Central Composite Type Experimental Designs for Multiple Responses with Different Models

Wilmina (Billie) Marget
Augsburg University,
Department of MSCS

Max Morris
Iowa State University,
Department of Statistics

Introduction

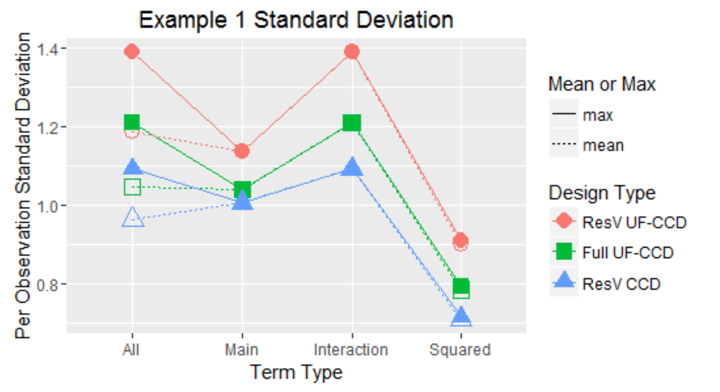
- New experimental designs based on CCD
- Multiple explanatory *and* response variables
- Previous info on model forms
  - Screening experiment
  - Process knowledge

Motivation

Unique Factor CCD

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Results & Future Research



Motivation

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Factor	1	2	3	4	5
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Response 1	X	X	X		
Response 2		X	X	X	
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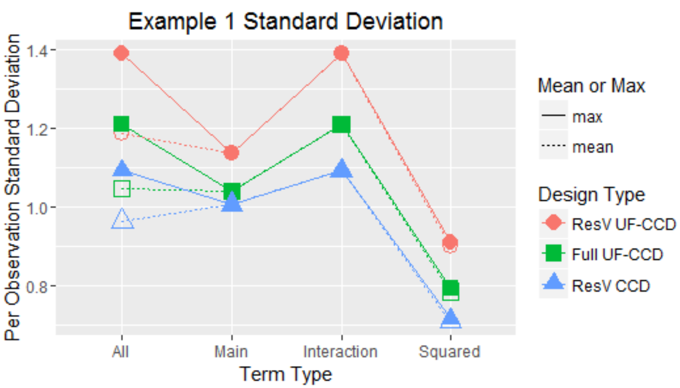
Response 4	X			X	

Results & Future Research



Bio-fuels Application [Friend (2013)]

- Factors: (15 total)
  - Coal particle size
  - Coal moisture content
  - Pellet aging temperature
  - Amount of bio-oil binder in pellet

- Response variables: (12 total)
  - Heating value
  - Moisture content
  - Carbon content
  - Strength

Bio-fuels Application

	Coal particle size	Coal moisture content	Pellet aging temp	Amt. of bio-oil binder	…
Heating value	X	X			
Moisture content		X		X	
Carbon content			X	X	
Strength		X			

Central Composite Design (CCD)

