Importance of the first design matrix in simplex optimization

Tomas Öberg

www.tomasoberg.com

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Introduction

- Simplex - efficient optimization techniques.
- A number of modifications and improvements have been published.
- Less interest in the first design matrix.

We have investigated the influence of the first design matrix under practical conditions, including noise and interaction effects.

Experimental - response functions

- RSM-models, polynomials with linear, interaction (all possible two-factor interactions) and quadratic terms.
- Noise added (1 and 5% proportional normally distributed).

Table 1
Polynomial test functions.

Control variables	Linear terms	Interaction terms	Quadratic terms
4	4	6	4
7	7	21	7

Experimental - first designs

- Three different setups of the first design matrices: Cornered, tilted and optimal.

Table 2
Evaluated first simplex design matrices with four variables (each row representing one trial).

Cornered				Tilted				Optimal			
9	9	9	9	9	9	9	9	9	9	9	10
10	9	9	9	9.9	9.2	9.2	9.2	9	10	10	9
9	10	9	9	9.2	9.9	9.2	9.2	10	10	10	10
9	9	10	9	9.2	9.2	9.9	9.2	10	9	10	9
9	9	9	10	9.2	9.2	9.2	9.9	10	10	9	9

Seven variable first designs specified in an equivalent manner, with a design space of 2-3 for each control variable.

Experimental - algorithms/calc.

- Basic and modified simplex algorithms were evaluated. The k+1 re-evaluation rule was used.
- The on-line module of the *MultiSimplex*™ software was used for calculations.
- Run as a minimization problem.
- 20 iterations were run 10 times for each combination. Average was used.
- Improvement calculated compared to the center of the available first design space.

Results and discussion

Table 3
Percentage improvement after 20 iterations.
Minimization of a 4 variable polynomial.

	Cornered	Tilted	Optimal
Basic, 5% noise	12%	15%	36%
Basic, 1% noise	25%	34%	49%
Modified, 5% noise	10%	15%	89%
Modified, 1% noise	49%	70%	98%

Results and discussion

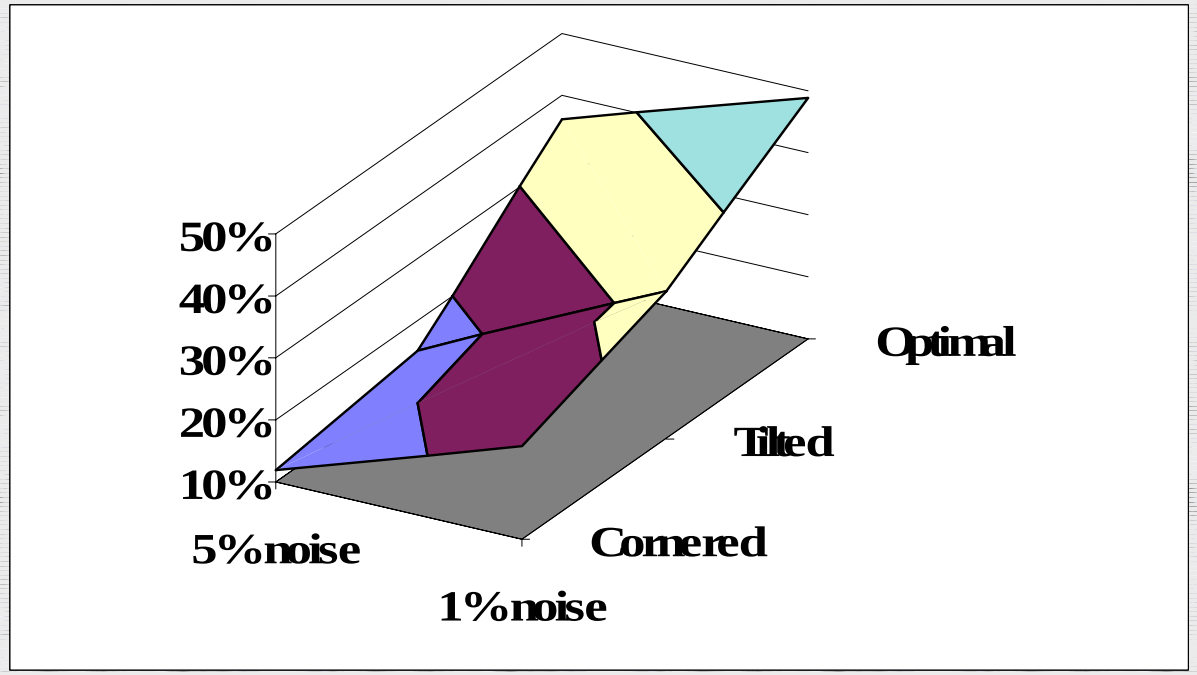

Figure 1
Comparison of performance of different first design matrices with the basic simplex algorithm. Minimization of a 4 variable polynomial.

