BIOS 835: Basic Matrix Algebra, Random Vectors, and the Covariance Matrix

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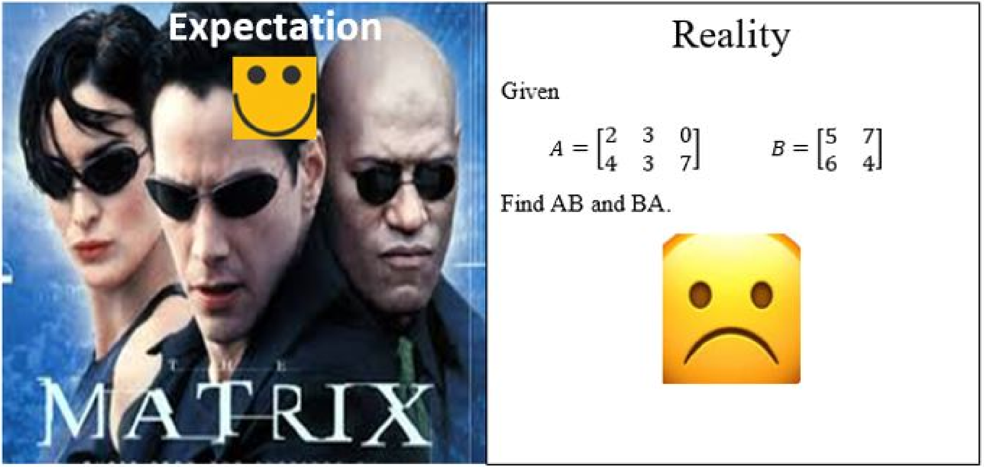
Outline

1. Basic Matrix Algebra
2. Random Vectors
3. Covariance Matrices

What is the Matrix?



Why linear algebra?

- Linear algebra is a branch of mathematics concerning:
  - linear equations,
  - linear functions, and
  - and their representations in vector spaces and through matrices
- Linear algebra is fundamental to many algorithms and concepts in machine learning; for example,
  - **Data Representation:** Datasets in machine learning are often represented as matrices.
  - **Transformations and Dimensionality Reduction:** Techniques like Principal Component Analysis (PCA) and Singular Value Decomposition (SVD) use linear algebra to project data into lower-dimensional spaces.

Why linear algebra?

- **Eigenvalues and Eigenvectors:** These are used in clustering, PCA, and in many optimization algorithms.
- **Distance and Similarity Computations:** Computing the distance between vectors or matrices is fundamental for many areas of ML.
- **Linear Regression:** Linear algebra is fundamental.
- **Regularization:** Techniques like L1 (Lasso) and L2 (Ridge) regularization in regression analysis can be described and implemented using linear algebra.
- **Support Vector Machines (SVMs):** utilize dot products, particularly with the kernel trick.
- **Neural Networks and Deep Learning:** Neural network operations involve matrix multiplications, activations, and transformations.

Introduction

- Some helpful resources:
  - Check out the **Matrix Algebra Tutorial** here,
  - A free text *"Linear Algebra"* is available here.
- Let $\boldsymbol{A}$ be a $m \times n$ matrix.
- Let a_{ij} be the element in row i column j

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}$$

  here $\boldsymbol{A}$ is a 2×3 matrix.
- Some special cases:
  - a Vector: $m \times 1$ or $1 \times n$:
  - a square matrix when $m = n$ (we'll deal with these often).
  - an identity matrix $\boldsymbol{I}$.
- Transpose of $\boldsymbol{A}$, $\boldsymbol{A}'$.

Basic Matrix Operation

- Matrix addition and subtraction: $\boldsymbol{A} + \boldsymbol{B}$ and $\boldsymbol{A} - \boldsymbol{B}$
- General properties:
  - $a\boldsymbol{A} = \boldsymbol{A}a$ where a is a scalar.
  - $\boldsymbol{A} + \boldsymbol{B} = \boldsymbol{B} + \boldsymbol{A}$
  - $a(\boldsymbol{A} + \boldsymbol{B}) = a\boldsymbol{A} + a\boldsymbol{B}$
  - $a(\boldsymbol{A} + \boldsymbol{B})' = a\boldsymbol{A}' + a\boldsymbol{B}'$
- Matrix multiplication, $\boldsymbol{AB}$
- General properties:
  - $\boldsymbol{C}(\boldsymbol{A} + \boldsymbol{B}) = \boldsymbol{CA} + \boldsymbol{CB}$
  - $\boldsymbol{IA} = \boldsymbol{A}$
  - $\boldsymbol{A}'\boldsymbol{A}$ is a square matrix
  - $(\boldsymbol{AB})' = \boldsymbol{B}'\boldsymbol{A}'$

