

# Mixed Algorithms

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Proposed models

Mixing the algorithms

# Criteria

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

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

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

## Revisiting the mixed algorithms 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: greedily 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  $s \in 2 : (S - 1)$ , choose the location of  $\mathbf{x}_j$  in the  $(s + 1)$ th stage's design:

$$\mathbf{x}_j^{s+1} = \arg \min_{\mathbf{x} \in \mathbf{C}_{s+1}^j} \max_{i=1:(j-1)} \frac{q^{\gamma_s}(\mathbf{x}_i)q^{\gamma_s}(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})}$$

## one-at-a-time method with fast criterion (mix1)

This is just fast algorithm with  $k = 1$ , but using max instead of sum over the design points:

$$\mathbf{x}_{n+1} = \arg \min_{\mathbf{c}} \max_{i=1:n} \frac{q(\mathbf{x}_i)q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})}$$

## fast method with one-at-a-time criterion (mix2)

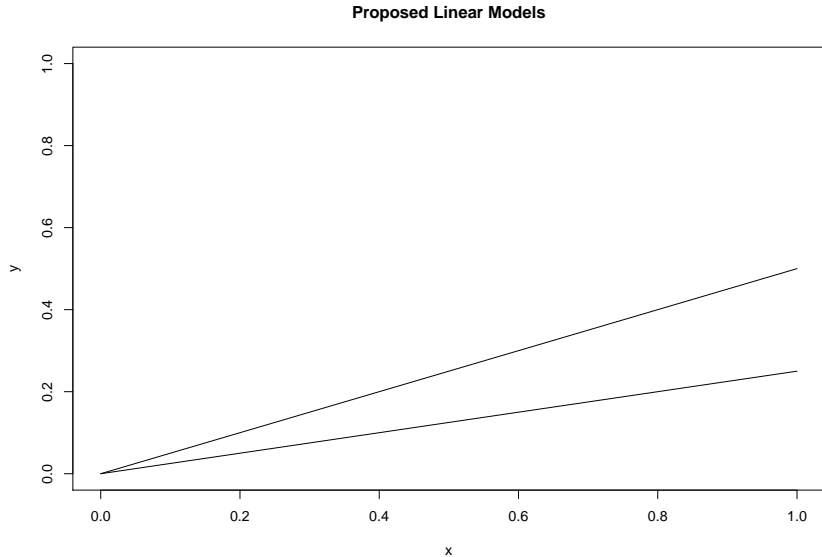
Have points converge to those which minimize the one-at-a-time algorithm's criterion (summation raised to  $k = 4$  power) over  $S$  stages. At design for stage  $s \in 2 : (S - 1)$ , choose the location of  $\mathbf{x}_j$  in the  $(s + 1)$ th design:

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

## Proposed models

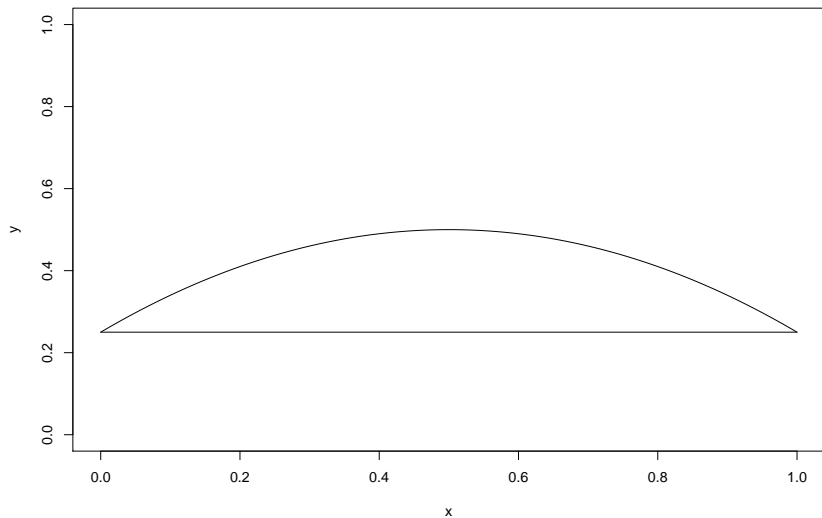


# I. Proposed Models



## VI. Proposed Models

Proposed Linear and Quadratic Models



## Mixing the algorithms

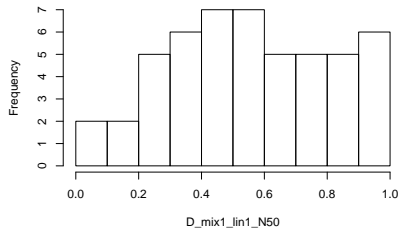
## one-at-a-time method with fast criterion (mix1)

This is just fast algorithm with  $k = 1$ , but using max instead of sum over the design points:

