

# Manual for Systematic Search and One Step

Department of Mathematics, Linköping University

**Johan Persson**

Credits: **16 hp**

Level: **G2**

Supervisor: **Frank Miller**,  
Department of Statistics, Stockholm University

Examiner: **Zhenxia Liu**,  
Department of Mathematics, Linköping University

Linköping: **July 2017**



# Models

In one dimension.

Linear,  $m_{1,L}$        $y = \beta_1 x_1 + \varepsilon$

Affine,  $m_{1,A}$        $y = \beta_1 + \beta_2 x_1 + \varepsilon$

Quadratic,  $m_{1,Q}$      $y = \beta_1 + \beta_2 x_1 + \beta_3 x_1^2 + \varepsilon$

Cubic,  $m_{1,C}$        $y = \beta_1 + \beta_2 x_1 + \beta_3 x_1^2 + \beta_4 x_1^3 + \varepsilon$

In two dimensions.

Linear,  $m_{2,L}$        $y = \beta_1 x_1 + \beta_2 x_2 + \varepsilon$

Affine,  $m_{2,A}$        $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \varepsilon$

Interaction,  $m_{2,I}$     $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1 x_2 + \varepsilon$

Quadratic,  $m_{2,Q}$     $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1 x_2 + \beta_5 x_1^2 + \beta_6 x_2^2 + \varepsilon$

Cubic,  $m_{2,C}$        $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1 x_2 + \beta_5 x_1^2 + \beta_6 x_2^2 + \beta_7 x_1^3 + \beta_8 x_2^3 + \varepsilon$

In three dimensions.

Linear,  $m_{3,L}$        $y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \varepsilon$

Affine,  $m_{3,A}$        $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_3 + \varepsilon$

Interaction,  $m_{3,I}$     $y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_3 + \beta_5 x_1 x_2 + \beta_6 x_1 x_3 + \beta_7 x_2 x_3 + \varepsilon$

Quadratic,  $m_{3,Q}$     $y = \text{Interaction} + \beta_8 x_1^2 + \beta_9 x_2^2 + \beta_{10} x_3^2 + \varepsilon$

Cubic,  $m_{3,C}$        $y = \text{Quadratic} + \beta_{11} x_1^3 + \beta_{12} x_2^3 + \beta_{13} x_3^3 + \varepsilon$



# Design regions

## One factor (d=1).

Full design space.

-1 ————— 1

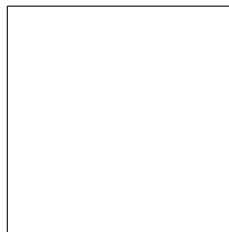
With only one factor the cut-off region and the cut-out region look the same as the full design space.

## Two factors (d=2).

Full design space.

$$\{\mathbf{x} = (x_1, x_2) : x_1, x_2 \in [-1, 1]\}$$

(-1, 1) (1, 1)



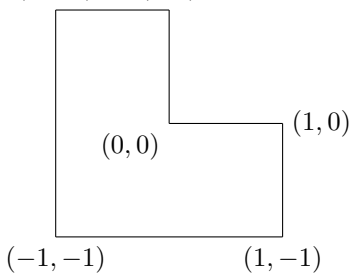
(-1, -1) (1, -1)

Cut-out region.

$$\{\mathbf{x} = (x_1, x_2) : x_1, x_2 \in [-1, 1], x_1 \vee x_2 \leq 0\}$$

$\vee$  meaning at least one of  $x_1$  and  $x_2 \leq 0$

$$(-1, 1) \quad (0, 1)$$

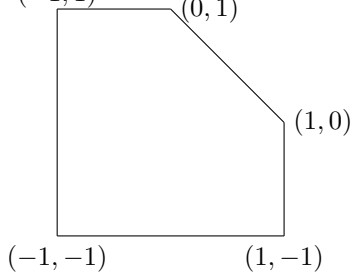


Cut-off region.

