Carnegie Mellon

18-660: Numerical Methods for Engineering Design and Optimization

Xin Li
Department of ECE
Carnegie Mellon University
Pittsburgh, PA 15213

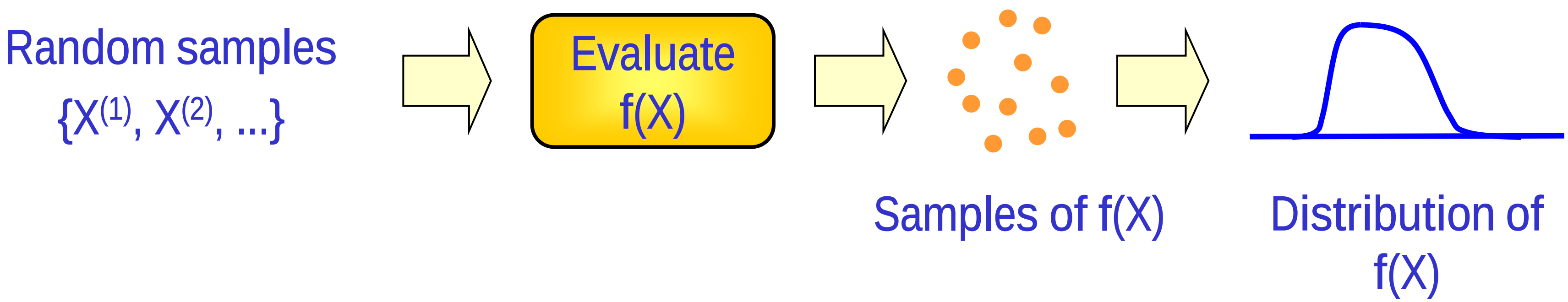
Electrical & Computer ENGINEERING

Overview

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

Monte Carlo Analysis

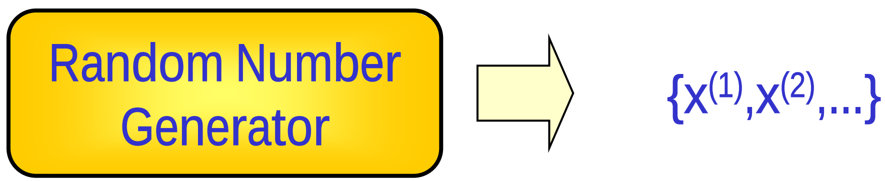
- Monte Carlo analysis for f(X)
  - Randomly select M samples for X
  - Evaluate function f(X) at each sampling point
  - Estimate distribution of f using these M samples



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

Monte Carlo Analysis

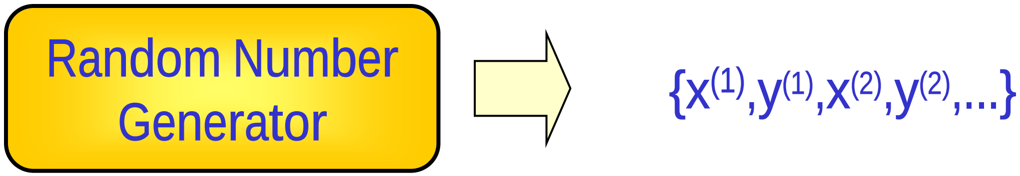
- A random number generator creates a pseudo-random sequence for which the period is extremely large
  - MATLAB function "randn(•)": period is ~2^{64}
  - MATLAB function "rand(•)": period is ~2^{1492}



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

Monte Carlo Analysis

- Example: sample independent random variables x and y



  - Generate random sequence $\{x^{(1)},y^{(1)},x^{(2)},y^{(2)},...\}$
  - Create sampling pair $\{(x^{(1)},y^{(1)}),(x^{(2)},y^{(2)}),...\}$
  - $x^{(i)}$ 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

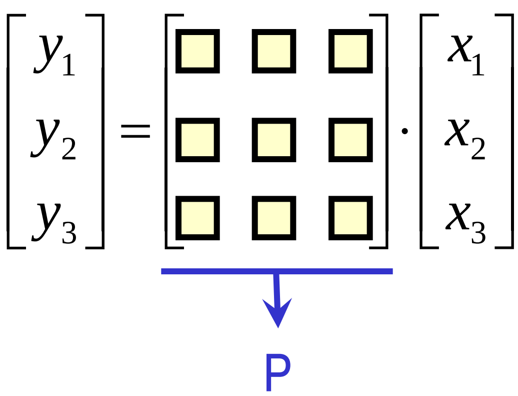
- We can decompose correlated random variables to a set of independent variables, if they are jointly Normal
  - Focus of this lecture

- 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



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

$$E\left[X \cdot X^T\right] = E\begin{bmatrix} x_1^2 & x_1x_2 & x_1x_3 \\ x_1x_2 & x_2^2 & x_2x_3 \\ x_1x_3 & x_2x_3 & x_3^2 \end{bmatrix}$$

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 $X = [x_1\ x_2\ \dots\ x_N]^T$ are N random variables with zero mean

$$y = Q^T X$$

scalar (y) — any real-value vector (Q)

$$E\left[y^2\right] = E\left[\left(Q^T X\right)\cdot\left(X^T Q\right)\right] = Q^T \cdot E\left[XX^T\right]\cdot Q \geq 0$$

$\left(Q^T X\right)$ → y $\left(X^T Q\right)$ → $y^T = y$

Principal Component Analysis (PCA)

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

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

$$AV_i = V_i \cdot \lambda_i$$

$$A \cdot V = V \cdot \Sigma$$

$$V = \begin{bmatrix} V_1 & V_2 & \cdots \end{bmatrix}$$

"Normalized" eigenvectors: $||V_i||_2 = 1$

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

Eigenvalues

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

$$A \cdot V = V \cdot \Sigma \quad \Rightarrow \quad V^T V = I$$

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

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

⇓

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

⇓

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

⇓

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

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

Eigenvalues

Principal Component Analysis (PCA)

- Define new random variables Y (principal components)

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

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

- 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

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

$$\Downarrow$$

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

$$\Downarrow \quad E[X] = 0$$

All random variables in X have zero mean

$$E[Y] = 0$$

Principal Component Analysis (PCA)

- All principal components are independent and standard Normal

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

$$\Downarrow$$

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

$$\Downarrow$$

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

Principal Component Analysis (PCA)

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

$$E\left[X \cdot X^T\right] = V \cdot \Sigma \cdot V^T$$

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

$$V^T V = I$$

$$E\left[Y \cdot Y^T\right] = \Sigma^{-0.5} \cdot \Sigma \cdot \Sigma^{-0.5} = I$$ Unit variance and uncorrelated

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

Principal Component Analysis (PCA)

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

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

Eigen decomposition

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

Principal Component Analysis (PCA)

- Example (continued):

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

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

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

Principal Component Analysis (PCA)

- Example (continued):

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

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

Principal Component Analysis (PCA)

- Example (continued):

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

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

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

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., $U^T U = I$

$$E\left[Z \cdot Z^T\right] = E\left[U \cdot Y \cdot Y^T \cdot U^T\right] = U \cdot E\left[Y \cdot Y^T\right] \cdot U^T = U \cdot U^T = I$$

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