Carnegie Mellon

18-660: Numerical Methods for Engineering Design and Optimization

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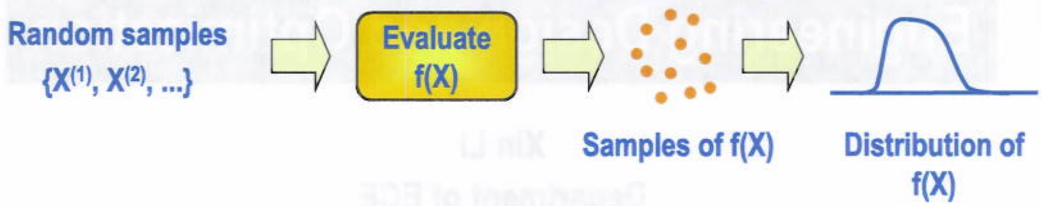
Overview

- Principal Component Analysis (PCA)
  - Correlation decomposition
  - Dimension reduction

Monte Carlo Analysis

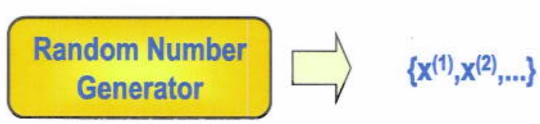
- **Monte Carlo analysis for f(X)**
  - Randomly select M samples for X
  - Evaluate function f(X) at each sampling point
  - Estimate distribution of f using these M samples



We assume that random samples can be easily created from a random number generator

Monte Carlo Analysis

- **A random number generator creates a pseudo-random sequence for which the period is extremely large**
  - MATLAB function "randn(•)": period is ~2^{64}
  - MATLAB function "rand(•)": period is ~2^{1492}



- **All samples in $\{x^{(1)},x^{(2)},\ldots\}$ are "almost" independent**

Monte Carlo Analysis

- **Example: sample independent random variables x and y**

Random Number Generator ⇒ $\{x^{(1)},y^{(1)},x^{(2)},y^{(2)},\ldots\}$

  - Generate random sequence $\{x^{(1)},y^{(1)},x^{(2)},y^{(2)},\ldots\}$
  - Create sampling pair $\{(x^{(1)},y^{(1)}),(x^{(2)},y^{(2)}),\ldots\}$
  - $x^{(i)}$ and $y^{(i)}$ in each pair are independent

However, how can we sample correlated random variables?

Monte Carlo Analysis

- **Correlated random variables cannot be directly sampled by a random number generator**

- **We can decompose correlated random variables to a set of independent variables, if they are jointly Normal**
  - Focus of this lecture

- **Other techniques also exist to sample correlated variables**
  - Details can be found in many text books on Monte Carlo analysis

Fishman, A First Course In Monte Carlo, 2006

Correlation Decomposition

- **Key idea: given the correlated random variables $\{x_1, x_2, \ldots\}$, find a linear transform $Y = P \cdot X$ such that $\{y_1, y_2, \ldots\}$ are independent**
  - Only applicable to jointly Normal random variables for which $\{y_1, y_2, \ldots\}$ just need to be uncorrelated
  - Otherwise, if the random variables are not jointly Normal, such a linear transform may not exist

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \underbrace{\begin{bmatrix} \square & \square & \square \\ \square & \square & \square \\ \square & \square & \square \end{bmatrix}}_{\mathbf{P}} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Principal Component Analysis (PCA)

- **Given a set of jointly Normal random variables**

$$X = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$$

  - Assume that all x_i's have zero mean

- **Covariance matrix is**

$$E\left[X \cdot X^T\right] = E\begin{bmatrix} x_1^2 & x_1 x_2 & x_1 x_3 \\ x_1 x_2 & x_2^2 & x_2 x_3 \\ x_1 x_3 & x_2 x_3 & x_3^2 \end{bmatrix}$$

The covariance matrix has many important properties, e.g., it is symmetric

Principal Component Analysis (PCA)

- **Covariance matrix is positive semi-definite**
- **A symmetric matrix A is called positive semi-definite if**

$$Q^T A Q \geq 0 \quad \text{for any real-valued vector Q}$$

Why is a covariance matrix positive semi-definite?