Results and discussion

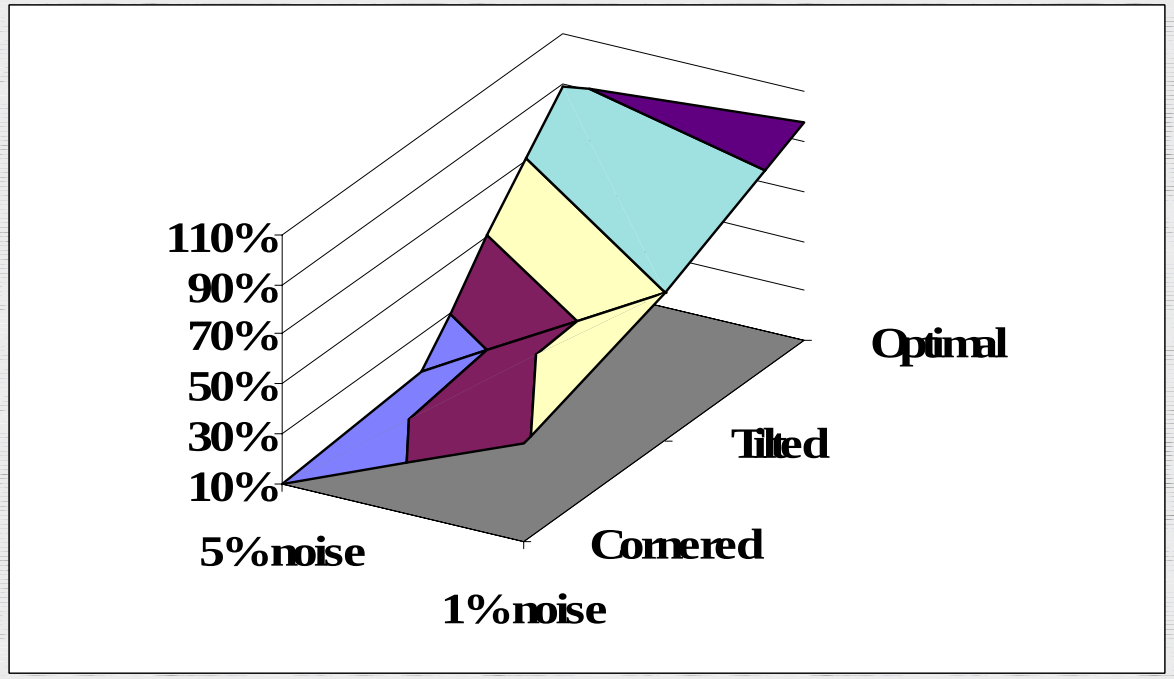

Figure 2
Comparison of performance of different first design matrices with the modified simplex algorithm. Minimization of a 4 variable polynomial.

Results and discussion

Table 4
Percentage improvement after 20 iterations.
Minimization of a 7 variable polynomial..

	Cornered	Tilted	Optimal
Basic, 5% noise	35%	43%	61%
Basic, 1% noise	41%	49%	62%
Modified, 5% noise	34%	49%	96%
Modified, 1% noise	43%	55%	96%