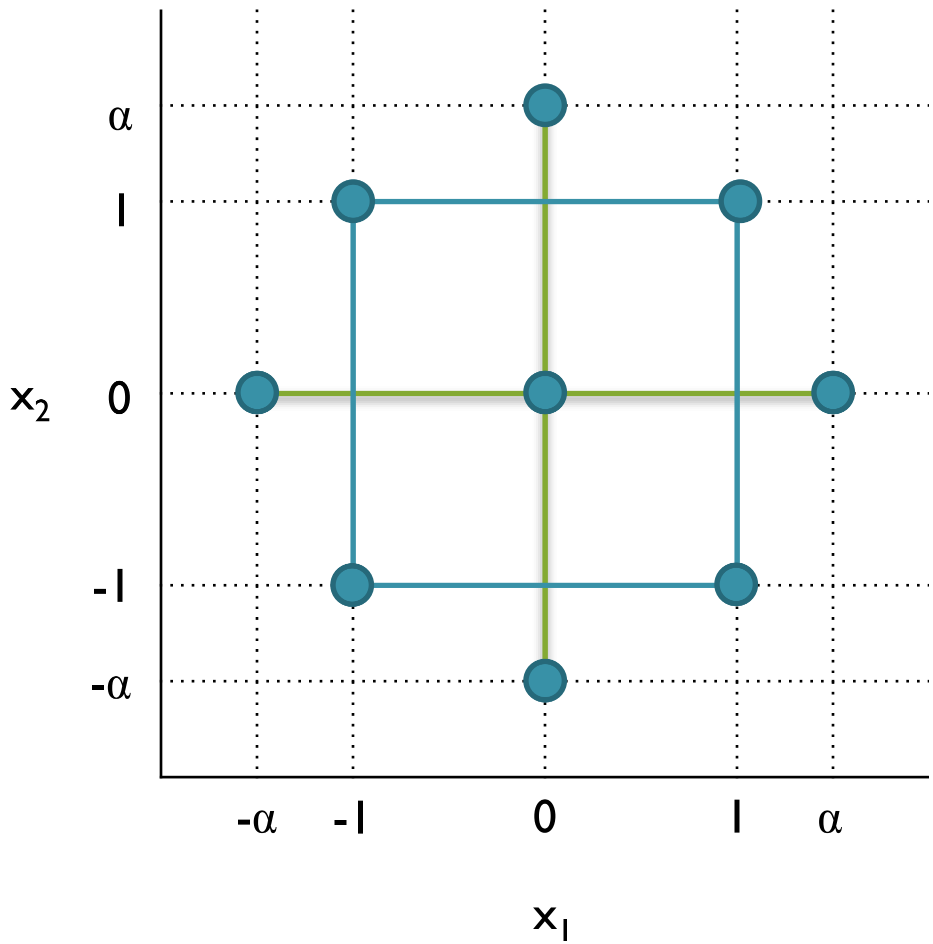
Used for estimating full quadratic.

- Two-level (full or fractional) factorial
- Axial points
- Center points

	1	2
Full Factorial (2^k)	+	+
	+	-
	-	+
	-	-
Axial Points (2k)	$+\alpha$	0
	$-\alpha$	0
	0	$+\alpha$
	0	$-\alpha$
Center Points (n_c)	0	0
	0	0
	0	0

[Box and Wilson (1951)]

Central Composite Design (CCD)



	1	2
Full Factorial (2^k)	+	+
	+	-
	-	+
	-	-
Axial Points (2k)	+α	0
	-α	0
	0	+α
	0	-α
Center Points (n_c)	0	0
	0	0
	0	0

Regular Fractional Factorial

- Subset of full factorial
- Confound certain effects with intercept
- **Resolution :** Lowest order interaction confounded with intercept

1	2	3	4	1234	123
+	+	+	+	+	+
+	+	-	-	+	-
+	-	+	-	+	-
+	-	-	+	+	+
-	+	+	-	+	-
-	+	-	+	+	+
-	-	+	+	+	+
-	-	-	-	+	-

Regular Fractional Factorial

- **Resolution V:** smallest effect confounded with intercept is 5-factor interaction
- Main effects: not confounded with 2- or 3-factor interactions
- 2-factor interactions: not confounded with other 2-factor interactions

Example: The standard solution is overkill.

	1	2	3	4	5	6	7	8	9	10
Response 1	X	X	X	X	X					
Response 2			X		X	X	X			
Response 3			X	X			X	X		
Response 4				X				X	X	X

Example: The standard solution is overkill.

	1	2	3	4	5	6	7	8	9	10
Response 1	X	X	X	X	X					
Response 2			X		X	X	X			
Response 3			X	X			X	X		
Response 4				X				X	X	X

Standard CCD:

- Resolution V fraction: 128
- Axial points: 20
- Center points: n_c
- Total runs needed: **148+n_c**

Example: The standard solution is overkill.