Principal Component Analysis (PCA)

- **Assume that X = $[x_1\ x_2 \ldots x_N]^T$ are N random variables with zero mean**

$\underbrace{y}_{\text{scalar}} = Q^T \underbrace{x}_{\text{vector}}$

$Q = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \end{bmatrix}$

$E[y^2] = E[(Q^T x)^2] = E[(Q^T x)^T \cdot (Q^T x)]$

$= x^T Q$

$E[Q^T x \cdot x^T Q]$

$= Q^T \cdot \underbrace{E[x x^T]}_{Cov(x,x)} \cdot Q \geq 0$

Principal Component Analysis (PCA)

- **To remove correlation, we decompose the covariance matrix by eigenvalues & eigenvectors**

$$\underline{A} = E\left[X \cdot X^T\right]$$

$$A v_i = v_i \lambda_i$$

v_i: eigenvector $\quad$ λ_i: eigenvalue

$$A\,[v_1 \; v_2 \cdots] = [A v_1 \; A v_2 \cdots] = [v_1 \lambda_1 \; v_2 \lambda_2 \cdots]$$

$$= \underbrace{[v_1 \; v_2 \cdots]}_{V} \underbrace{\begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{bmatrix}}_{\Sigma}$$

$$AV = V\Sigma$$

Principal Component Analysis (PCA)

- **The eigen-decomposition of a covariance matrix A has a number of important properties**
  - A is symmetric $\rightarrow$ all eigenvalues are real
  - A is symmetric $\rightarrow$ all eigenvectors are real and orthogonal

V: orthogonal matrix

$$A \cdot V = V \cdot \Sigma \quad \Longrightarrow \quad \boxed{V^T V = I}$$

Identity matrix

Principal Component Analysis (PCA)

- **The eigen-decomposition of a covariance matrix A has a number of important properties**
  - A is positive semi-definite ↔ all eigenvalues are non-negative

$$A \cdot V = V \cdot \Sigma \qquad V^T V = I$$

$V^{-1} = V^T$

$A V V^{-1} = V \Sigma V^{-1}$

$V = [V_1\ V_2 \ldots]$

$A = V \Sigma V^T$

$\Sigma = [\lambda_1\ \lambda_2 \ldots]$

Principal Component Analysis (PCA)

- **Define new random variables Y (principal components)**

$$Y = \Sigma^{-0.5} \cdot V^T \cdot X$$
$$X = V \cdot \Sigma^{0.5} \cdot Y$$

$P = \Sigma^{-0.5} V^T$

$x = P^{-1} \cdot Y$

- **All principal components (also called principal factors) are jointly Normal**
  - They are linear combination of jointly Normal random variables

- **We will theoretically prove that all principal components are independent and standard Normal**

Principal Component Analysis (PCA)

- **All principal components have zero mean**

$$Y = \Sigma^{-0.5} \cdot V^T \cdot X$$

$$E[Y] = E[\Sigma^{-0.5} V^T X]$$

$$= \Sigma^{-0.5} V^T \underbrace{E[X]}_{=0}$$

Principal Component Analysis (PCA)

- **All principal components are independent and standard Normal**

$$Y = \Sigma^{-0.5} \cdot V^T \cdot X$$

$$E[YY^T] = E[\Sigma^{-0.5} V^T X X^T \cdot V \cdot \Sigma^{-0.5}]$$

$$(Y)^T = (\Sigma^{-0.5} V^T X)^T$$

$$= X^T V \cdot \Sigma^{-0.5}$$

$$= \Sigma^{-0.5} \cdot V^T \cdot \underbrace{E[XX^T]}_{A} \cdot V \cdot \Sigma^{-0.5}$$

Principal Component Analysis (PCA)

$$E\left[Y\cdot Y^T\right]=\Sigma^{-0.5}\cdot V^T\cdot E\left[X\cdot X^T\right]\cdot V\cdot\Sigma^{-0.5}$$

$A = V\cdot\Sigma V^T$

$$E[Y\cdot Y^T] = \Sigma^{-0.5}\cdot \underbrace{V^T\cdot V}_{I}\cdot\Sigma\cdot \underbrace{V^T V}_{I}\cdot\Sigma^{-0.5}$$

$$= \Sigma^{-0.5}\cdot\Sigma\cdot\Sigma^{-0.5}$$

$= I$ unit variance uncorrelate

"Uncorrelated" = "independent" for jointly Normal random variables

Principal Component Analysis (PCA)

- Example: x_1 and x_2 are zero mean and jointly Normal

$X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$$E\left[X\cdot X^T\right]=\begin{bmatrix}5 & 4\\ 4 & 5\end{bmatrix}$$

Eigen decomposition

$$\Sigma=\begin{bmatrix}1 & 0\\ 0 & 9\end{bmatrix}\quad and\quad V=\begin{bmatrix}-1/\sqrt{2} & 1/\sqrt{2}\\ 1/\sqrt{2} & 1/\sqrt{2}\end{bmatrix}$$

