MACHINE LEARNING

Dimensionality reduction

Corso di Laurea Magistrale in Informatica

Università di Roma Tor Vergata

Prof. Giorgio Gambosi

a.a. 2023-2024

In general, many features: high-dimensional spaces.

- *•* sparseness of data
- *•* increase in the number of coefficients, for example for dimension *D* and order 3 of the polynomial,

$$
y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D} \sum_{j=1}^{D} w_{ij} x_i x_j + \sum_{i=1}^{D} \sum_{j=1}^{D} \sum_{k=1}^{D} w_{ijk} x_i x_j x_k
$$

number of coefficients is *O*(*D M*)

High dimensions lead to difficulties in machine learning algorithms (lower reliability or need of large number of coefficients) this is denoted as curse of dimensionality

DIMENSIONALITY REDUCTION

- for any given classifier, the training set size required to obtain a certain accuracy grows exponentially wrt the number of features
- *•* it is important to bound the number of features, identifying the less discriminant ones

DIMENSIONALITY REDUCTION

- *•* Feature selection: identify a subset of features which are still discriminant, or, in general, still represent most dataset variance
- *•* Feature extraction: identify a projection of the dataset onto a lower-dimensional space, in such a way to still represent most dataset variance
	- *•* Linear projection: principal component analysis, probabilistic PCA, factor analysis
	- *•* Non linear projection: manifold learning, autoencoders

SEARCHING HYPERPLANES FOR THE DATASET

• verifying whether training set elements lie on a hyperplane (a space of lower dimensionality), apart from a limited variability (which could be seen as noise)

- \bullet principal component analysis looks for a d' -dimensional subspace ($d' < d$) such that the projection of elements onto such suspace is a "faithful" representation of the original dataset
- *•* as "faithful" representation we mean that distances between elements and their projections are small, even minimal

• Objective: represent all *d*-dimensional vectors x_1, \ldots, x_n by means of a unique vector x_0 , in the most faithful way, that is so that

$$
J(\mathbf{x}_0) = \sum_{i=1}^n ||\mathbf{x}_0 - \mathbf{x}_i||^2
$$

is minimum

• it is easy to show that

$$
\mathbf{x}_0 = \mathbf{m} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i
$$

• In fact,

 $J(\mathbf{x}_0) = \sum^{n} ||(\mathbf{x}_0 - \mathbf{m}) - (\mathbf{x}_i - \mathbf{m})||^2$ *i*=1 $= \sum_{i=1}^{n} ||\mathbf{x}_0 - \mathbf{m}||^2 - 2 \sum_{i=1}^{n} (\mathbf{x}_0 - \mathbf{m})^T (\mathbf{x}_i - \mathbf{m}) + \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{m}||^2$ *i*=1 *i*=1 *i*=1 $= \sum_{i=1}^{n} ||\mathbf{x}_0 - \mathbf{m}||^2 - 2(\mathbf{x}_0 - \mathbf{m})^T \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{m}) + \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{m}||^2$ *i*=1 *i*=1 *i*=1 $=$ $\sum_{i=1}^{n} ||\mathbf{x}_0 - \mathbf{m}||^2 + \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{m}||^2$ *i*=1 *i*=1

• since

$$
\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{m}) = \sum_{i=1}^{n} \mathbf{x}_i - n \cdot \mathbf{m} = n \cdot \mathbf{m} - n \cdot \mathbf{m} = 0
$$

• the second term is independent from x_0 , while the first one is equal to zero for $x_0 = m$

- *•* a single vector is too concise a representation of the dataset: anything related to data variability gets lost
- a more interesting case is the one when vectors are projected onto a line passing through m

• let u_1 be unit vector ($||u_1|| = 1$) in the line direction: the line equation is then

