

# Simple Linear Model Selection Experiments for Unknown Intercept and Unknown Slope: $N = 50,$ 75

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I. intercept at 0

III. intercept at 0.5

II. space in-between

IV. intercept at 0.5 with space in-between

V. less space in-between

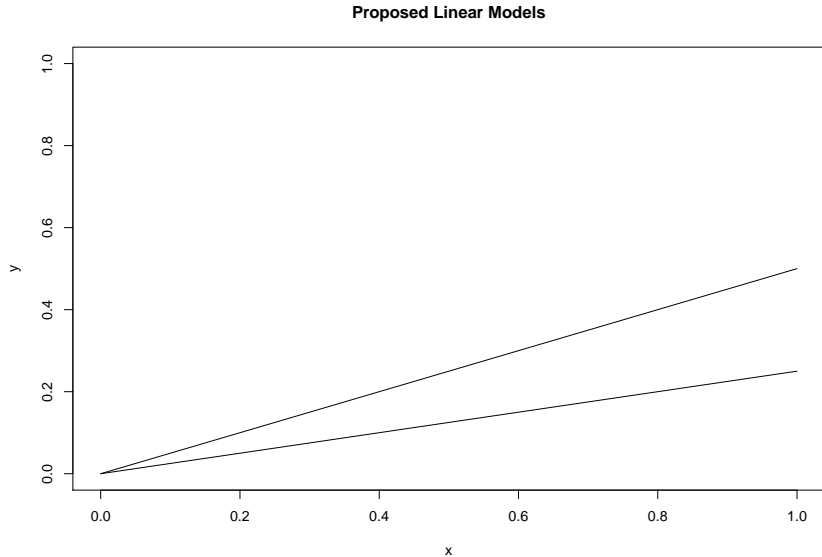
VI. linear vs quadratic

## Some Observations

1. Call the criteria for the One-at-a-Time algorithm and the Fast algorithm G-Crit and F-Crit, resp. For any design  $\mathbf{D}$ ,  $\text{G-Crit}_{k \rightarrow \infty}\{\mathbf{D}\} = \text{F-Crit}\{\mathbf{D}\}$ .
2. Call the MED generated by the One-at-a-Time algorithm  $\mathbf{D}_G$ , and the MED generated by the Fast algorithm  $\mathbf{D}_F$ . Both designs  $\mathbf{D}_G$  and  $\mathbf{D}_F$  are invariant to y-intercept. All that seems to matter in generating the design is the Wasserstein distance between  $f_0$  and  $f_1$  at each point  $\mathbf{x} \in \mathbf{D}_\ell, \ell = \{G, F\}$ .
3. Calculating an MED algorithm's criteria in log space (using logSumExp trick) might prevent any overflow that may be happening due to dividing by small values of  $d(\mathbf{x}, \mathbf{y})$ .
4. Sometimes  $\mathbf{D}_G$  does not seem to approach  $\mathbf{D}_F$  as  $k$  gets larger (from observing the histograms). This seems to be the case when  $N = 50$ , but not when  $N = 75$ . i.e.  $N$  needs to be large enough?

I. intercept at 0

# I. Proposed Linear Models



# Histograms

The following slides show histograms of:

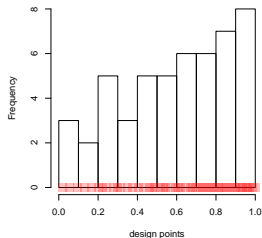
- ▶ design points:  $\mathbf{x} \in \mathbf{D}$
- ▶ charge function evaluated for each design point:  $q(\mathbf{x}), \forall \mathbf{x} \in \mathbf{D}$
- ▶ pairwise distances:  $d(\mathbf{x}_i, \mathbf{x}_j), \forall \mathbf{x}_i, \mathbf{x}_j \in \mathbf{D}$
- ▶ pairwise potential energies:  $\frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}, \forall \mathbf{x}_i, \mathbf{x}_j \in \mathbf{D}$

for each of the MED designs considered:

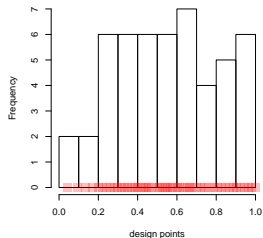
- ▶ MED generated by the One-at-a-Time algorithm, with power  $k = 1, 4, 20, 50, 100$
- ▶ MED generated by the Fast algorithm, with number of stages  $S = 20$

# Designs, $N = 50$

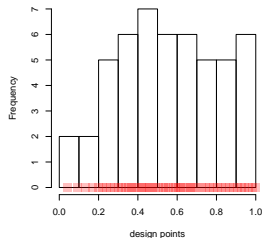
One-at-a-Time,  $k = 1$



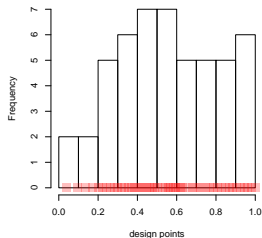
One-at-a-Time,  $k = 4$



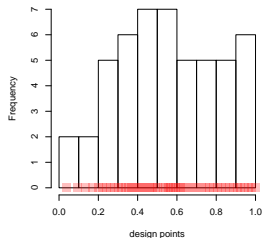
One-at-a-Time,  $k = 20$



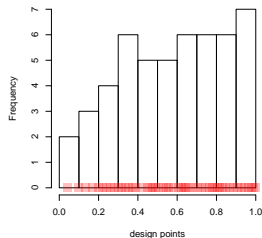
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

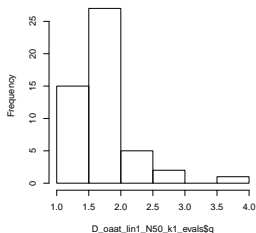


Fast,  $S = 20$

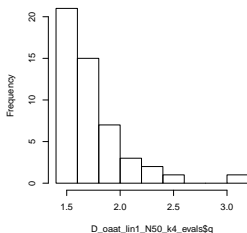


# Evaluations of q(.)

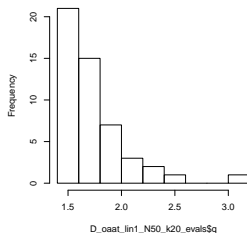
Histogram of D\_oaat\_lin1\_N50\_k1\_evals\$q



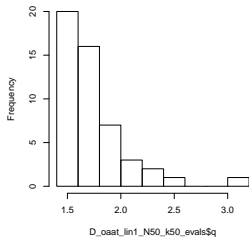
Histogram of D\_oaat\_lin1\_N50\_k4\_evals\$q



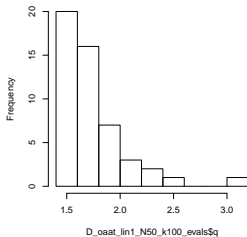
Histogram of D\_oaat\_lin1\_N50\_k20\_evals\$q



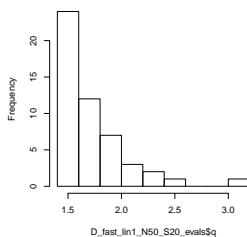
Histogram of D\_oaat\_lin1\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin1\_N50\_k100\_evals\$q



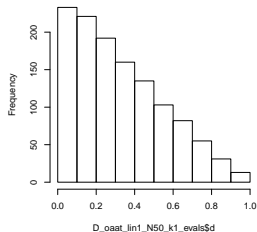
Histogram of D\_fast\_lin1\_N50\_S20\_evals\$q



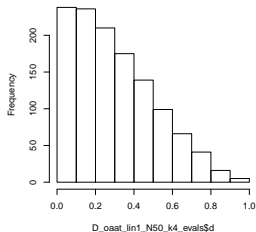


# Pairwise distances of design points

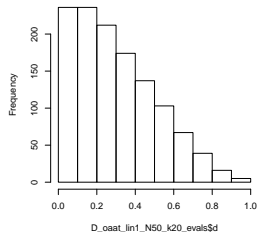
Histogram of D\_oaat\_lin1\_N50\_k1\_evals\$d



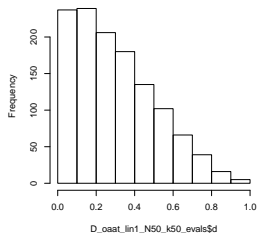
Histogram of D\_oaat\_lin1\_N50\_k4\_evals\$d



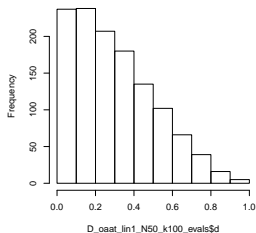
Histogram of D\_oaat\_lin1\_N50\_k20\_evals\$d



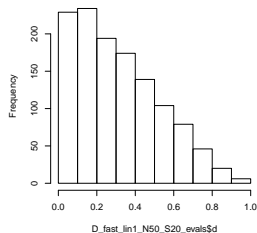
Histogram of D\_oaat\_lin1\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin1\_N50\_k100\_evals\$d

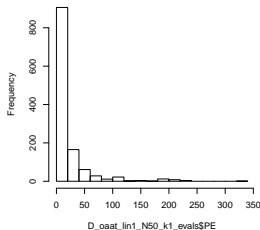


Histogram of D\_fast\_lin1\_N50\_S20\_evals\$d

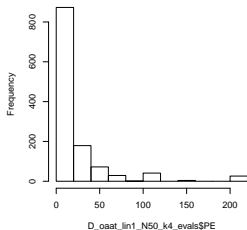


# Pairwise potential energies of design points

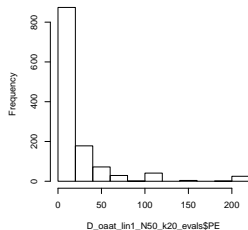
Histogram of D\_oaat\_lin1\_N50\_k1\_evals\$PE



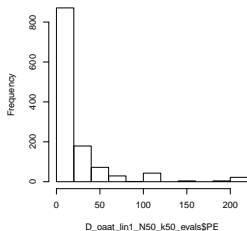
Histogram of D\_oaat\_lin1\_N50\_k4\_evals\$PE



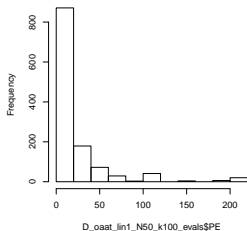
Histogram of D\_oaat\_lin1\_N50\_k20\_evals\$PE



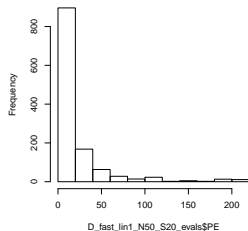
Histogram of D\_oaat\_lin1\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin1\_N50\_k100\_evals\$PE



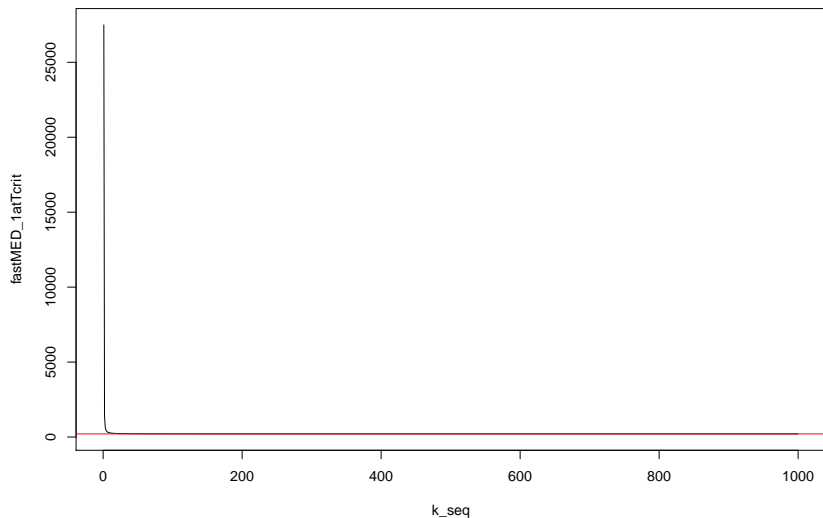
Histogram of D\_fast\_lin1\_N50\_S20\_evals\$PE



# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	27.105	28.693	28.57	28.757	28.749	27.492
Fast	335.26	209.63	208.43	208.1	208.06	208.15
1atT(k=4)	502.21	484.28	480.28	480.12	479.88	469.12
Mean(D)	0.59672	0.55135	0.55316	0.55152	0.55167	0.5767
sd(D)	0.28173	0.25876	0.25893	0.25844	0.25845	0.26824

