Meeting : 14 May 2019

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Criterions

1. The total potential energy, which both algorithms aim to minimize:

$$\sum_{i \neq j} \frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

2. One-at-a-Time Algorithm criterion tries to minimize:

$$\left\{ \sum_{i \neq j} \left(\frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)} \right)^k \right\}^{1/k}$$

3. Fast Algorithm Algorithm tries to minimize:

$$\max_{i \neq j} \frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

or, taking into account the simulated annealing at each step k, tries to minimize

$$\max_{i \neq j} \frac{1}{f^{\gamma_k}(\mathbf{x}_i) f^{\gamma_k}(\mathbf{x}) d^{2p}(\mathbf{x}_i, \mathbf{x})}$$

when producing the $(k+1)$th design.

Computational issues

- Well, we saw that, for the one-at-a-time algorithm, when `k` is large, there were some computational issues: it was getting stuck at particular locations.
- This seemed to be the case in both the original implementation (for densities) and for the model selection case.
- We talked about potentially working around this by mixing the two algorithms:
  - use the criterion of the one-at-a-time algorithm
  - with the method of the fast algorithm (re: annealing)

One-at-a-Time Algorithm: choose the next $(n+1)$th design point:

$$\mathbf{x}_{n+1} = \arg\min_{\mathbf{C}} \sum_{i=1}^{n} \left(\frac{q(\mathbf{x}_i)q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \right)^k$$

Fast Algorithm: At design $k \in 2 : (K-1)$, choose the location of x_j in the $(k+1)$th design:

$$\mathbf{x}_j^{k+1} = \arg\min_{\mathbf{x} \in \mathbf{C}_{k+1}^j} \max_{i=1:(j-1)} \frac{1}{f^{\gamma_k}(\mathbf{x}_i) f^{\gamma_k}(\mathbf{x}) d^{2p}(\mathbf{x}_i, \mathbf{x})}$$

Revisiting the Mixed Algorithm Idea

- Mixing the two algorithms:
  - use the criterion of the one-at-a-time algorithm
  - with the method of the fast algorithm (re: annealing)

One-at-a-Time Algorithm: choose the next $(n+1)$th design point:

$$\mathbf{x}_{n+1} = \arg\min_{\mathbf{C}} \sum_{i=1}^{n} \left(\frac{q(\mathbf{x}_i) q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \right)^k$$

Fast Algorithm: At design $k \in 2 : (K-1)$, choose the location of x_j in the $(k+1)$th design:

$$\mathbf{x}_j^{k+1} = \arg\min_{\mathbf{x} \in \mathbf{C}_{k+1}^j} \max_{i=1:(j-1)} \frac{1}{f^{\gamma_k}(\mathbf{x}_i) f^{\gamma_k}(\mathbf{x}) d^{2p}(\mathbf{x}_i, \mathbf{x})}$$

- But what would this look like? Idea: at design $k \in 2 : (K-1)$, choose the location of x_j in the $(k+1)$th design:

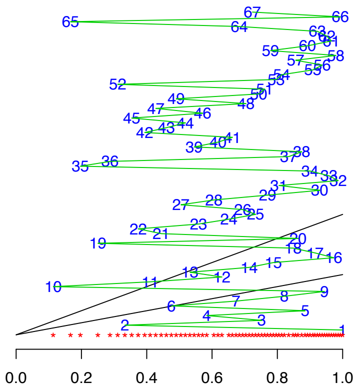
$$\mathbf{x}_j^{k+1} = \arg\min_{\mathbf{x} \in \mathbf{C}_{k+1}^j} \sum_{i=1}^{j-1} \left(\frac{1}{f^{\gamma_k}(\mathbf{x}_i) f^{\gamma_k}(\mathbf{x}) d^{2p}(\mathbf{x}_i, \mathbf{x})} \right)^k$$

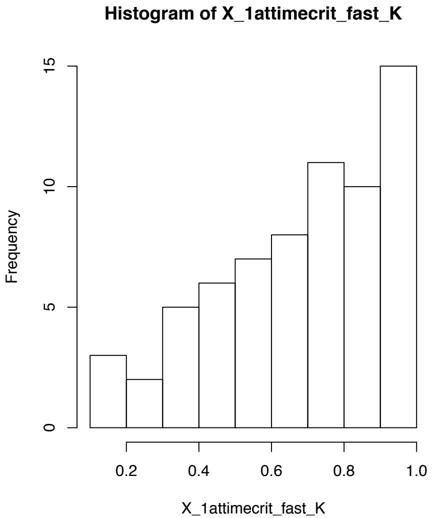
Mixed Algorithms

Criterion of One-at-a-Time Algorithm with Method of Fast Algorithm

$$\mathbf{x}_j^{k+1} = \arg\min_{\mathbf{x} \in \mathbf{C}_{k+1}^{j}} \sum_{i=1}^{j-1} \left(\frac{1}{f^{\gamma_k}(\mathbf{x}_i) f^{\gamma_k}(\mathbf{x}) d^{2p}(\mathbf{x}_i, \mathbf{x})} \right)^k$$

Design generated by this method






```r
mean(X_1attimecrit_fast_K)
```

```
## [1] 0.6799633
```

```r
sd(X_1attimecrit_fast_K)
```

```
## [1] 0.2346713
```

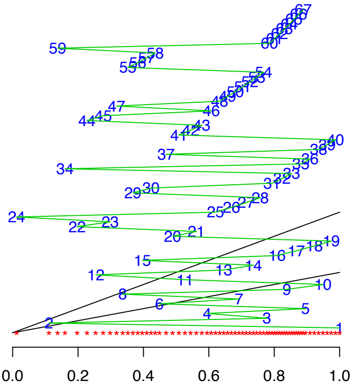
Criterion of Fast Algorithm with Method of One-at-a-Time Algorithm

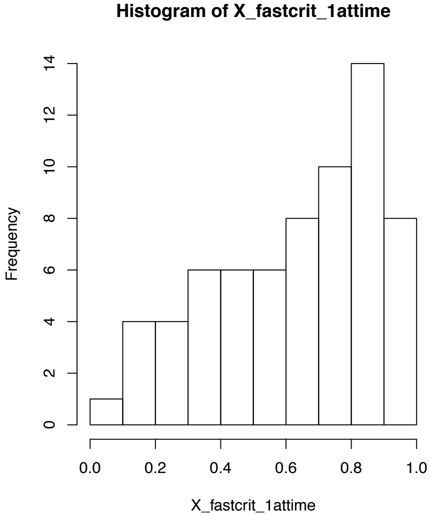
One-at-a-Time Algorithm: choose the next $(n+1)$th design point:

Fast Algorithm: At design $k \in 2:(K-1)$, choose the location of x_j in the $(k+1)$th design:

$$\mathbf{x}_j^{k+1} = \arg\min_{\mathbf{C}} \max_{i=1:(j-1)} \frac{1}{f(\mathbf{x}_i)f(\mathbf{x})d^{2p}(\mathbf{x}_i, \mathbf{x})}$$

Design generated by this method






```r
mean(X_fastcrit_1attime)
```

```
## [1] 0.6279951
```

```r
sd(X_fastcrit_1attime)
```

```
## [1] 0.253249
```

The Table

Results!

	FastCrit_1atTime	1atTimeCrit_Fast
Var Slope	2.00e-03	3.00e-03
TPE	2.55e+06	2.77e+06
Fast Crit	4.68e+04	5.57e+04
1atTime Crit	9.15e+04	9.45e+04