

COMS 4721: Machine Learning for Data Science

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PRINCIPAL COMPONENT ANALYSIS

DIMENSIONALITY REDUCTION

We're given data x_1, \dots, x_n , where $x \in \mathbb{R}^d$. This data is often high-dimensional, but the “information” doesn't use the full d dimensions.



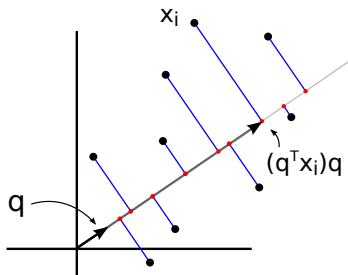
For example, we could represent the above images with three numbers since they have three degrees of freedom. Two for shifts and a third for rotation.

Principal component analysis can be thought of as a way of automatically mapping data x_i into some new low-dimensional coordinate system.

- ▶ It captures most of the information in the data in a few dimensions
- ▶ Extensions allow us to handle missing data, and “unwrap” the data

PRINCIPAL COMPONENT ANALYSIS

Example: How can we approximate this data using a unit-length vector q ?



q is a unit-length vector, $q^T q = 1$.

Red dot: The length, $q^T x_i$, to the axis after projecting x onto the line defined by q .

The vector $(q^T x_i)q$ takes q and stretches it to the corresponding red dot.

So what's a good q ? How about minimizing the squared approximation error,

$$q = \arg \min_q \sum_{i=1}^n \|x_i - qq^T x_i\|^2 \quad \text{subject to} \quad q^T q = 1$$

$qq^T x_i = (q^T x_i)q$: The approximation of x_i by stretching q to the “red dot.”

PCA : THE FIRST PRINCIPAL COMPONENT

This is related to the problem of finding the largest eigenvalue,

$$\begin{aligned} q &= \arg \min_q \sum_{i=1}^n \|x_i - qq^T x_i\|^2 \quad \text{s.t.} \quad q^T q = 1 \\ &= \arg \min_q \sum_{i=1}^n x_i^T x_i - q^T \underbrace{\left(\sum_{i=1}^n x_i x_i^T \right)}_{= XX^T} q \end{aligned}$$

We've defined $X = [x_1, \dots, x_n]$. Since the first term doesn't depend on q and we have a negative sign in front of the second term, equivalently we solve

$$q = \arg \max_q q^T (XX^T) q \quad \text{subject to} \quad q^T q = 1$$

This is the eigendecomposition problem:

- ▶ q is the first eigenvector of XX^T
- ▶ $\lambda = q^T (XX^T) q$ is the first eigenvalue

PCA: GENERAL

The general form of PCA considers K eigenvectors,

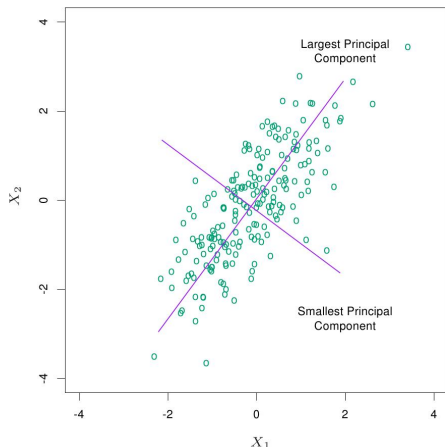
$$\begin{aligned} q &= \arg \min_q \sum_{i=1}^n \left\| x_i - \underbrace{\sum_{k=1}^K (x_i^T q_k) q_k}_{\text{approximates } x} \right\|^2 \quad \text{s.t. } q_k^T q_{k'} = \begin{cases} 1, & k = k' \\ 0, & k \neq k' \end{cases} \\ &= \arg \min_q \sum_{i=1}^n x_i^T x_i - \sum_{k=1}^K q_k^T \underbrace{\left(\sum_{i=1}^n x_i x_i^T \right)}_{= XX^T} q_k \end{aligned}$$

The vectors in $Q = [q_1, \dots, q_K]$ give us a K -dimensional subspace with which to represent the data:

$$x_{\text{proj}} = \begin{bmatrix} q_1^T x \\ \vdots \\ q_K^T x \end{bmatrix}, \quad x \approx \sum_{k=1}^K (q_k^T x) q_k = Q x_{\text{proj}}$$

The eigenvectors of (XX^T) can be learned using built-in software.

