StatEase
statistics made easy
*Make the most from every experiment!*℠

# Multiple Response Optimization Unveiled

Shari Kraber, MS Applied Statistics
shari@statease.com

August 2020

1

## Making the most of this learning opportunity

Hide the Control Panel
Mute your line

To prevent audio disruptions, all attendees will be muted.

Questions can be posted in the Question area. If they are not addressed during the webinar, I will reply via email afterwards.

Questions may also be sent to stathelp@statease.com. Please provide your company name and, if you are using Design-Expert, the serial number (found under Help, About).

**Note:** The slides and a recording of this webinar will be posted on the Webinars page of the Stat-Ease website within a few days.



2

## Agenda

- **Response surface methods case** *(based on RSM software tutorial*)*
  - **RSM analysis**
  - Numerical Optimization
    - Desirability function
    - Searching the design space
    - Solutions found
  - Graphical Optimization

*Data in Design-Expert Software Help – Tutorials Data: "Conversion"





## Response Surface Method Case
Highlights

This case study on a chemical process features two key responses:

- $y_1$ - Conversion (%)
- $y_2$ - Activity

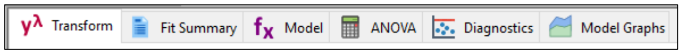
There are three process factors:

- A - time (minutes)
- B - temperature (degrees C)
- C - catalyst (percent)

Central composite design runs are conducted in two blocks:

1. 8 factorial points, plus 4 center points (12 runs total)
2. 6 star points, plus 2 center points (8 runs).

## Response Surface Methods Case
Analysis Procedure




1. Transform: Without prior knowledge start with none.
2. Fit Summary: Comparative statistics on polynomial models. *Generally, start with the suggested model.*
3. Model: Choose best model for in-depth analysis.
4. ANOVA: Examine ANOVA and summary statistics.
5. Diagnostics: Use diagnostic graphs to validate model chosen.
6. Model Graphs: If model adequately represents response, generate contour and 3D plots.
7. *Move on to next response.*

Multiple Response Optimization in Design-Expert software

5

5

## First Step: Develop Good Models
*Don't Over Interpret the Statistics!*

Be sure the fitted surface adequately represents your process before you use it for optimization. Check for:

1. A significant model: Large F-value with $p<0.05$.
2. Insignificant lack-of-fit: F-value with $p>0.10$.
3. Reasonable agreement between adjusted/predicted R-squares.
4. Adequate precision >4.
5. Well behaved residuals: Check diagnostic plots!

*Let's review the ANOVA tables for the two responses to make sure they meet criteria 1-4.*

Multiple Response Optimization in Design-Expert software

6

6

## First Step: Develop Good Models
Conversion

**ANOVA for Quadratic model**

| Source | Sum of Squares | df | Mean Square | F-value | p-value | |
|---|---|---|---|---|---|---|
| Block | 64.53 | 1 | 64.53 | | | |
| **Model** | 2561.82 | 9 | 284.65 | 16.87 | 0.0001 | significant |
| **Residual** | 151.85 | 9 | 16.87 | | | |
| Lack of Fit | 46.60 | 5 | 9.32 | 0.3542 | 0.8574 | not significant |
| Pure Error | 105.25 | 4 | 26.31 | | | |
| **Cor Total** | 2778.20 | 19 | | | | |

| | | | | |
|---|---|---|---|---|
| **Std. Dev.** | 4.11 | | **$R^2$** | 0.9440 |
| **Mean** | 78.30 | | **Adjusted $R^2$** | 0.8881 |
| **C.V. %** | 5.25 | | **Predicted $R^2$** | 0.7891 |
| | | | **Adeq Precision** | 16.2944 |

*Looks OK*

Multiple Response Optimization in Design-Expert software

7

7

## First Step: Develop Good Models
Activity

**ANOVA for Linear model**

| Source | Sum of Squares | df | Mean Square | F-value | p-value | |
|---|---|---|---|---|---|---|
| Block | 0.3967 | 1 | 0.3967 | | | |
| **Model** | 316.70 | 3 | 105.57 | 109.78 | < 0.0001 | significant |
| **Residual** | 14.42 | 15 | 0.9617 | | | |
| Lack of Fit | 10.77 | 11 | 0.9793 | 1.07 | 0.5197 | not significant |
| Pure Error | 3.65 | 4 | 0.9131 | | | |
| **Cor Total** | 331.53 | 19 | | | | |

| | | | | |
|---|---|---|---|---|
| **Std. Dev.** | 0.9806 | | **$R^2$** | 0.9564 |
| **Mean** | 60.23 | | **Adjusted $R^2$** | 0.9477 |
| **C.V. %** | 1.63 | | **Predicted $R^2$** | 0.9202 |
| | | | **Adeq Precision** | 29.2274 |

*Looks good!*

Multiple Response Optimization in Design-Expert software

8

8

## Agenda

- Response surface methods case *(based on RSM software tutorial)*
  - RSM analysis
  - **Numerical Optimization**
    - Desirability function
    - Searching the design space
    - Solutions found
  - Graphical Optimization

