MED for Model Selection : Linear Regression

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Simple Linear Regression without Intercept

One-at-a-Time Algorithm

Fast Algorithm

Other Designs

The Table

Simple Linear Regression with Intercept

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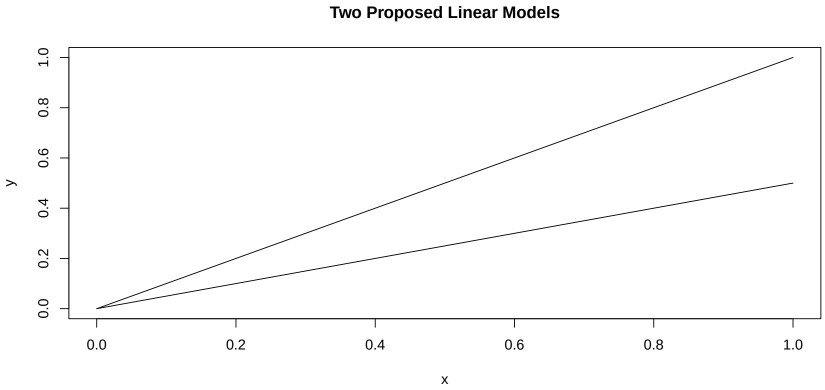
Design an Experiment that Estimates Slope



- Want to choose design $\mathbf{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ to gather data that will
  1. help distinguish these two slopes
  2. allow adequate estimation of β.
- Idea: Minimum Energy Design!

Minimum Energy Design

Minimum energy design (MED) is a deterministic sampling method which makes use of evaluations of the target distribution f to obtain a weighted space-filling design.

Definition:

Design $\mathbf{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ is a minimum energy design if it minimizes the total potential energy given by:

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

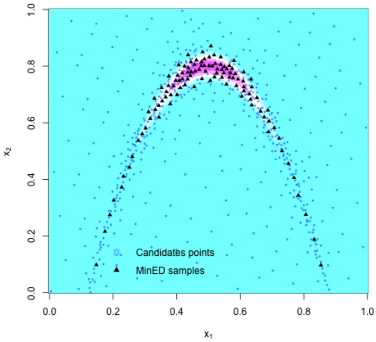
Choose the charge function, $q = \frac{1}{f^{1/2p}}$ so that the limiting distribution of the design points is target distribution, f.

Objective:

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

Example: The “Banana” Function

- $N = 109$
- $K = 6$
- $\Longrightarrow$ number of evaluations of f is $NK = 654$



Advantages of MED

Compared to other sampling or experiment design methods, MED

- has fewer points since it avoids repeated samples and points that are too close together (unlike MCMC).
- requires fewer evaluations of the posterior (unlike MCMC).
- is not prone to missing high-density regions (unlike other deterministic methods, e.g. QMC)

Simple Linear Regression without Intercept

- Assume $y_i = x_i\beta + \varepsilon_i$ with $\varepsilon_i \sim N(0, \sigma^2)$ and $\beta \sim N(\mu, \tau^2)$.
- $y_i|\beta \sim N(x_i\beta, \sigma^2)$
- $y_i \sim N(x_i\mu, \sigma^2 + x_i^2\tau^2)$ after marginalizing out β
- Here, we are assuming that the intercept is 0 (or known, in which case we can scale from 0).

Hypotheses

Suppose we suspect $\beta = \mu_0$ or $\beta = \mu_1$, i.e.

$$
\begin{aligned}
H_0 &: \beta \sim N(\mu_0, \tau_0^2) \\
H_1 &: \beta \sim N(\mu_1, \tau_1^2)
\end{aligned}
$$

Evaluating the Designs

Evaluating Methods

- Posterior Variance, i.e. $Var[\beta|y, X]$
- Expected Posterior Probabilities of H_ℓ, $\ell \in \{0, 1\}$ and Expected Bayes Factor
- Design Criteria:
  - Total Potential Energy
  - Criterion for One-at-a-Time Algorithm
  - Criterion for Fast Algorithm

Interpretations

- A design that is better for estimating β might have smaller regression variance.
- A design that is better for hypothesis testing will give larger expected values of BF_{01} for simulated data Y under H_0.