# Fast MED Evaluated at One-at-a-Time Criterion

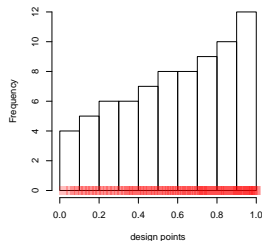


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## [1] "Fast Criterion : 208.149982615237"
```

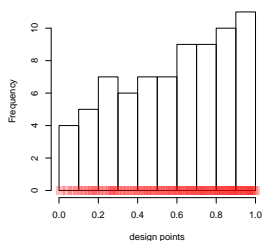
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## [1] "One-at-a-Time Criterion at max k : 208.175089060583"
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# Designs, $N = 75$

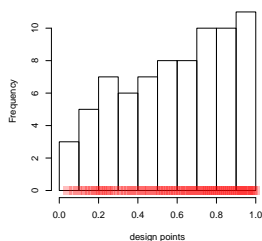
One-at-a-Time,  $k = 1$



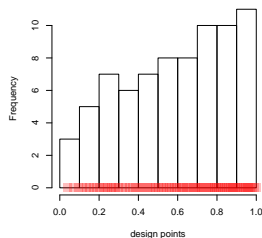
One-at-a-Time,  $k = 4$



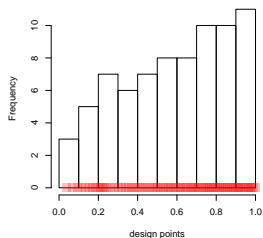
One-at-a-Time,  $k = 20$



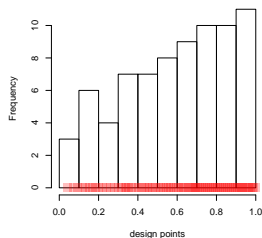
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

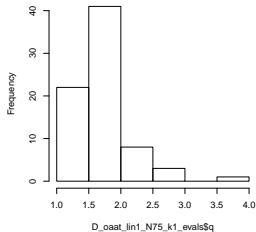


Fast,  $S = 20$

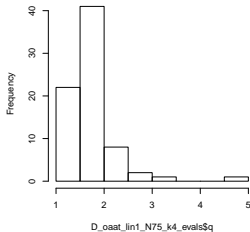


# Evaluations of q(.)

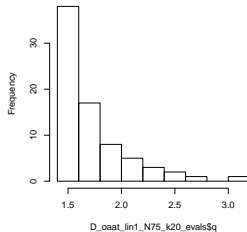
Histogram of D\_oaat\_lin1\_N75\_k1\_evals\$q



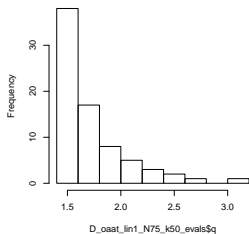
Histogram of D\_oaat\_lin1\_N75\_k4\_evals\$q



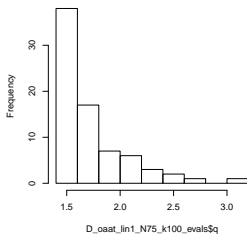
Histogram of D\_oaat\_lin1\_N75\_k20\_evals\$q



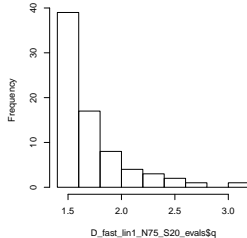
Histogram of D\_oaat\_lin1\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin1\_N75\_k100\_evals\$q

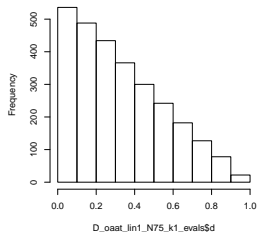


Histogram of D\_fast\_lin1\_N75\_S20\_evals\$q

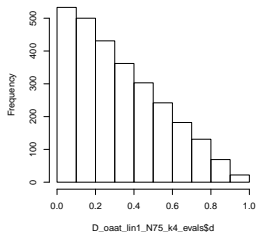


# Pairwise distances of design points

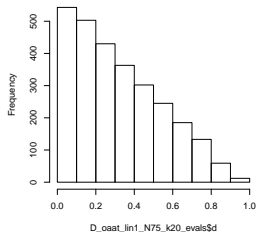
Histogram of D\_oaat\_lin1\_N75\_k1\_evals\$d



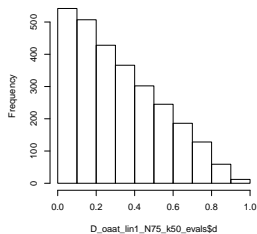
Histogram of D\_oaat\_lin1\_N75\_k4\_evals\$d



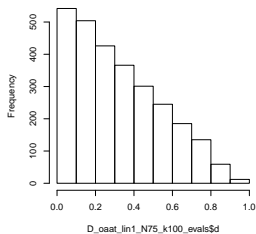
Histogram of D\_oaat\_lin1\_N75\_k20\_evals\$d



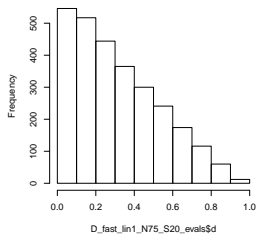
Histogram of D\_oaat\_lin1\_N75\_k50\_evals\$d



Histogram of D\_oaat\_lin1\_N75\_k100\_evals\$d

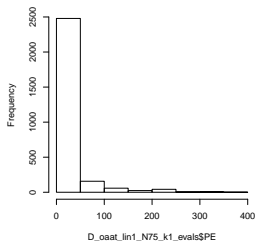


Histogram of D\_fast\_lin1\_N75\_S20\_evals\$d

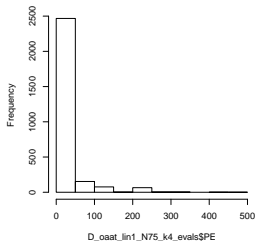


# Pairwise potential energies of design points

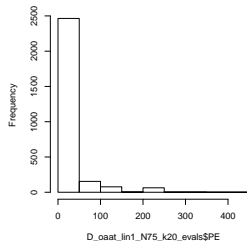
Histogram of D\_oaat\_lin1\_N75\_k1\_evals\$PE



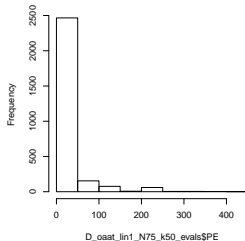
Histogram of D\_oaat\_lin1\_N75\_k4\_evals\$PE



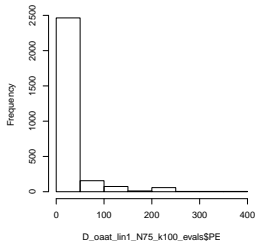
Histogram of D\_oaat\_lin1\_N75\_k20\_evals\$PE



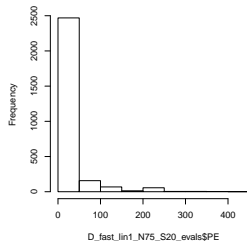
Histogram of D\_oaat\_lin1\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin1\_N75\_k100\_evals\$PE



Histogram of D\_fast\_lin1\_N75\_S20\_evals\$PE

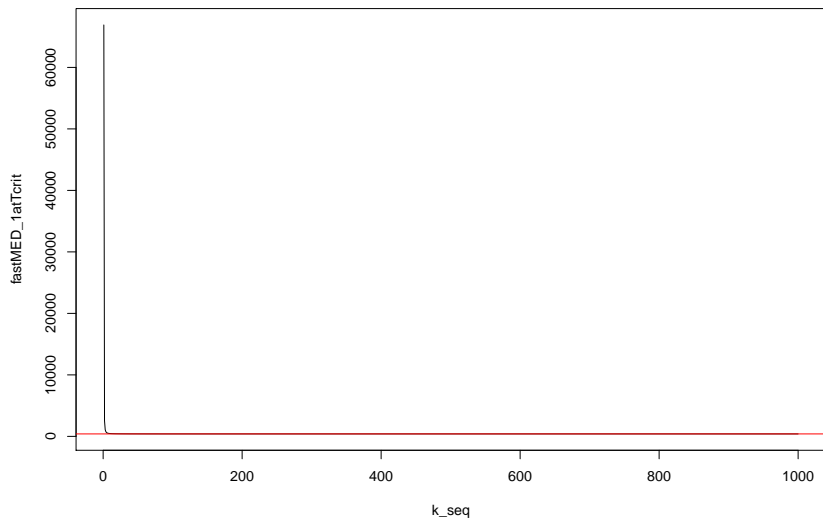




# Comparing Evaluations for each $N = 75$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	66.27	66.737	66.912	66.844	67.018	66.905
Fast	373.54	451.94	402	400.01	399.65	401.03
1atT(k=4)	733.35	742.62	745.74	745.07	745.91	744.47
Mean(D)	0.5874	0.58103	0.58511	0.58596	0.58528	0.59326
sd(D)	0.28154	0.28039	0.27604	0.27536	0.2764	0.27154

# Fast MED Evaluated at One-at-a-Time Criterion

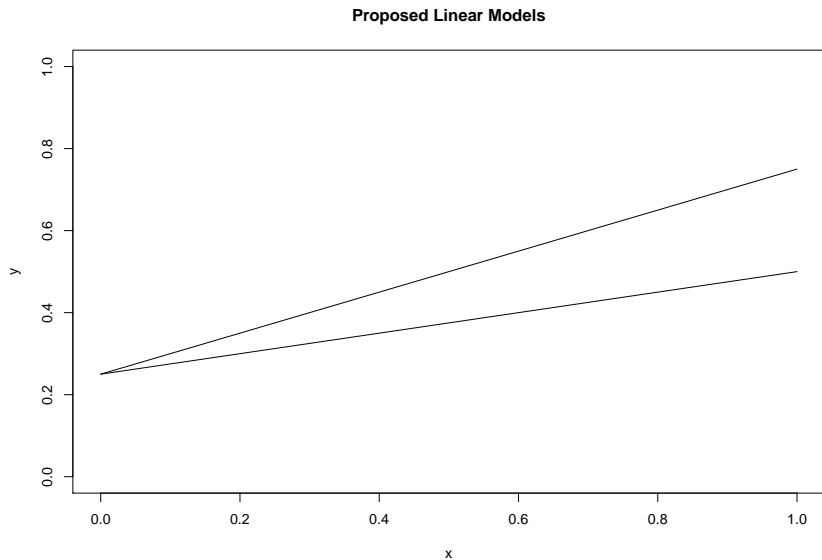


```
## [1] "Fast Criterion : 401.030941543323"
```

```
## [1] "One-at-a-Time Criterion at max k : 401.030941880717"
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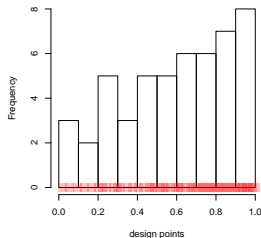
III. intercept at 0.5

### III. Proposed Linear Models

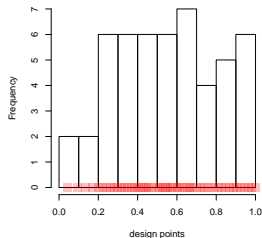


# Designs, $N = 50$

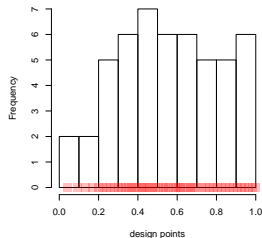
One-at-a-Time,  $k = 1$



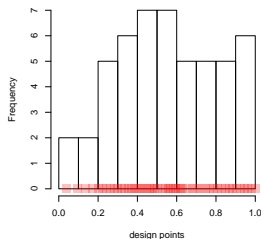
One-at-a-Time,  $k = 4$



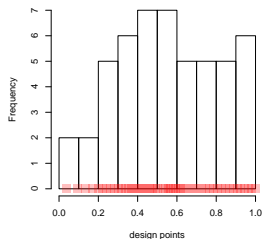
One-at-a-Time,  $k = 20$



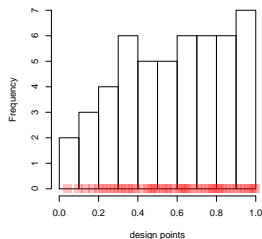
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

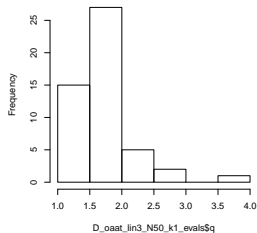


Fast,  $S = 20$

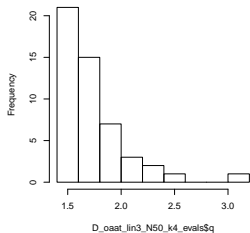


# Evaluations of q(.)

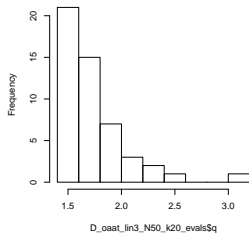
Histogram of D\_oaat\_lin3\_N50\_k1\_evals\$q



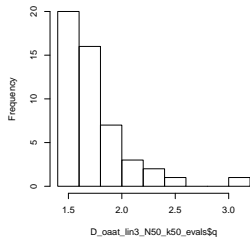
Histogram of D\_oaat\_lin3\_N50\_k4\_evals\$q



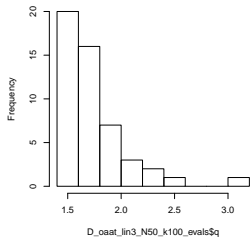
Histogram of D\_oaat\_lin3\_N50\_k20\_evals\$q



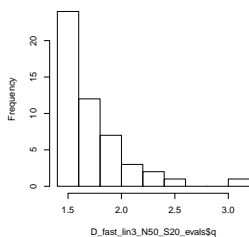
Histogram of D\_oaat\_lin3\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin3\_N50\_k100\_evals\$q

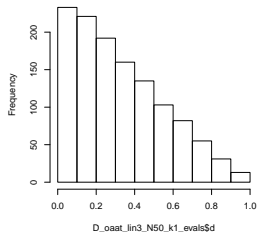


Histogram of D\_fast\_lin3\_N50\_S20\_evals\$q

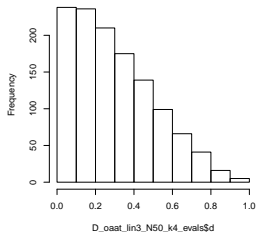


# Pairwise distances of design points

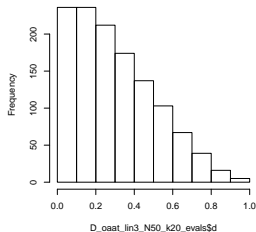
Histogram of D\_oaat\_lin3\_N50\_k1\_evals\$d



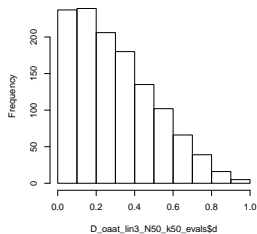
Histogram of D\_oaat\_lin3\_N50\_k4\_evals\$d



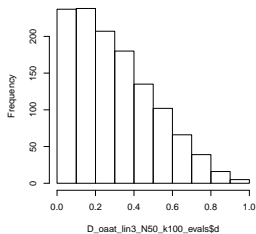
Histogram of D\_oaat\_lin3\_N50\_k20\_evals\$d



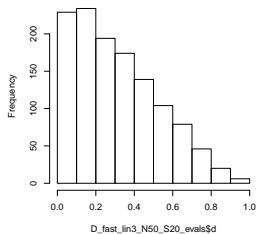
Histogram of D\_oaat\_lin3\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin3\_N50\_k100\_evals\$d

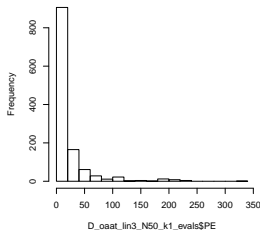


Histogram of D\_fast\_lin3\_N50\_S20\_evals\$d

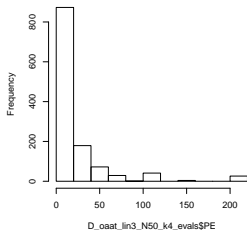


# Pairwise potential energies of design points

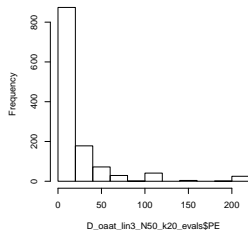
Histogram of D\_oaat\_lin3\_N50\_k1\_evals\$PE



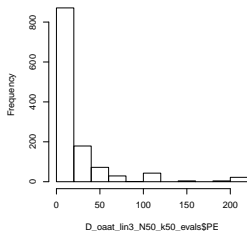
Histogram of D\_oaat\_lin3\_N50\_k4\_evals\$PE



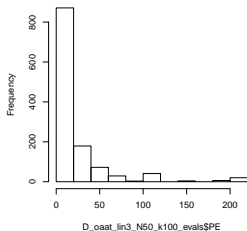
Histogram of D\_oaat\_lin3\_N50\_k20\_evals\$PE



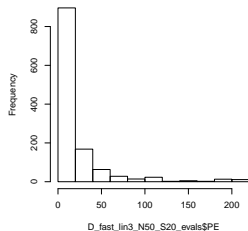
Histogram of D\_oaat\_lin3\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin3\_N50\_k100\_evals\$PE