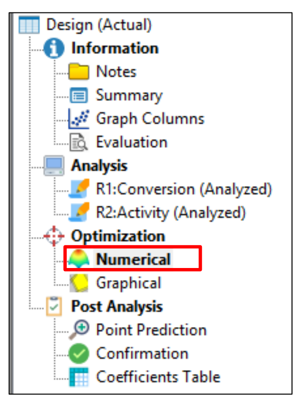


9

## Optimization Case Study
Getting Started

Click the **Numerical** node under the Optimization branch to work on achieving goals for the multiple responses:

- ✓ Maximize Conversion (> 80%)
- ✓ Target Activity (= 63 ± 3)





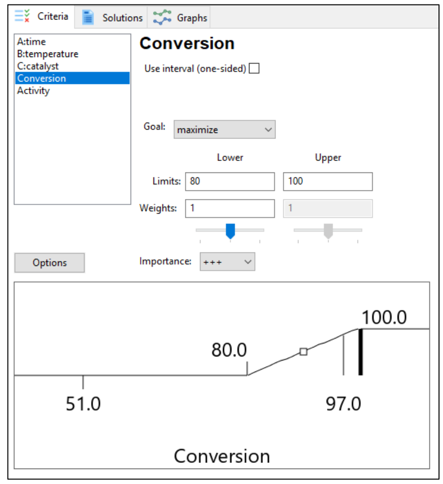

10

# Optimization Case Study

Setting Goals: Conversion

Conversion must be 80 percent or better, ideally 100 percent.

1. Click Conversion.
2. Set Goal to "**maximize**".
3. Make the lower limit "**80**".
4. S t r e t c h the upper limit to a perfect "**100**".




Multiple Response Optimization in Design-Expert software

11

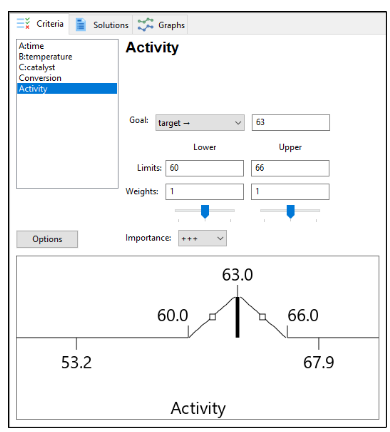
11

# Optimization Case Study

Setting Goals: Activity

Activity at 63 is the goal but anywhere from 60 to 66 is OK.

1. Click Activity.
2. Set Goal to "**target**" of "**63**"
3. Enter Limits:
   - Lower "**60**" and
   - Upper "**66**".




Multiple Response Optimization in Design-Expert software

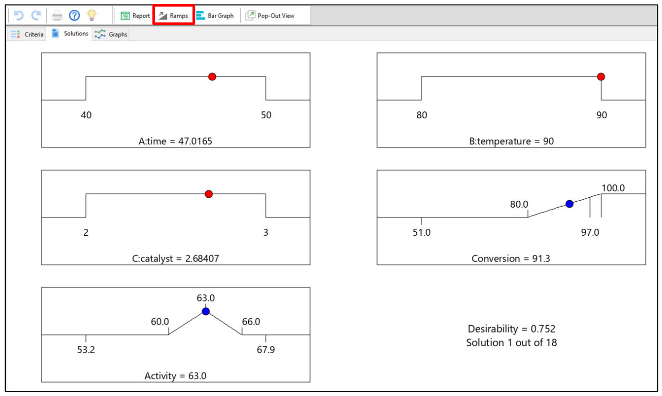
12

12

# Optimization Case Study

## Solution for Multiple Responses: Ramps View

This provides a clear picture of where to set each factor to get most desirable response levels. The number of solutions *(ranked by overall desirability)* varies for reasons we will discuss.




Multiple Response Optimization in Design-Expert software

13

13

# Optimization Case Study

## Solution for Multiple Responses: Report

*Solutions are reported by desirability – most to least, based on how well the specified goals are met.*

*The closer all goals are met, the higher the overall desirability will be.*

| Number | time | temperature | catalyst | Conversion | Activity | Desirability | |
|---|---|---|---|---|---|---|---|
| **1** | **47.018** | **90.000** | **2.684** | **91.317** | **63.000** | **0.752** | **Selected** |
| 2 | 47.038 | 90.000 | 2.680 | 91.316 | 63.000 | 0.752 | |
| 3 | 47.001 | 90.000 | 2.688 | 91.322 | 63.004 | 0.752 | |
| 4 | 47.105 | 90.000 | 2.667 | 91.304 | 63.000 | 0.752 | |
| 5 | 46.925 | 90.000 | 2.701 | 91.303 | 63.000 | 0.752 | |
| 6 | 47.139 | 90.000 | 2.661 | 91.291 | 63.000 | 0.751 | |
| 7 | 47.214 | 90.000 | 2.646 | 91.250 | 63.000 | 0.750 | |
| 8 | 46.782 | 90.000 | 2.729 | 91.224 | 63.000 | 0.749 | |
| 9 | 46.752 | 90.000 | 2.735 | 91.198 | 63.000 | 0.748 | |
| 10 | 47.412 | 90.000 | 2.609 | 91.049 | 63.000 | 0.743 | |
| 11 | 47.104 | 89.997 | 2.655 | 91.209 | 62.946 | 0.742 | |
| 12 | 46.173 | 90.000 | 2.842 | 90.116 | 62.986 | 0.710 | |
| 13 | 46.320 | 80.000 | 2.931 | 87.392 | 63.000 | 0.608 | |
| 14 | 46.355 | 80.000 | 2.925 | 87.390 | 63.000 | 0.608 | |
| 15 | 46.386 | 80.000 | 2.919 | 87.385 | 63.000 | 0.608 | |
| 16 | 46.440 | 80.000 | 2.909 | 87.370 | 63.001 | 0.607 | |
| 17 | 46.164 | 80.000 | 2.961 | 87.349 | 63.000 | 0.606 | |
| 18 | 46.541 | 80.000 | 2.889 | 87.310 | 63.000 | 0.605 | |
| 19 | 45.978 | 80.000 | 2.997 | 87.188 | 63.000 | 0.600 | |

