CHE384, From Data to Decisions: Measurement, Uncertainty, Analysis, and Modeling

Lecture 7
Appendix: Matrix Math

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Why Care About Matrices?

- Regression software almost universally uses matrix methods for model fitting
  - Inputs and results are discussed using the terminology of matrices
- Regression textbooks and journal papers frequently refer to matrix methods
- The covariance matrix will be central to much of what we do next

Matrix Math Review

- m x n matrix (m rows and n columns)

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{2m} & \cdots & a_{nm} \end{bmatrix}$$

a_{ij} = element of the matrix

(i = row index, j = column index)

- Two matrices are equal if they have the same number of rows and columns (i.e., are the same size), and all the elements are equal

Adding Matrices

- We can add matrices only of they have the same number of rows and columns (i.e., they are the same size)
  - Add together the corresponding elements:

$$\boldsymbol{A} + \boldsymbol{B} = \boldsymbol{C} \qquad a_{ij} + b_{ij} = c_{ij}$$

- We can multiply a matrix by a scalar
  - The resulting matrix will have every element multiplied by the scalar

Multiplying Matrices

- We can multiply two matrices $\boldsymbol{AB}$ if the number of columns of $\boldsymbol{A}$ equals the number of rows of $\boldsymbol{B}$
  - If $\boldsymbol{A}$ is m x n and $\boldsymbol{B}$ is n x p then $\boldsymbol{AB}$ will be m x p

$$\boldsymbol{AB} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{12} \end{bmatrix}$$

$$\boldsymbol{AB} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \\ a_{31}b_{11} + a_{32}b_{21} & a_{31}b_{12} + a_{32}b_{22} \end{bmatrix}$$

- Matrix multiplication is not commutative ($\boldsymbol{AB} \neq \boldsymbol{BA}$)

Matrix Math Review

- The identity matrix $\boldsymbol{I}$ is a square matrix where all diagonal elements are 1 and all off-diagonal elements are 0
- The transpose of an m x n matrix $\boldsymbol{A}$ is an n x m matrix $\boldsymbol{A}^T$ where the rows and columns are swapped:

$$a_{ij} = a^T_{ji}$$

Trace and Determinan

- The trace of a square matrix $\boldsymbol{A}$, $\mathrm{tr}(\boldsymbol{A})$, is the sum of its diagonal entries
- The determinant of a square matrix $\boldsymbol{A}$, $\det(\boldsymbol{A})$ or $|\boldsymbol{A}|$, for a 2x2 is

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

  - For larger matrices, we use various permutations to calculate the determinant

Inverse of a Matrix

- The inverse of a square matrix $\boldsymbol{A}$, written as $\boldsymbol{A}^{-1}$, is defined by $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$
  - The inverse of $\boldsymbol{A}$ exists if the determinant of $\boldsymbol{A}$ is non-zero (otherwise, we say the matrix is singular or degenerate)
- Properties of the inverse (if it exists):

$$(\boldsymbol{A}^{-1})^{-1} = \boldsymbol{A} \qquad (\boldsymbol{A}^{T})^{-1} = (\boldsymbol{A}^{-1})^{T}$$

$$(\boldsymbol{A}\boldsymbol{B})^{-1} = \boldsymbol{B}^{-1}\boldsymbol{A}^{-1} \qquad \det(\boldsymbol{A}^{-1}) = 1/\det(\boldsymbol{A})$$

Orthogonal Matrix

- An orthogonal matrix is a square matrix such that $\boldsymbol{A}\boldsymbol{A}^{T} = \boldsymbol{A}^{T}\boldsymbol{A} = \boldsymbol{I}$
- Thus, its transpose is equal to its inverse: $\boldsymbol{A}^{T} = \boldsymbol{A}^{-1}$
- Properties of an orthogonal matrix:
  - Its determinant is either +1 or -1
  - Examples include rotation, reflection, and axis permutation matrices