Histogram of D\_fast\_lin3\_N50\_S20\_evals\$PE

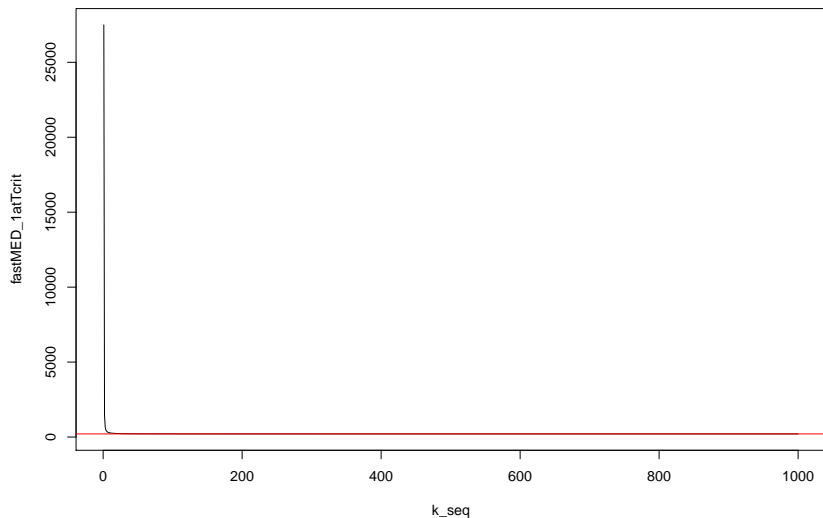




# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	27.105	28.693	28.57	28.757	28.749	27.492
Fast	335.26	209.63	208.43	208.1	208.06	208.15
1atT(k=4)	502.21	484.28	480.28	480.12	479.88	469.12
Mean(D)	0.59672	0.55135	0.55316	0.55152	0.55167	0.5767
sd(D)	0.28173	0.25876	0.25893	0.25844	0.25845	0.26824

# Fast MED Evaluated at One-at-a-Time Criterion

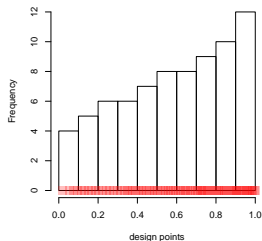


```
## [1] "Fast Criterion : 208.149982615237"
```

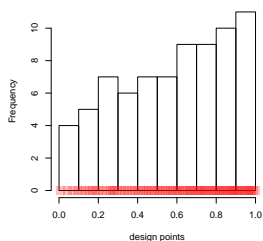
```
## [1] "One-at-a-Time Criterion at max k : 208.175089060583"
```

# Designs, $N = 75$

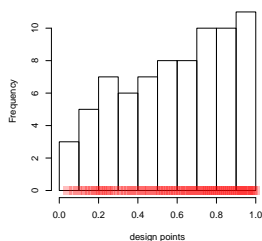
One-at-a-Time,  $k = 1$



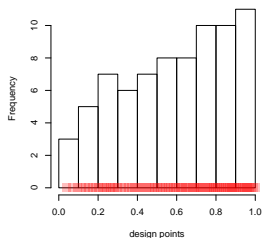
One-at-a-Time,  $k = 4$



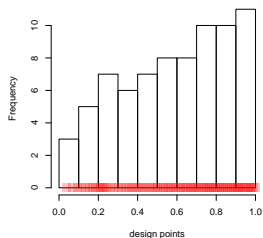
One-at-a-Time,  $k = 20$



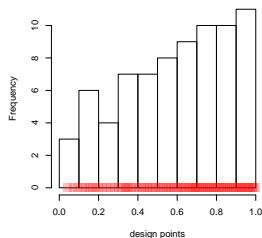
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

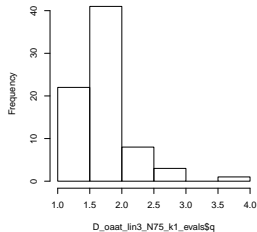


Fast,  $S = 20$

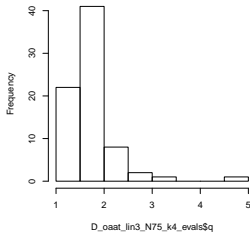


# Evaluations of q(.)

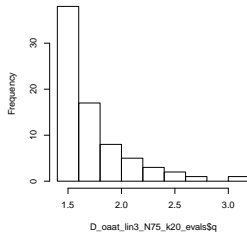
Histogram of D\_oaat\_lin3\_N75\_k1\_evals\$q



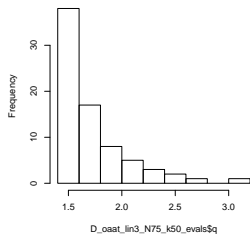
Histogram of D\_oaat\_lin3\_N75\_k4\_evals\$q



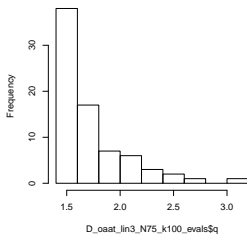
Histogram of D\_oaat\_lin3\_N75\_k20\_evals\$q



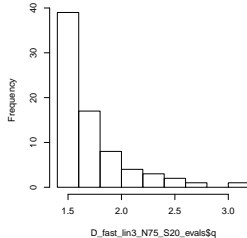
Histogram of D\_oaat\_lin3\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin3\_N75\_k100\_evals\$q

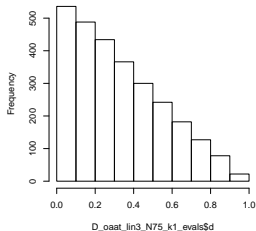


Histogram of D\_fast\_lin3\_N75\_S20\_evals\$q

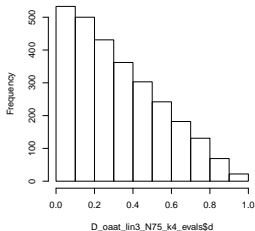


# Pairwise distances of design points

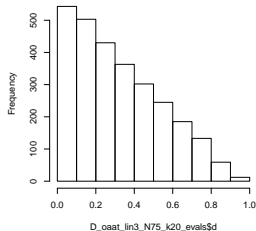
Histogram of D\_oaat\_lin3\_N75\_k1\_evals\$d



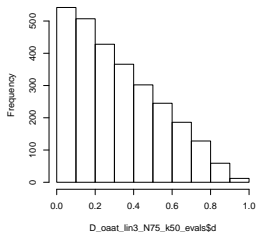
Histogram of D\_oaat\_lin3\_N75\_k4\_evals\$d



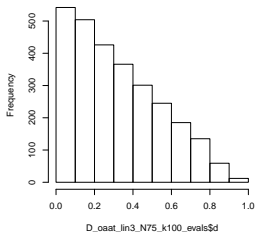
Histogram of D\_oaat\_lin3\_N75\_k20\_evals\$d



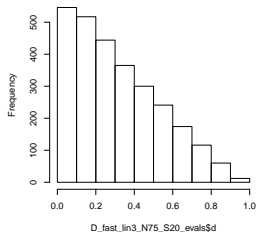
Histogram of D\_oaat\_lin3\_N75\_k50\_evals\$d



Histogram of D\_oaat\_lin3\_N75\_k100\_evals\$d

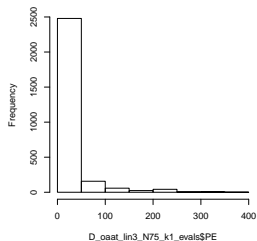


Histogram of D\_fast\_lin3\_N75\_S20\_evals\$d

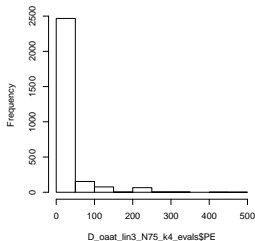


# Pairwise potential energies of design points

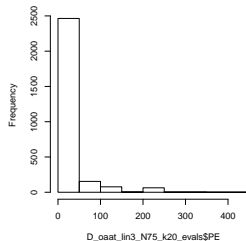
Histogram of D\_oaat\_lin3\_N75\_k1\_evals\$PE



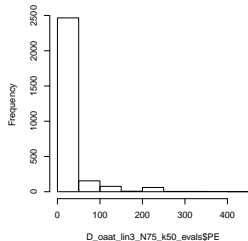
Histogram of D\_oaat\_lin3\_N75\_k4\_evals\$PE



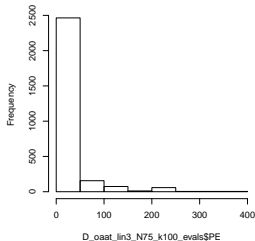
Histogram of D\_oaat\_lin3\_N75\_k20\_evals\$PE



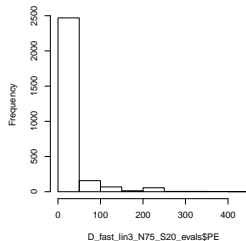
Histogram of D\_oaat\_lin3\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin3\_N75\_k100\_evals\$PE



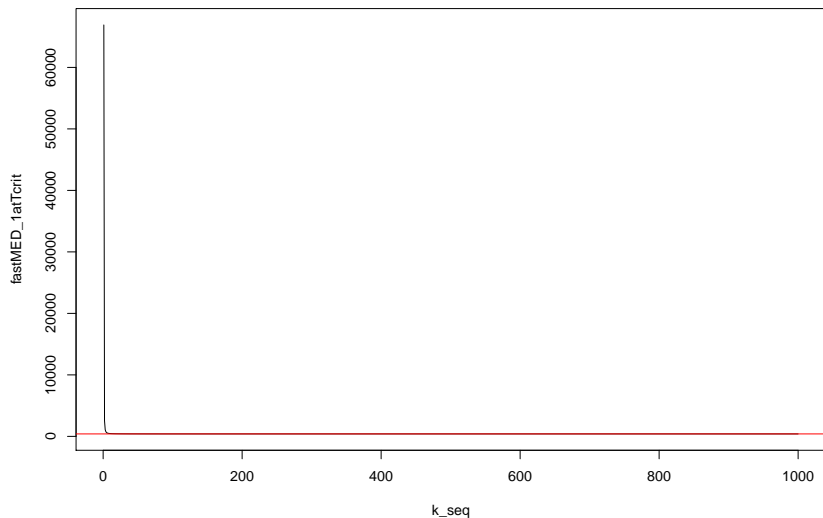
Histogram of D\_fast\_lin3\_N75\_S20\_evals\$PE



# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	66.27	66.737	66.912	66.844	67.018	66.905
Fast	373.54	451.94	402	400.01	399.65	401.03
1atT(k=4)	733.35	742.62	745.74	745.07	745.91	744.47
Mean(D)	0.5874	0.58103	0.58511	0.58596	0.58528	0.59326
sd(D)	0.28154	0.28039	0.27604	0.27536	0.2764	0.27154

# Fast MED Evaluated at One-at-a-Time Criterion



```
## [1] "Fast Criterion : 401.030941543323"
```

```
## [1] "One-at-a-Time Criterion at max k : 401.030941880717"
```

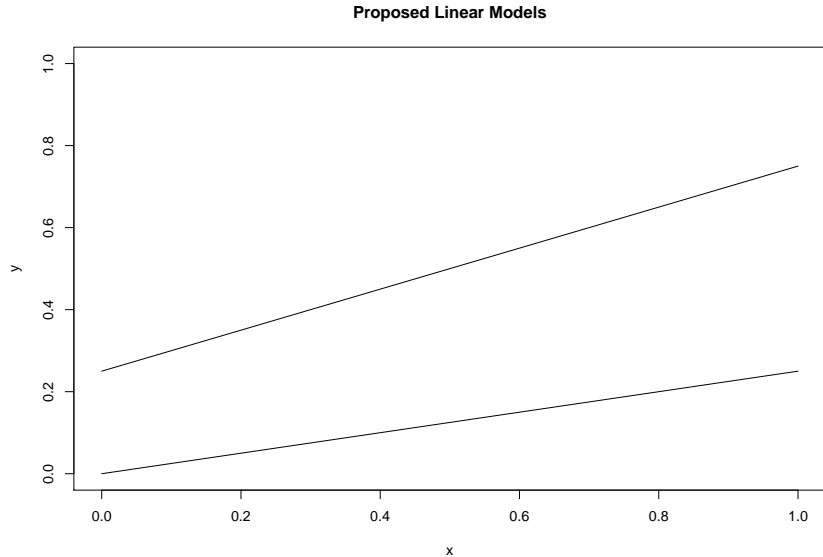


## Comparing I and III

- ▶ The designs are exactly the same, whether the intercept is at 0, or at 0.5 (or anywhere else)!
- ▶ All that matters for MED is how much distance there is between the two functions  $f_1(x)$  and  $f_2(x)$ , at a given point  $x$ .

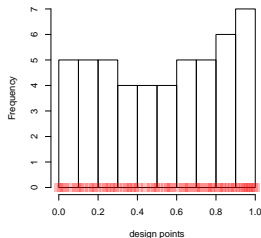
## II. space in-between

## II. Proposed Linear Models

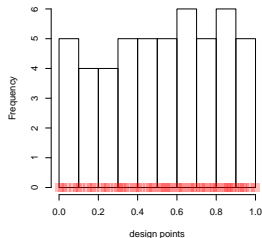


# Designs, $N = 50$

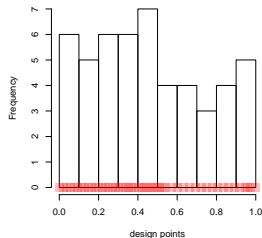
One-at-a-Time,  $k = 1$



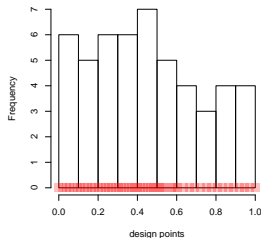
One-at-a-Time,  $k = 4$



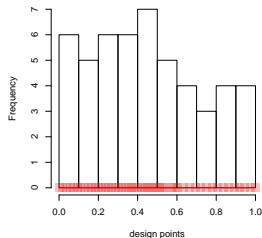
One-at-a-Time,  $k = 20$



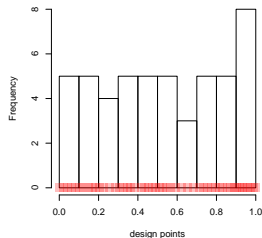
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

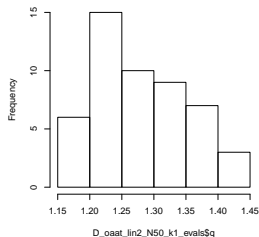


Fast,  $S = 20$

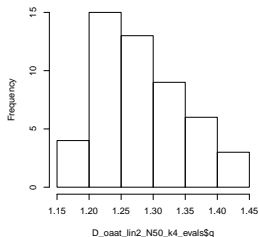


# Evaluations of $q(.)$

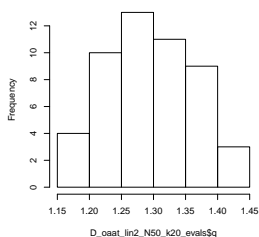
Histogram of D\_oaat\_lin2\_N50\_k1\_evals\$q