$\mathbf{x} = \alpha \mathbf{u}_1 + \mathbf{m}$

where α is the distance of x from m along the line

• let $\tilde{\mathbf{x}}_i = \alpha_i \mathbf{u}_1 + \mathbf{m}$ be the projection of \mathbf{x}_i $(i = 1, \ldots, n)$ onto the line: given $\mathbf{x}_1, \ldots, \mathbf{x}_n$, we wish to find the set of projections minimizing the quadratic error

The quadratic error is defined as

$$
J(\alpha_1, ..., \alpha_n, \mathbf{u}_1) = \sum_{i=1}^n ||\tilde{\mathbf{x}}_i - \mathbf{x}_i||^2
$$

=
$$
\sum_{i=1}^n ||(\mathbf{m} + \alpha_i \mathbf{u}_1) - \mathbf{x}_i||^2
$$

=
$$
\sum_{i=1}^n ||\alpha_i \mathbf{u}_1 - (\mathbf{x}_i - \mathbf{m})||^2
$$

=
$$
\sum_{i=1}^n +\alpha_i^2 ||\mathbf{u}_1||^2 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2 - 2 \sum_{i=1}^n \alpha_i \mathbf{u}_1^T (\mathbf{x}_i - \mathbf{m})
$$

=
$$
\sum_{i=1}^n \alpha_i^2 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2 - 2 \sum_{i=1}^n \alpha_i \mathbf{u}_1^T (\mathbf{x}_i - \mathbf{m})
$$

Its derivative wrt *α^k* is

$$
\frac{\partial}{\partial \alpha_k} J(\alpha_1, \dots, \alpha_n, \mathbf{u}_1) = 2\alpha_k - 2\mathbf{u}_1^T(\mathbf{x}_k - \mathbf{m})
$$

which is zero when $\alpha_k = \mathbf{u}_1^T(\mathbf{x}_k - \mathbf{m})$ (the orthogonal projection of \mathbf{x}_k onto the line).

The second derivative turns out to be positive

$$
\frac{\partial}{\partial \alpha_k^2} J(\alpha_1, \ldots, \alpha_n, \mathbf{u}_1) = 2
$$

showing that what we have found is indeed a minimum.

To derive the best direction u_1 of the line, we consider the covariance matrix of the dataset

$$
\mathbf{S} = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^T
$$

By plugging the values computed for α_i into the definition of $\jmath(\alpha_1,\ldots,\alpha_n,\mathbf{u}_1)$, we get

$$
J(\mathbf{u}_1) = \sum_{i=1}^n \alpha_i^2 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2 - 2 \sum_{i=1}^n \alpha_i^2
$$

= $-\sum_{i=1}^n [\mathbf{u}_1^T(\mathbf{x}_i - \mathbf{m})]^2 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2$
= $-\sum_{i=1}^n \mathbf{u}_1^T(\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^T \mathbf{u}_1 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2$
= $-\mathbf{n}\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 + \sum_{i=1}^n ||\mathbf{x}_i - \mathbf{m}||^2$

- *•* u *T* ¹(x*ⁱ −* m) is the projection of x*ⁱ* onto the line
- *•* the product

$$
\mathbf{u}_1^T(\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^T \mathbf{u}_1
$$

is then the variance of the projection of x_i wrt the mean m

• the sum

$$
\sum_{i=1}^n \mathbf{u}_1^T(\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^T \mathbf{u}_1 = n\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1
$$

is the overall variance of the projections of vectors x_i wrt the mean m

Minimizing $\bm{\mathit{J}}(\mathbf{u}_1)$ is equivalent to maximizing $\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$. That is, $\bm{\mathit{J}}(\mathbf{u}_1)$ is minimum if \mathbf{u}_1 is the direction which keeps the maximum amount of variance in the dataset

Hence, we wish to maximize $\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1$ (wrt \mathbf{u}_1), with the constraint $||\mathbf{u}_1|| = 1$.