	1	2	3	4	5	6	7	8	9	10
Response 1	X	X	X	X	X					
Response 2			X		X	X	X			
Response 3			X	X			X	X		
Response 4				X				X	X	X

CCD (with **148+n_c**):

- 10 main effects
- 10 squared
- 45 2-factor interactions
- 72 higher order interactions

We need:

- 10 main effects
- 10 squared
- 24 2-factor interactions
- **Not all in same model**

Objective

- Develop design w/ fewer runs
- Estimation of:
  - Main effects
  - Quadratic
  - Needed 2-factor interactions
- Use previous info on model forms
- Same structure as CCD

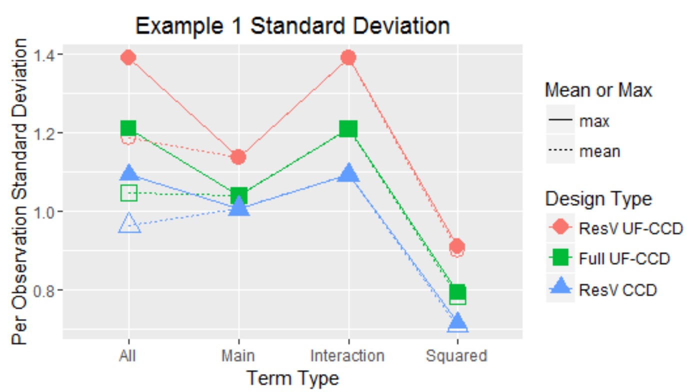
CCD = Central Composite Design

Motivation

Unique Factor CCD

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Results & Future Research



Overview of UF Algorithm

1. Consider each factor in order.
2. Assign factor 1 to new unique factor 1^*
3. For factor $l = 2, \ldots, k$
   a) If such a unique factor exists, assign to an existing unique factor s.t. no other factor related to the same response has been assigned to that unique factor.
   b) If not, assign to a new unique factor.
4. Construct a resolution $(\max_i k_i+1)$ or V fractional factorial in all k^* unique factors, and add axial and center points.
5. For each factor l assigned to unique factor m^*, set $l = m^*$.

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor					
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*				
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*	2*			
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*		
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Algorithm 2 Example

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

- Resolution IV fractional factorial in $k^* = 4$ unique factors.
- Full factorial in each response model.

1	2	3	4	5
1*	2*	3*	4*	2*
+	+	+	+	+
+	+	-	-	+
+	-	+	-	-
+	-	-	+	-
-	+	+	-	+
-	+	-	+	+
-	-	+	+	-
-	-	-	-	-
$\pm\alpha$				
	$\pm\alpha$			$\pm\alpha$
		$\pm\alpha$		
			$\pm\alpha$	
0	0	0	0	0

Summary of Algorithm 2

- Assign each factor to a unique factor so that no 2 factors related to the same response are assigned to the same unique factor.
- Construct a fractional factorial design in the set of unique factors.
  - Resolution $\max_i k_i + 1$ or
  - Resolution V

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Order matters

- If we reorder the factors, the assignment of unique factors changes.
- How do we know this is the smallest number of factors we could get from the algorithm? (Illustrated in examples later)

Factor	**4**	**1**	**2**	**3**	**5**
Unique Factor	1*	2*	3*	4*	1*
Response 1		X	X	X	
Response 2	X		X	X	
Response 3		X		X	X
Response 4	X	X			

What do we get?

- Design with fewer runs
- Each response:
  - CCD
  - (replicated) full/fractional factorial
- All responses:
  - CCD with fractional factorial
  - Main effects confounded
    - Only across models
- Only use when you are sure of the model

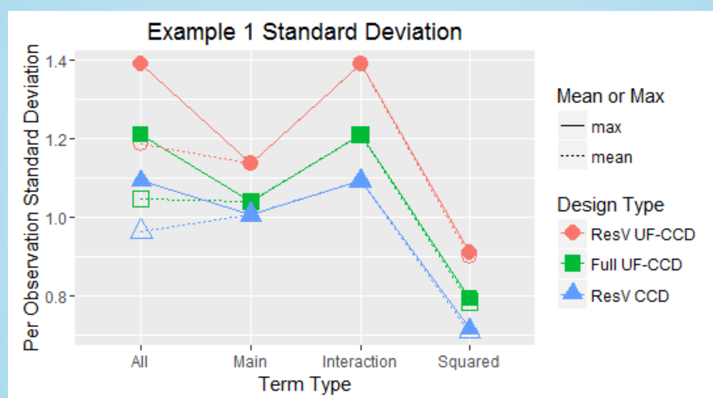
CCD = Central Composite Design

Motivation

Unique Factor CCD

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Results & Future Research



Example 1

	1	2	3	4	5	6	7	8	9	10
	1*	2*	3*	4*	5*	1*	2*	1*	2*	3*
Response 1	X	X	X	X	X					
Response 2			X		X	X	X			
Response 3			X	X			X	X		
Response 4				X				X	X	X