Multiple Response Optimization in Design-Expert software

14

14

## Agenda

- Response surface methods case *(based on RSM software tutorial)*
  - RSM analysis
  - **Numerical Optimization**
    - **Desirability function**
    - Searching the design space
    - Solutions found
  - Graphical Optimization





## Numerical Optimization
Desirability Objective Function *(page 1 of 2)*

To search for "good" combinations of responses, we use an objective function, D, that involves the use of a geometric mean:

$$D = \left(d_1 \times d_2 \times \ldots \times d_n\right)^{\frac{1}{n}} = \left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}$$

- The $d_i$, which range from 0 to 1 (least to most desirable respectively), represents the desirability of each individual (i) response.
- n is the number of responses being optimized.

*Desirability is not a statistic but is a numerical tool to evaluate how closely all the responses met the criteria you assigned.*

## Numerical Optimization

### Desirability Objective Function *(page 2 of 2)*

Now you can search for the greatest overall desirability D, for responses and factors.

*(E.g. if time is a factor, you may want to minimize it.)*

- D = 1 indicates that all the goals are perfectly satisfied. *(If this happens, you're probably not asking for enough!)*
- D = 0 when one or more responses fall outside acceptable limits. *(Hopefully this will not happen, but if does, try relaxing some of your criteria!)*



## Numerical Optimization

### Assigning Optimization Parameters *(page 1 of 2)*

The crucial phase of numerical optimization is assignment of various parameters that define the application of individual desirabilities ($d_i$'s). The most important are:

- Goal (none, maximize, minimize, target or in range)
- Limits (lower and upper)

In this example:

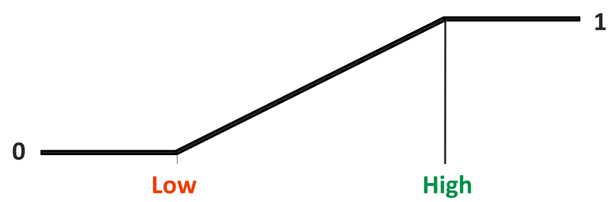
- Conversion should be maximized, and it must exceed a lower limit of 80%. The theoretical upper limit is 100%
- Activity is targeted at 63, and must be within limits of 60 to 66

## Numerical Optimization

### Options for Setting Goals: Maximize

If you choose the goal "maximize", the desirability is assigned:

| | |
|---|---|
| $d_i = 0$ | if y < low limit |
| $0 \leq d_i \leq 1$ | as y varies from low to high |
| $d_i = 1$ | if y > high limit |




*This is the goal set for conversion, with 'stretch' to 100%.*



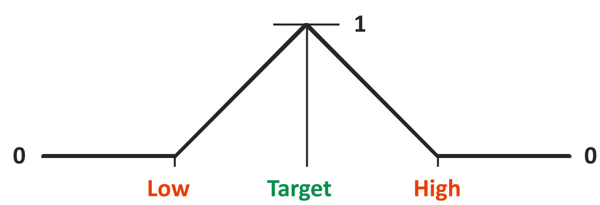


## Numerical Optimization

### Options for Setting Goals: Target

If you choose the goal "target", the desirability is assigned:

| | |
|---|---|
| $d_i = 0$ | if y < low limit |
| $0 \leq d_i \leq 1$ | as y varies from low to target |
| $1 \geq d_i \geq 0$ | as y varies from target to high |
| $d_i = 0$ | if y > high limit |




*This goal, used for activity, forms a "tent" of desirability.*

## Numerical Optimization

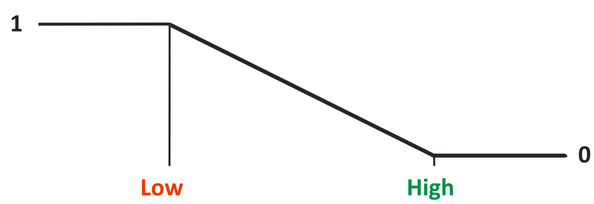
Options for Setting Goals: Minimize

If you choose the goal "minimize", the desirability is assigned:

$d_i = 1$ if y < low limit

$1 \geq d_i \geq 0$ as y varies from low to high

$d_i = 0$ if y > high limit




*The ramp for minimum is flipped over from that for maximum.*





## Numerical Optimization

Options for Setting Goals: In Range

If you choose the goal "in range", the desirability is assigned:

$d_i = 0$ if y < low limit

$d_i = 1$ as y varies from low to high

$d_i = 0$ if y > high limit

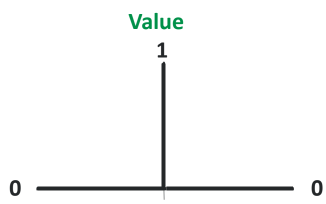

*This is the default Goal for the factors.*

## Numerical Optimization
Options for Setting Goals: Equal to

If you choose the goal "equal to", the desirability is assigned:

$d_i = 0$ if $y \neq$ value

$d_i = 1$ if $y =$ value




*This goal applies only to factors.*





## Numerical Optimization
Options for Setting Goals: None

If you choose the goal "none", the response is ignored during optimization. This is the default setting.