EIGENVALUES, EIGENVECTORS AND THE SVD



An equivalent formulation of the problem is to find (λ, q) such that

$$(XX^T)q = \lambda q$$

Since (XX^T) is a PSD matrix, there are $r \leq \min\{d, n\}$ eigenpairs (λ_i, q_i) such that

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r \geq 0,$$

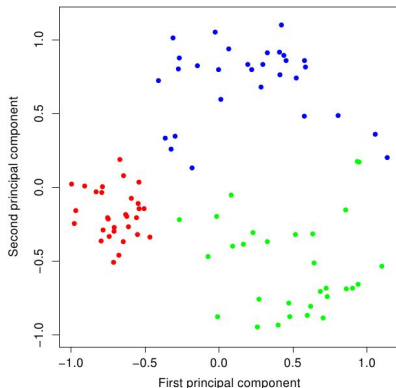
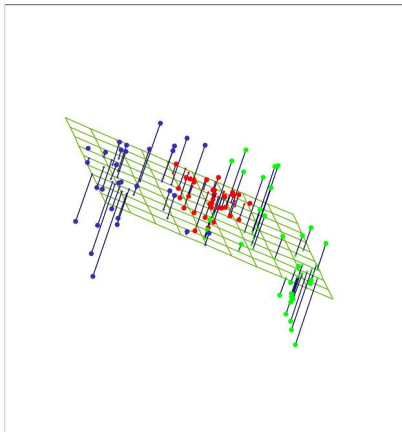
$$q_k^T q_k = 1, \quad q_k^T q_{k'} = 0$$

Why is (XX^T) PSD? Using the SVD, $X = USV^T$, we have that

$$(XX^T) = US^2U^T \Rightarrow Q = U, \quad \lambda_i = (S^2)_{ii} \geq 0$$

(Preprocessing: Usually first subtract off the mean of each dimension of x .)

PCA: EXAMPLE OF PROJECTING FROM \mathbb{R}^3 TO \mathbb{R}^2



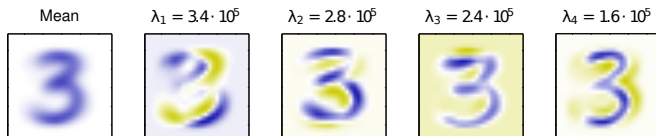
For this data, most information (structure in the data) can be captured in \mathbb{R}^2 .

(left) The original data in \mathbb{R}^3 . The hyperplane is defined by q_1 and q_2 .

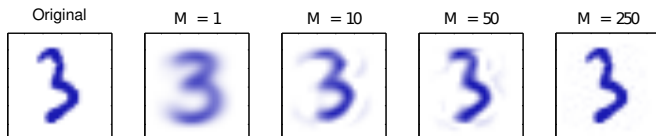
(right) The new coordinates for the data: $x_i \rightarrow x_i^{proj} = \begin{bmatrix} x_i^T q_1 \\ x_i^T q_2 \end{bmatrix}$.

EXAMPLE: DIGITS

Data: 16×16 images of handwritten 3's (treat as vectors in \mathbb{R}^{256})



Above: The first four eigenvectors q and their eigenvalues λ .



Above: Reconstructing a 3 using the first $M - 1$ eigenvectors plus the mean.

Let $\bar{x} = x - \text{mean}$, then

$$x \approx \text{mean} + \sum_{k=1}^{M-1} (\bar{x}^T q_k) q_k$$

PROBABILISTIC PCA

PCA AND THE SVD

We've discussed how any matrix X has a singular value decomposition,

$$X = USV^T, \quad U^T U = I, \quad V^T V = I$$

and S is a diagonal matrix with non-negative entries.

Therefore,

$$XX^T = US^2U^T \quad \Leftrightarrow \quad (XX^T)U = US^2$$

U is a matrix of eigenvectors, and S^2 is a diagonal matrix of eigenvalues.

A MODELING APPROACH TO PCA

Using the SVD perspective of PCA, we can also derive a probabilistic model for the problem and use the EM algorithm to learn it.

This model will have the advantages of:

- ▶ Handling the problem of missing data
- ▶ Allowing us to learn additional parameters such as noise
- ▶ Provide a framework that could be extended to more complex models
- ▶ Gives distributions used to characterize uncertainty in predictions
- ▶ etc.

