AI505

Optimization

Sampling Plans

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Outline

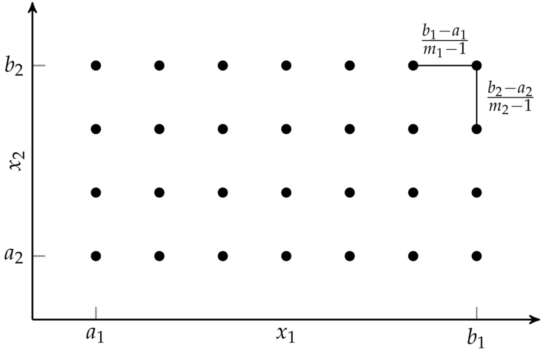
Sampling Plans

- In all nonlinear non convex optimization, to generate good initial design points
- With computationally costly functions, to create an initial set of design points from where to build a **surrogate models** to optimize in place of the original function
- In hyperparameter tuning

Full Factorial Design

- Factors and levels, terms from the field of Experimental Design in Statistics
- Uniform and evenly spaced samples across domain
- Simple, easy to implement, and covers domain
- Optimization over the points known as **grid search**
- Sample count grows exponentially with dimension

$a_i \leq x_i \leq b_i$ for each component i.
grid with m_i samples in the ith dimension

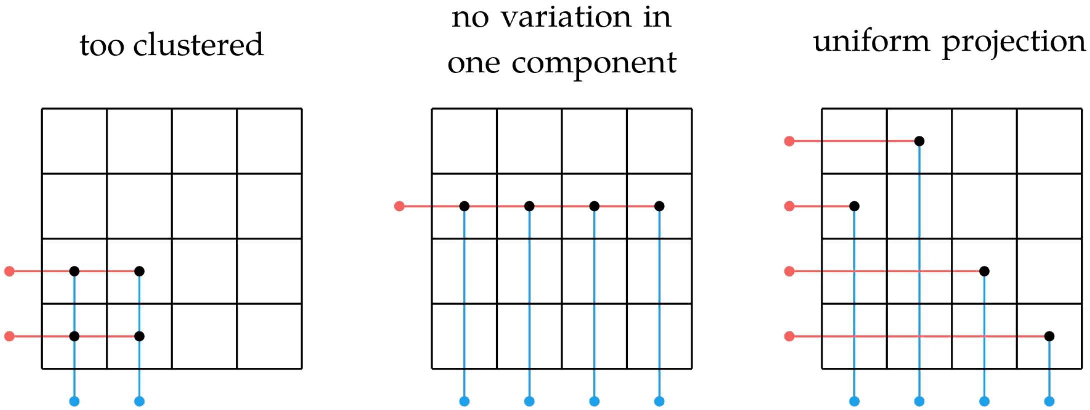


Random Sampling

- Uses pseudorandom number generator to define samples according to our desired distribution
- If variable bounds are known, a common choice is a uniform distribution across domain of possible values
- Ideally, if enough points are sampled and the right distribution is chosen, the design space will be covered

Uniform Projection Plans

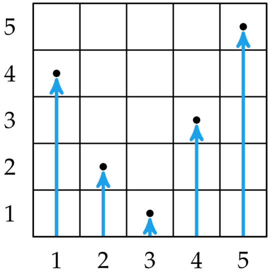
- Sample locations are random, but their projection onto a particular subspace is uniform



Uniform Projection Plans

- Examples: Random permutation, Latin square

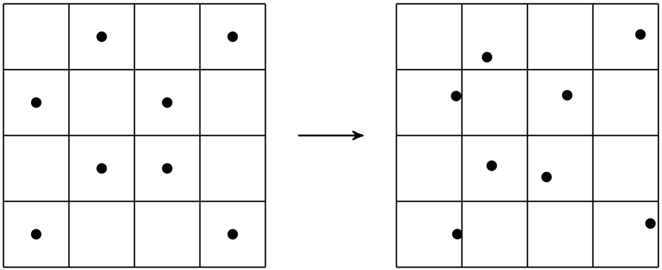
$$p \;=\; 4 \quad 2 \quad 1 \quad 3 \quad 5$$

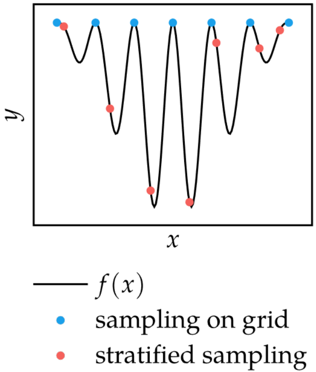


4	1	3	2
1	4	2	3
3	2	1	4
2	3	4	1

Stratified Sampling

- Each point is sampled uniformly at random within each grid cell instead of the center
- Can capture details that regularly-spaced samples might miss

