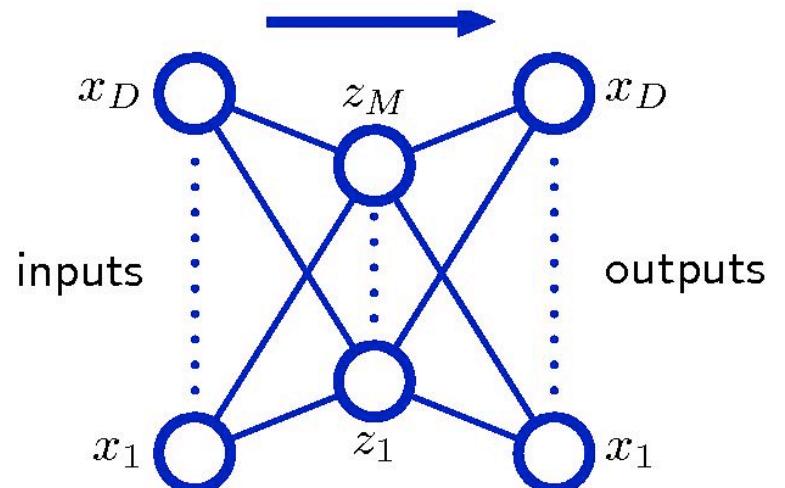
$$p(\mathbf{z}) = \prod_k p(z_k)$$
$$\mathbf{x} = \mathbf{V}\mathbf{z}$$



- Learning in this case can be done with **gradient descent** (plus some tricks to make the updates faster and more stable).
- If we keep \mathbf{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

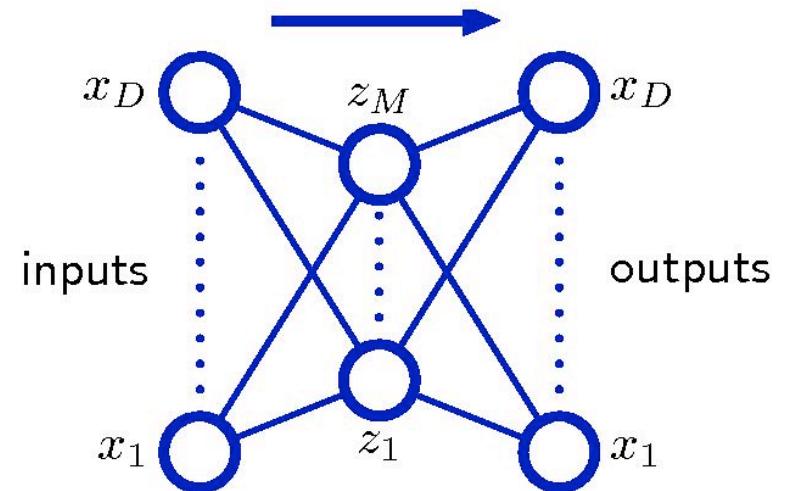
- Given an input x , its corresponding reconstruction is given by:

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

- We can determine the network parameters \mathbf{w} by minimizing the reconstruction error:

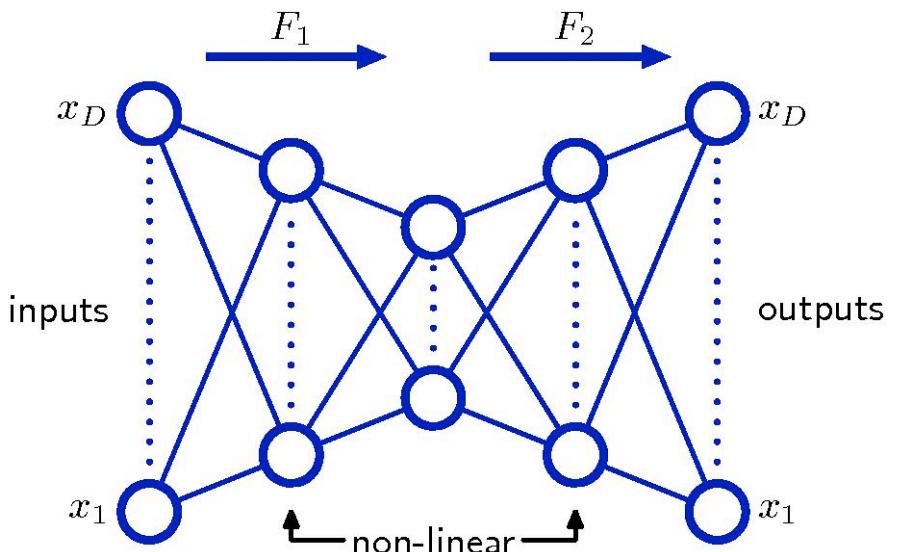
$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \|y(\mathbf{x}_n, \mathbf{w}) - \mathbf{x}_n\|^2.$$

- 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.