Posterior Variance

In the simple linear regression model with no intercept, $y \sim N(X\beta + \sigma^2 I)$ with $\beta \sim N(\mu, \tau^2)$,

- $\hat{\beta} = \frac{1}{\sigma^2}\Sigma_B(X^T y + \frac{\sigma^2}{\tau^2}\mu)$ with posterior distribution

$$\beta | y, X \sim N\left(m_B, \Sigma_B\right)$$

where

$$\Sigma_B = \sigma^2(X^T X + \frac{\sigma^2}{\tau^2} I)^{-1}$$

$$m_B = \frac{1}{\sigma^2}\Sigma_B(X^T y + \frac{\sigma^2}{\tau^2}\mu)$$

Posterior Probabilities of Hypotheses and Bayes Factors

- Posterior Probability of model $H_\ell, \ell \in 1, ..., M$:

$$P(H_\ell|Y) = \frac{\pi_\ell P(Y|H_\ell)}{\sum_{m=1}^{M} \pi_m P(Y|H_m)}$$

  where π_m is the prior on H_m (typically $\pi_m = \frac{1}{M}$), and $P(Y|H_m)$ is the model evidence.
- The posterior probability of hypotheses tells which hypothesis is more likely to give the correct model.
- If we have only 2 hypotheses, i.e. $M = 2$, we can also calculate the Bayes Factor, $BF_{01} = \frac{P(H_0|Y)}{P(H_1|Y)}$.

Expected Posterior Probabilities of Hypotheses

- We want to calculate the posterior probabilities of our hypotheses given a design, **D**.
- Since we don't have any data Y to calculate the model evidence, instead we estimate the *expected* model evidence $E_Y[P(Y|H_m)]$ from simulations under a chosen hypothesis.

Estimate Expected Posterior Probability of a Hypothesis

Estimate the expected posterior probability of hypothesis H_ℓ for data $Y = \{y_1, \ldots, y_N\}$ simulated under H_r:

1. Obtain design $\mathbf{D} = \{x_1, ..., x_N\}$.
2. Draw $\beta \sim N(\mu_r, \tau_r^2)$
3. For J simulations of Y under H_r, draw $y_i^{(j)} \sim N(\mathbf{x}\beta, \sigma_r^2)$, $\forall \mathbf{x}_i \in \mathbf{D}$, $j = 1, \ldots, J$.
4. $\forall m \in \{1, ..., M\}$, estimate model evidence $E[P(Y|H_m)|H_r] \approx \frac{1}{J}\sum_{j=1}^{J} P(Y|H_m, \mathbf{D}) \approx \frac{1}{JN}\sum_{j=1}^{J}\sum_{i=1}^{N} P(y_i^{(j)}|H_m, \mathbf{x}_i)$
   - $P(y_i|H_m, \mathbf{x}_i)$ is the density of $N(\mathbf{x}\mu_m, \sigma_m^2 + \mathbf{x}^2\tau_m^2)$ evaluated at y_i and $\mathbf{x_i}$.
5. Estimate the posterior probability of H_ℓ: $E[P(H_\ell|Y)|H_r]$

$$E_Y[P(H_\ell|Y)|H_r] \approx \frac{\pi_\ell E_Y[P(Y|H_\ell)|H_r]}{\sum_{m=1}^{M} \pi_m E_Y[P(Y|H_m)|H_r]}$$

MED Criteria

1. The Total Potential Energy, which both algorithms aim to minimize:

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

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

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

which becomes the Total Potential Energy Criterion when $k = 1$.

3. Fast Algorithm tries to minimize:

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

One-at-a-Time Algorithm

One-at-a-Time Algorithm (2015)

Steps to obtain MED using One-at-a-Time algorithm:

1. Obtain *numCandidates* candidate points, $\mathbf{x}$, in $[0, 1]$.
2. Initialize D_N by choosing $\mathbf{x}_j$ to be the candidate $\mathbf{x}$ which optimizes f, where $f(\mathbf{x}) = \text{Wasserstein}(\phi_{0,\mathbf{x}}, \phi_{1,\mathbf{x}})$ and