*You may want to set real goals (maximize, minimize, target, range) only on the most critical response first. If you get any solutions, go ahead and add the next most important response, and so forth.*

*This non-goal applies only to responses.*

## Numerical Optimization
### Adding Weights to Goals

An additional parameter, called “weight”, can be added to emphasize upper and/or lower bounds or a target value. Weight, which can vary from 0.1 to 10, affects individual desirabilities as follows:

- = 1, the $d_i$ go up or down on straight (linear) ramps: This is the default.
- > 1, the $d_i$ get pulled down into a concave curve that increases close to the goal.
- < 1, the curve goes the opposite direction (convex) going up immediately after the threshold limit, well before reaching the goal.

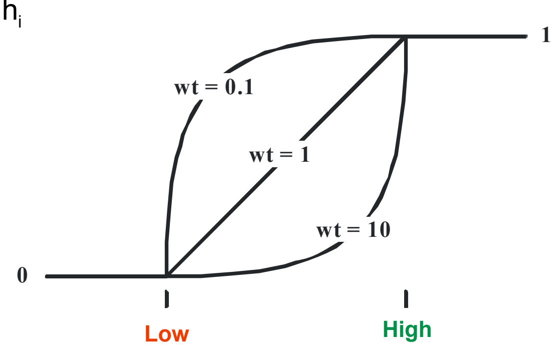


## Numerical Optimization
### Adding Weights to Goals: Maximize

$$d_i = 0 \quad \text{at } y_i \le \text{Low}_i$$

$$d_i = \left[\frac{y_i - \text{Low}_i}{\text{High}_i - \text{Low}_i}\right]^{wt1_i} \quad \text{when } \text{Low}_i < y_i < \text{High}_i$$

$$d_i = 1 \quad \text{at } y_i \ge \text{High}_i$$

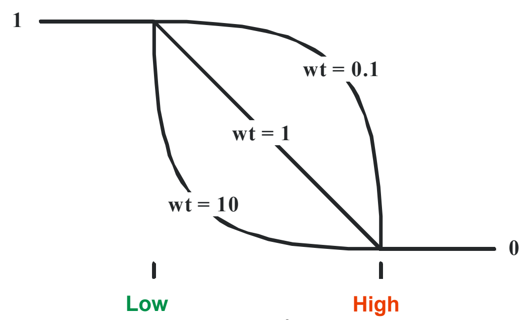


## Numerical Optimization
### Adding Weights to Goals: Minimize

$$d_i = 1 \text{ at } y_i \le Low_i$$

$$d_i = \left[\frac{High_i - y_i}{High_i - Low_i}\right]^{wt1_i} \text{ at } Low_i < y_i < High_i$$

$$d_i = 0 \text{ at } y_i \ge High_i$$




Multiple Response Optimization in Design-Expert software

27

27

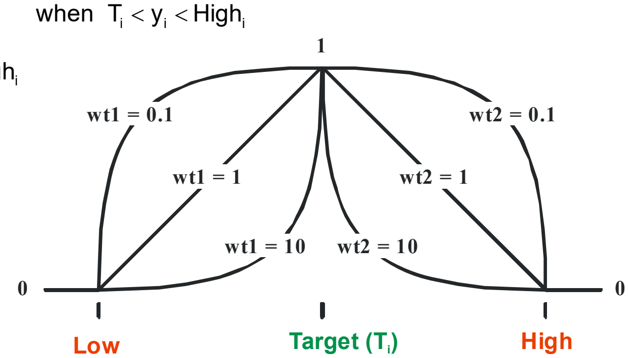
## Numerical Optimization
### Adding Weights to Goals: Target

$$d_i = 0 \text{ at } y_i \le Low_i$$

$$d_i = \left[\frac{y_i - Low_i}{T_i - Low_i}\right]^{wt1_i} \text{ when } Low_i < y_i < T_i$$

$$d_i = \left[\frac{y_i - High_i}{T_i - High_i}\right]^{wt2_i} \text{ when } T_i < y_i < High_i$$

$$d_i = 0 \text{ at } y_i \ge High_i$$

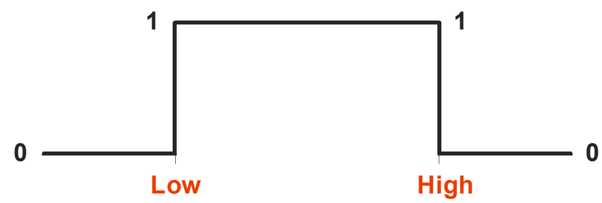



Multiple Response Optimization in Design-Expert software

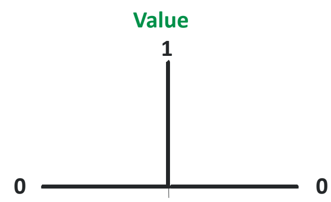
28

28

## Numerical Optimization
Adding Weights to Goals: ~~In Range, Equal to~~




*Weights do not apply to "in range" or "equal to" goals.*




Multiple Response Optimization in Design-Expert software

29

29

## Numerical Optimization
Adding Importance to Goals

In our objective function D, each response can be assigned a relative "importance" ($r_i$) that varies from 1 plus ( + ) least to 5 plus ( +++++ ) most. If varying degrees of importance are assigned to the different responses, the objective function is:

$$D = \left(d_1^{r_1} \times d_2^{r_2} \times \ldots \times d_n^{r_n}\right)^{\frac{1}{\sum r_i}} = \left(\prod_{i=1}^{n} d_i^{r_i}\right)^{\frac{1}{\sum r_i}}$$

where n is the number of responses in D.

If the importance values do not differ, then the function reduces to:

$$D = \left(d_1 \times d_2 \times \ldots \times d_n\right)^{\frac{1}{n}} = \left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}$$

Multiple Response Optimization in Design-Expert software

30

30

## Numerical Optimization


Recap:

- Desirability of one means…
  - Your wildest dreams have come true!
  - You should set more demanding criteria.
- Desirability between one and zero means…
  - All of the responses were within acceptable limits.
  - At least one was not perfect.
- Desirability of zero indicates…
  - One or more responses fall outside acceptable limits.



## Agenda

- Response surface methods case *(based on RSM software tutorial)*
  - RSM analysis
  - **Numerical Optimization**
    - Desirability function
    - **Searching the design space**
    - Solutions found
  - Graphical Optimization

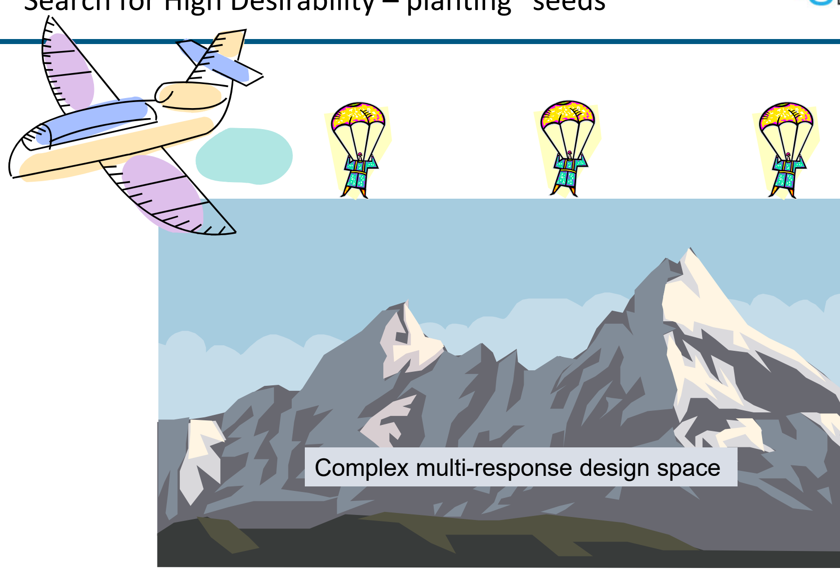
## Numerical Optimization
### Search for High Desirability

- Numerical Optimization is basically a hill climbing technique.
- More than one hill can exist. The optimum found (the hill climbed) depends on where the numerical optimization starts.
- To increase the chances of finding multiple optimums, several optimization cycles should be done using different starting points.
- In this illustration 109 cycles (started at one hundred randomly selected coordinates and the nine unique design points in the cube) are run and two unique optimums (hills) found.



33

## Numerical Optimization
### Search for High Desirability – planting “seeds”

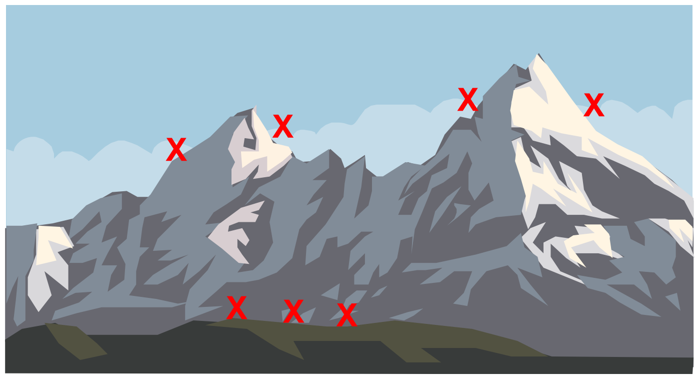





34

## Numerical Optimization
Search for High Desirability

Skydivers landed randomly, then look around and walk up (towards increasing desirability).




How do they choose which direction to walk?

Multiple Response Optimization in Design-Expert software

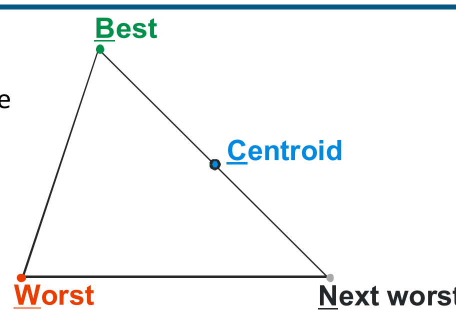
35

35

## Numerical Optimization
Details on Hill-Climbing Algorithm: Simplex

Rules:

1. Construct first simplex about the random coordinates.
2. Use selected models to predict responses at each vertex, then compute desirability.