Linear Dependence

- The columns $c_1, \ldots, c_k$ of a matrix are linearly dependent if there exists a set of scalar values $\lambda_1, \ldots, \lambda_k$ (at least one is none zero) such that

$$\lambda_1 c_1 + \ldots + \lambda_k c_k = 0$$

- An example

$$\boldsymbol{A} = \begin{bmatrix} 1 & 1 & 1 \\ 3 & 1 & 5 \\ 2 & 3 & 1 \end{bmatrix}$$

- Linearly independent: if the only set of λ_j values to satisfy the above equation is a set of all zeros.

Rank

- The **rank** of a matrix is a fundamental concept in linear algebra, and it holds significant importance in various machine-learning contexts.
- **Definition:**
  - The rank of a matrix A is the maximum number of linearly independent row vectors (or equivalently, column vectors) in the matrix. It provides a measure of the "information content" of the matrix.
- Mathematically, if a matrix has a rank r, it means that:
  1. There are r linearly independent rows (or columns) in the matrix.
  2. Any other row (or column) can be represented as a linear combination of these r rows (or columns).
- If a matrix X is $n \times p$ with $p \gg n$, what is the maximum rank of X.

Determinant and Inverse Matrix

- The determinant of $\boldsymbol{A}$ is denoted by $det(\boldsymbol{A}) = |\boldsymbol{A}|$.
- The inverse of $\boldsymbol{A}$ is denoted by $\boldsymbol{A}^{-1}$.
- Example, let

$$\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

then

  - $|\boldsymbol{A}| = ad - bc$,
  - and

$$\boldsymbol{A}^{-1} = \frac{1}{|\boldsymbol{A}|} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

Determinant and Inverse Matrix

Some properties of the determinants and inverses:

- $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$ This is the main property of the inverse (check for the above $\boldsymbol{A}$).
- $|\boldsymbol{A}| = |\boldsymbol{A}'|$, and $|\boldsymbol{A}| = 1/|\boldsymbol{A}^{-1}|$
- $|\boldsymbol{A}\boldsymbol{B}| = |\boldsymbol{A}||\boldsymbol{B}|$
- $(\boldsymbol{A}\boldsymbol{B})^{-1} = \boldsymbol{B}^{-1}\boldsymbol{A}^{-1}$
- $(\boldsymbol{A}')^{-1} = (\boldsymbol{A}^{-1})'$

Some required properties for $\boldsymbol{A}$ to have an inverse are: $\boldsymbol{A}$ is linearly independent, square matrix, non-zero determinant, and full rank.

Positive Definite Matrix

- A matrix A is said to be symmetric positive definite if it meets the following criteria:
  1. **Symmetry:** The matrix A is symmetric, which means it is equal to its transpose, $A = A^T$
  2. **Positive Definiteness:** For any non-zero column vector x, the scalar $x^T Ax$ is positive.
- Some of the useful properties of these include:
  - All eigenvalues of a symmetric positive definite matrix are positive.
  - It is invertible, and its inverse is also symmetric positive definite.

Orthogonal and Orthonormal Matrices

- A square matrix $\boldsymbol{Q}$ is called orthogonal if its transpose is its inverse: $\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{Q}^T = I$ where I is the identity matrix of the same order as $\boldsymbol{Q}$.
- Properties of orthogonal matrices:
  - The columns (and rows) of an orthogonal matrix form an orthogonal set of vectors, meaning their dot product is zero
  - The determinant of an orthogonal matrix is either 1 or -1.
  - The inverse of an orthogonal matrix is also orthogonal.
- An orthonormal matrix is an orthogonal matrix, but one where each vector has a unit length (norm of 1).

Matrix Decompositions

LR Decomposition

- $\boldsymbol{A} = \boldsymbol{LR}$ with $\boldsymbol{L}-$lower-triangular and $\boldsymbol{R}-$upper-triangular

Cholesky Decomposition

- If $\boldsymbol{A}$ is symmetric positive definite $\boldsymbol{A} = \boldsymbol{LL}'$

QR Decomposition

- $\boldsymbol{A} = \boldsymbol{QR}$ where $\boldsymbol{Q}$ is an orthogonal matrix, i.e., $det(\boldsymbol{Q}) = 1$