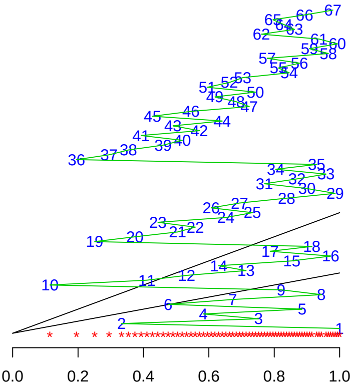
$$\phi_{0,\mathbf{x}} = N(\tilde{\beta_0}\mathbf{x}, \sigma_{\epsilon_0}^2 + \mathbf{x}^2\sigma_{\beta_0}^2),$$
$$\phi_{1,\mathbf{x}} = N(\tilde{\beta_1}\mathbf{x}, \sigma_{\epsilon_1}^2 + \mathbf{x}^2\sigma_{\beta_1}^2)$$

3. Choose the next point $\mathbf{x}_{j+1}$ by:

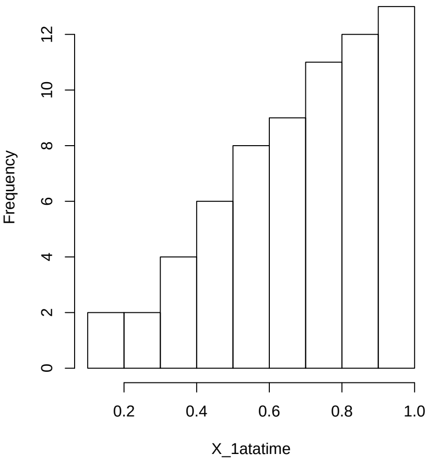
$$\mathbf{x}_{j+1} = \arg\min_{\mathbf{x}} \sum_{i=1}^{j} \left(\frac{q(\mathbf{x}_i)q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \right)^k$$

where $q = 1/f^{(1/2p)}$, $d(x, y)$ is Euclidean distance and (suggested) $k = 4p$.

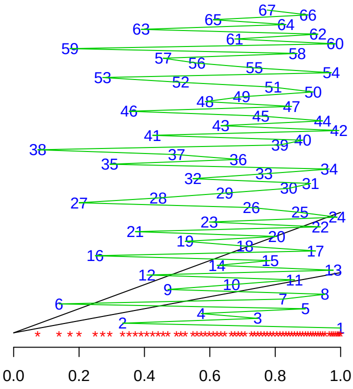
Design generated by One-at-a-Time Algorithm (k = 4)

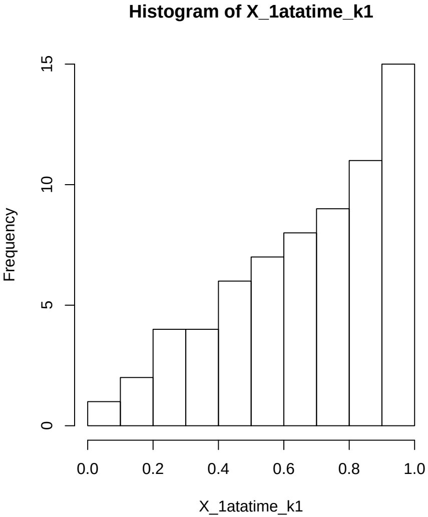


Histogram of X_1atatime



Design generated by One-at-a-Time Algorithm (k = 1)





Fast Algorithm

Fast Algorithm (2018)

In each of K stages, create a new design to iteratively minimize

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

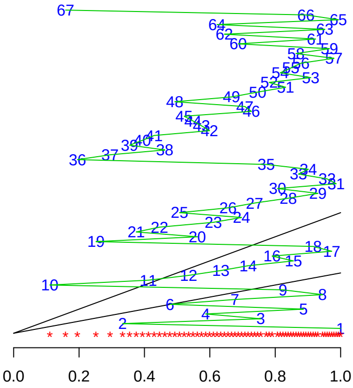
1. Initialize space-filling design $\mathbf{D}_1 = \{\mathbf{x}_1^{(1)} \ldots \mathbf{x}_N^{(1)}\}$
2. For $k = 1, \ldots, K-1$ steps, obtain each design point $\mathbf{x}_j^{(k+1)}$ of the next stage $\mathbf{D}_{k+1}$ by:

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

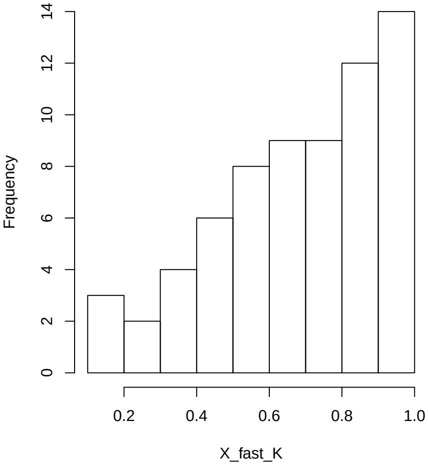
where $\gamma_k = k/(K-1)$ and $\mathbf{C}_j^{k+1}$ is the candidate set for design point $\mathbf{x}_j$ at stage $k+1$.

