18.650 – Fundamentals of Statistics

8. Principal Component Analysis (PCA)

Multivariate statistics

- Let $\mathbf{X}$ be a d-dimensional random vector and $\mathbf{X}_1, \ldots, \mathbf{X}_n$ be n independent copies of $\mathbf{X}$.

- Write $\mathbf{X}_i = (X_i^{(1)}, \ldots, X_i^{(d)})^\top, \quad i = 1, \ldots, n.$
- Denote by $\mathbb{X}$ the random $n \times d$ matrix

$$\begin{array}{cc} & \text{d: features} \\ \text{n: samples} & \mathbb{X} = \begin{pmatrix} \cdots & \mathbf{X}_1^\top & \cdots \\ & \vdots & \\ \cdots & \mathbf{X}_n^\top & \cdots \end{pmatrix}. \end{array}$$

Multivariate statistics

- Assume that $\mathbb{E}[\|\mathbf{X}\|_2^2] < \infty$.
- Mean of $\mathbf{X}$:

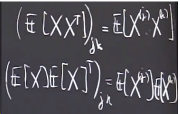
$$\mathbb{E}[\mathbf{X}] = \left(\mathbb{E}[X^{(1)}], \ldots, \mathbb{E}[X^{(d)}]\right)^\top.$$

- Covariance matrix of $\mathbf{X}$: the matrix $\Sigma = (\sigma_{j,k})_{j,k=1,\ldots,d}$, where

$$\sigma_{j,k} = \mathrm{cov}(\mathbf{X}^{(j)}, \mathbf{X}^{(k)}).$$

- It is easy to see that

$$\Sigma = \mathbb{E}[\mathbf{X}\mathbf{X}^\top] - \mathbb{E}[\mathbf{X}]\mathbb{E}[\mathbf{X}]^\top = \mathbb{E}\Big[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top\Big].$$



Multivariate statistics

- Empirical mean of $\mathbf{X}_1, \ldots, \mathbf{X}_n$:

$$\bar{\mathbf{X}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i = \left(\bar{X}^{(1)}, \ldots, \bar{X}^{(d)} \right)^\top .$$

- Empirical covariance of $\mathbf{X}_1, \ldots, \mathbf{X}_n$: the matrix $S = (s_{j,k})_{j,k=1,\ldots,d}$ where $s_{j,k}$ is the empirical covariance of the $X_i^{(j)}$, $X_i^{(h)}$, $i = 1 \ldots, n$.

- It is easy to see that

$$S = \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i^\top - \bar{\mathbf{X}} \bar{\mathbf{X}}^\top = \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{X}_i - \bar{\mathbf{X}} \right) \left(\mathbf{X}_i - \bar{\mathbf{X}} \right)^\top .$$

Multivariate statistics

- Note that $\bar{\mathbf{X}} = \dfrac{1}{n}\mathbb{X}^\top \mathbb{1}$, where $\mathbb{1} = (1, \dots, 1)^\top \in \mathbb{R}^d$.

- Note also that

$$S = \frac{1}{n}\mathbb{X}^\top \mathbb{X} - \frac{1}{n^2}\mathbb{X}\mathbb{1}\mathbb{1}^\top \mathbb{X} = \frac{1}{n}\mathbb{X}^\top H \mathbb{X},$$

  where $H = I_n - \frac{1}{n}\mathbb{1}\mathbb{1}^\top$.

- H is an orthogonal projector: $H^2 = H, H^\top = H$. *(on what subspace ?)*

- If $\mathbf{u} \in \mathbb{R}^d$,
  - $\mathbf{u}^\top \Sigma \mathbf{u} = \text{var}(\mathbf{u}^\top \mathbf{X})$
  - $\mathbf{u}^\top S \mathbf{u}$ is the sample variance of $\mathbf{u}^\top \mathbf{X}_1, \dots, \mathbf{u}^\top \mathbf{X}_n$.

Multivariate statistics

- In particular, $\mathbf{u}^\top S\mathbf{u}$ measures how spread (i.e., diverse) the points are in direction $\mathbf{u}$.

- If $\mathbf{u}^\top S\mathbf{u} = 0$, then all $\mathbf{X}_i$' s are in an affine subspace orthogonal to $\mathbf{u}$.

- If $\mathbf{u}^\top \Sigma\mathbf{u} = 0$, then $\mathbf{X}$ is almost surely in an affine subspace orthogonal to $\mathbf{u}$.