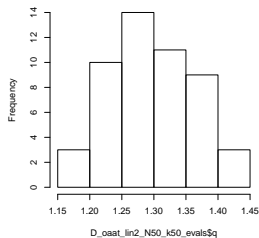
Histogram of D\_oaat\_lin2\_N50\_k4\_evals\$q



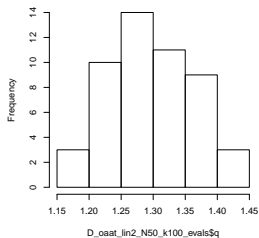
Histogram of D\_oaat\_lin2\_N50\_k20\_evals\$q



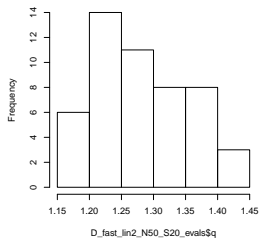
Histogram of D\_oaat\_lin2\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin2\_N50\_k100\_evals\$q

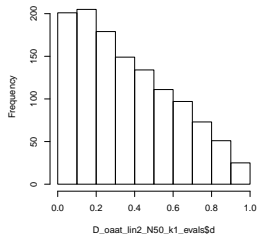


Histogram of D\_fast\_lin2\_N50\_S20\_evals\$q

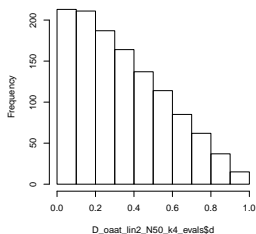


# Pairwise distances of design points

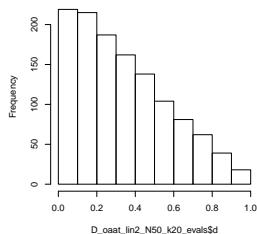
Histogram of D\_oaat\_lin2\_N50\_k1\_evals\$d



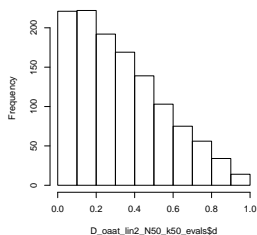
Histogram of D\_oaat\_lin2\_N50\_k4\_evals\$d



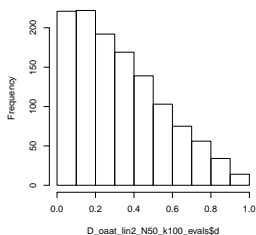
Histogram of D\_oaat\_lin2\_N50\_k20\_evals\$d



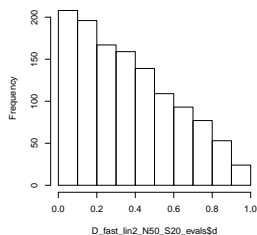
Histogram of D\_oaat\_lin2\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin2\_N50\_k100\_evals\$d

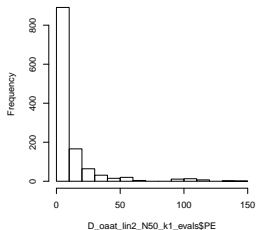


Histogram of D\_fast\_lin2\_N50\_S20\_evals\$d

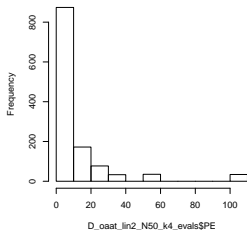


# Pairwise potential energies of design points

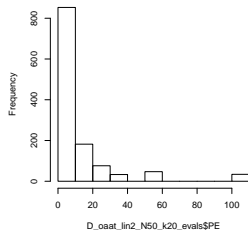
Histogram of D\_oaat\_lin2\_N50\_k1\_evals\$PE



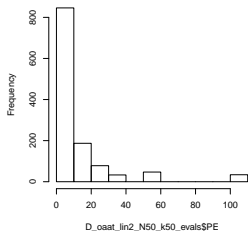
Histogram of D\_oaat\_lin2\_N50\_k4\_evals\$PE



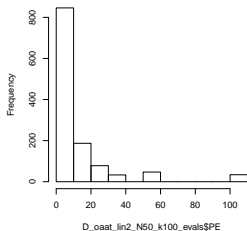
Histogram of D\_oaat\_lin2\_N50\_k20\_evals\$PE



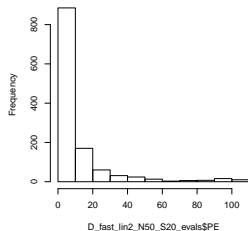
Histogram of D\_oaat\_lin2\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin2\_N50\_k100\_evals\$PE



Histogram of D\_fast\_lin2\_N50\_S20\_evals\$PE

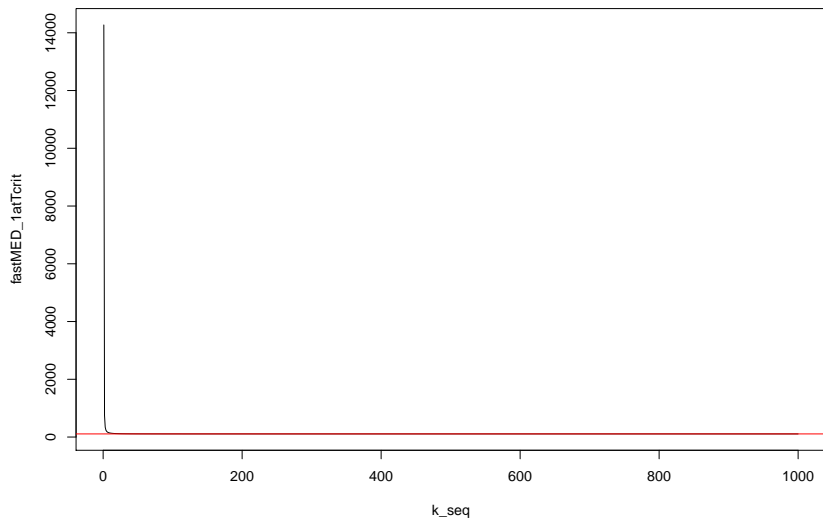


# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	14.448	14.712	15.394	15.558	15.558	14.271
Fast	144.42	105.58	105.23	105.32	105.32	108.16
1atT(k=4)	266.3	258.43	259.47	259.44	259.44	240.49
Mean(D)	0.53194	0.5202	0.45769	0.45036	0.45036	0.52515
sd(D)	0.3106	0.2927	0.29233	0.28393	0.28393	0.31158



# Fast MED Evaluated at One-at-a-Time Criterion

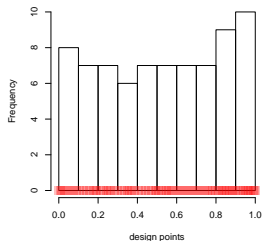


```
## [1] "Fast Criterion : 108.156988894383"
```

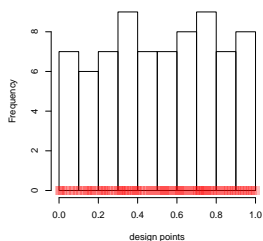
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## [1] "One-at-a-Time Criterion at max k : 108.160369698106"
```

# Designs, $N = 75$

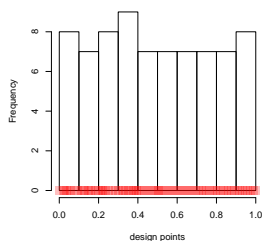
One-at-a-Time,  $k = 1$



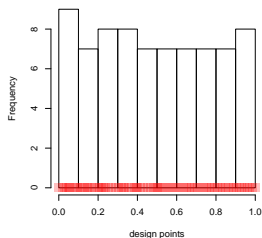
One-at-a-Time,  $k = 4$



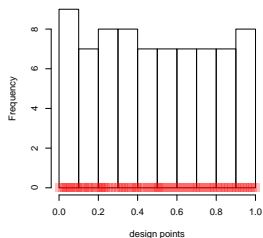
One-at-a-Time,  $k = 20$



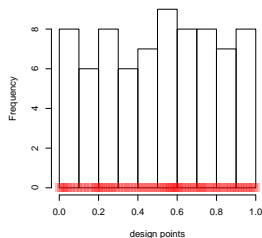
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

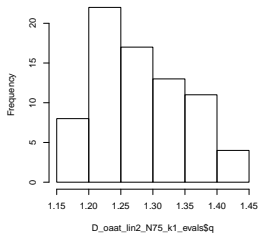


Fast,  $S = 20$

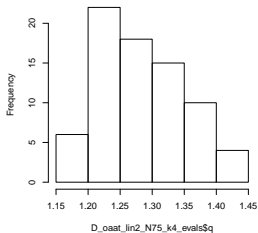


# Evaluations of q(.)

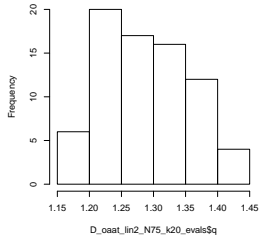
Histogram of D\_oaat\_lin2\_N75\_k1\_evals\$q



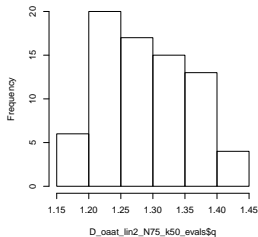
Histogram of D\_oaat\_lin2\_N75\_k4\_evals\$q



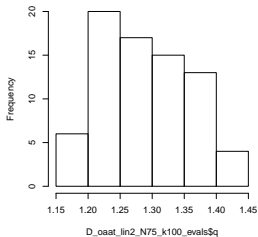
Histogram of D\_oaat\_lin2\_N75\_k20\_evals\$q



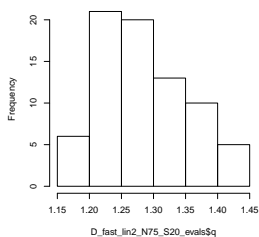
Histogram of D\_oaat\_lin2\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin2\_N75\_k100\_evals\$q

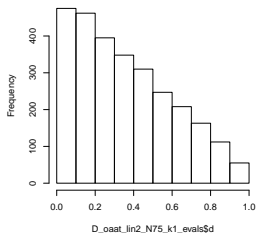


Histogram of D\_fast\_lin2\_N75\_S20\_evals\$q

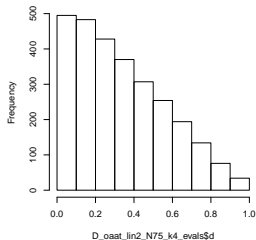


# Pairwise distances of design points

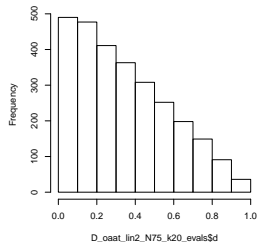
Histogram of D\_oaat\_lin2\_N75\_k1\_evals\$d



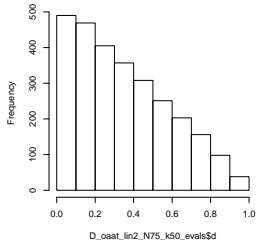
Histogram of D\_oaat\_lin2\_N75\_k4\_evals\$d



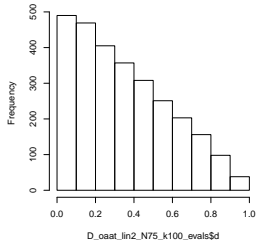
Histogram of D\_oaat\_lin2\_N75\_k20\_evals\$d



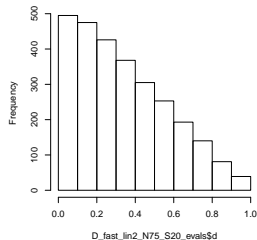
Histogram of D\_oaat\_lin2\_N75\_k50\_evals\$d



Histogram of D\_oaat\_lin2\_N75\_k100\_evals\$d

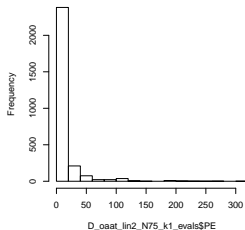


Histogram of D\_fast\_lin2\_N75\_S20\_evals\$d

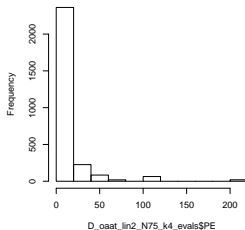


# Pairwise potential energies of design points

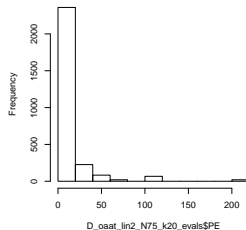
Histogram of D\_oaat\_lin2\_N75\_k1\_evals\$PE



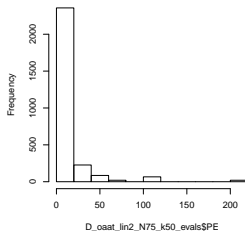
Histogram of D\_oaat\_lin2\_N75\_k4\_evals\$PE



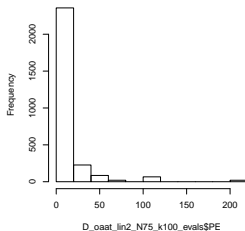
Histogram of D\_oaat\_lin2\_N75\_k20\_evals\$PE



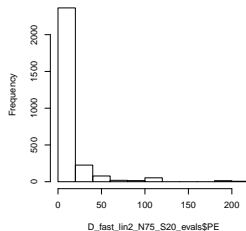
Histogram of D\_oaat\_lin2\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin2\_N75\_k100\_evals\$PE



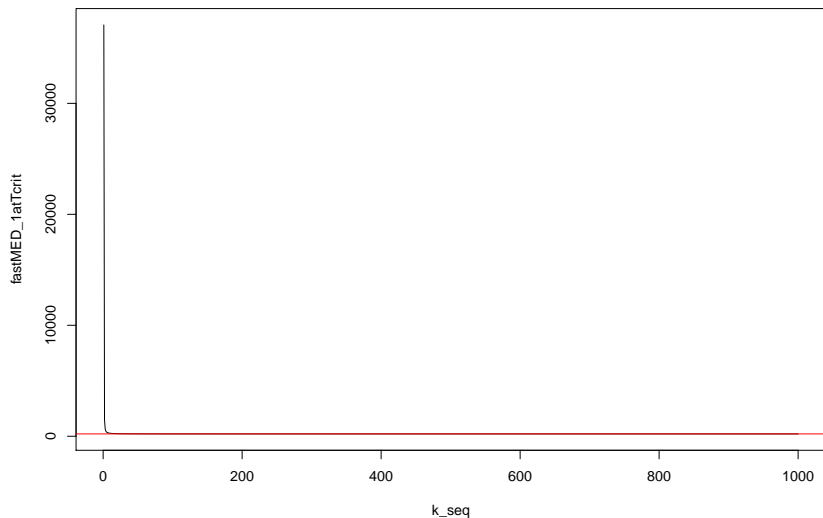
Histogram of D\_fast\_lin2\_N75\_S20\_evals\$PE



# Comparing Evaluations for each $N = 75$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	36.335	37.069	37.248	37.135	37.135	37.067
Fast	302.5	210.13	210.08	209.66	209.66	209.51
1atT(k=4)	492.53	465.92	466.77	466.43	466.43	451.56
Mean(D)	0.52681	0.51185	0.48986	0.48604	0.48604	0.50762
sd(D)	0.30757	0.28924	0.2955	0.29894	0.29894	0.2923

# Fast MED Evaluated at One-at-a-Time Criterion



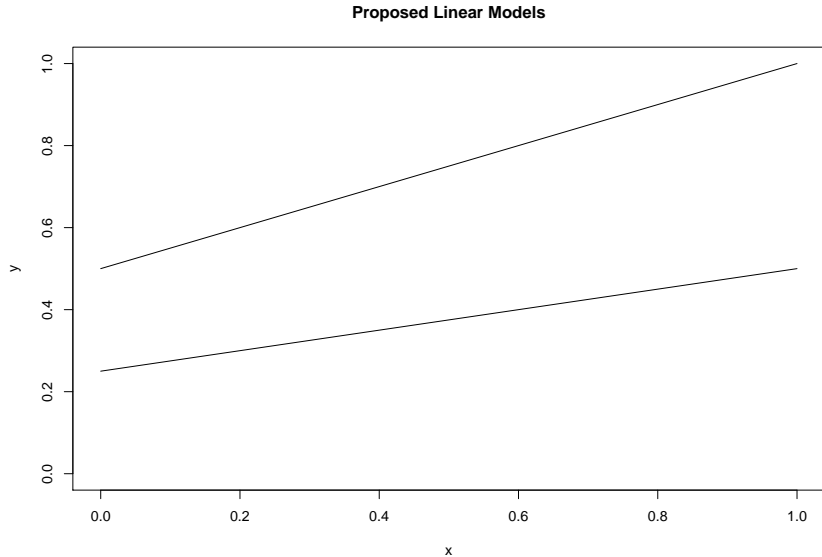
```
## [1] "Fast Criterion : 209.513428140087"
```