- points are no longer picked sequentally
- candidates are different for each design point

Design generated by Fast Algorithm (K = 20)



Histogram of X_fast_K



Other Designs

Random Designs

10 simulated random designs ($\mathbf{x} \sim U([0,1]^p)$, $\forall \mathbf{x} \in \mathbf{D}_{\text{random}}$).

- There is large variability for the criteria in designs with randomly chosen design points.

```
# Mean Slope Variance
v_rand
```

```
## [1] 0.001926288
```

```
# Mean Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_rand, crit1_rand, crit2_rand)
```

```
## [1] 7279551279 7046112509 7046949313
```

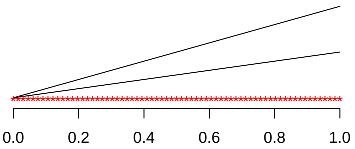
```
# SD Slope Variance
v_rand_sd
```

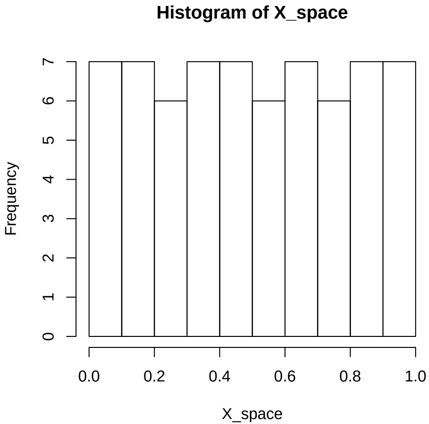
```
## [1] 0.000139415
```

```
# SD Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_rand_sd, crit1_rand_sd, crit2_rand_sd)
```

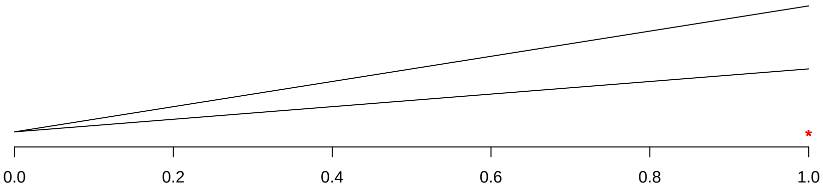
```
## [1] 13290670154 13228511528 13228052751
```

Space-Filling Design





Design at 1



D-Optimal Design

- The D-optimal design seeks to minimize the variance of the estimated regression coefficients (i.e. maximize $\det(X^T X)$, which occurs in the denominator of variance of each of the regression coefficients):

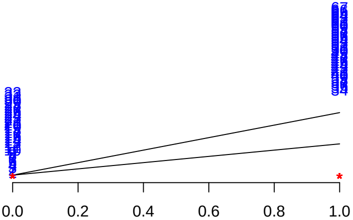
  $$\det(X^T X)^{-1}) = 1/\det(X^T X)$$

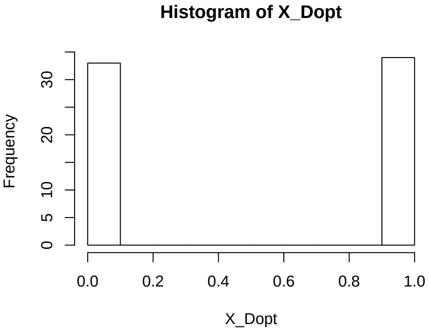
  where X is the data matrix of independent variables.
- It is considered a sequential algorithm, since one can specify fixed points in the design while choosing the rest of the design points.
- It can be interpreted as minimizing the volume of the confidence ellipsoid of the regression estimates of the linear model parameters.
- It is model-dependent, which raises the question of robustness. Here, the model is assumed to be $y = \beta_0 + \beta_1 x_i$ hence why the points are approximately evenly split between 0 and 1 (since $X = [1\ D]$, i.e. $f(X) = (1, x)^T$ in the literature).