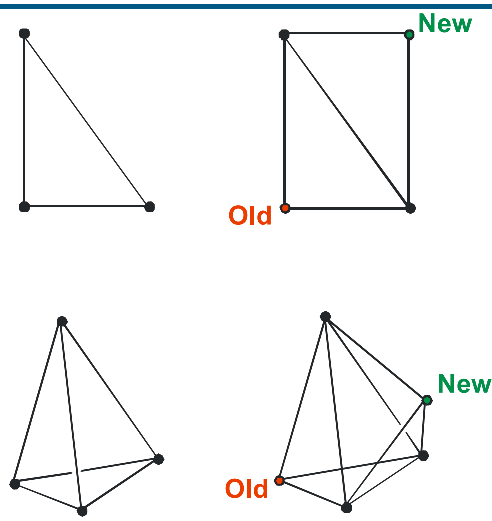

3. Initially, reflect away from the worst vertex (W). Then move away from the next-to-worst vertex (N), from the previous simplex.
4. Continue until the change in desirability, or the change in the movement of the vertices, becomes very small.

Multiple Response Optimization in Design-Expert software

36

36

## Numerical Optimization
Simplex Moves in 2D and 3D

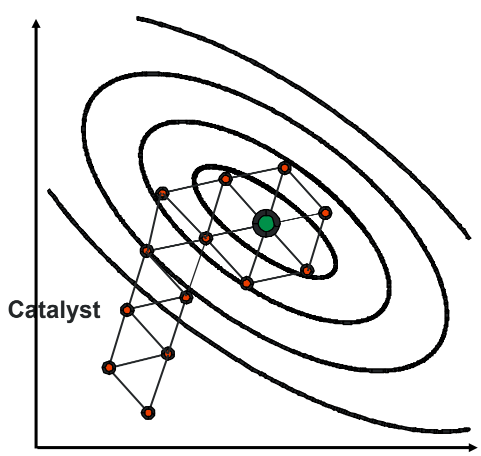



Multiple Response Optimization in Design-Expert software

37

37

## Numerical Optimization
Simplex Moves on RSM Contours




Multiple Response Optimization in Design-Expert software

38

38

## Variable Size Simplex

Nelder-Mead (1965)

Reflection: if N ≤ R ≤ B

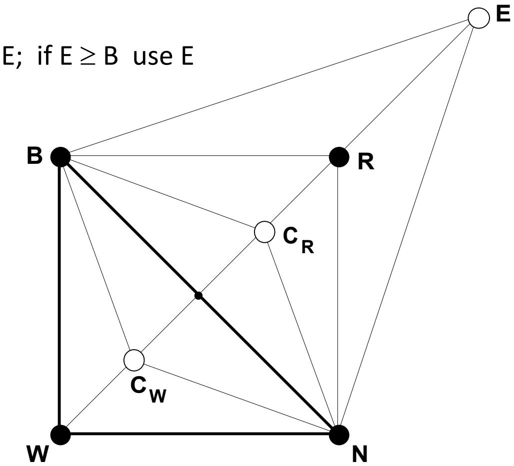
Expansion: if R > B evaluate E; if E ≥ B use E

if E < B use R

Contraction: if R < N and

if R ≥ W use CR

if R < W use CW



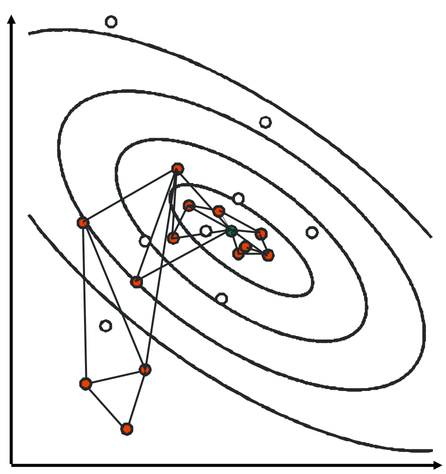

Multiple Response Optimization in Design-Expert software

39

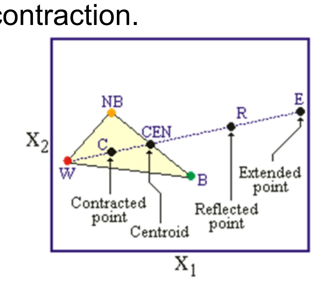
39

## Numerical Optimization

Enhanced – Simplex: Variable-Sized



Open circles (o) were abandoned due to being either: 1) Better than any point in that simplex, so it expanded, or 2) Worse, causing a contraction.




Multiple Response Optimization in Design-Expert software

40

40

## Numerical Optimization
### Search for High Desirability (Recap)

- Numerical Optimization is basically a hill climbing technique.
- More than one hill can exist. The optimum found (the hill climbed) depends on where the numerical optimization starts.
- To increase the chances of finding multiple optimums, several optimization cycles should be done using different starting points.
- Due to the variable step size, the final stopping point of each cycle will differ by small amounts. This results in the multiple "solutions" that are very similar to each other.