PROBABILISTIC PCA

In effect, this is a new matrix factorization model.

- ▶ With the SVD, we had $X = USV^T$.
- ▶ We now approximate $X \approx WZ$, where
 - ▶ W is a $d \times K$ matrix. In different settings this is called a “factor loadings” matrix, or a “dictionary.” It’s like the eigenvectors, but no orthonormality.
 - ▶ The i th column of Z is called $z_i \in \mathbb{R}^K$. Think of it as a low-dimensional representation of x_i .

The generative process of Probabilistic PCA is

$$x_i \sim N(Wz_i, \sigma^2 I), \quad z_i \sim N(0, I).$$

In this case, we don’t know W or any of the z_i .

THE LIKELIHOOD

Maximum likelihood

Our goal is to find the maximum likelihood solution of the matrix W under the marginal distribution, i.e., with the z_i vectors integrated out,

$$W_{\text{ML}} = \arg \max_W \ln p(x_1, \dots, x_n | W) = \arg \max_W \sum_{i=1}^n \ln p(x_i | W).$$

This is intractable because $p(x_i | W) = N(x_i | 0, \sigma^2 I + WW^T)$,

$$N(x_i | 0, \sigma^2 I + WW^T) = \frac{1}{(2\pi)^{\frac{d}{2}} |\sigma^2 I + WW^T|^{\frac{1}{2}}} e^{-\frac{1}{2} x^T (\sigma^2 I + WW^T)^{-1} x}$$

We can set up an EM algorithm that uses the vectors z_1, \dots, z_n .

EM FOR PROBABILISTIC PCA

Setup

The marginal log likelihood can be expressed using EM as

$$\begin{aligned} \sum_{i=1}^n \ln \int p(x_i, z_i | W) dz_i &= \sum_{i=1}^n \int q(z_i) \ln \frac{p(x_i, z_i | W)}{q(z_i)} dz_i && \leftarrow \mathcal{L}(W) \\ &+ \sum_{i=1}^n \int q(z_i) \ln \frac{q(z_i)}{p(z_i | x_i, W)} dz_i && \leftarrow \text{KL} \end{aligned}$$

EM Algorithm: Remember that EM has two steps. At iteration t ,

1. Set $q(z_i) = p(z_i | x_i, W_{t-1})$ for each i and calculate $\mathcal{L}(W)$
2. Maximize \mathcal{L} with respect to W

Again, for this to work well we need that

- ▶ we can calculate the conditional posterior distribution $p(z_i | x_i, W)$, and
- ▶ maximizing \mathcal{L} is easy, i.e., we update W using a simple equation

THE ALGORITHM

EM for Probabilistic PCA

Given: Data $x_{1:n}$, $x_i \in \mathbb{R}^d$ and model $x_i \sim N(Wz_i, \sigma^2)$, $z_i \sim N(0, I)$, $z \in \mathbb{R}^K$

Output: Point estimate of W and posterior distribution on each z_i

E-Step: Set each $q(z_i) = p(z_i|x_i, W) = N(z_i|\mu_i, \Sigma_i)$ where

$$\Sigma_i = (I + W^T W / \sigma^2)^{-1}, \quad \mu_i = \Sigma_i W^T x_i / \sigma^2$$

M-Step: Update W by maximizing the objective \mathcal{L} from the E-step

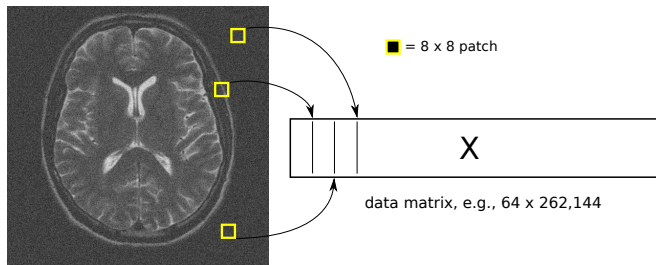
$$W = \left[\sum_{i=1}^n x_i \mu_i^T \right] \left[\sigma^2 I + \sum_{i=1}^n (\mu_i \mu_i^T + \Sigma_i) \right]^{-1}$$

Iterate E and M steps until increase in $\sum_{i=1}^n \ln p(x_i|W)$ is “small.”

Comment:

- The probabilistic framework gives a way to learn K and σ^2 as well.