Design generated by D-Optimal Criterion

Using `AlgDesign` package (using Federov's exchange algorithm),

where the points are in no particular order. It is assumed that they will be randomized.





```
mean(X_Dopt)
```

```
## [1] 0.5074578
```

```
sd(X_Dopt)
```

```
## [1] 0.5035538
```

I-Optimal Design

- I-Optimal design seeks to minimize the average prediction variance over the entire design space. (In contrast, D-optimality focuses on reducing prediction variance at the design points.)
- The criterion:

$$\int_{\chi} f(x)^T (X^T X)^{-1} f(x)\, dx = \text{tr}((X^T X)^{-1}) M$$

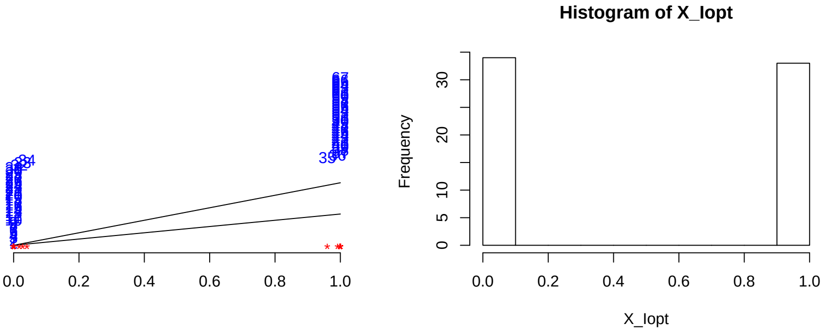
  where $M = \int_{\chi} f(x)^T f(x)\, dx$ and where row vector $f(x)^T$ consists of a 1 followed by the effects corresponding to the assumed model: here, $f(x)^T = (1, x)$.
- This can be approximated (and scaled) by

$$\frac{1}{M} \sum_{i \in \mathbf{C}} \mathbf{x}_i^T \frac{(X^T X)^{-1}}{N} \mathbf{x}_i$$

  where M is the number of candidate points in **C** and N is the number of design points in **D**.
- It is more naturally applied when you know the form of the model and want “good” prediction over your design space
- I-Optimal design is also invariant under linear transformations

Design generated by I-Optimal Criterion

Using `AlgDesign` package (using Federov's exchange algorithm),



```r
mean(X_Iopt)
```

```
## [1] 0.4931015
```

```r
sd(X_Iopt)
```

```
## [1] 0.5016174
```

The Table

Results!

	Fast	1atT,k=4	1atT,k=1	Random	Space	X = 1	D-opt	I-opt
E[H0 | Y0]	0.875	0.883	0.861	0.732	0.737	0.998	0.67	0.67
E[H1 | Y0]	0.125	0.117	0.139	0.268	0.263	0.00181	0.33	0.33
E[BF01 | Y0]	7	7.58	6.18	2.77	2.8	550	2.03	2.03
E[H0 | Y1]	0.123	0.115	0.138	0.269	0.262	0.00193	0.33	0.33
E[H1 | Y1]	0.877	0.885	0.862	0.731	0.738	0.998	0.67	0.67
E[BF01 | Y1]	0.141	0.13	0.16	0.369	0.355	0.00194	0.492	0.492
Var Slope	0.00299	0.0033	0.00259	0.00193	0.00181	NaN	0.000627	0.000633
TPE	2820000	2870000	2760000	7.28e+09	Inf	Inf	Inf	Inf
Fast Crit	44500	43700	80400	7.05e+09	Inf	Inf	Inf	Inf
1atT Crit (k=4)	94100	92200	109000	7.05e+09	Inf	Inf	Inf	Inf
Mean(D)	0.684	0.689	0.674	NA	0.5	1	0.507	0.493
sd(D)	0.23	0.219	0.247	NA	0.295	0	0.504	0.502

- Design at $X = 1$ has highest expected Bayes Factor, and hence is best for testing hypotheses on slope.
- MEDs (designs from Fast & One-at-a-Time algorithms) have second expected Bayes Factors (when H_0 is true)
- Variances on slope, i.e. $Var[\hat{\beta}]$, are all fairly small except for that of design $X = 1$ which cannot be computed.
- `Inf` for the space-filling and D-optimal designs in the evaluations of each of the 3 criteria are from including `0`, which has gives as Wasserstein distance of 0 (in the denominator).