41

## Agenda

- Response surface methods case *(based on RSM software tutorial)*
  - RSM analysis
  - **Numerical Optimization**
    - Desirability function
    - Searching the design space
    - **Solutions found**
  - Graphical Optimization



42

## Numerical Optimization
### Numerical Solutions for Case Study

Two distinct solutions for Conversion found at temps 90 & 80.

Constraints

| Name | Goal | Lower Limit | Upper Limit | Lower Weight | Upper Weight | Importance |
|---|---|---|---|---|---|---|
| time | is in range | 40 | 50 | 1 | 1 | 3 |
| temperature | is in range | 80 | 90 | 1 | 1 | 3 |
| catalyst | is in range | 2 | 3 | 1 | 1 | 3 |
| Conversion | maximize | 80 | 100 | 1 | 1 | 3 |
| Activity | is target = 63.0 | 60 | 66 | 1 | 1 | 3 |

Solutions

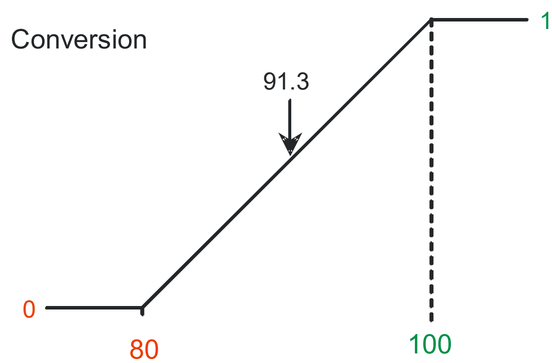
| Number | time | temperature | catalyst | Conversion | Activity | Desirability |
|---|---|---|---|---|---|---|
| 1 | 47.02 | 90.00 | 2.68 | 91.3 | 63.0 | 0.752 |
| 2 | 46.70 | 90.00 | 2.74 | 91.2 | 63.0 | 0.747 |
| … | | | | | | |
| 10 | 46.32 | 80.00 | 2.93 | 87.4 | 63.0 | 0.608 |
| 11 | 46.35 | 80.00 | 2.93 | 87.4 | 63.0 | 0.608 |
| … | | | | | | |

Multiple Response Optimization in Design-Expert software

43

43

## Numerical Optimization
### First Optimum: Temp = 90° Conversion




$$d_1 = \left(\frac{91.3 - 80}{100 - 80}\right) = 0.565$$

Multiple Response Optimization in Design-Expert software

44

44

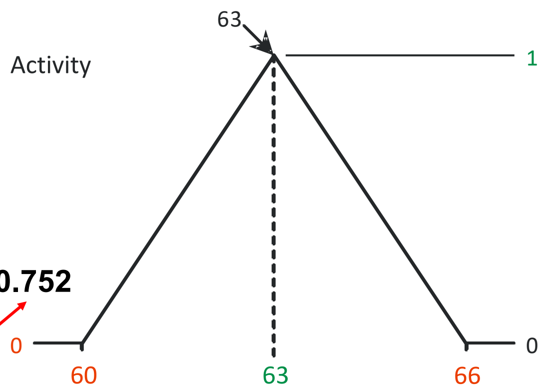
## Numerical Optimization

First Optimum: Temp = 90° Activity

$$d_2 = 1$$

$$D = \left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}$$

$$D = (0.565 \times 1)^{\frac{1}{2}} = 0.752$$




**Overall Desirability** *Activity on target ($d_2$=1), but this gets multiplied by lesser desirability ($d_1$=0.565) for Conversion.*

Multiple Response Optimization in Design-Expert software

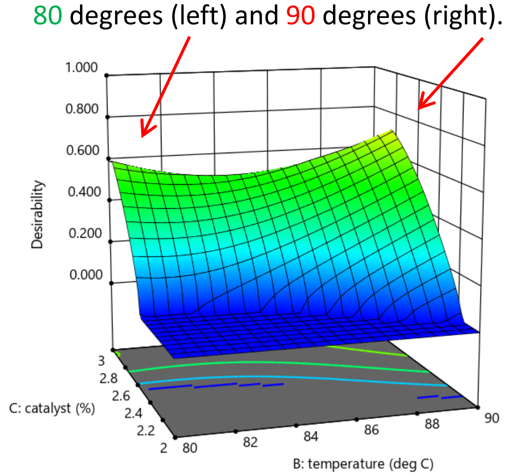
45

45

## Numerical Optimization

Two Optimums: 80° and 90°

Two shoulders on ridge parallel to temperature at 80 degrees (left) and 90 degrees (right).




Multiple Response Optimization in Design-Expert software

46

46

## Numerical Optimization
Tips for Use

- Change the default upper/lower limits to represent your expectations, especially cutting off the unacceptable response values.
- Use Importance to prioritize your responses.
- If you have many solutions, tighten up the criteria on the responses, or add criteria for a few factors.
- Remember, desirability is NOT a statistical function that must be high – it is simply a mathematical tool to rank solutions according to how closely they met the goals you set.



