An Efficient Algorithm for Generating Space-filling Designs When the Region of Experimentation is Not Cubic

Latin Hypercube designs (LHD) are in standard use as plans for deterministic computer experiments. However, these designs depend on the ability of the investigator to set each factor independently of all the others. To be specific, the implied design region for an LHD is a square, cube or hypercube. However, there are cases where some parts of such a design region may be inaccessible or even nonsensical. In such cases it is useful to be able to produce a design that is both space-filling while obeying constraints on the design region.

In this talk I will present an efficient algorithm for generating space-filling designs in an arbitrary k-dimensional region assuming that it is possible to generate a random sample of a large number of points inside the region. The construction uses a fast clustering algorithm to create n clusters of points where n is the desired number of design points. The design is then composed of the cluster centroids of each of the clusters. This construction approach leads to some desirable properties. Using cluster centroid forces the design points away from each other in the space of the design. Using a random sample of points results in designs that do not replicate in projection. When applied to design regions without constraints, this design approach yields designs that are nearly orthogonal.

I will present several examples including designs on a simplex. I will also compare these designs to maximin LHDs for various measures of space-fillingness.