```
## [1] "One-at-a-Time Criterion at max k : 209.545525843194"
```

IV. intercept at 0.5 with space in-between

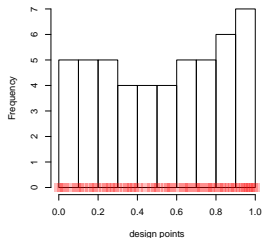


## IV. Proposed Linear Models

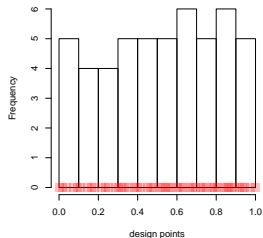


# Designs, $N = 50$

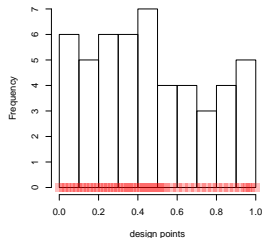
One-at-a-Time,  $k = 1$



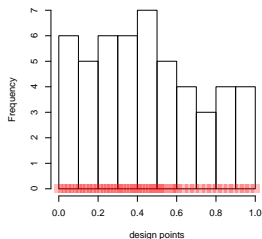
One-at-a-Time,  $k = 4$



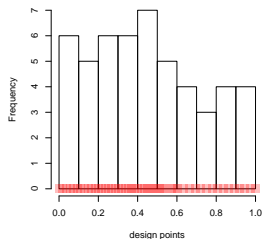
One-at-a-Time,  $k = 20$



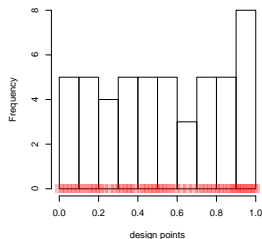
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

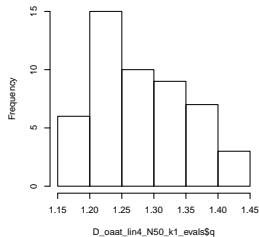


Fast,  $S = 20$

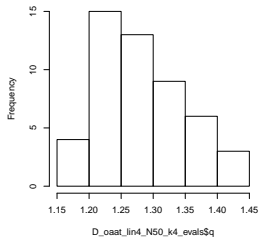


# Evaluations of $q(.)$

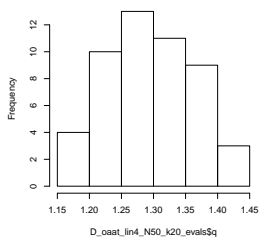
Histogram of D\_oaat\_lin4\_N50\_k1\_evals\$q



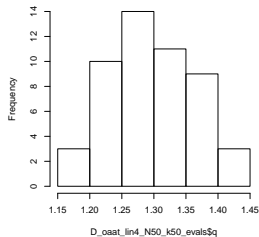
Histogram of D\_oaat\_lin4\_N50\_k4\_evals\$q



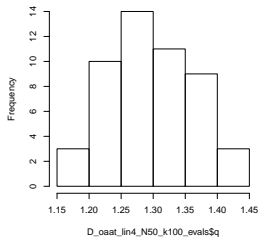
Histogram of D\_oaat\_lin4\_N50\_k20\_evals\$q



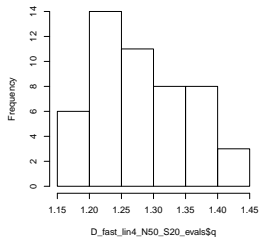
Histogram of D\_oaat\_lin4\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin4\_N50\_k100\_evals\$q

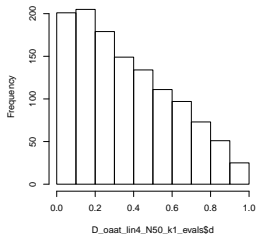


Histogram of D\_fast\_lin4\_N50\_S20\_evals\$q

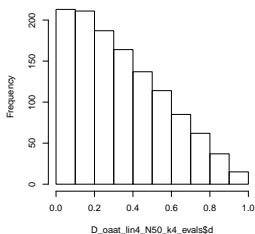


# Pairwise distances of design points

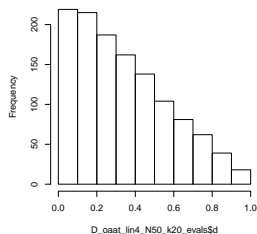
Histogram of D\_oaat\_lin4\_N50\_k1\_evals\$d



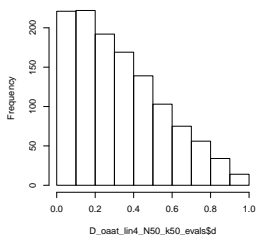
Histogram of D\_oaat\_lin4\_N50\_k4\_evals\$d



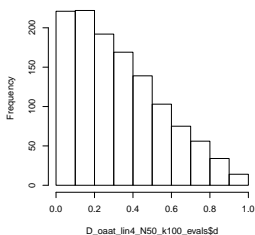
Histogram of D\_oaat\_lin4\_N50\_k20\_evals\$d



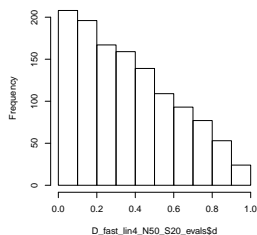
Histogram of D\_oaat\_lin4\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin4\_N50\_k100\_evals\$d

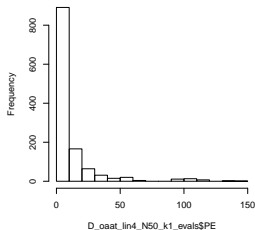


Histogram of D\_fast\_lin4\_N50\_S20\_evals\$d

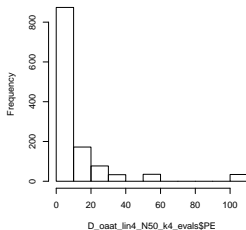


# Pairwise potential energies of design points

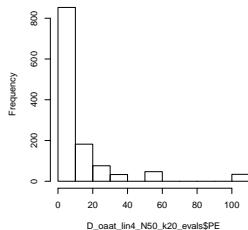
Histogram of D\_oaat\_lin4\_N50\_k1\_evals\$PE



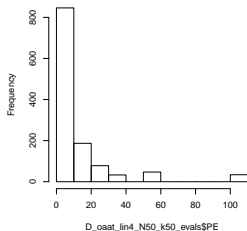
Histogram of D\_oaat\_lin4\_N50\_k4\_evals\$PE



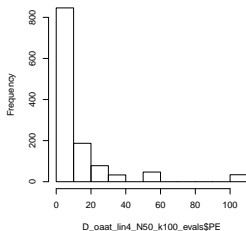
Histogram of D\_oaat\_lin4\_N50\_k20\_evals\$PE



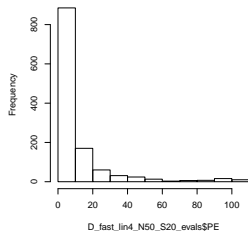
Histogram of D\_oaat\_lin4\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin4\_N50\_k100\_evals\$PE



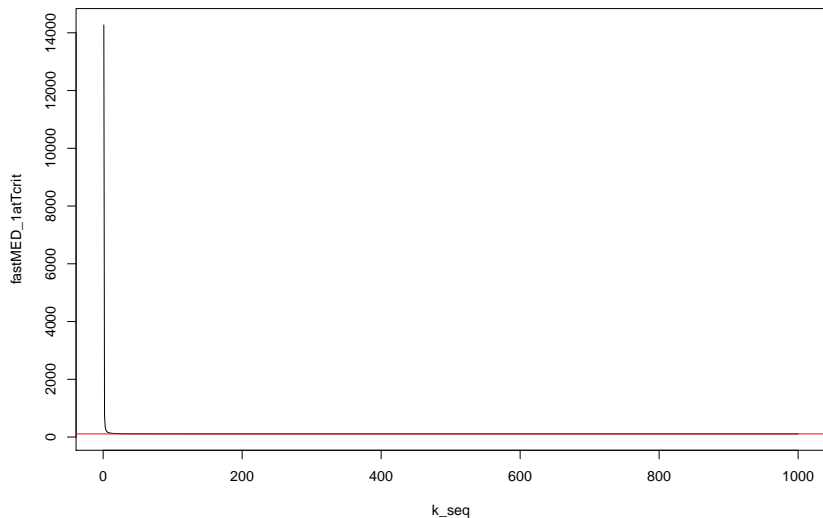
Histogram of D\_fast\_lin4\_N50\_S20\_evals\$PE



# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	14.448	14.712	15.394	15.558	15.558	14.271
Fast	144.42	105.58	105.23	105.32	105.32	108.16
1atT(k=4)	266.3	258.43	259.47	259.44	259.44	240.49
Mean(D)	0.53194	0.5202	0.45769	0.45036	0.45036	0.52515
sd(D)	0.3106	0.2927	0.29233	0.28393	0.28393	0.31158

# Fast MED Evaluated at One-at-a-Time Criterion

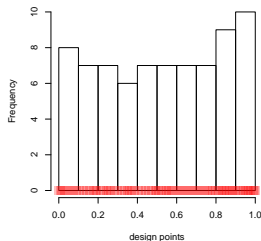