Eigenvalues and Eigenvectors

- $\boldsymbol{A}$ is $J \times J$.
- A scalar λ is called an eigenvalue of $\boldsymbol{A}$ then there is a nontrivial solution $\boldsymbol{x}$ to $\boldsymbol{Ax} = \lambda\boldsymbol{x}$. Such an $\boldsymbol{x}$ is called an eigenvector corresponding to the eigenvalue λ.
  - Note that if $\boldsymbol{Ax} = \lambda\boldsymbol{x}$ then $(\boldsymbol{A} - \lambda\boldsymbol{I})\boldsymbol{x} = \boldsymbol{0}$
- If $\boldsymbol{A}$ is positive definite then $\boldsymbol{A}$ will have J eigenvalues where $\lambda_j > 0$ for all $j = 1, \ldots, J$.
  - and are usually ordered such that $\lambda_1 > \lambda_2 > \ldots > \lambda_J$
- Let $\boldsymbol{x}_j$ and $\boldsymbol{x}_k$ be eigenvectors from $\lambda_j \neq \lambda_k$ then
  - $\boldsymbol{x}_j$ and $\boldsymbol{x}_k$ are orthogonal, i.e. $\boldsymbol{x}_j'\boldsymbol{x}_k = \boldsymbol{0}$

Spectral theorm

- For a given real symmetric matrix A, there exists $\boldsymbol{AQ} = \boldsymbol{Q}\Lambda$ or

$$\boldsymbol{A} = \boldsymbol{Q}\Lambda\boldsymbol{Q}' = \sum_{j=1}^{J} \lambda_j \boldsymbol{q}_j \boldsymbol{q}_j',$$

  where
  - $\boldsymbol{Q}$ is a $J \times J$ matrix with $\boldsymbol{Q}'\boldsymbol{Q} = \boldsymbol{I}_J$, i.e., $\boldsymbol{Q}$ is orthogonal, and
  - $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_J)$ and $\lambda_1 > \lambda_2 > \ldots > \lambda_J$.
- $trace(\boldsymbol{A}) = \sum_j \lambda_j$
- $det(\boldsymbol{A}) = \prod_j \lambda_j$

Singular Value Decomposition

- Singular Value Decomposition (SVD) of a matrix A of size $m \times n$ is given by:

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

Where:

- U (of size $m \times m$) is the left singular vector matrix. Its columns are the eigenvectors of AA^T.
- Σ (of size $m \times n$) is a diagonal matrix. The elements on its diagonal are the singular values of A, and they are non-negative and usually sorted in descending order. These values are the square roots of the eigenvalues of $A^T A$ (or equivalently, AA^T).
- V^T (of size $n \times n$) is the right singular vector matrix. Its rows are the eigenvectors of $A^T A$.

Functions of matrices

- $\boldsymbol{A}$ is $J \times J$ and $\phi : \mathbb{R}^J \Rightarrow \mathbb{R}^J$ then

$$\phi(\boldsymbol{A}) = \sum_{j=1}^{J} \phi(\lambda_j)\boldsymbol{x}_j\boldsymbol{x}_j'$$

  where λ_j and $\boldsymbol{x}_j$ are normalized to have norm 1.
- Example, $\boldsymbol{A}^{1/2} = \sum_{j=1}^{J} \sqrt{\lambda_j}\boldsymbol{x}_j\boldsymbol{x}_j'$ or $\boldsymbol{A}^{-1} = \sum_{j=1}^{J} \frac{1}{\lambda_j}\boldsymbol{x}_j\boldsymbol{x}_j'$

Matrix Norms

- $\boldsymbol{A}$ is $J \times J$, how do we measure the size of $\boldsymbol{A}$?

Properties of a Norm $||\cdot||$

1. $||\boldsymbol{A}|| \geq 0$
2. $||\boldsymbol{A}|| = 0 \Leftrightarrow \boldsymbol{A} = \boldsymbol{0}$
3. $||\boldsymbol{A} + \boldsymbol{B}|| \leq ||\boldsymbol{A}|| + ||\boldsymbol{B}||$
4. $||\alpha\boldsymbol{A}|| = |\alpha|||\boldsymbol{A}||$

Examples of Matrix Norms

- Frobenius Norm: often referred to as the Euclidean norm for matrices, it is the square root of the sum of the absolute squares of its elements.

$$||A||_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2}$$

  where A is an $m \times n$ matrix.
- Lp Norm: for vectors (a special case of matrices), the Lp norm is defined as:

$$||v||_p = \left(\sum_i |v_i|^p \right)^{\frac{1}{p}}$$

- Max Norm: the maximum absolute row sum of the matrix. For vectors, it's the maximum absolute value of the elements.