- If $\mathbf{u}^\top S\mathbf{u}$ is large with $\|\mathbf{u}\|_2 = 1$, then the direction of $\mathbf{u}$ explains well the spread (i.e., diversity) of the sample.

Review of linear algebra

- In particular, Σ and S are symmetric, positive semi-definite.

- Any real symmetric matrix $A \in \mathbb{R}^{d \times d}$ has the spectral decomposition
$$A = PDP^\top,$$
where:
  - P is a $d \times d$ orthogonal matrix, i.e., $PP^\top = P^\top P = I_d$;
  - D is diagonal.

- The diagonal elements of D are the eigenvalues of A and the columns of P are the corresponding eigenvectors of A.

- A is semi-definite positive iff all its eigenvalues are nonnegative.

Principal Component Analysis

- The sample $\mathbf{X}_1, \ldots, \mathbf{X}_n$ makes a cloud of points in $\mathbb{R}^d$.
- In practice, d is large. If $d > 3$, it becomes impossible to represent the cloud on a picture.
- **Question:** Is it possible to project the cloud onto a linear subspace of dimension $d' < d$ by keeping as much information as possible ?
- **Answer:** PCA does this by keeping as much covariance structure as possible by keeping orthogonal directions that discriminate well the points of the cloud.

Variances

- Idea: Write $S = PDP^\top$, where
  - $P = (\mathbf{v}_1, \ldots, \mathbf{v}_d)$ is an orthogonal matrix, i.e., $\|\mathbf{v}_j\|_2 = 1, \mathbf{v}_j^\top \mathbf{v}_k = 0, \forall j \neq k$.
  - $$D = \mathrm{diag}(\lambda_1, \ldots, \lambda_d) = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & \mathbf{0} & \\ & & \ddots & & \\ & \mathbf{0} & & \ddots & \\ & & & & \lambda_d \end{pmatrix}$$

    with $\lambda_1 \geq \ldots \geq \lambda_d \geq 0$.
- Note that D is the empirical covariance matrix of the $P^\top \mathbf{X}_i$'s, $i = 1, \ldots, n$.
- In particular, λ_1 is the empirical variance of the $\mathbf{v}_1^\top \mathbf{X}_i$'s; λ_2 is the empirical variance of the $\mathbf{v}_2^\top \mathbf{X}_i$'s, etc...

Projection

- So, each λ_j measures the spread of the cloud in the direction $\mathbf{v}_j$.
- In particular, $\mathbf{v}_1$ is the direction of maximal spread.
- Indeed, $\mathbf{v}_1$ maximizes the empirical covariance of $\mathbf{a}^\top \mathbf{X}_1, \ldots, \mathbf{a}^\top \mathbf{X}_n$ over $\mathbf{a} \in \mathbb{R}^d$ such that $\|\mathbf{a}\|_2 = 1$.
- *Proof:* For any unit vector $\mathbf{a}$, show that

  $$\mathbf{a}^\top \Sigma \mathbf{a} = \left(P^\top \mathbf{a}\right)^\top D \left(P^\top \mathbf{a}\right) \le \lambda_1,$$

  with equality if $\mathbf{a} = \mathbf{v}_1$.

Principal Component Analysis: Main principle

- Idea of the PCA: Find the collection of orthogonal directions in which the cloud is much spread out.

Theorem

$$
\begin{aligned}
\mathbf{v}_1 &\in \underset{\|\mathbf{u}\|=1}{\operatorname{argmax}} \ \mathbf{u}^\top S \mathbf{u}, \\
\mathbf{v}_2 &\in \underset{\|\mathbf{u}\|=1, \mathbf{u}\perp\mathbf{v}_1}{\operatorname{argmax}} \ \mathbf{u}^\top S \mathbf{u}, \\
&\cdots \\
\mathbf{v}_d &\in \underset{\|\mathbf{u}\|=1, \mathbf{u}\perp\mathbf{v}_j, j=1,\ldots,d-1}{\operatorname{argmax}} \ \mathbf{u}^\top S \mathbf{u}.
\end{aligned}
$$

Hence, the k orthogonal directions in which the cloud is the most spread out correspond exactly to the eigenvectors associated with the k largest values of S. They are called **principal directions**

Principal Component Analysis: Algorithm

1. Input: $\mathbf{X}_1, \ldots, \mathbf{X}_n$: cloud of n points in dimension d.

2. Step 1: Compute the empirical covariance matrix.

3. Step 2: Compute the spectral decomposition $S = PDP^\top$, where $D = \text{diag}(\lambda_1, \ldots, \lambda_d)$, with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$ and $P = (\mathbf{v}_1, \ldots, \mathbf{v}_d)$ is an orthogonal matrix.