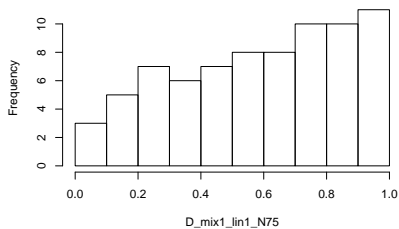
$$\mathbf{x}_{n+1} = \arg \min_{\mathbf{c}} \max_{i=1:n} \frac{q(\mathbf{x}_i)q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})}$$

# Design Points

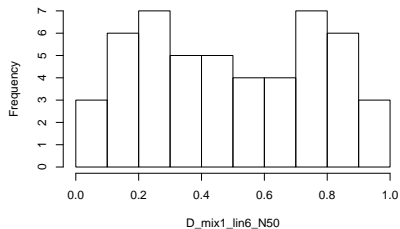
**I, N=50**



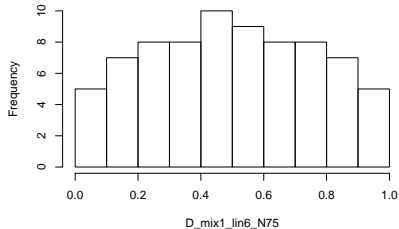
**I, N=75**



**VI, N=50**



**VI, N=75**



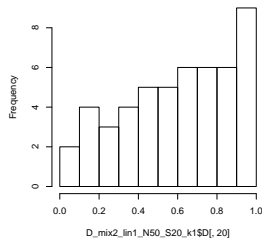
## fast method with one-at-a-time criterion (mix2)

Have points converge to those which minimize the one-at-a-time algorithm's criterion (summation raised to  $k = 4$  power) over  $S$  stages. At design for stage  $s \in 2 : (S - 1)$ , choose the location of  $\mathbf{x}_j$  in the  $(s + 1)$ th design:

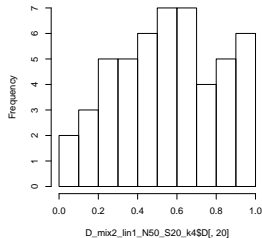
$$\mathbf{x}_j^{s+1} = \arg \min_{\mathbf{x} \in \mathbf{C}_{s+1}^j} \sum_{i=1}^{j-1} \left( \frac{q^{\gamma_s}(\mathbf{x}_i) q^{\gamma_s}(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \right)^k$$

# Design Points, I

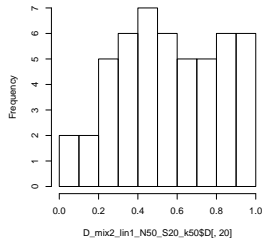
**k = 1, N=50**



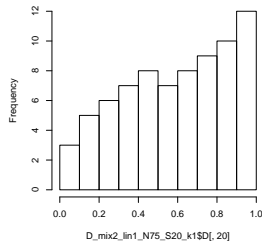
**k = 4, N=50**



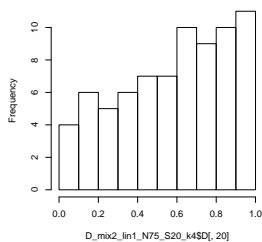
**k = 50, N=50**



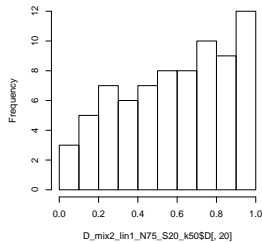
**k = 1, N=75**



**k = 4, N=75**

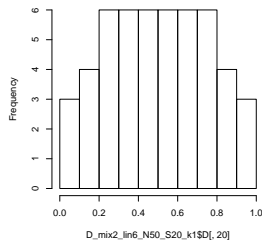


**k = 50, N=75**

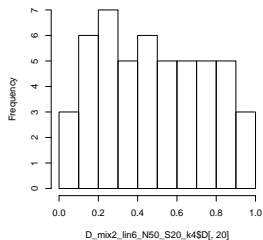


# Design Points, VI

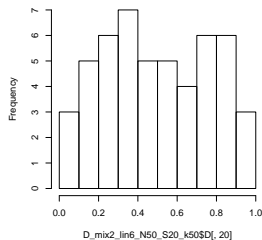
**k = 1, N=50**



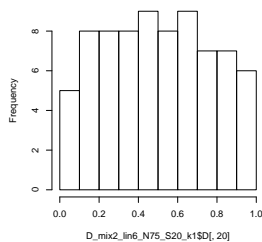
**k = 4, N=50**



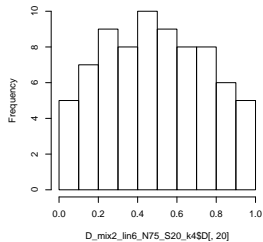
**k = 50, N=50**



**k = 1, N=75**



**k = 4, N=75**



**k = 50, N=75**