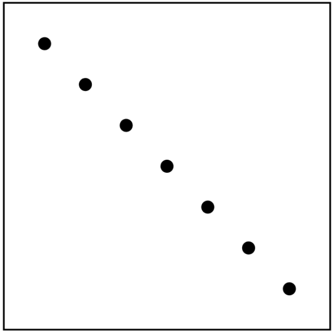




Space Filling Metrics

- A sampling plan may cover a search space fully, but still leave large areas unexplored
- Space-filling metrics quantify this aspect of sampling-plan performance

Example (Uniform Projection)

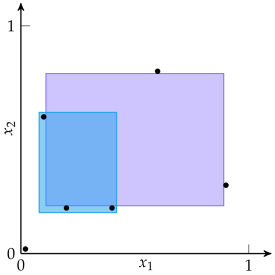


Space-Filling Metrics: Discrepancy

- The maximum difference between the fraction of samples in a hyper-rectangular subset H and that subset's volume

- Often very difficult to compute directly

$$d(X) = \underset{\mathcal{H}}{\text{supremum}} \left| \frac{\#(X \cap \mathcal{H})}{\#X} - \lambda(\mathcal{H}) \right|$$



Space-Filling Metrics: Pairwise Distances

- Method of measuring relative space-filling performance of two-point sampling plans
- Better spread-out plans will have larger pairwise distances
- The pairwise distances of each set are sorted in ascending order
- The plan with the first pairwise distance exceeding the other is considered more space-filling
- Suggests simple algorithm of producing a set of randomly distributed sampling plans, then picking the one with greatest pairwise distances

Space-Filling Metrics: Morris-Mitchell

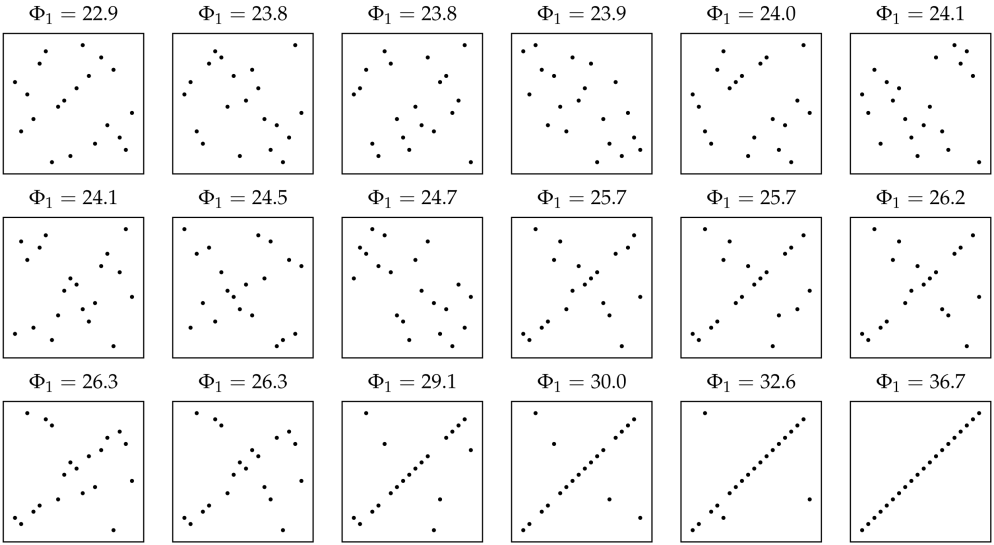
- Alternative to previously suggested algorithm that simplifies optimization problem

$$\underset{X}{\text{minimize}} \underset{q \in \{1,2,3,10,20,50,100\}}{\text{maximize}} \Phi_q(X)$$

