**Calculating Minimum-Energy Reaction Pathways**

**Rob Sanchez**

**Programming Assignment 1**

**CIS 677 F2017**

**1 Overview**

The graph in Figure 1 represents a biochemical reaction system with multiple reaction pathways. Each node represents a compound, and each directed edge a specific reaction’s energy requirement. To compute the minimum-energy reaction cost needed to get from node 1 (the start) to node 4 (the end) several approaches can be used. The Julia[1] program described in this document, *pathways.jl*, explores two: 1) a brute-force “edge-linking” method, and 2) Dijkstra’s shortest-path algorithm.

**2 Canonical Correlation**

**3 Unsupervised Learning**

**3.1 K-Means Clustering**

**3.2 Hierarchical Clustering**

**4 Response Variable Selection**

**5 Supervised Learning**

**5.1 Multivariate Normality**

**5.2 Linear Regression**

**5.3 Logistic Regression**

**5.4 Random Forest Regression**

**5.5 Random Forest Classification**

**6 Results**

**References**