By applying Lagrange multipliers this results equivalent to maximizing

 $u = \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 - \lambda_1 (\mathbf{u}_1^T \mathbf{u}_1 - 1)$

This can be done by setting the first derivative wrt \mathbf{u}_1 :

$$
\frac{\partial u}{\partial \mathbf{u}_1} = 2\mathbf{S}\mathbf{u}_1 - 2\lambda_1\mathbf{u}_1
$$

to 0, obtaining

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

Note that:

- *is maximized if is an eigenvector of S*
- *•* the overall variance of the projections is then equal to the corresponding eigenvalue

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

• the variance of the projections is then maximized (and the error minimized) if u_1 is the eigenvector of S corresponding to the maximum eigenvalue *λ*¹

- *•* The quadratic error is minimized by projecting vectors onto a hyperplane defined by the directions associated to the *d'* eigenvectors corresponding to the *d'* largest eigenvalues of S
- *•* If we assume data are modeled by a *d*-dimensional gaussian distribution with mean *µ* and covariance matrix **Σ**, PCA returns a *d ′* -dimensional subspace corresponding to the hyperplane defined by the eigenvectors associated to the *d ′* largest eigenvalues of **Σ**
- *•* The projections of vectors onto that hyperplane are distributed as a *d ′* -dimensional distribution which keeps the maximum possible amount of data variability

AN EXAMPLE OF PCA

• Digit recognition $(D = 28 \times 28 = 784)$
Original $M = 1$

CHOOSING *d ′*

Eigenvalue size distribution is usually characterized by a fast initial decrease followed by a small decrease

This makes it possible to identify the number of eigenvalues to keep, and thus the dimensionality of the projections.

CHOOSING *d ′*

Eigenvalues measure the amount of distribution variance kept in the projection.

Let us consider, for each $k < d$, the value

$$
r_k = \frac{\sum_{i=1}^k \lambda_i^2}{\sum_{i=1}^n \lambda_i^2}
$$

which provides a measure of the variance fraction associated to the *k* largest eigenvalues.

When $r_1 < \ldots < r_d$ are known, a certain amount p of variance can be kept by setting

 $d' = \text{argmin} \; r_i > p$ *i∈{*1*,...,d}*

PROBABILISTIC APPROACH TO PCA: IDEA

Introduce a latent variable model to relate a *d*-dimensional observation vector to a corresponding *d ′* -dimensional gaussian latent variable (with *d ′ < d*)

 $x = Wz + \mu + \epsilon$

where

- \bullet z is a d'-dimensional gaussian latent variable (the "projection" of x on a lower-dimensional subspace)
- \bullet $\,$ **W** is a $d \times d'$ matrix, relating the original space with the lower-dimensional subspace
- *• ϵ* is a *d*-dimensional gaussian noise: noise covariance on different dimensions is assumed to be 0. Noise variance is assumed equal on all dimensions: hence $p(\epsilon) = \mathcal{N}(0, \sigma^2 \mathbf{I})$
- *• µ* is the *d*-dimensional vector of the means

 ϵ and μ are assumed independent.

GRAPHICAL MODEL

1. $z \in \mathbb{R}^{d'}$, $x, \epsilon \in \mathbb{R}^{d}$, $d' < d$ 2. $p(z) = \mathcal{N}(0, I)$ 3. $p(\epsilon) = \mathcal{N}(0, \sigma^2 I)$, (isotropic gaussian noise)

GENERATIVE PROCESS

This can be interpreted in terms of a generative process

1. sample the latent variable $z \in \mathbb{R}^{d'}$ from

$$
p(\mathbf{z}) = \frac{1}{(2\pi)^{d'/2}} e^{-\frac{||\mathbf{z}||^2}{2}}
$$

2. linearly project onto \mathbb{R}^d

$$
\mathbf{y} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu}
$$

3. sample the noise component $\epsilon \in \mathbb{R}^d$ from

$$
p(\epsilon) = \frac{1}{(2\pi)^{d/2}} e^{-\frac{||\epsilon||^2}{2\sigma^2}}
$$

4. add the noise component *ϵ*

 $x = y + \epsilon$

This results into $p(x|z) = \mathcal{N}(Wz + \mu, \sigma^2I)$

GENERATIVE PROCESS

LATENT VARIABLE MODEL

The joint distribution is

$$
p\left(\left[\begin{array}{c} {\bf z} \\ {\bf x} \end{array} \right] \right) = \mathcal{N}(\mu_{{\bf z}x}, \Sigma)
$$