Examples of Matrix Norms

- Spectral Norm: for a matrix A with singular value decomposition $A = U\Sigma V^T$, the spectral norm is the largest entry in Σ.
- Nuclear (or trace) Norm: the sum of the singular values of a matrix.
- Condition Number: (not actually a norm) is the ratio of its largest singular value to its smallest singular value.
  - gives an indication of the numerical stability of matrix inversion and the sensitivity of the system's solution to changes in the input.

Matrix Calculus

- $\boldsymbol{y}$: J-vector
- $\boldsymbol{x}$: K-vector
- Let $f(\boldsymbol{x}) = \boldsymbol{y}$ be a mapping (i.e., a function) from $\mathbb{R}^K \to \mathbb{R}^J$.
- The partial of $\boldsymbol{y}$ with respect to $\boldsymbol{x}$ is

$$J_x\boldsymbol{y} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{dy_1}{dx_1} & \cdots & \frac{dy_1}{dx_K} \\ \vdots & \ddots & \vdots \\ \frac{dy_J}{dx_1} & \cdots & \frac{dy_J}{dx_K} \end{pmatrix}_{J\times K}$$

which is call the Jacobian matrix

Matrix Calculus

- $\boldsymbol{y}$: 1-vector
- $\boldsymbol{x}$: K-vector
- Hessian Matrix of $\boldsymbol{y}$ with respect to $\boldsymbol{x}$ is

$$H_x y = \frac{\partial^2 \boldsymbol{y}}{\partial \boldsymbol{x}^2} = \begin{pmatrix} \frac{dy}{dx_1^2} & \cdots & \frac{dy_1}{dx_1 dx_K} \\ \vdots & \ddots & \vdots \\ \frac{dy}{dx_1 dx_K} & \cdots & \frac{dy}{dx_K^2} \end{pmatrix}_{K \times K}$$

Taylor series approximation

- $\boldsymbol{y}$: 1-vector
- $\boldsymbol{x}$: K-vector
- Let $f(\boldsymbol{x}) = \boldsymbol{y}$ be a mapping (i.e., a function) from $\mathbb{R}^K \to \mathbb{R}$.
- The Taylor series approximation of $f(\boldsymbol{x})$ at $\boldsymbol{c}$ is

$$f(\boldsymbol{x}) = f(\boldsymbol{c}) + [J_x f(\boldsymbol{c})](\boldsymbol{x} - \boldsymbol{c}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{c})^T [H_x f(\boldsymbol{c})](\boldsymbol{x} - \boldsymbol{c})$$

Random Vectors

Example: 10-week-old guinea pigs

- $\boldsymbol{X} = (X_1, X_2, X_3, X_4, X_5)$
  - X_1 - weight
  - X_2 - length
  - X_3 - cholesterol
  - X_4 - time on maze test
  - X_5 - Wheel distance

Multivariate Distributions

- $F_x(\boldsymbol{x}) = F_x(x_1, x_2, x_3, x_4, x_5) = \Pr(X_1 \leq x_1, X_2 \leq x_2, X_3 \leq x_3, X_4 \leq x_4, X_5 \leq x_5)$
- If $\boldsymbol{X}$ is all continuous

$$f_x(\boldsymbol{x}) = \frac{\partial^5 F_x(\boldsymbol{x})}{\partial x_1 \partial x_2 \cdots \partial x_5}$$

where

$$F_x(\boldsymbol{x}) = \int_{-\infty}^{x_1} \int_{-\infty}^{x_2} \cdots \int_{-\infty}^{x_5} f_x(\boldsymbol{x}) dx_1 dx_2 \cdots dx_5$$

- If $\boldsymbol{X}$ is all discrete

$$p_x(\boldsymbol{x}) = \Pr(X_1 = x_1, X_2 = x_2, \cdots X_5 = x_5)$$

Expectation and Variance

- In general $E(\boldsymbol{X}) = \boldsymbol{\mu}$.
- For each element of $\boldsymbol{X}$ we have

$$E(X_j) = \mu_j, \quad \text{var}(X_j) = E\{(X_j - \mu_j)^2\} = \sigma_j^2$$

- If we think of the elements of $\boldsymbol{X}$ together, we must consider the possible relationship among different elements of $\boldsymbol{X}$. This leads us to covariance.

