15.095 Project Proposal

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Problem Summary:
Currently, K-Means Clustering (KMN) is performed using a heuristic algorithm, so the results rely on random initialization. We thus aim to develop a mixed-integer optimization (MIO) model that determines optimal cluster configurations. Implementing this model in a solver such as Gurobi will improve the stability and performance of the existing algorithm. Accomplishing this task will deepen our understanding on the application of optimization to machine learning tasks.

Dataset(s) you plan to use (for applied projects):
We plan on comparing several different metrics (computation time, number of iterations, average distance across clusters, etc.) of our method to the typical heuristic results for several different datasets:

Dataset	N (rows)	P (predictors)
Abalone	4177	9
Auto MPG	392	8
Comp Hard	209	7
Concrete	1030	8
Housing	506	13
Space Shuttle	23	4
WPBC	46	32

Note: We may attempt different datasets as well, but this list came from Dr. Bertsimas' lectures when comparing a heuristic algorithm to optimal MIO algorithms

Methods that you will use and how these relate to our class:

- K-Means Clustering: KMN is an unsupervised ML algorithm that we have not discussed in-depth in this course. Having a better understanding of this method (and, more generally, unsupervised methods) would extend our knowledge beyond the scope of the course into new ML territory.
- Mixed-integer optimization: MIO has been at the heart of many discussions this semester. Applying MIO in a new setting would be a great way to get novel hands-on experience with applying optimization methods to new machine learning tasks.

Challenges, and ideas to overcome them:

Challenge #1: Reporting and Comparing Results

- It may be difficult to initially compare results from our algorithm to the heuristic one (from scikit-learn, or other libraries),
- Resolution: Be very intentional and clear with reporting results to allow for accurate comparisons

Challenge #2: Potential Non-Linearity

- If we decide to use Euclidean (L-2 norm) distance instead of a linear measure, it may be difficult to find solutions using Gurobi,
- Resolution: Begin to develop our algorithm using Manhattan (L-1 norm) distances and extend capabilities to other distance measures (L-2, L-∞ norm, etc.), if possible.