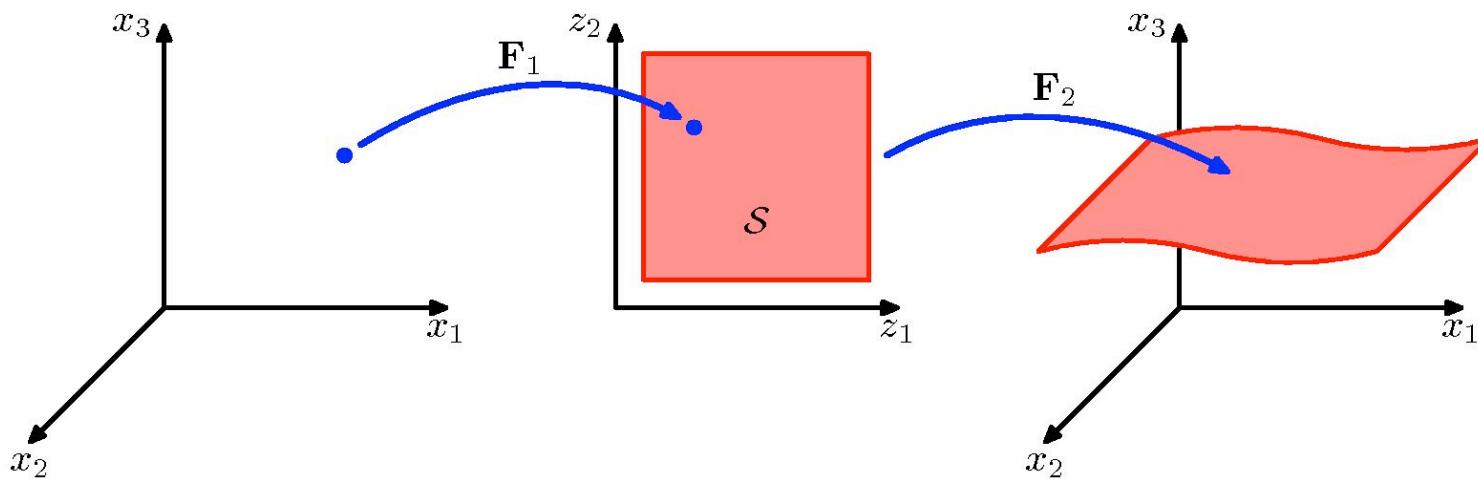
Deep Autoencoders

- 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

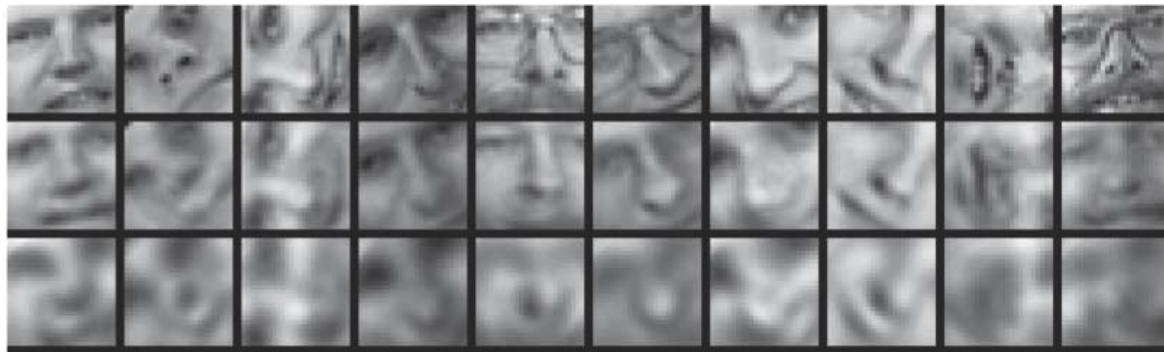
- Geometrical interpretation of the mappings performed by the network with 2 hidden layers for the case of $D=3$ and $M=2$ units in the middle layer.