$\Sigma = \begin{bmatrix}\lambda_1 & \\ & \lambda_2\end{bmatrix}$

$\Sigma^{-0.5} = \begin{bmatrix}\lambda_1^{-0.5} & \\ & \lambda_2\end{bmatrix}$

Principal Component Analysis (PCA)

- **Example (continued):**

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix} \quad and \quad V = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$$Y = \Sigma^{-0.5} \cdot V^T \cdot X = \begin{bmatrix} 1 & 0 \\ 0 & 1/3 \end{bmatrix} \cdot \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \cdot X$$

$$\Sigma = \begin{bmatrix} \lambda_1 & \\ & \lambda_2 \end{bmatrix}$$

$$\Sigma^{-0.5} = \begin{bmatrix} \lambda_1^{-0.5} & \\ & \lambda_2^{-0.5} \end{bmatrix}$$

$$Y = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \end{bmatrix} \cdot X$$

Principal Component Analysis (PCA)

- **Example (continued):**

$$Y = \underbrace{\begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \end{bmatrix}}_{P} \cdot X$$

$$E\left[Y \cdot Y^T\right] = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \end{bmatrix} \cdot E\left[X \cdot X^T\right] \cdot \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \end{bmatrix}^T$$

Principal Component Analysis (PCA)

- **Example (continued):**

$$E\left[Y\cdot Y^T\right]=\begin{bmatrix}-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}}\end{bmatrix}\cdot E\left[X\cdot X^T\right]\cdot\begin{bmatrix}-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}}\end{bmatrix}^T \qquad E\left[X\cdot X^T\right]=\begin{bmatrix}5 & 4\\ 4 & 5\end{bmatrix}$$

$$E\left[Y\cdot Y^T\right]=\begin{bmatrix}-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}}\end{bmatrix}\cdot\begin{bmatrix}5 & 4\\ 4 & 5\end{bmatrix}\cdot\begin{bmatrix}-\frac{1}{\sqrt{2}} & \frac{1}{3\sqrt{2}}\\ \frac{1}{\sqrt{2}} & \frac{1}{3\sqrt{2}}\end{bmatrix}=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

All principal components in Y are independent and standard Normal

Principal Component Analysis (PCA)

- **The decomposition for independence is not unique**
  - Define

$$Z=U\cdot Y$$

U is an orthogonal matrix, i.e., $U^TU = I$

$Y = \Phi X$

$E[ZZ^T] = E[U\cdot Y\cdot (UY)^T] = E[UYY^TU^T]$

$= U\cdot \underbrace{E[YY^T]}_{I}\, U^T = U\cdot U^T = I$

All random variables in Z are also independent and standard Normal

Dimension Reduction by PCA

- **Example: x_1, x_2 and x_3 are zero mean and jointly Normal**

$$E\left[X \cdot X^T\right] = \begin{bmatrix} 5 & 4 & 3 \\ 4 & 5 & 3 \\ 3 & 3 & 2 \end{bmatrix}$$

Eigen decomposition

$$\Sigma = \begin{bmatrix} 11 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad and \quad V = \begin{bmatrix} 0.6396 & 0.7071 & 0.3015 \\ 0.6396 & -0.7071 & 0.3015 \\ 0.4264 & 0 & -0.9045 \end{bmatrix}$$

One of the eigenvalues is 0

Dimension Reduction by PCA

- **Example (continued):**
  - In this case, the 3x3 covariance matrix has a rank of 2
  - Only 2 independent principal components (Y) are required to EXACTLY represent the 3-dimensional random space

$$X = V \cdot \Sigma^{0.5} \cdot Y = \begin{bmatrix} 0.6396 & 0.7071 & 0.3015 \\ 0.6396 & -0.7071 & 0.3015 \\ 0.4264 & 0 & -0.9045 \end{bmatrix} \cdot \begin{bmatrix} \sqrt{11} & 0 & 0 \\ 0 & \sqrt{1} & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot Y$$

$$X = \begin{bmatrix} 2.1213 & 0.7071 & 0 \\ 2.1213 & -0.7071 & 0 \\ 1.4142 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

Only y_1 and y_2 are required

y_3 does not affect X

Dimension Reduction by PCA

- **In general, if some of the eigenvalues are small, they can be ignored to reduce the random space dimension**
  - Allows us to use a compact set of independent principal components to approximate the original high-dimensional space
  - E.g., only two random variables y_1 and y_2 are required to represent the variations of x_1, x_2 and x_3 in the previous example

- **PCA is useful to reduce problem size in many applications**
  - But applicable to jointly Normal variables only

Summary

- **Principal component analysis (PCA)**
  - Correlation decomposition
  - Dimension reduction