4. Step 3: Choose $k < d$ and set $P_k = (\mathbf{v}_1, \ldots, \mathbf{v}_k) \in \mathbb{R}^{d \times k}$.

5. Output: $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$, where

$$\mathbf{Y}_i = P_k^\top \mathbf{X}_i \in \mathbb{R}^k, \quad i = 1, \ldots, n.$$

Question: How to choose k ?

How to choose the number of principal components k?

- Experimental rule: Take k where there is an inflection point in the sequence $\lambda_1, \ldots, \lambda_d$ (scree plot).

- Define a criterion: Take k such that

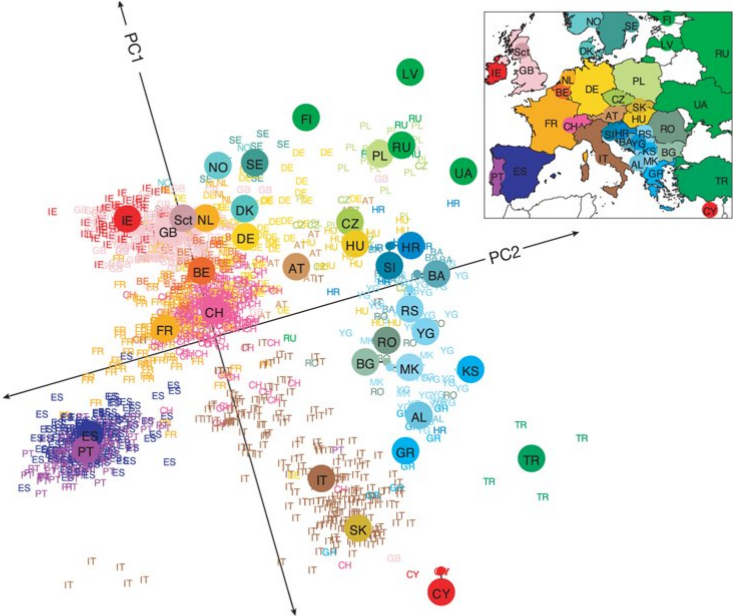
$$\text{proportion of explained variance} = \frac{\lambda_1 + \ldots + \lambda_k}{\lambda_1 + \ldots + \lambda_d} \geq 1 - \alpha,$$

  for some $\alpha \in (0, 1)$ that determines the approximation error that the practitioner wants to achieve.

- Remark: $\lambda_1 + \ldots + \lambda_k$ is called *the variance explained by the PCA* and $\lambda_1 + \ldots + \lambda_d = \mathrm{tr}(S)$ is *the total variance*.

- Data visualization: Take $k = 2$ or 3.

Example: Expression of 500,000 genes among 1400 Europeans



Principal Component Analysis - Beyond practice

- PCA is an algorithm that reduces the dimension of a cloud of points and keeps its covariance structure as much as possible.

- In practice this algorithm is used for clouds of points that are not necessarily random.

- In statistics, PCA can be used for estimation.

- If $\mathbf{X}_1, \ldots, \mathbf{X}_n$ are i.i.d. random vectors in $\mathbb{R}^d$, how to estimate their population covariance matrix Σ ?

- If $n \gg d$, then the empirical covariance matrix S is a consistent estimator.

- In many applications, $n \ll d$ (e.g., gene expression). Solution: sparse PCA

Principal Component Analysis - Beyond practice

- It may be known beforehand that Σ has (almost) low rank.
- Then, run PCA on S: Write $S \approx S'$, where

$$S' = P \begin{pmatrix} \lambda_1 & & & & & & \\ & \lambda_2 & & & \text{\Huge 0} & & \\ & & \ddots & & & & \\ & & & \lambda_k & & & \\ & & & & 0 & & \\ & \text{\Huge 0} & & & & \ddots & \\ & & & & & & 0 \end{pmatrix} P^\top.$$

- S' will be a better estimator of S under the low-rank assumption.
- A theoretical analysis would lead to an optimal choice of the tuning parameter k.