Discrete OED Criteria

Benoît Chachuat

We propose two alternative criteria for operable space maximization with design of experiments, as introduced by Chen et al. [2018]. Given a finite set of candidate points $\mathbf{p}_i \in \mathbb{R}^n, i = 1 \ldots N$—possibly rescaled in the unit hypercube $[0,1]^n$—the goal is now to select of subset of M points that minimize or maximize a certain metric.

Maximal Covering This criterion selects M centroids among the N candidates in such a way that the maximal distance between any candidate point to the closest centroid is minimized. A mixed-integer (linear) programming (MIP) formulation for this criterion is the following:

$$\begin{aligned}
\min_{\mathbf{y},\mathbf{z},\eta}\ & \eta \\
\text{s.t. }\ & \eta \geq \sum_{i=1}^{N} z_{ij} \|\mathbf{p}_i - \mathbf{p}_j\|, \ \ j = 1 \ldots N \\
& 1 = \sum_{i=1}^{N} z_{ij}, \ \ j = 1 \ldots N \\
& y_i \geq z_{ij}, \ \ i,j = 1 \ldots N \\
& M \geq \sum_{i=1}^{N} y_i \\
& y_i, z_{ij} \in \{0,1\}, \ \ i,j = 1 \ldots N
\end{aligned}$$

where the selected centroids $\mathbf{p}_i$ are those with $y_i = 1$; and $z_{ij} = 1$ indicates the closest centroid $\mathbf{p}_i$ to point $\mathbf{p}_j$. This problem is also known as the uncapacitated vertex k-center problem [Daskin, 2013], for which heuristics algorithms exist that could be used to warm-start the MIP solution.

Maximal Spread This criterion selects M extreme points among the N candidates in such a way that the minimal distance between any pair of extreme points is maximized. A MIP formulation for this criterion is the following:

$$\begin{aligned}
\max_{\mathbf{y},\eta}\ & \eta \\
\text{s.t. }\ & \eta \leq \|\mathbf{p}_i - \mathbf{p}_j\| + (1-y_i)D + (1-y_j)D, \ \ i,j = 1 \ldots N \\
& M \geq \sum_{i=1}^{N} y_i \\
& y_i \in \{0,1\}, \ \ i = 1 \ldots N
\end{aligned}$$

where the selected extreme points $\mathbf{p}_i$ are those with $y_i = 1$; and the scalar D should be no smaller than the diameter of the set of candidate points—e.g., upper bounded by $\sqrt{n}$ if the candidate points are rescaled within the unit hypercube $[0,1]^n$.

References

Q. Chen, R Paulavičius, C. S. Adjiman, and S. García-Muñoz. An optimization framework to combine operable space maximization with design of experiments. *AIChE Journal*, 64(11):3944–3957, 2018. doi: 10.1002/aic.16214.

M. S. Daskin. *Network and Discrete Location: Models, Algorithms, and Applications*. John Wiley & Sons, Ltd, 2nd edition, 2013. doi: 10.1002/9781118537015.