Covariance Matix

- Covariance: a measure of how two random variables vary together.
- Mathematically we have,

$$\mathrm{cov}(X_j, X_k) = E\{(X_j - \mu_j)(X_k - \mu_k)\}$$

- The covariance matrix of a random vector is defined by $E\{(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})\}$

$$= \begin{pmatrix} E(X_1 - \mu_1)^2 & E(X_1 - \mu_1)(X_2 - \mu_2) & \dots & E(X_1 - \mu_1)(X_n - \mu_n) \\ E(X_2 - \mu_2)(X_1 - \mu_1) & E(X_2 - \mu_2)^2 & \dots & E(X_2 - \mu_2)(X_n - \mu_n) \\ \vdots & \vdots & \ddots & \vdots \\ E(X_n - \mu_n)(X_1 - \mu_1) & E(X_n - \mu_n)(X_2 - \mu_2) & \dots & E(X_n - \mu_n)^2 \end{pmatrix}$$

Covariance Matix

- Let $\text{cov}(X_j, X_k) = E(X_j - \mu_j)(X_k - \mu_k) = \sigma_{jk}$ with $\sigma_{jj} = \sigma_j^2$

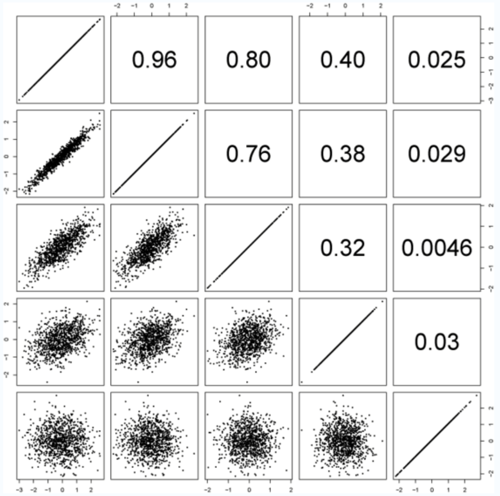
$$\boldsymbol{\Sigma} = E\{(\boldsymbol{Y} - \boldsymbol{\mu})(\boldsymbol{Y} - \boldsymbol{\mu})\} = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1n} \\ \sigma_{21} & \sigma_2^2 & \dots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \dots & \sigma_n^2 \end{pmatrix}$$

- The population correlation of two elements is

$$\rho_{jk} = \frac{\sigma_{jk}}{\sqrt{\sigma_j^2 \sigma_k^2}}$$

with corresponding correlation matrix.

Correlation Matix Example



Multivariate Normal Distribution

- If a random vector $\boldsymbol{X}$ has a multivariate normal distribution we write this as $\boldsymbol{X} \sim MVN_n(\boldsymbol{\mu}, \Sigma)$ or $\boldsymbol{X} \sim N(\boldsymbol{\mu}, \Sigma)$ where $\boldsymbol{\mu}$ is the mean and Σ is the covariance.
- The density can be written as

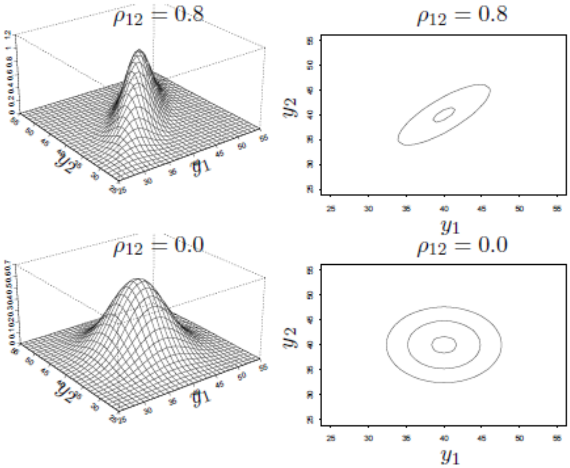
$$f(\boldsymbol{X}) = \frac{|\Sigma|^{-1/2}}{(2\pi)^{n/2}} \exp\left\{-(\boldsymbol{X}-\boldsymbol{\mu})'\Sigma^{-1}(\boldsymbol{X}-\boldsymbol{\mu})/2\right\}$$

- A simple case is the bivariate normal (where n=2)

$$\boldsymbol{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}, \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}.$$

and Σ^{-1} can be found using the equation for the inverse given above.

Multivariate Normal Distribution



Random Matricies

- Let $\boldsymbol{X} \sim MVN_r(\mathbf{0}, \Sigma)$
- We have data $\boldsymbol{X}_i$ for $i = 1, \ldots, n$ where $\boldsymbol{X}_i$ is an r-vector.
- Let

$$W = n\hat{\Sigma} = \sum_{i=1}^{n} \boldsymbol{X}_i \boldsymbol{X}_i^T$$

- Then W has a central Wishart distribution with n degrees of freedom and associated matrix Σ.
- Written as $W \sim W_r(n, \Sigma)$.