Results and discussion

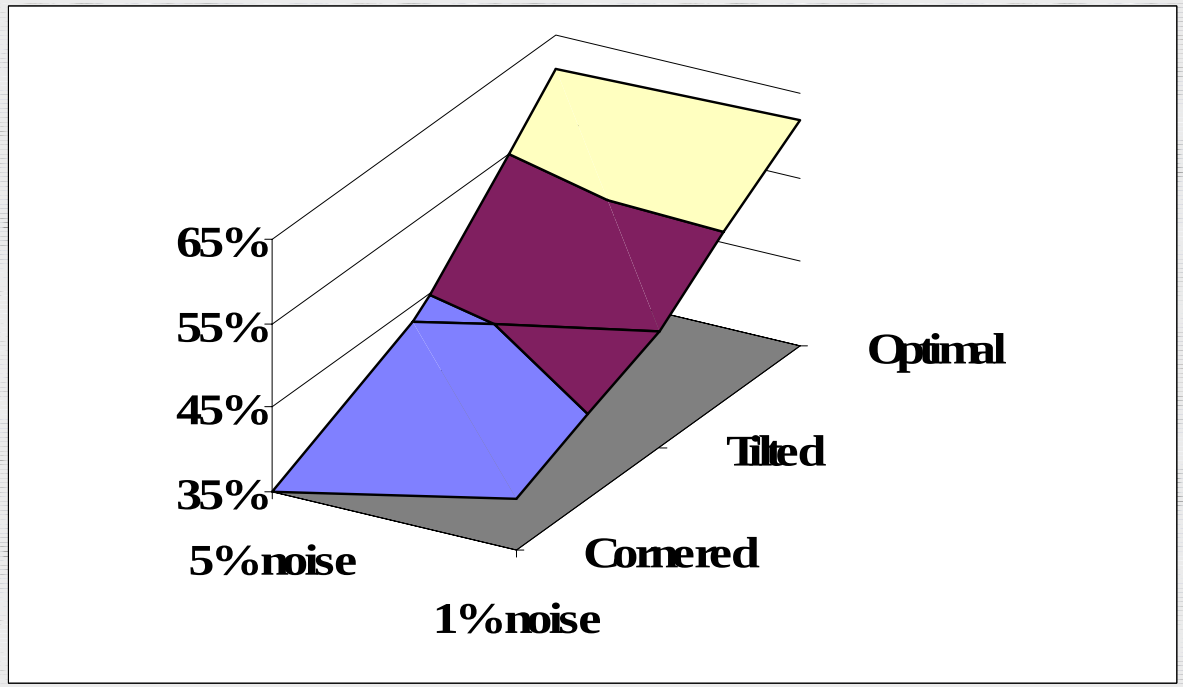

Figure 3
Comparison of performance of different first design matrices with the basic simplex algorithm. Minimization of a 7 variable polynomial.