$$\Phi_q(X) = \left(\sum_i d_i^{-q} \right)^{\frac{1}{q}}$$

- is the th pairwise distance and is a tunable parameter

Space-Filling Metrics: Morris-Mitchell



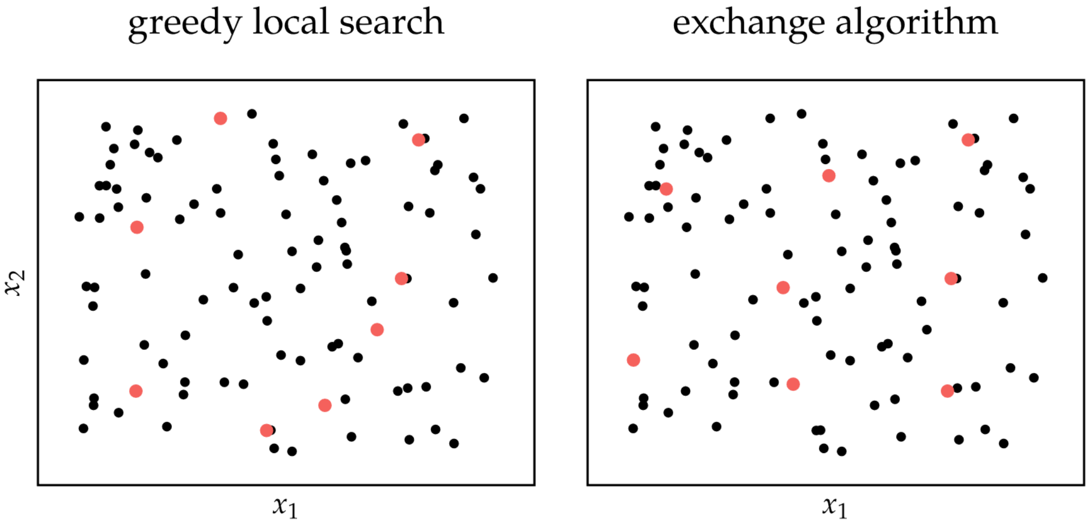
Space-Filling Subsets

- Often, the set of possible sample points is constrained to be a subset of available choices
- A space-filling metric for a subset S within a finite set X is the maximum distance between a point in X and the closest point in S using a norm to measure distance

$$d_{\max}(X, S) = \underset{\mathbf{x} \in X}{\text{maximize}} \; \underset{\mathbf{s} \in S}{\text{minimize}} \; \|\mathbf{s} - \mathbf{x}\|_q$$

- A space-filling subset minimizes this metric
- Often computationally intractable, but heuristics like greedy search and exchange often produce acceptable results

Space-Filling Subsets



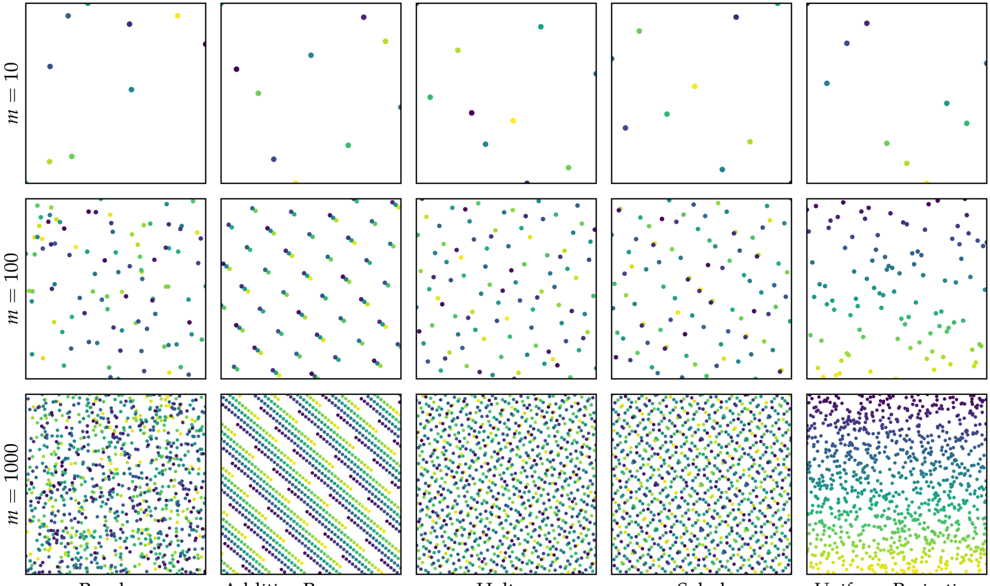
Quasi-Random Sequences

- Also called low-discrepancy sequences, quasi-random sequences are deterministic sequences that systematically fill a space such that their integral over the space converges as fast as possible
- Used for fast convergence in Monte Carlo integration, which approximates an integral by sampling points in a domain

Quasi-Random Sequences

- Additive Recurrence: recursively adds irrational numbers
- Halton Sequence: sequence of fractions generated with coprime numbers
- Sobol Sequence: recursive XOR operation with carefully chosen numbers

Quasi-Random Sequences



Summary

- Sampling plans are used to cover search spaces with a limited number of points
- Full factorial sampling, which involves sampling at the vertices of a uniformly discretized grid, requires a number of points exponential in the number of dimensions
- Uniform projection plans, which project uniformly over each dimension, can be efficiently generated and can be optimized to be space-filling
- Greedy local search and the exchange algorithm can be used to find a subset of points that maximally fill a space
- Quasi-random sequences are deterministic procedures by which space-filling sampling plans can be generated