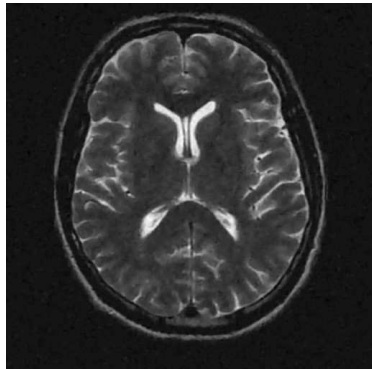
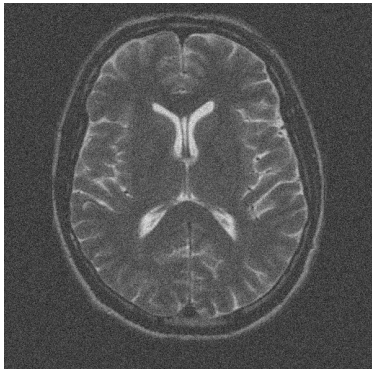
EXAMPLE: IMAGE PROCESSING



For image problems such as denoising or inpainting (missing data)

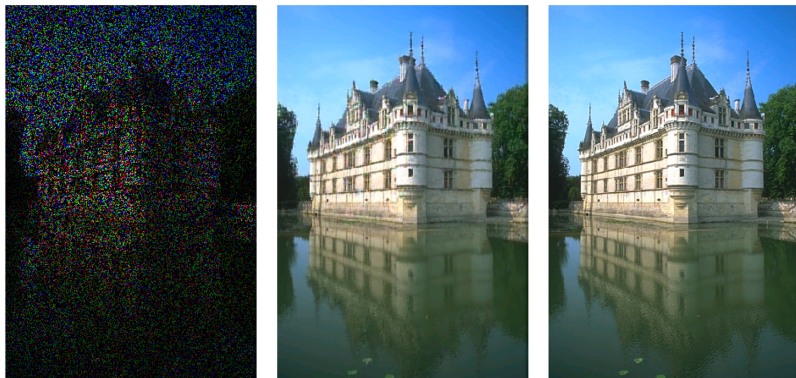
- ▶ Extract overlapping patches (e.g., 8×8) and vectorize to construct X
- ▶ Model with a factor model such as Probabilistic PCA
- ▶ Approximate $x_i \approx W\mu_i$, where μ_i is the posterior mean of z_i
- ▶ Reconstruct the image by replacing x_i with $W\mu_i$ (and averaging)

EXAMPLE: DENOISING



Noisy image on left, denoised image on right. The noise variance parameter σ^2 was learned for this example.

EXAMPLE: MISSING DATA



Another somewhat extreme example:

- ▶ Image is $480 \times 320 \times 3$ (RGB dimension)
- ▶ Throw away 80% at random
- ▶ (left) Missing data, (middle) reconstruction, (right) original image

KERNEL PCA

KERNEL PCA

We've seen how we can take an algorithm that uses dot products, $x^T x$, and generalize with a nonlinear kernel. This generalization can be made to PCA.

Recall: With PCA we find the eigenvectors of the matrix $\sum_{i=1}^n x_i x_i^T = XX^T$.

- ▶ Let $\phi(x)$ be a feature mapping from \mathbb{R}^d to \mathbb{R}^D , where $D \gg d$
- ▶ We want to solve the eigendecomposition

$$\left[\sum_{i=1}^n \phi(x_i) \phi(x_i)^T \right] q_k = \lambda_k q_k$$

without having to work in the higher dimensional space.

- ▶ That is, how can we do PCA without explicitly using $\phi(\cdot)$ and q ?

Notice that we can reorganize the operations of the eigendecomposition

$$\sum_{i=1}^n \phi(x_i) \underbrace{(\phi(x_i)^T q_k)}_{= a_{ki}} / \lambda_k = q_k$$

That is, the eigenvector $q_k = \sum_{i=1}^n a_{ki} \phi(x_i)$ for some vector $\mathbf{a}_k \in \mathbb{R}^n$.

The trick is that instead of learning q_k , we'll learn \mathbf{a}_k . Plug the above equation for q_k back into the equation on the previous slide:

$$\sum_{i=1}^n \phi(x_i) \sum_{j=1}^n a_{kj} \underbrace{\phi(x_i)^T \phi(x_j)}_{= K(x_i, x_j)} = \lambda_k \sum_{i=1}^n a_{ki} \phi(x_i)$$

Let's try to write this in matrix-vector form. . .