$$\{\mathbf{x} = (x_1, x_2) : x_1, x_2 \in [-1, 1], x_1 + x_2 \leq 1\}$$

$$(-1, 1)$$

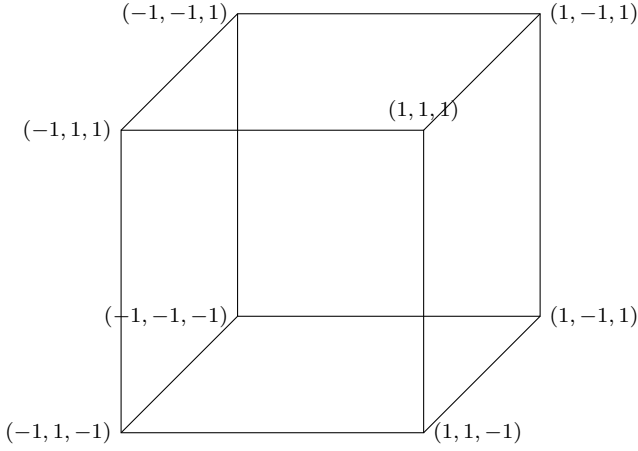
$$(0, 1)$$



### Three factors (d=3).

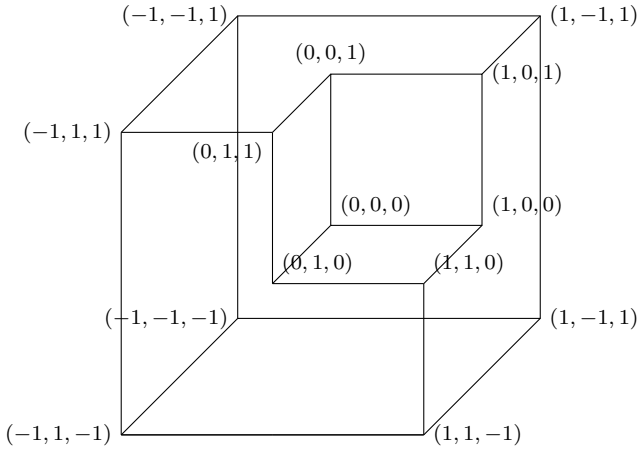
Full design space.

$$\{\mathbf{x} = (x_1, x_2, x_3) : x_1, x_2, x_3 \in [-1, 1]\}$$



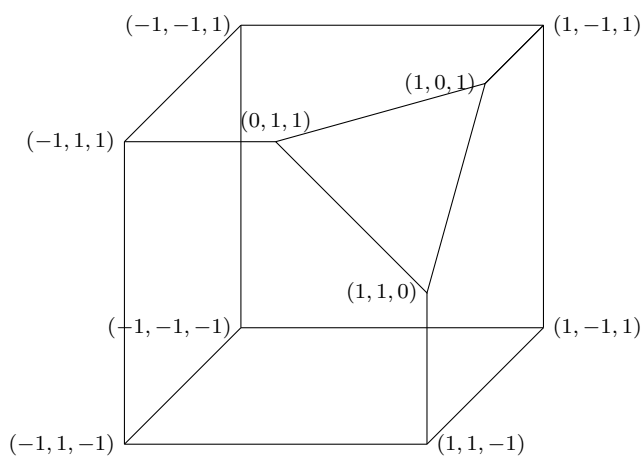
Cut out-design region.

$$\{\mathbf{x} = (x_1, x_2, x_3) : x_1, x_2, x_3 \in [-1, 1], x_1 \vee x_2 \vee x_3 \leq 0\}$$



Cut off-design region.

$$\{\mathbf{x} = (x_1, x_2, x_3) : x_1, x_2, x_3 \in [-1, 1], x_1 + x_2 + x_3 \leq 1\}$$