	# of runs		
	Ex 1	Ex 2	Ex 3
Res V UF-CCD	$26+n_c$		
Full UF-CCD	$42+n_c$		
Res V CCD	$148+n_c$		

Example 1

	1	2	3	4	5	6	7	8	9	10
	1*	2*	3*	4*	5*	1*	2*	1*	2*	3*
Response 1	X	X	X	X	X					
Response 2			X		X	X	X			
Response 3			X	X			X	X		
Response 4				X				X	X	X

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	1	2	5	3	9	6	8	4	10	7
	1*	2*	3*	4*	1*	1*	2*	5*	3*	6*
Response 1	X	X	X	X				X		
Response 2			X	X		X				X
Response 3				X			X	X		X
Response 4					X		X	X	X	

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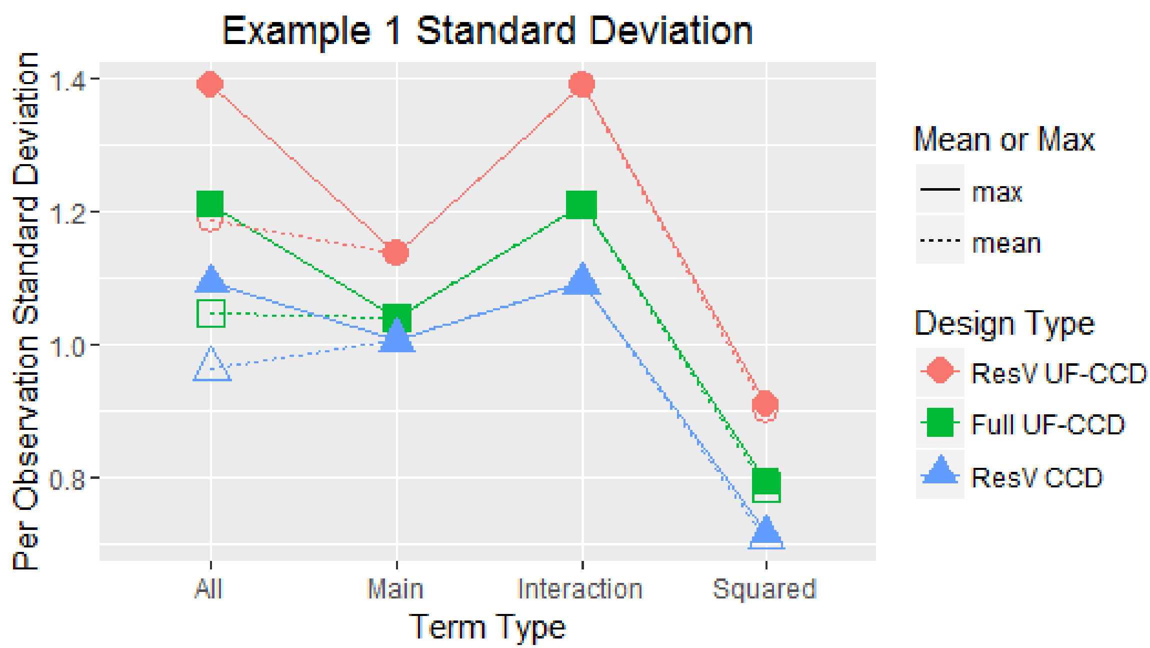
Example 1



	N	All Effects		Main Effects		Interactions		Squared	
		mean	max	mean	max	mean	max	mean	max
Res V UF-CCD	26+n_c	0.213	0.250	0.204	0.204	0.250	0.250	0.162	0.164
Full UF-CCD	42+n_c	0.153	0.177	0.152	0.152	0.177	0.177	0.115	0.116
Res V CCD	148+n_c	0.078	0.088	0.081	0.081	0.088	0.088	0.057	0.058