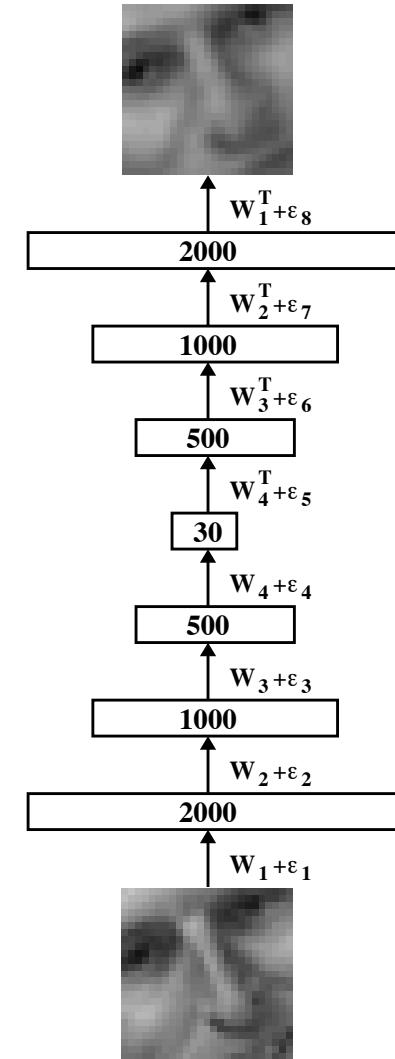
- The mapping F_1 defines a nonlinear projection of points in the original D -space into the M -dimensional subspace.
- The mapping F_2 maps from an M -dimensional space into D -dimensional space .

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 MNIST handwritten digits:



Real data

30-d deep autoencoder

30-d logistic PCA

30-d PCA

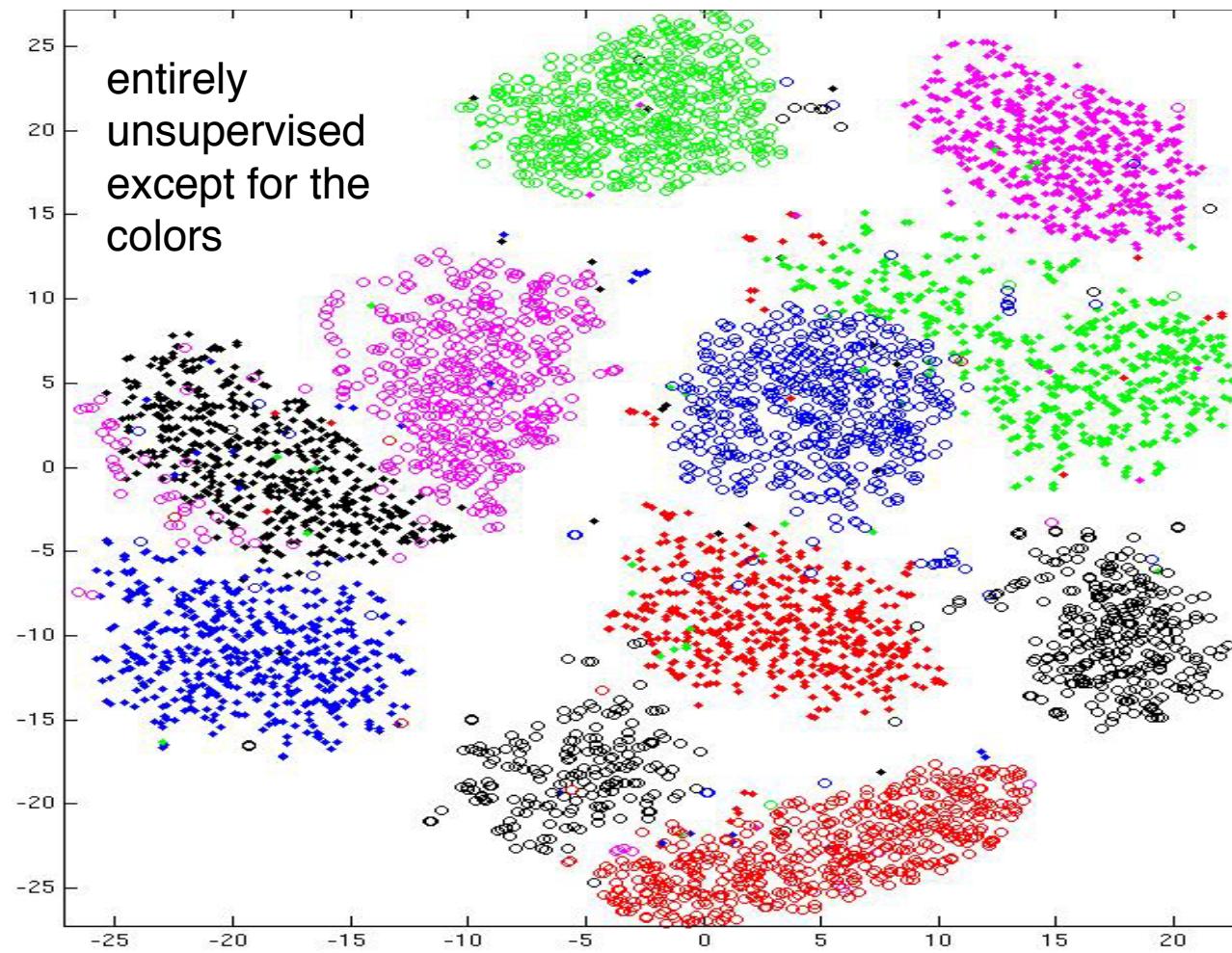
- Deep auto produces much better reconstructions.