Results and discussion

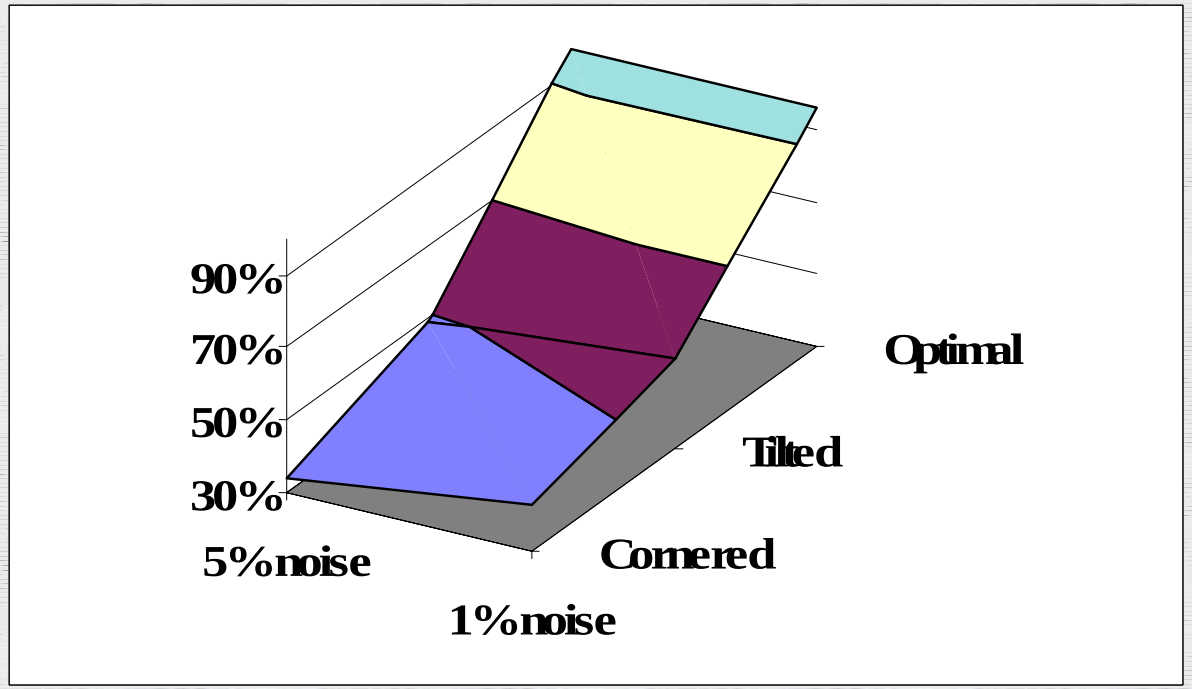

Figure 4
Comparison of performance of different first design matrices with the modified simplex algorithm. Minimization of a 7 variable polynomial.

Results and discussion

- The performance, under given conditions, of the optimal first simplex is superior to the classical tilted first simplex and the cornered first simplex.
- The performance of the tilted first simplex is better than the cornered first simplex.

Results and discussion

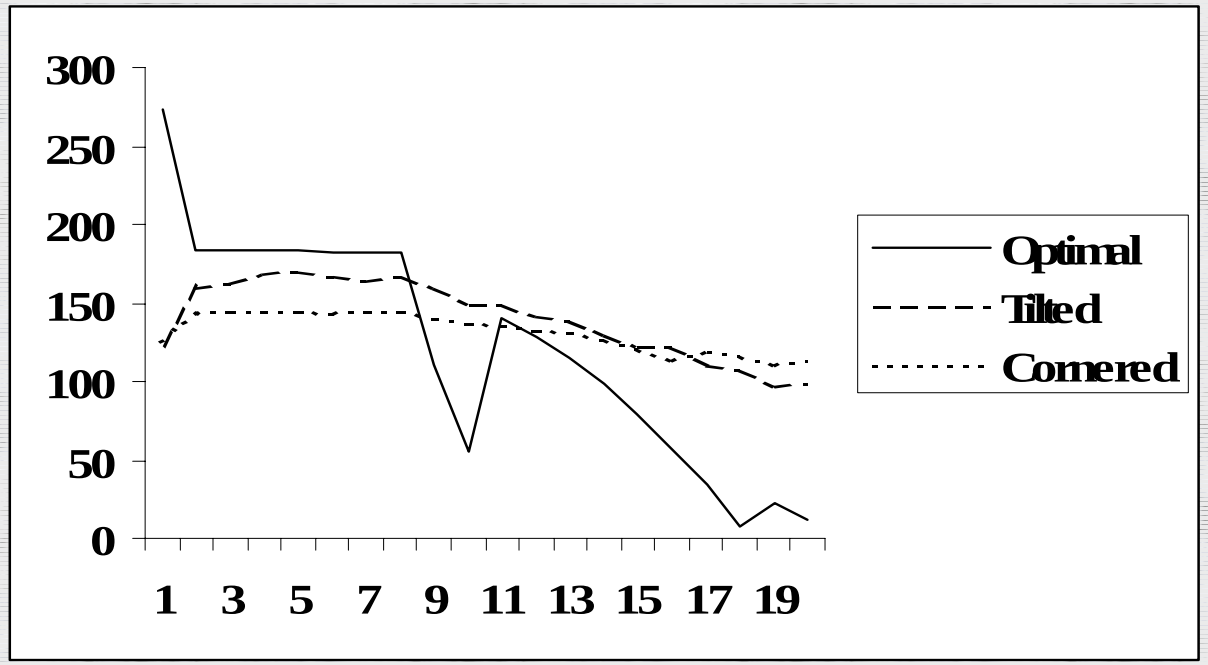

Figure 5
Average response vs. iteration number, first simplex = 1-8, using the modified simplex algorithm. Minimization of a 7 variable polynomial with 35 terms and a noise level of 1%.

Conclusions

- Simulation results will depend on the test functions evaluated.
- We feel that the test functions we have used in this study are closer to reality than those found in previously reported evaluations.
- We therefore expect the choice of the optimal first design matrix to give faster convergence in most practical situations, as compared to other types of first design matrices.

Conclusions cont.

- The choice of a first simplex that efficiently cover the available design space is also obvious when we consider available experience from using statistical experimental design.
- Optimal first design matrices have therefore been implemented as the preset alternative in the new *MultiSimplex*™ experimental design and optimization software.