By definition,

$$
\mu_{zx} = \left[\begin{array}{c} \mu_z \\ \mu_x \end{array}\right]
$$

- Since $p(z) = \mathcal{N}(0, I)$, then $\mu_z = 0$.
- Since $p(x) = Wz + \mu + \epsilon$, then

$$
\mu_{\mathbf{x}} = E[\mathbf{x}] = E[W\mathbf{z} + \mu + \epsilon] = \mathbf{W}E[\mathbf{z}] + \mu + E[\epsilon] = \mu
$$

Hence

$$
\mu_{zx}=\left[\begin{array}{c}0\\ \mu\end{array}\right]
$$

LATENT VARIABLE MODEL

For what concerns the distribution covariance

$$
\boldsymbol{\Sigma} = \left[\begin{array}{cc} \boldsymbol{\Sigma}_{\text{zz}} & \boldsymbol{\Sigma}_{\text{zx}} \\ \boldsymbol{\Sigma}_{\text{zx}} & \boldsymbol{\Sigma}_{\text{xx}} \end{array} \right]
$$

where

$$
\Sigma_{zz} = E[zz^T] = I
$$

\n
$$
\Sigma_{zx} = W^T
$$

\n
$$
\Sigma_{xx} = WW^T + \sigma^2 I
$$

LATENT VARIABLE MODEL

As a consequence, we get, for the joint distribution,

$$
\mu_{\text{zx}} = \left[\begin{array}{c} 0 \\ \mu \end{array} \right] \hspace{3cm} \Sigma = \left[\begin{array}{cc} \textbf{I} & \textbf{W}^{\textsf{T}} \\ \textbf{W} & \textbf{W} \textbf{W}^{\textsf{T}} + \sigma^2 \textbf{I} \end{array} \right]
$$

The marginal distribution of x is then $p(x) = \mathcal{N}(\mu, WW^{T} + \sigma^{2}I)$

The conditional distribution of z given x is $p(z|x) = \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$ with

$$
\mu_{\mathbf{z}|\mathbf{x}} = \mathbf{W}^{\mathsf{T}} (\mathbf{W}\mathbf{W}^{\mathsf{T}} + \sigma^2 \mathbf{I})^{-1} (\mathbf{x} - \boldsymbol{\mu})
$$

$$
\Sigma_{\mathbf{z}|\mathbf{x}} = \mathbf{I} - \mathbf{W}^{\mathsf{T}} (\mathbf{W}\mathbf{W}^{\mathsf{T}} + \sigma^2 \mathbf{I})^{-1} \mathbf{W} = \sigma^2 (\sigma^2 \mathbf{I} + \mathbf{W}^{\mathsf{T}} \mathbf{W})^{-1}
$$

MAXIMUM LIKELIHOOD FOR PCA

Setting $\mathbf{C} = \mathbf{W}\mathbf{W}^{\intercal} + \sigma^2 \mathbf{I}$, the log-likelihood of the dataset in the model is

$$
\log p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) = \sum_{i=1}^n \log p(\mathbf{x}_i|\mathbf{W}, \boldsymbol{\mu}, \sigma^2)
$$

=
$$
-\frac{nd}{2} \log(2\pi) - \frac{n}{2} \log |\mathbf{C}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_n - \boldsymbol{\mu}) \mathbf{C}^{-1} (\mathbf{x}_i - \boldsymbol{\mu})^T
$$