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?

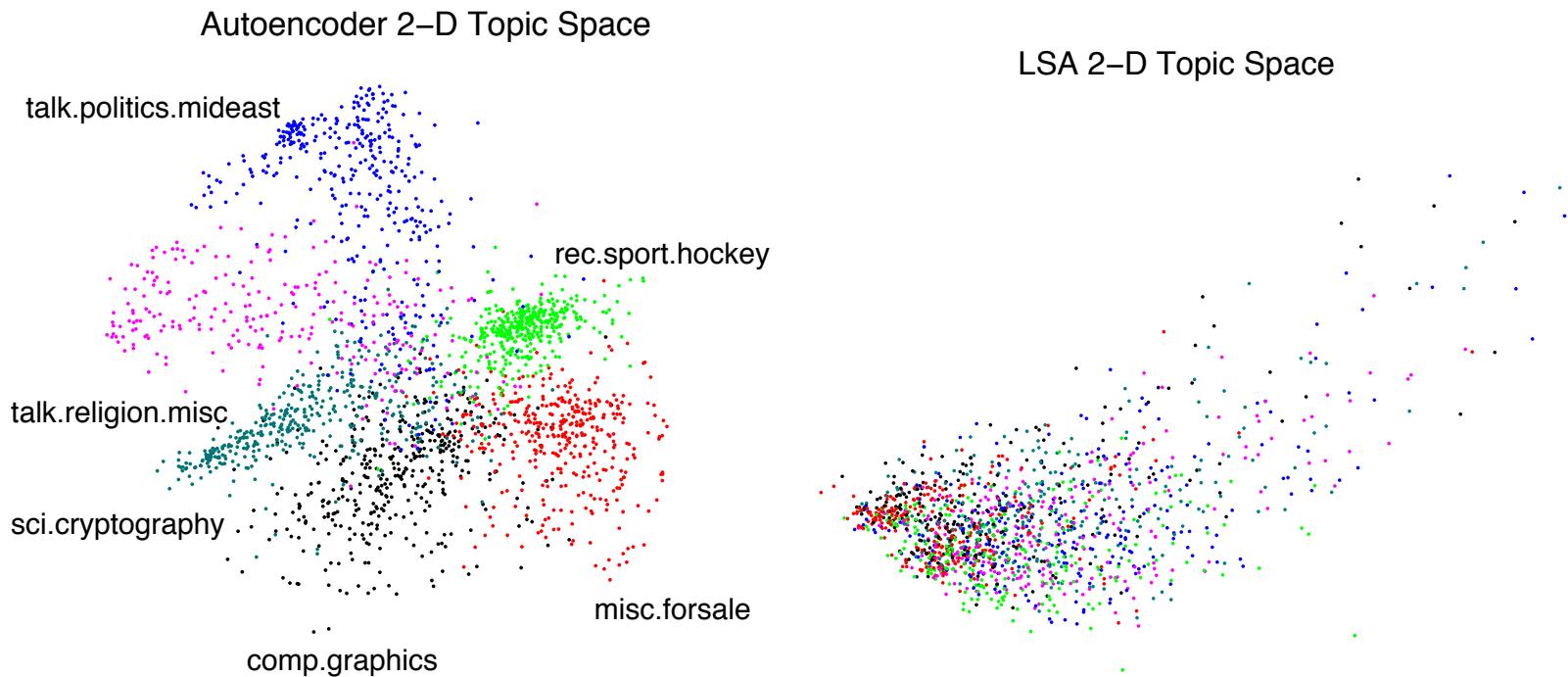


Learning 2-D topic Space

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

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

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



Reuters dataset

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