KERNEL PCA

Let $\Phi = [\phi(x_1), \dots, \phi(x_n)]$. Then the previous equation:

$$\sum_{i=1}^n \phi(x_i) \sum_{j=1}^n a_{kj} \underbrace{\phi(x_i)^T \phi(x_j)}_{= K(x_i, x_j)} = \lambda_k \sum_{i=1}^n a_{ki} \phi(x_i)$$

is equal to $\Phi K \mathbf{a}_k = \lambda_k \Phi \mathbf{a}_k$, where K is the $n \times n$ kernel matrix of the data.

Assuming ϕ is a high-dimensional, we often can (and will) assume that

$$\Phi K \mathbf{a}_k = \lambda_k \Phi \mathbf{a}_k \quad \Longleftrightarrow \quad K \mathbf{a}_k = \lambda_k \mathbf{a}_k$$

We now perform “regular” PCA, but on the kernel matrix K instead of the data matrix XX^T . We summarize the algorithm on the following slide.

KERNEL PCA ALGORITHM

Kernel PCA

Given: Data $x_1, \dots, x_n, x \in \mathbb{R}^d$, and a kernel function $K(x_i, x_j)$.

Construct: The kernel matrix on the data, e.g., $K_{ij} = b \exp \left\{ -\frac{\|x_i - x_j\|^2}{c} \right\}$.

Solve: The eigendecomposition

$$K\mathbf{a}_k = \lambda_k \mathbf{a}_k$$

for the first $r \ll n$ eigenvector/eigenvalue pairs $(\lambda_1, \mathbf{a}_1), \dots, (\lambda_r, \mathbf{a}_r)$.

Output: A new coordinate system for x_i by (implicitly) mapping $\phi(x_i)$ and then projecting $q_k^T \phi(x_i)$

$$x_i \xrightarrow{\text{projection}} \begin{bmatrix} \lambda_1 a_{1i} \\ \vdots \\ \lambda_r a_{ri} \end{bmatrix}$$

where a_{ki} is the i th dimension of the k th eigenvector \mathbf{a}_k .

KERNEL PCA AND NEW DATA

Q: How do we handle new data, x_0 ? Before, we projected $x_0^T q_k$, but $\mathbf{a}_k \neq q_k$.

A: Recall the relationship of \mathbf{a}_k to q_k in kernel PCA is

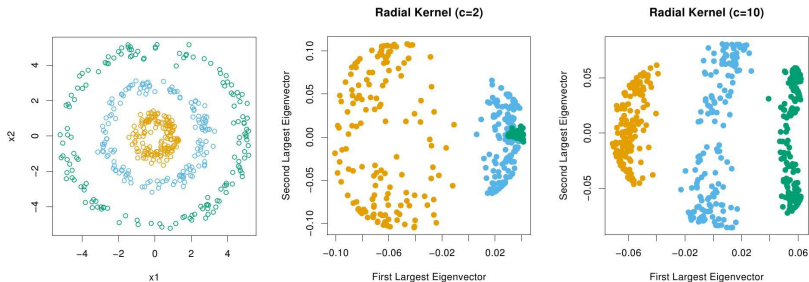
$$q_k = \sum_{i=1}^n a_{ki} \phi(x_i).$$

We used the “kernel trick” to avoid working with or even defining $\phi(x_i)$. As with regular PCA, after mapping x_0 we want to project onto eigenvectors

$$x_0 \xrightarrow{\text{projection}} \begin{bmatrix} \phi(x_0)^T q_1 \\ \vdots \\ \phi(x_0)^T q_r \end{bmatrix}$$

Plugging in for q_k gives $\phi(x_0)^T q_k = \sum_{i=1}^n a_{ki} \phi(x_0)^T \phi(x_i) = \sum_{i=1}^n a_{ki} K(x_0, x_i)$.

EXAMPLE RESULTS



An example of kernel PCA using the Gaussian kernel.

(left) Original data, colored for reference (but could be class labels)

(middle) New coordinates using kernel width $c = 2$

(right) New coordinates using kernel width $c = 10$

Terminology: What we are doing is closely related to “spectral clustering” and can be considered an instance of “manifold learning.”