Setting the derivative wrt μ to zero results into

$$
\mu = \overline{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i
$$

Maximization wrt ${\bf W}$ and σ^2 is more complex: however, a closed form solution exists:

$$
\mathbf{W} = \mathbf{U}_{d'} (\mathbf{L}_{d'} - \sigma^2 \mathbf{I})^{1/2}
$$

where

- $U_{d'}$ is the $d \times d'$ matrix whose columns are the eigenvectors corresponding to the d' largest eigenvalues
- *•* L*^d′* is the *d ′ [×] ^d ′* diagonal matrix of the largest eigenvalues

The columns of W are the principal components eigenvectors scaled by the variance $\lambda_i - \sigma^2$

For what concerns maximization wrt σ^2 , it results

$$
\sigma^2 = \frac{1}{\mathbf{d} - \mathbf{d}'} \sum_{i = \mathbf{d}' + 1}^{\mathbf{d}} \lambda_i
$$

since eigenvalues provide measures of the dataset variance along the corresponding eigenvector direction, this corresponds to the average variance along the discarded directions.

MAPPING POINTS TO SUBSPACE

The conditional distribution

$$
p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu}), \sigma^2(\sigma^2 \mathbf{I} + \mathbf{W}^T \mathbf{W})^{-1})
$$

can be applied.

In particular, the conditional expectation

$$
E[\mathbf{z}|\mathbf{x}] = \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu})
$$

can be assumed as the latent space point corresponding to x. The projection onto the d'-dimensional subspace can then be performed as

$$
\mathbf{x}' = \mathbf{W}\mathbf{E}[\mathbf{z}|\mathbf{x}] + \boldsymbol{\mu} = \mathbf{W}\mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu}) + \boldsymbol{\mu}
$$

Even if the log-likelihood has a closed form maximization, applying EM can sometimes be useful.

FACTOR ANALYSIS

Noise components still gaussian and independent, but with different variance.

\n- 1.
$$
z \in \mathbb{R}^d
$$
, $x, \epsilon \in \mathbb{R}^p$, $d \lt\lt D$
\n- 2. $p(z) = \mathcal{N}(0, I)$
\n- 3. $p(\epsilon) = \mathcal{N}(0, \Psi)$, Ψ diagonal (independent gaussian noise)
\n

FACTOR ANALYSIS

Model distribution are modified accordingly.

Joint distribution

$$
\rho\left(\left[\begin{array}{c}z\\x\end{array}\right]\right)=\mathcal{N}\left(\left[\begin{array}{c}0\\W\end{array}\right],\left[\begin{array}{cc}I & W^{\text{T}}\\ \Lambda & WW^{\text{T}}+\Psi\end{array}\right]\right)
$$

Marginal distribution

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

Conditional distribution

The conditional distribution of z given x is now $p(z|x) = \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$ with

$$
\begin{aligned} \boldsymbol{\mu}_{z|x} &= \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi})^{-1}(\mathbf{x} - \boldsymbol{\mu}) \\ \boldsymbol{\Sigma}_{z|x} &= \mathbf{I} - \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi})^{-1}\mathbf{W} \end{aligned}
$$

MAXIMUM LIKELIHOOD FOR FA

The log-likelihood of the dataset in the model is now

$$
\log p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \boldsymbol{\Psi}) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\mathbf{W}, \boldsymbol{\mu}, \boldsymbol{\Psi})
$$

= $-\frac{n d}{2} \log(2\pi) - \frac{n}{2} \log |\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi}| - \frac{1}{2} \sum_{i=1}^{n} (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi})^{-1} (\mathbf{x}_i - \boldsymbol{\mu})^T$

Setting the derivative wrt μ to zero results gain into

$$
\mu = \overline{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i
$$

Estimating parameters through log-likelihood maximization does not provide a closed form solution for W and **Ψ**. Iterative techniques such as EM must be applied.