```
## [1] "Fast Criterion : 108.156988894383"
```

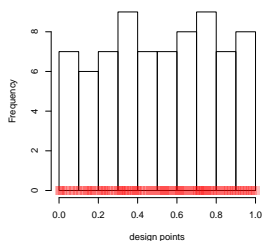
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## [1] "One-at-a-Time Criterion at max k : 108.160369698106"
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# Designs, $N = 75$

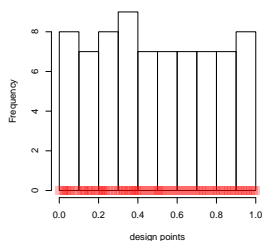
One-at-a-Time,  $k = 1$



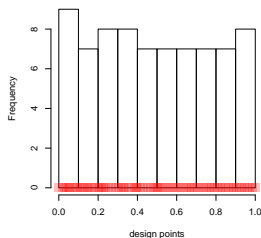
One-at-a-Time,  $k = 4$



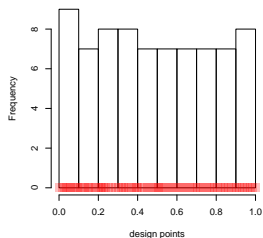
One-at-a-Time,  $k = 20$



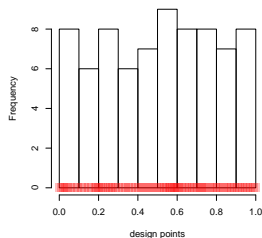
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$



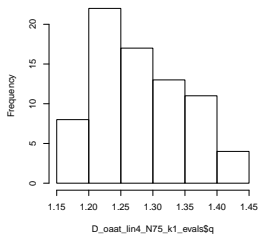
Fast,  $S = 20$



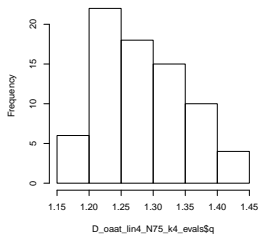


# Evaluations of q(.)

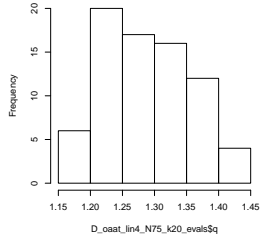
Histogram of D\_oaat\_lin4\_N75\_k1\_evals\$q



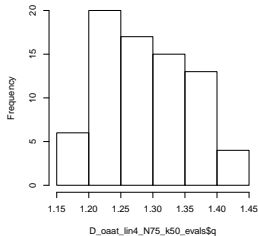
Histogram of D\_oaat\_lin4\_N75\_k4\_evals\$q



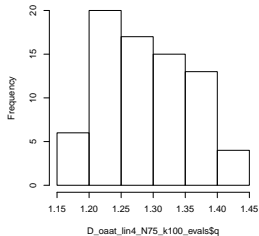
Histogram of D\_oaat\_lin4\_N75\_k20\_evals\$q



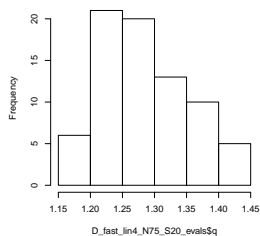
Histogram of D\_oaat\_lin4\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin4\_N75\_k100\_evals\$q

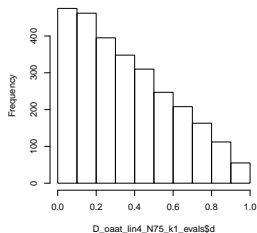


Histogram of D\_fast\_lin4\_N75\_S20\_evals\$q

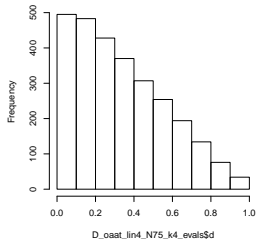


# Pairwise distances of design points

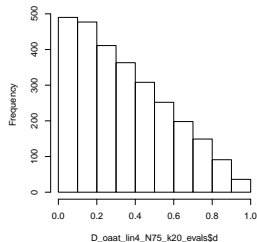
Histogram of D\_oaat\_lin4\_N75\_k1\_evals\$d



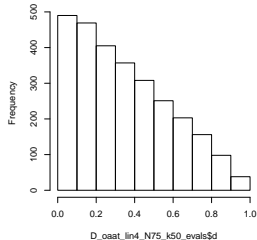
Histogram of D\_oaat\_lin4\_N75\_k4\_evals\$d



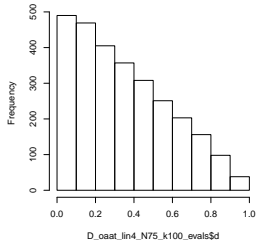
Histogram of D\_oaat\_lin4\_N75\_k20\_evals\$d



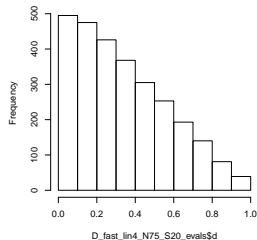
Histogram of D\_oaat\_lin4\_N75\_k50\_evals\$d



Histogram of D\_oaat\_lin4\_N75\_k100\_evals\$d

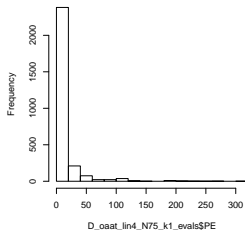


Histogram of D\_fast\_lin4\_N75\_S20\_evals\$d

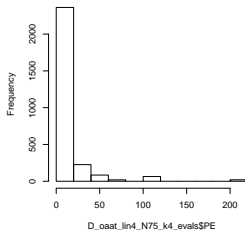


# Pairwise potential energies of design points

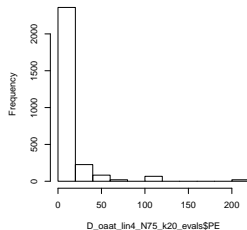
Histogram of D\_oaat\_lin4\_N75\_k1\_evals\$PE



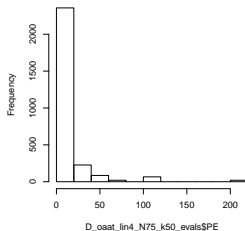
Histogram of D\_oaat\_lin4\_N75\_k4\_evals\$PE



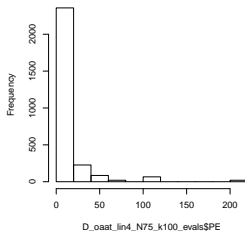
Histogram of D\_oaat\_lin4\_N75\_k20\_evals\$PE



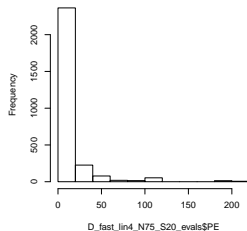
Histogram of D\_oaat\_lin4\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin4\_N75\_k100\_evals\$PE



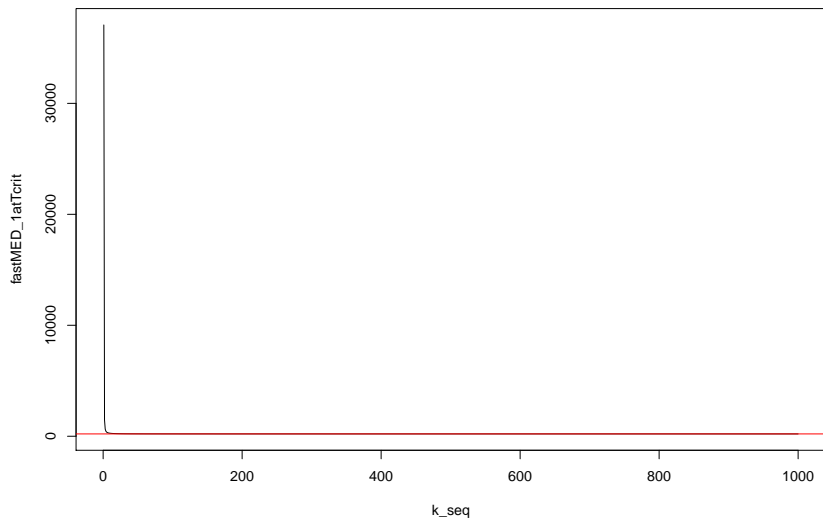
Histogram of D\_fast\_lin4\_N75\_S20\_evals\$PE



# Comparing Evaluations for each $N = 75$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	36.335	37.069	37.248	37.135	37.135	37.067
Fast	302.5	210.13	210.08	209.66	209.66	209.51
1atT(k=4)	492.53	465.92	466.77	466.43	466.43	451.56
Mean(D)	0.52681	0.51185	0.48986	0.48604	0.48604	0.50762
sd(D)	0.30757	0.28924	0.2955	0.29894	0.29894	0.2923

# Fast MED Evaluated at One-at-a-Time Criterion



```
## [1] "Fast Criterion : 209.513428140087"
```

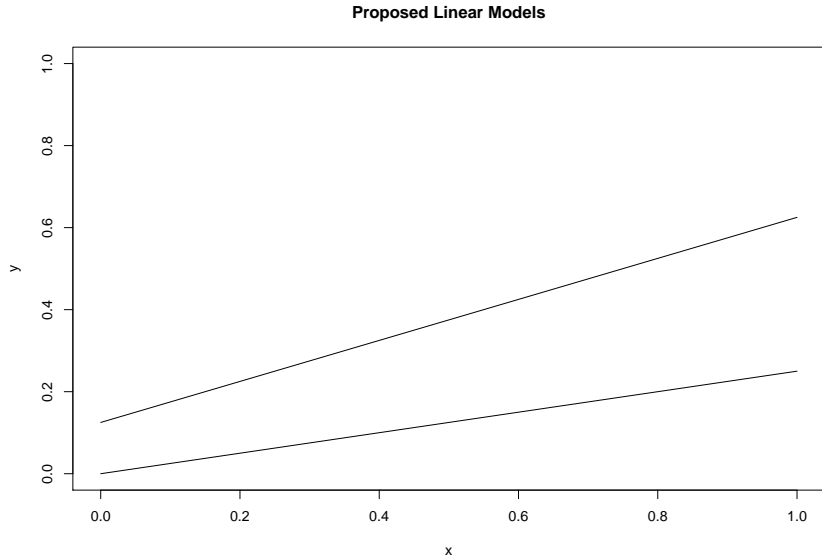
```
## [1] "One-at-a-Time Criterion at max k : 209.545525843194"
```

## Comparing I and III

- ▶ The designs are exactly the same here as well, regardless of where the intercept is!
- ▶ As with the comparison of I and III, all that matters is how much distance there is between the two functions  $f_1(x)$  and  $f_2(x)$ , at a given point  $x$ .

V. less space in-between

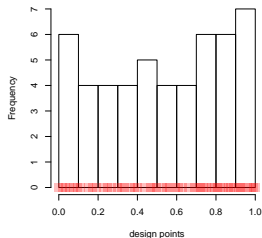
## V. Proposed Linear Models



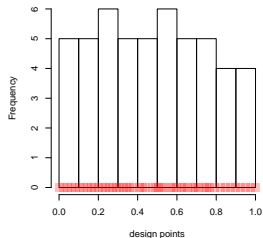


# Designs, $N = 50$

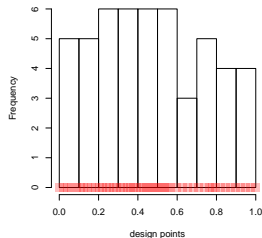
One-at-a-Time,  $k = 1$



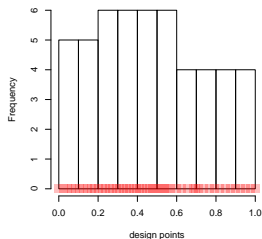
One-at-a-Time,  $k = 4$



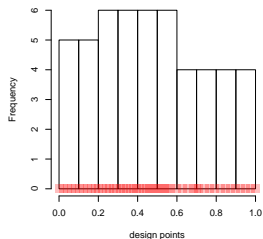
One-at-a-Time,  $k = 20$



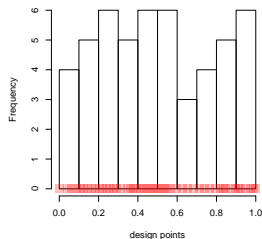
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

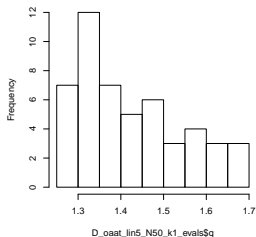


Fast,  $S = 20$

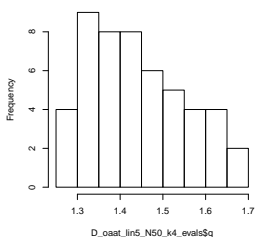


# Evaluations of q(.)

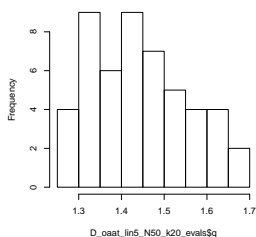
Histogram of D\_oaat\_lin5\_N50\_k1\_evals\$q



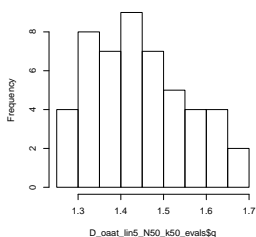
Histogram of D\_oaat\_lin5\_N50\_k4\_evals\$q



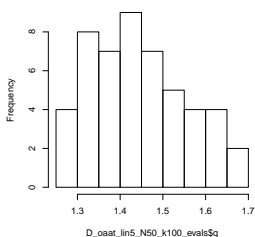
Histogram of D\_oaat\_lin5\_N50\_k20\_evals\$q



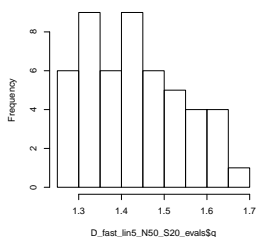
Histogram of D\_oaat\_lin5\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin5\_N50\_k100\_evals\$q

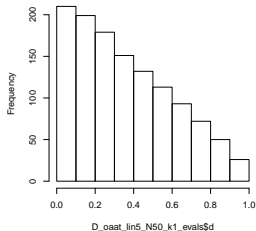


Histogram of D\_fast\_lin5\_N50\_S20\_evals\$q

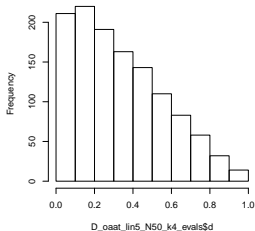


# Pairwise distances of design points

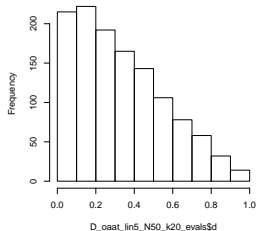
Histogram of D\_oaat\_lin5\_N50\_k1\_evals\$d



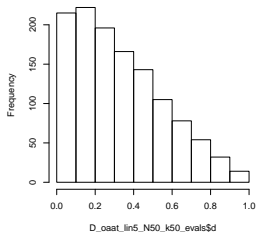
Histogram of D\_oaat\_lin5\_N50\_k4\_evals\$d



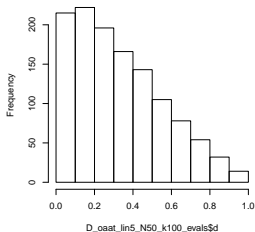
Histogram of D\_oaat\_lin5\_N50\_k20\_evals\$d



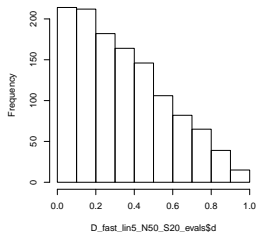
Histogram of D\_oaat\_lin5\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin5\_N50\_k100\_evals\$d

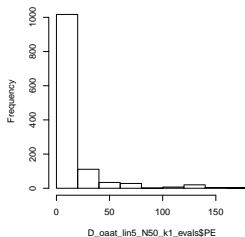


Histogram of D\_fast\_lin5\_N50\_S20\_evals\$d

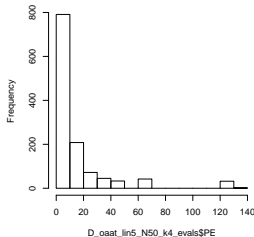


# Pairwise potential energies of design points

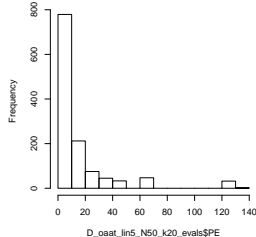
Histogram of D\_oaat\_lin5\_N50\_k1\_evals\$PE



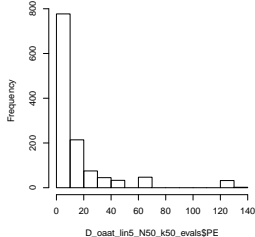
Histogram of D\_oaat\_lin5\_N50\_k4\_evals\$PE



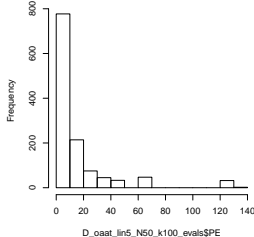
Histogram of D\_oaat\_lin5\_N50\_k20\_evals\$PE



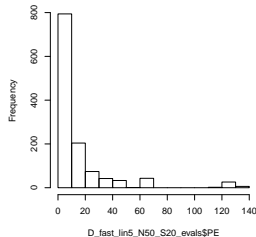
Histogram of D\_oaat\_lin5\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin5\_N50\_k100\_evals\$PE



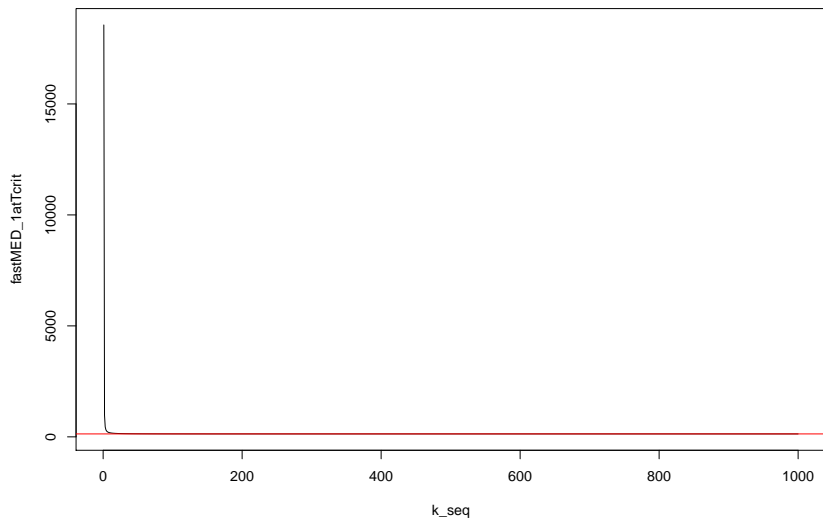
Histogram of D\_fast\_lin5\_N50\_S20\_evals\$PE



# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	17.834	18.691	19.038	19.067	19.064	18.559
Fast	179.04	130.52	130.62	130.94	130.93	132.39
1atT(k=4)	328.02	318.2	317.77	317.62	317.56	317.09
Mean(D)	0.53486	0.48047	0.47149	0.47004	0.47008	0.5038
sd(D)	0.30937	0.2875	0.28524	0.28363	0.28367	0.29313

# Fast MED Evaluated at One-at-a-Time Criterion

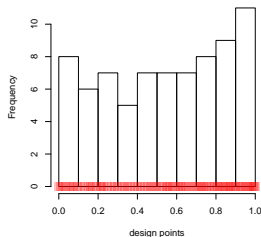