47

## Agenda

- Response surface methods case *(RSM software tutorial)*
  - Sizing for precision
  - RSM analysis
  - Numerical Optimization
    - Desirability function
    - Searching the design space
    - Solutions found
  - **Graphical Optimization**

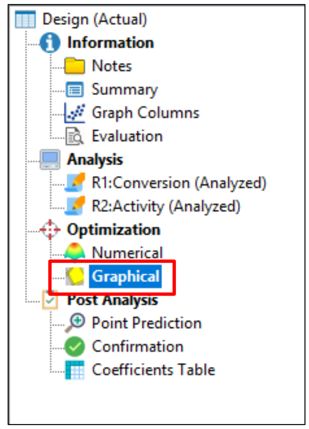


48

## Optimization Case Study *(Instructor Led)*
### Part 2 – Graphical Optimization

Click the Graphical node under the Optimization branch to frame out a window ("sweet spot") that achieves goals for the multiple responses:

- ✓ Maximize Conversion (> 80%)
- ✓ Target Activity (= 63 ± 3)

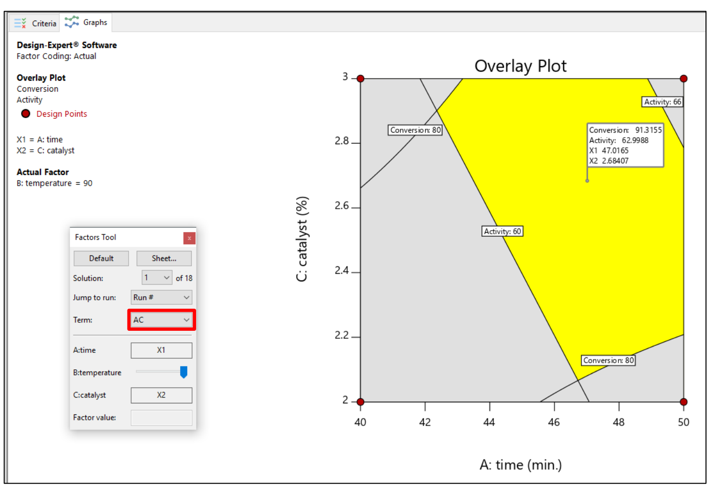



Multiple Response Optimization in Design-Expert software

49

49

## Graphical Optimization
### First Optimum: Temp = 90°




Multiple Response Optimization in Design-Expert software

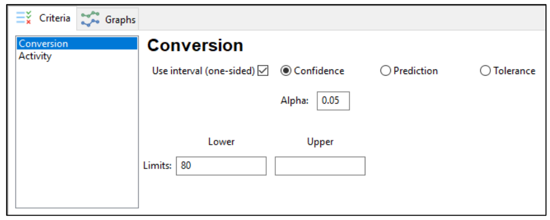
50

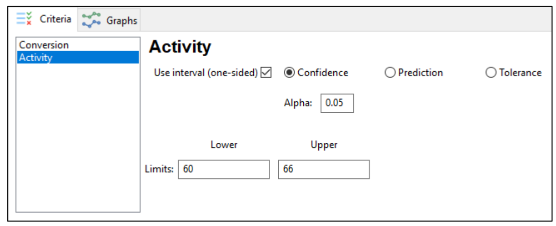
50

# Graphical Optimization

Overlay with Intervals *(page 1 of 2)*

Add a 95% ($\alpha$ = 5%) confidence interval to Conversion and Activity.



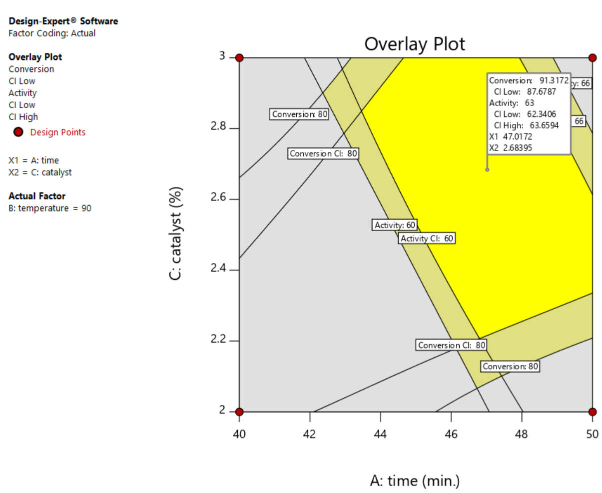

Multiple Response Optimization in Design-Expert software

51



# Graphical Optimization

Overlay with Intervals *(page 2 of 2)*




Multiple Response Optimization in Design-Expert software

52

## Multiple Response Optimization Wrap-Up

1. Numerical optimization: find where response requirements are simultaneously satisfied.
2. Graphical optimization: Superimpose response contours graphically to learn which response criteria constrain each optimum.
3. Add confidence intervals to build robustness into the design space, keeping you away from the edges.

Multiple Response Optimization in Design-Expert software

53

53

## Stat-Ease Training:
## Sharpen Up Your DOE Skills

**Modern DOE for Process Optimization**

**Mixture Design for Optimal Formulations**

| Individuals | Teams (6+ people) |
|---|---|
| Improve your DOE skills | Choose your date & time |
| Topics applicable to both novice and advanced practitioners | Add company case studies |

Learn more: **www.statease.com**

Contact: **workshops@statease.com**

DX Software Intro for New Users

54

54

StatEase®
statistics made easy®

*Make the most from every experiment!*[SM]

55