Example 2

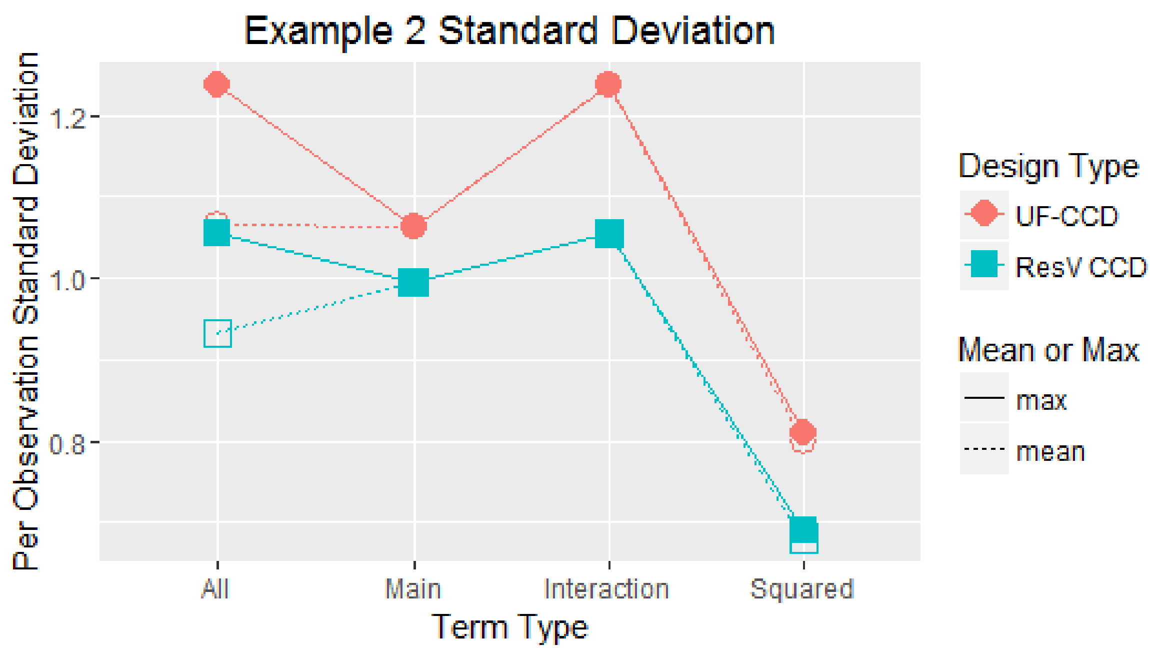
	1	2	3	4	5	6	7	8	9	10	11	12
Response 1	X	X	X	X	X							
Response 2		X	X	X		X	X					
Response 3		X	X					X	X			
Response 4			X	X		X				X		
Response 5						X			X	X	X	
Response 6					X	X	X					
Response 7								X				X

	# of runs		
	Ex 1	Ex 2	Ex 3
Res V UF-CCD	$26+n_c$	$44+n_c$	
Full UF-CCD	$42+n_c$	$44+n_c$	
Res V CCD	$148+n_c$	$280+n_c$	

Example 2

	1	2	3	4	5	6	7	8	9	10	11	12
	1*	2*	3*	4*	5*	1*	6*	1*	4*	2*	3*	2*
Response 1	X	X	X	X	X							
Response 2		X	X	X		X	X					
Response 3		X	X					X	X			
Response 4			X	X		X				X		
Response 5						X			X	X	X	
Response 6					X	X	X					
Response 7								X				X