# Program description

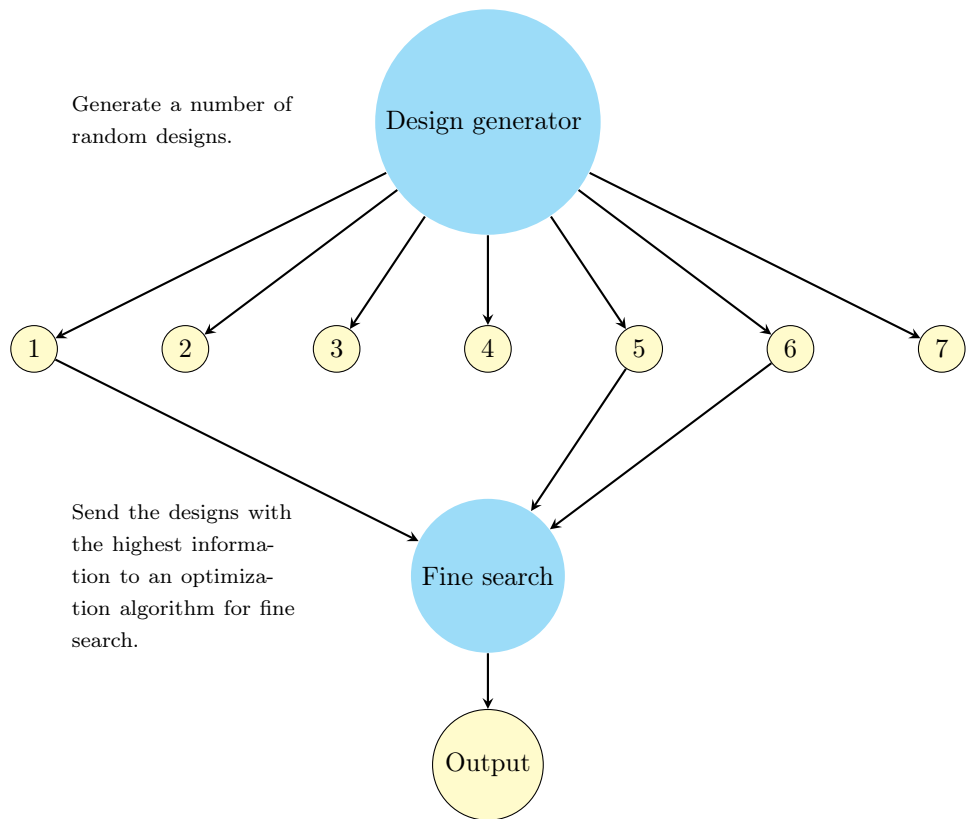


Figure 1: A schematic of what the program does.



## 0.0.1 Program description

### Function description

Spans a 1, 2 or 3-dimensional space.

Restricts the design space due to technical or medical reasons.

Randomly generates designs, D. The entries in D are the number of repetitions  $N_i$  at each design point  $x_i$ .