```
## [1] "Fast Criterion : 132.385179772763"
```

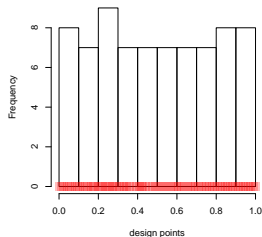
```
## [1] "One-at-a-Time Criterion at max k : 132.385408213725"
```

# Designs, $N = 75$

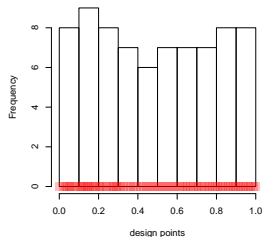
One-at-a-Time,  $k = 1$



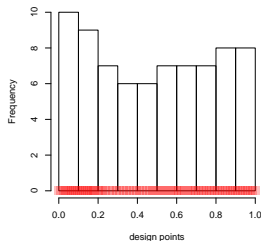
One-at-a-Time,  $k = 4$



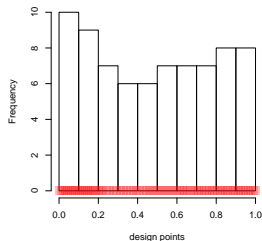
One-at-a-Time,  $k = 20$



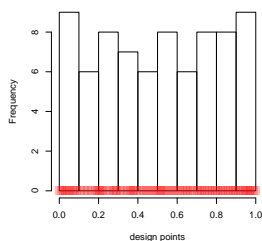
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

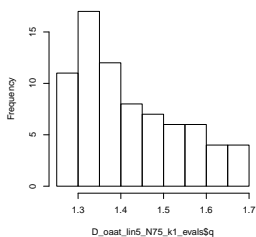


Fast,  $S = 20$

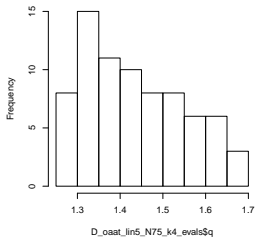


# Evaluations of $q(.)$

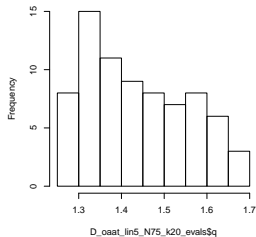
Histogram of D\_oaat\_lin5\_N75\_k1\_evals\$q



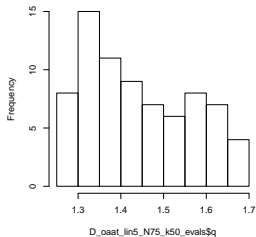
Histogram of D\_oaat\_lin5\_N75\_k4\_evals\$q



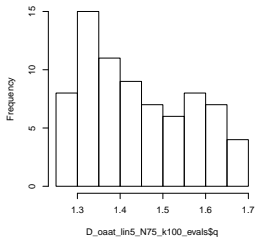
Histogram of D\_oaat\_lin5\_N75\_k20\_evals\$q



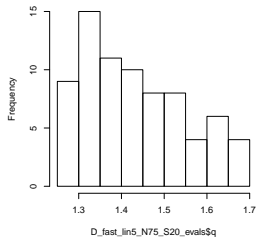
Histogram of D\_oaat\_lin5\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin5\_N75\_k100\_evals\$q

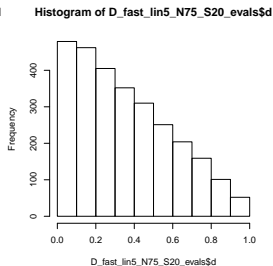
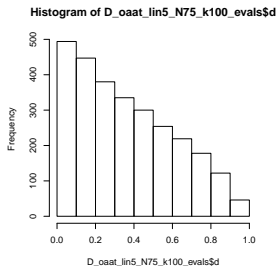
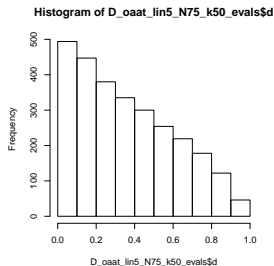
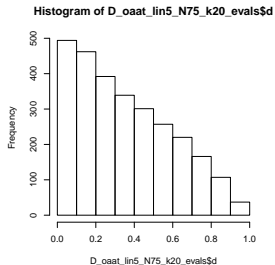
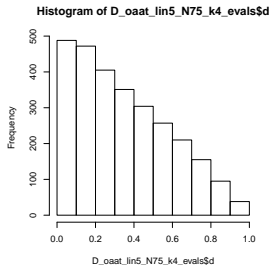
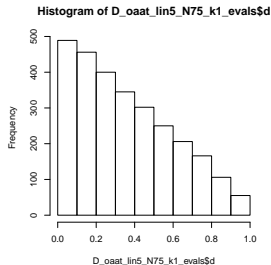


Histogram of D\_fast\_lin5\_N75\_S20\_evals\$q



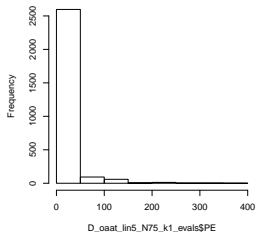


# Pairwise distances of design points

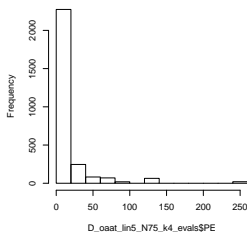


# Pairwise potential energies of design points

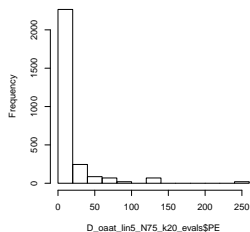
Histogram of D\_oaat\_lin5\_N75\_k1\_evals\$PE



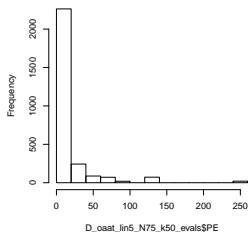
Histogram of D\_oaat\_lin5\_N75\_k4\_evals\$PE



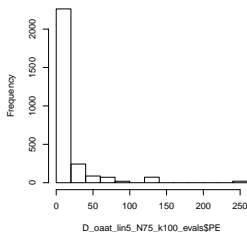
Histogram of D\_oaat\_lin5\_N75\_k20\_evals\$PE



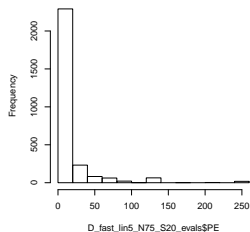
Histogram of D\_oaat\_lin5\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin5\_N75\_k100\_evals\$PE



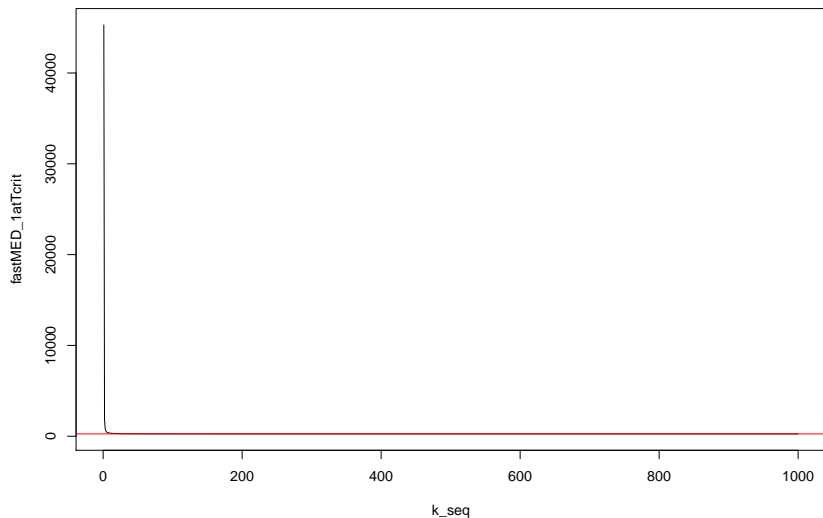
Histogram of D\_fast\_lin5\_N75\_S20\_evals\$PE



# Comparing Evaluations for each $N = 75$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	44.825	45.667	46.168	46.274	46.273	45.291
Fast	377.04	257.68	256.01	255.9	255.9	256.54
1atT(k=4)	606.54	571.78	571.35	571.96	571.96	567.94
Mean(D)	0.53962	0.49804	0.49274	0.48676	0.4868	0.50897
sd(D)	0.30624	0.29905	0.30355	0.31011	0.31014	0.30376

# Fast MED Evaluated at One-at-a-Time Criterion



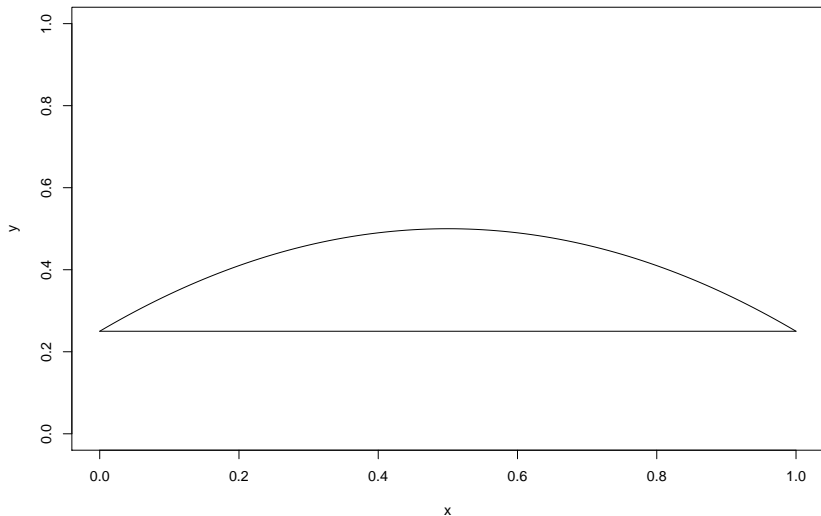
```
## [1] "Fast Criterion : 256.544891845871"
```

```
## [1] "One-at-a-Time Criterion at max k : 256.70600793309"
```

## VI. linear vs quadratic

# VI. Proposed Linear Models

## Proposed Linear and Quadratic Models

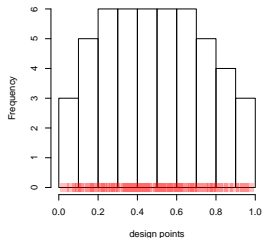


