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A Global Optimization Algorithm for Clustering Problems

We present a reduced-space spatial branch and bound strategy for two-stage stochastic nonlinear programs. At each node, a lower bound is constructed by relaxing the non-anticipativity constraints, and an upper bound is constructed by fixing the first-stage variables. Both lower and upper bounds can be computed by solving individual scenario subproblems. Another key property is that we only need to perform branching on the first-stage variables to guarantee convergence.

We also extend this algorithm to address clustering problems (a class of unsupervised learning). Preliminary numerical results have demonstrated that our algorithm is able to solve problems with hundreds of samples to global optimality within a reasonable amount of time, while state-of-the-art global solvers can only deal with tens of samples. Moreover, global optimization can significantly improve performance on several datasets compared with local optimal algorithms, such as k-means.