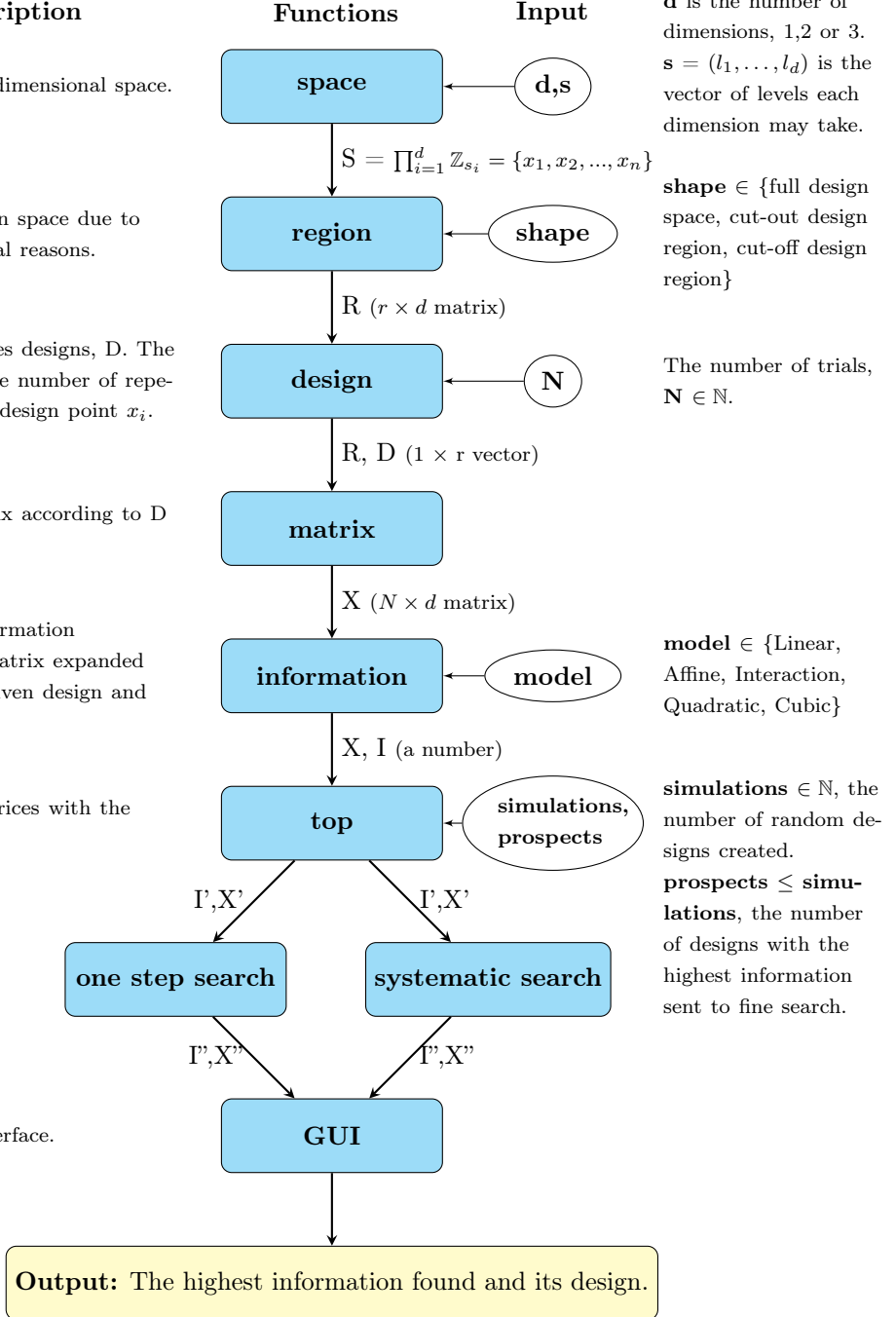
Constructs a matrix according to D and R.

Calculates the information  $\det(M^T M)$  of a matrix expanded according to the given design and model.

Takes out the matrices with the most information.

Two different ways of finding designs with maximum information.

Graphical user interface.



We'll now describe in detail what our program does and how each algorithm works. The program starts of by generating a number of random designs, this is done by the code modules *shape*, *region* and *design*. In the program implementation the random designs are called *simulations*. The code modules *matrix* and *information* creates model matrices and calculates the designs's information. The number of highest information designs to be sent to an algorithm is given by the number of *prospects*. The module *top* picks out this (prospect) number of best designs and sends it to one of the two algorithms. Which algorithm is used depends on if you've opened the program *Systematic Search* or *One Step*.

This is how *One Step* works:

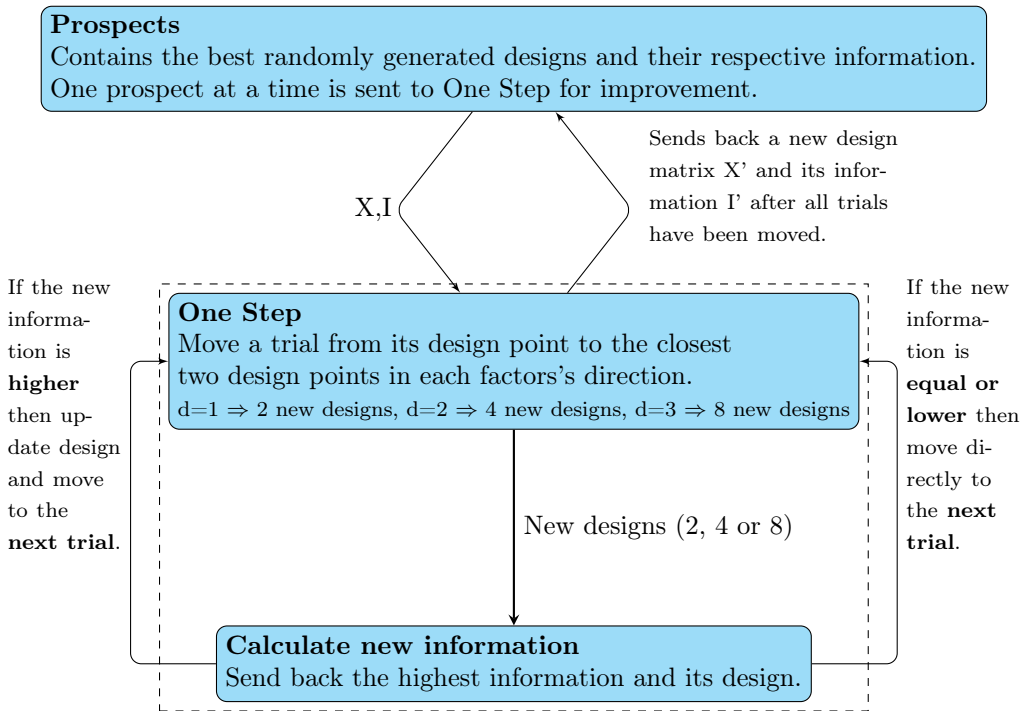


Figure 2: The functions inside the dashed box are iterated as long as the designs improve. This is done until the design have found an information/design maxima, that is the algorithm can't improve the design any more.

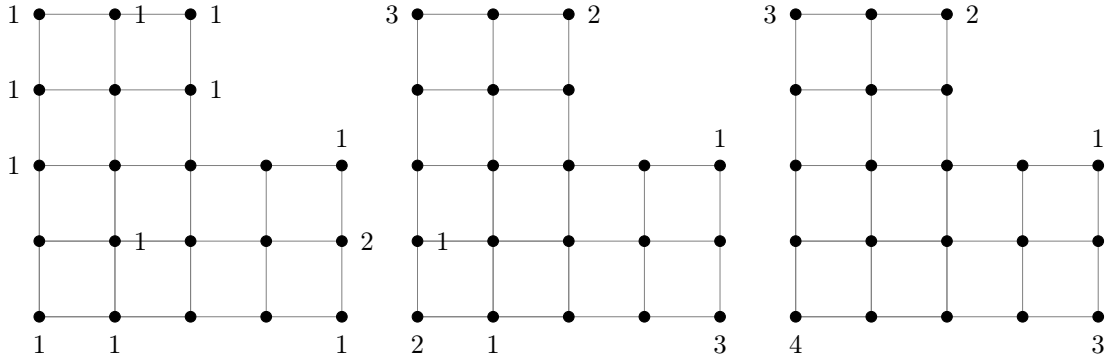


Figure 3: A design that goes through *One Step* and ends up in a sub-optimal design.

In the above figure the first design is a randomly generated design which is among the  $\frac{\text{prospects}}{\text{simulations}}$  highest information designs out of the randomly generated designs. The second design has gone through the *One Step* algorithm once. The third design has gone through *One Step* once more and has ended up in a local maxima that it can't get out from.