```
## Warning in calculateEvals(D_oaat_lin6_N50_k1, N, mean_beta0, mean_beta1, :  
## var_mean0 != var_mean1. posterior variance will be calculated wrt H1
```

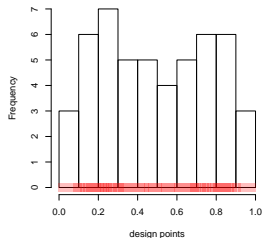
```
## Warning in calculateEvals(D_oaat_lin6_N50_k4, N, mean_beta0, mean_beta1, :  
## var_mean0 != var_mean1. posterior variance will be calculated wrt H1
```

# Designs, $N = 50$

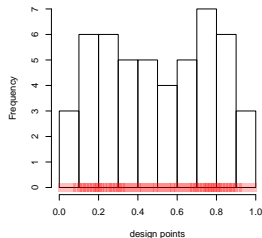
One-at-a-Time,  $k = 1$



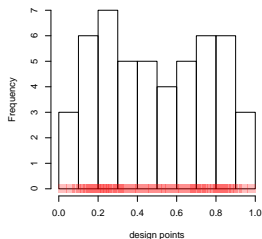
One-at-a-Time,  $k = 4$



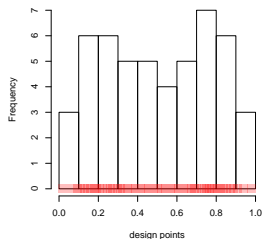
One-at-a-Time,  $k = 20$



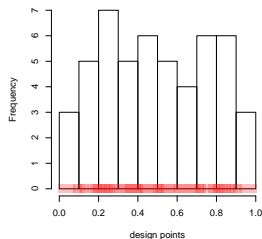
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

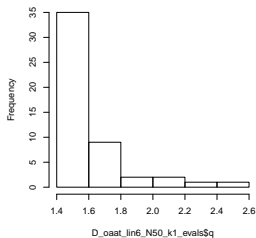


Fast,  $S = 20$

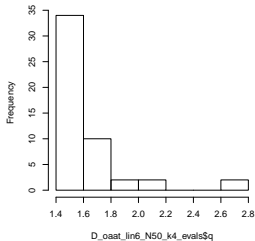


# Evaluations of $q(.)$

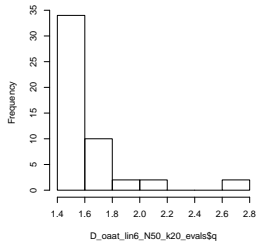
Histogram of D\_oaat\_lin6\_N50\_k1\_evals\$q



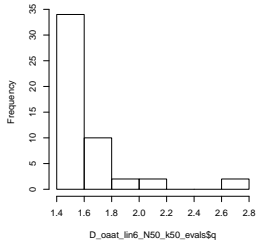
Histogram of D\_oaat\_lin6\_N50\_k4\_evals\$q



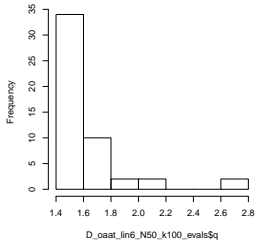
Histogram of D\_oaat\_lin6\_N50\_k20\_evals\$q



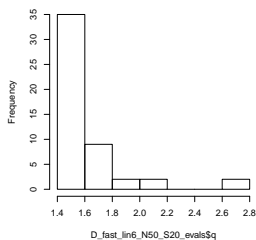
Histogram of D\_oaat\_lin6\_N50\_k50\_evals\$q



Histogram of D\_oaat\_lin6\_N50\_k100\_evals\$q



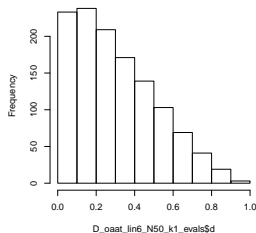
Histogram of D\_fast\_lin6\_N50\_S20\_evals\$q



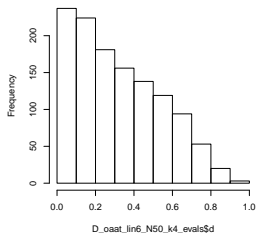


# Pairwise distances of design points

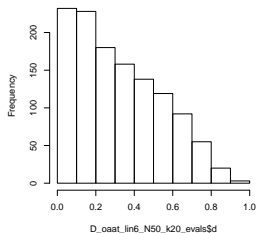
Histogram of D\_oaat\_lin6\_N50\_k1\_evals\$d



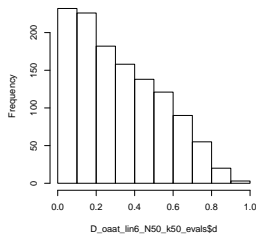
Histogram of D\_oaat\_lin6\_N50\_k4\_evals\$d



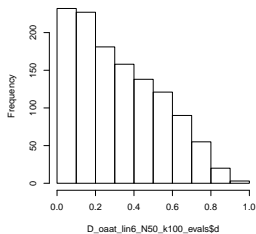
Histogram of D\_oaat\_lin6\_N50\_k20\_evals\$d



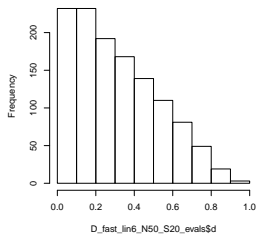
Histogram of D\_oaat\_lin6\_N50\_k50\_evals\$d



Histogram of D\_oaat\_lin6\_N50\_k100\_evals\$d

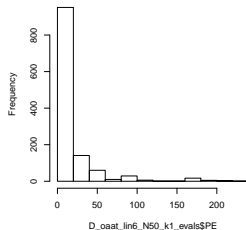


Histogram of D\_fast\_lin6\_N50\_S20\_evals\$d

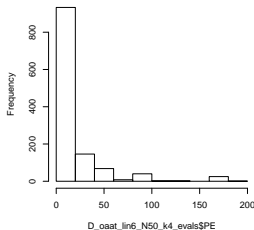


# Pairwise potential energies of design points

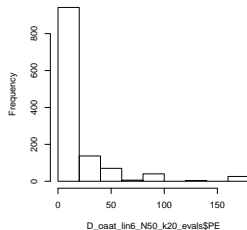
Histogram of D\_oaat\_lin6\_N50\_k1\_evals\$PE



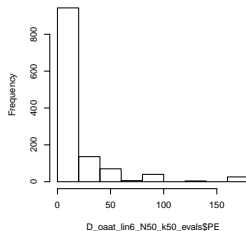
Histogram of D\_oaat\_lin6\_N50\_k4\_evals\$PE



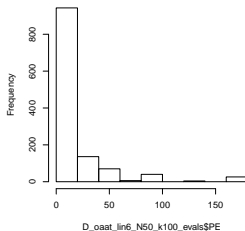
Histogram of D\_oaat\_lin6\_N50\_k20\_evals\$PE



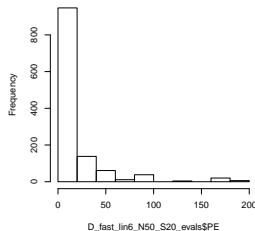
Histogram of D\_oaat\_lin6\_N50\_k50\_evals\$PE



Histogram of D\_oaat\_lin6\_N50\_k100\_evals\$PE



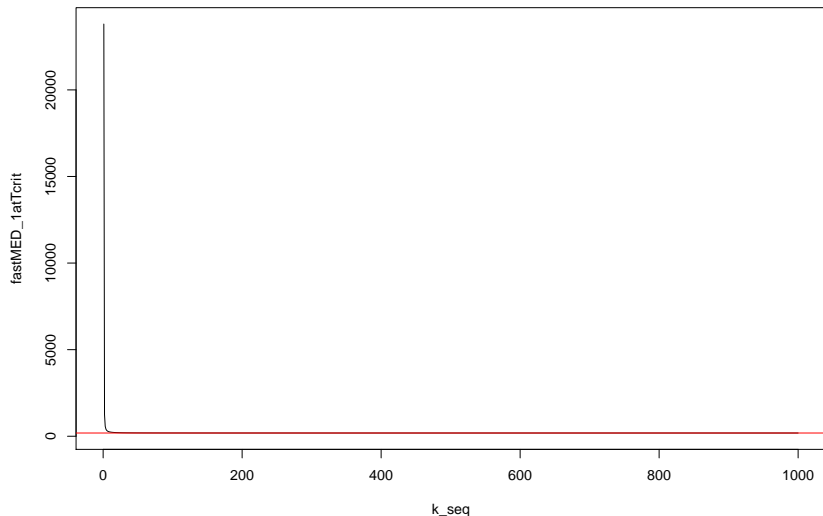
Histogram of D\_fast\_lin6\_N50\_S20\_evals\$PE



# Comparing Evaluations for each $N = 50$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	23.673	24.021	23.902	23.888	23.884	23.803
Fast	226.43	180.72	177.07	176.99	176.97	186.59
1atT(k=4)	426.78	414.73	409.09	408.43	408.23	413.16
Mean(D)	0.49045	0.49371	0.5053	0.4947	0.5053	0.49669
sd(D)	0.26054	0.27526	0.27563	0.27547	0.27544	0.26875

# Fast MED Evaluated at One-at-a-Time Criterion



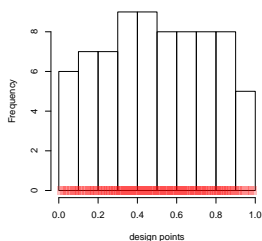
```
## [1] "Fast Criterion : 186.591526705804"
```

```
## [1] "One-at-a-Time Criterion at max k : 186.593304308173"
```

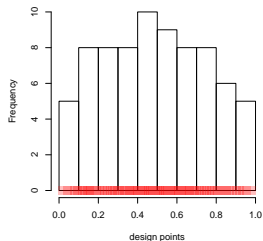
```
## Warning in calculateEvals(D_oaat_lin6_N75_k1, N, mean_beta0, mean_beta1, :  
## var_mean0 != var_mean1. posterior variance will be calculated wrt H1
```

# Designs, $N = 75$

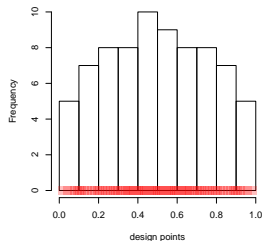
One-at-a-Time,  $k = 1$



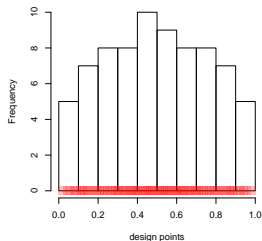
One-at-a-Time,  $k = 4$



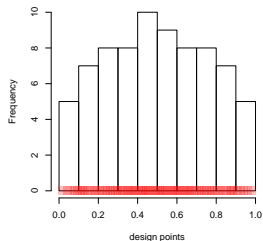
One-at-a-Time,  $k = 20$



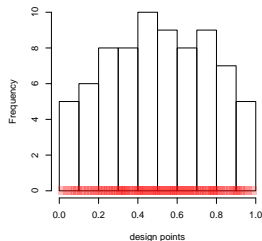
One-at-a-Time,  $k = 50$



One-at-a-Time,  $k = 100$

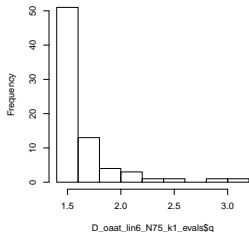


Fast,  $S = 20$

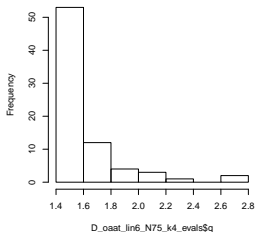


# Evaluations of q(.)

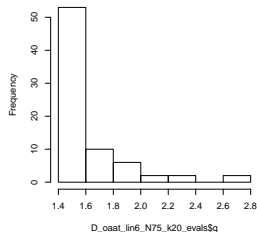
Histogram of D\_oaat\_lin6\_N75\_k1\_evals\$q



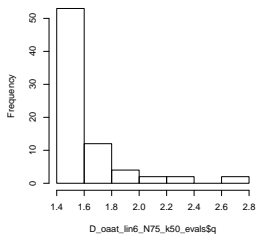
Histogram of D\_oaat\_lin6\_N75\_k4\_evals\$q



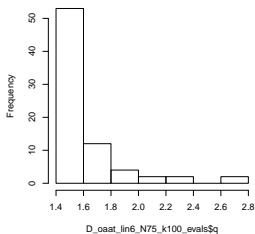
Histogram of D\_oaat\_lin6\_N75\_k20\_evals\$q



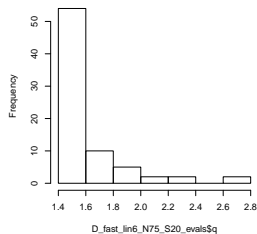
Histogram of D\_oaat\_lin6\_N75\_k50\_evals\$q



Histogram of D\_oaat\_lin6\_N75\_k100\_evals\$q

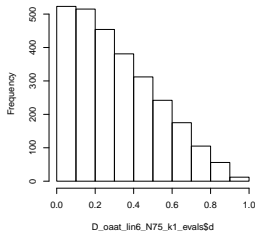


Histogram of D\_fast\_lin6\_N75\_S20\_evals\$q

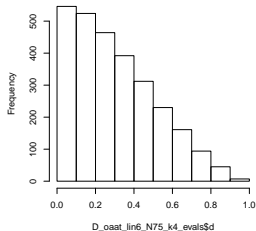


# Pairwise distances of design points

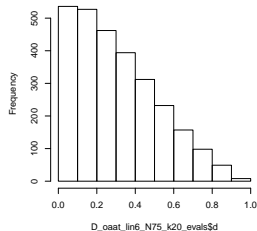
Histogram of D\_oaat\_lin6\_N75\_k1\_evals\$d



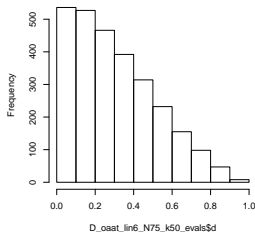
Histogram of D\_oaat\_lin6\_N75\_k4\_evals\$d



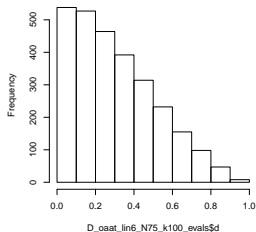
Histogram of D\_oaat\_lin6\_N75\_k20\_evals\$d



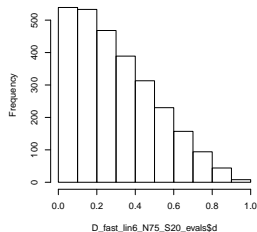
Histogram of D\_oaat\_lin6\_N75\_k50\_evals\$d



Histogram of D\_oaat\_lin6\_N75\_k100\_evals\$d

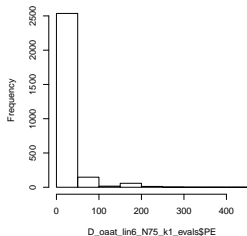


Histogram of D\_fast\_lin6\_N75\_S20\_evals\$d

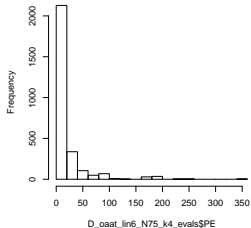


# Pairwise potential energies of design points

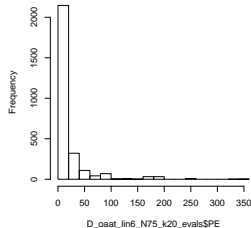
Histogram of D\_oaat\_lin6\_N75\_k1\_evals\$PE



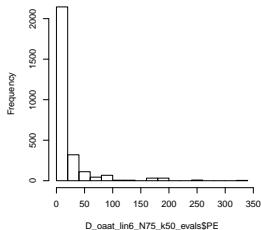
Histogram of D\_oaat\_lin6\_N75\_k4\_evals\$PE



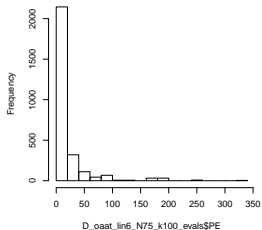
Histogram of D\_oaat\_lin6\_N75\_k20\_evals\$PE



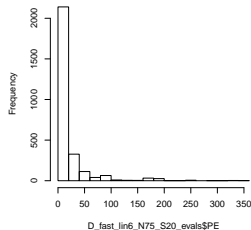
Histogram of D\_oaat\_lin6\_N75\_k50\_evals\$PE



Histogram of D\_oaat\_lin6\_N75\_k100\_evals\$PE



Histogram of D\_fast\_lin6\_N75\_S20\_evals\$PE

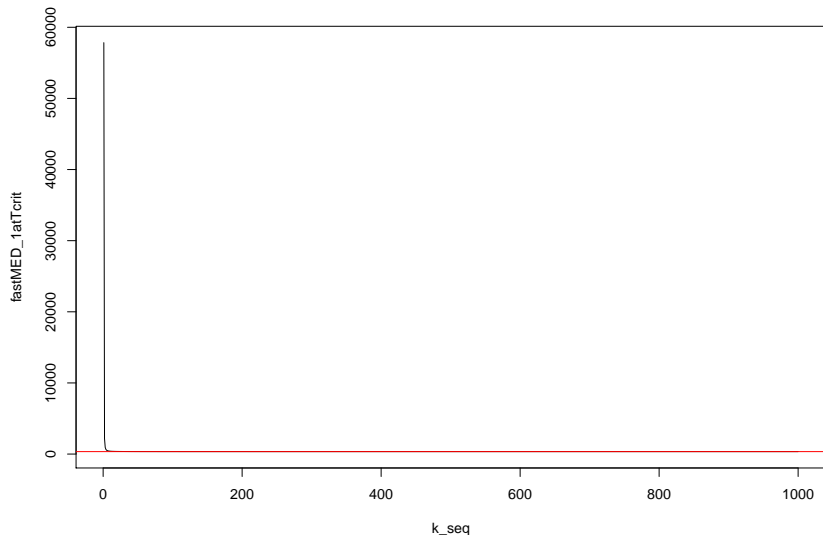




# Comparing Evaluations for each $N = 75$ Design

	1atT,k=1	1atT,k=4	1atT,k=20	1atT,k=50	1atT,k=100	Fast
TPE $\times 10e-3$	57.335	57.565	57.528	57.483	57.485	57.841
Fast	424.36	348.11	341.87	339.98	339.98	344.89
1atT(k=4)	641.68	632.38	632.58	631.56	631.58	651.87
Mean(D)	0.49943	0.4895	0.49999	0.5	0.5	0.50883
sd(D)	0.2703	0.26168	0.26357	0.26268	0.26265	0.26129

# Fast MED Evaluated at One-at-a-Time Criterion



```
## [1] "Fast Criterion : 344.892996988244"
```

```
## [1] "One-at-a-Time Criterion at max k : 344.922205119827"
```