More Evaluations (D, De, A, I, Ge)

- D-efficiency, $De = \frac{\det(X^TX)^{(1/p)}}{N}$, is the relative number of runs (expressed as a percent) required by a hypothetical orthogonal design to achieve the same determinant value. It provides a way of comparing designs across different sample sizes.
  - When a design is orthogonal (all parameters can be estimated independently of each other), $De = 1$
  - De is proportional to the criterion of D-Optimal design, which seeks to maximize $\det(X^TX)$ (or minimize $\det((X^TX)^{-1})$). Hence, we want De close to 1.
- The A-Optimal design minimizes the average variance of the estimates of the regression coefficients: $\mathrm{tr}((X^TX)^{-1})/p$.
- The I-Optimal design seeks to minimize the average prediction variance over the design space.
- Ge, or G-efficiency, is available as a standard of design quality. It is good for minimizing the maximum variance of the predicted values.
  - Ge provides a lower bound on De for approximate theory: $De \geq exp(1 - \frac{1}{Ge})$. Hence, the closer to 1, the better.

When the model is given by $f(x) = (x)^T$,

	Fast	1atT,k=4	1atT,k=1	Space	$X = 1$	D-opt	I-opt
D	34.8	34.9	34.4	22.5	67	34	32.9
De	0.519	0.521	0.514	0.336	1	0.507	0.491
A	1.93	1.92	1.95	2.98	1	1.97	2.04
I	0.642	0.639	0.649	0.992	0.333	0.657	0.679
Ge	0.519	0.521	0.514	0.336	1	0.507	0.491

- Best performances:
  - Highest *De*: $X = 1$ design (MEDs were next best, but D-optimal design was close)
  - Lowest *A*: $X = 1$ design (MEDs were next best)
  - Lowest *I*: $X = 1$ design (MEDs were next best)
  - Highest *Ge*: $X = 1$ design (MEDs were next best)
- Note: Optimal designs were not optimized to this form.

When $f(x) = (1, x)^T$,

	Fast	1atT,k=4	1atT,k=1	Space	X = 1	D-opt	I-opt
D	233	212	269	385	0	1120	1110
De	0.228	0.217	0.245	0.293	0	0.5	0.498
A	14.6	16.1	12.6	7.78	NA	3.02	3.01
I	3.25	3.52	2.89	1.97	NA	1.33	1.34
Ge	0.2	0.181	0.233	0.511	NA	0.985	0.982

- Here, MEDs did not do so well, but they weren't optimized for this model.
  - Highest *De*: D-optimal design (MEDs $>$ space-filling design)
  - Lowest *A*: I-optimal design (space-filling $>$ MEDs)
  - Lowest *I*: D-optimal design (space-filling $>$ MEDs)
  - Highest *Ge*: I-optimal design (space-filling $>$ MEDs)
  - This may suggest that MED might not be very robust...
- Note: `NA`s for $X = 1$ design are due to invertibility of $X^T X$ for design matrix $X = (\mathbf{I}_N \; \mathbf{I}_N)$

Simple Linear Regression with Intercept

SetUp

The set-up is similar, but there are some slight differences:

- Assume $y_i = \beta_0 + x_i\beta_1 + \varepsilon_i$ with $\varepsilon_i \sim N(0, \sigma^2)$ and $\beta \sim N(\mu, \tau^2 I)$, where $\mu = (\beta_0, \beta_1)^T$.
- $y_i|\beta \sim N(\beta_0 + x_i\beta_1, \sigma^2)$
- $y_i \sim N(\tilde{\beta}_0 + x_i\tilde{\beta}_1, \sigma^2 + (x_i^2 + 1)\tau^2)$ after marginalizing out β (iterated expectation and variance again)

Hypotheses

Suppose we suspect $\beta = \mu_0$ or $\beta = \mu_1$, i.e.

$$H_0 : \beta \sim N\left(\mu_0, \tau_0^2 I\right)$$
$$H_1 : \beta \sim N\left(\mu_1, \tau_1^2 I\right)$$

where $\mu_0 = (\beta_0^{(0)}, \beta_0^{(0)})^T$ and $\mu_1 = (\beta_0^{(1)}, \beta_0^{(1)})^T$.