Here's how *Systematic Search* works:

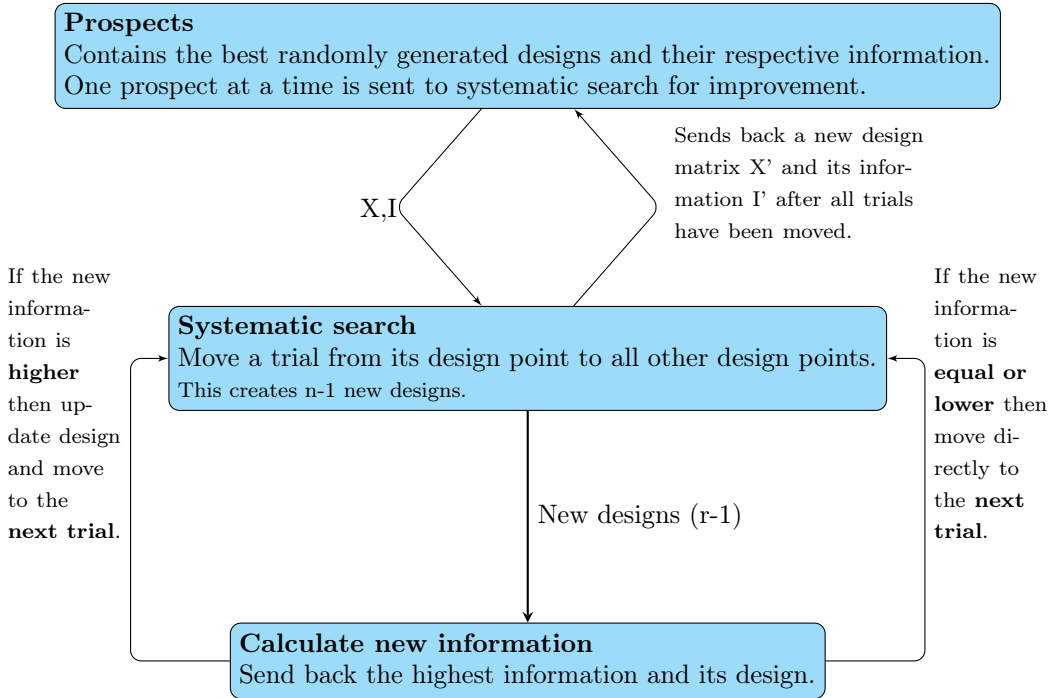


Figure 4: Notice that the *Systematic Search* is not iterated. As long as simulations and prospects are large it only needs one iteration to find a maxima. An advantage over *One Step* is that it is far less likely to end up in a local maxima.

When *Systematic search* has moved all trials once and when *One Step* has moved all trials until the algorithm can't improve the designs any more, then the program produces output.







## Copyright

The publishers will keep this document online on the Internet – or its possible replacement – from the date of publication barring exceptional circumstances.

The online availability of the document implies permanent permission for anyone to read, to download, or to print out single copies for his/her own use and to use it unchanged for non-commercial research and educational purpose. Subsequent transfers of copyright cannot revoke this permission. All other uses of the document are conditional upon the consent of the copyright owner. The publisher has taken technical and administrative measures to assure authenticity, security and accessibility.

According to intellectual property law the author has the right to be mentioned when his/her work is accessed as described above and to be protected against infringement.

For additional information about the Linköping University Electronic Press and its procedures for publication and for assurance of document integrity, please refer to its www home page: <http://www.ep.liu.se/>.

## Upphovsrätt

Detta dokument hålls tillgängligt på Internet – eller dess framtida ersättare – från publiceringsdatum under förutsättning att inga extraordinära omständigheter uppstår.

Tillgång till dokumentet innebär tillstånd för var och en att läsa, ladda ner, skriva ut enstaka kopior för enskilt bruk och att använda det oförändrat för ickekommersiell forskning och för undervisning. Överföring av upphovsrätten vid en senare tidpunkt kan inte upphäva detta tillstånd. All annan användning av dokumentet kräver upphovsmannens medgivande. För att garantera äktheten, säkerheten och tillgängligheten finns lösningar av teknisk och administrativ art.

Upphovsmannens ideella rätt innefattar rätt att bli nämnd som upphovsman i den omfattning som god sed kräver vid användning av dokumentet på ovan beskrivna sätt samt skydd mot att dokumentet ändras eller presenteras i sådan form eller i sådant sammanhang som är kränkande för upphovsmannens litterära eller konstnärliga anseende eller egenart.

För ytterligare information om Linköping University Electronic Press se förlagets hemsida <http://www.ep.liu.se/>.