Example 2



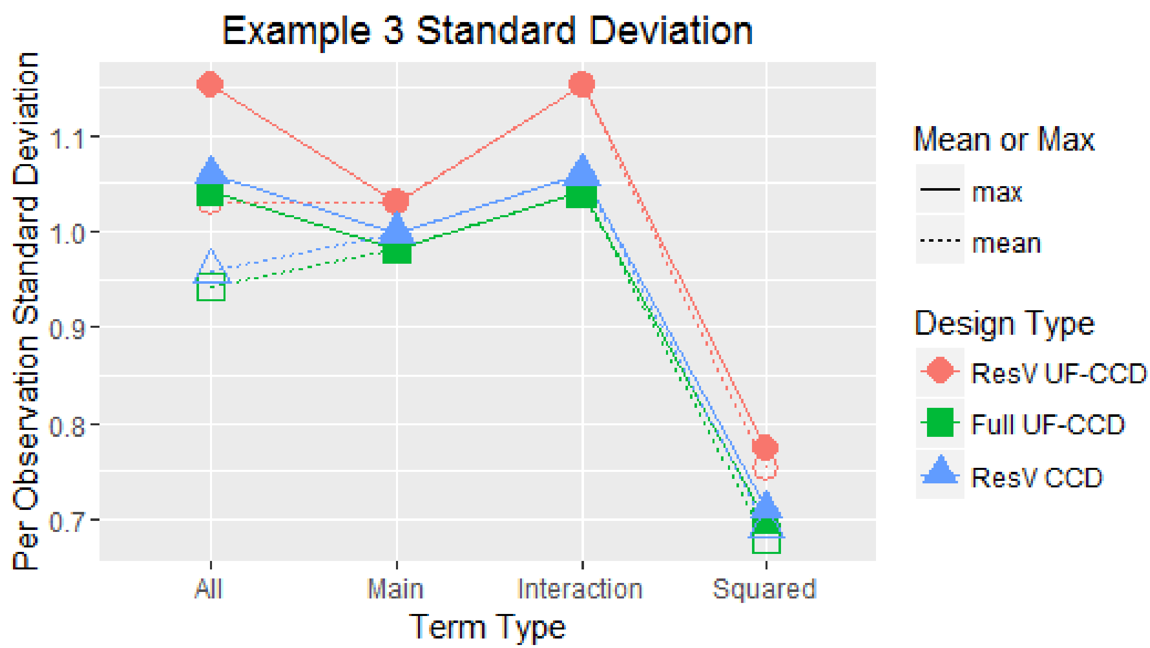
	N	All Effects		Main Effects		Interactions		Squared	
		mean	max	mean	max	mean	max	mean	max
UF-CCD	$44+n_c$	0.152	0.177	0.152	0.152	0.177	0.177	0.114	0.116
Res V CCD	$280+n_c$	0.055	0.063	0.059	0.059	0.063	0.063	0.040	0.041

Example 3

	1	2	3	4	5	6	7	8	9	10	11	12	13
Response 1	X	X	X	X	X	X	X	X					
Response 2						X	X	X	X	X			
Response 3				X	X			X			X	X	
Response 4					X							X	X
Response 5							X					X	

	# of runs		
	Ex 1	Ex 2	Ex 3
Res V UF-CCD	$26+n_c$	$44+n_c$	$80+n_c$
Full UF-CCD	$42+n_c$	$44+n_c$	$272+n_c$
Res V CCD	$148+n_c$	$280+n_c$	$282+n_c$

Example 3



	N	All Effects		Main Effects		Interactions		Squared	
		mean	max	mean	max	mean	max	mean	max
Res V UF-CCD	80+n_c	0.112	0.125	0.112	0.112	0.125	0.125	0.082	0.084
Full UF-CCD	272+n_c	0.057	0.063	0.059	0.059	0.063	0.063	0.041	0.042
Res V CCD	282+n_c	0.057	0.063	0.059	0.059	0.063	0.063	0.041	0.042

Conclusion

- These designs reduce cost
- For each response, CCD with
  - full factorial
  - resolution V fractional factorial
- Use when variance is small and runs are expensive.

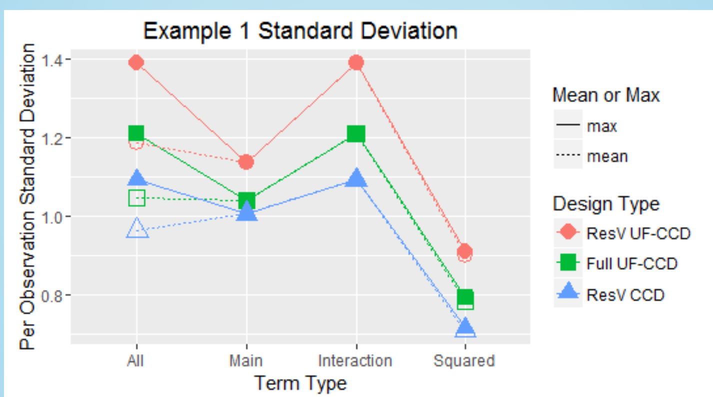
CCD = Central Composite Design

Motivation

Unique Factor CCD

Factor	1	2	3	4	5
Unique Factor	1*	2*	3*	4*	2*
Response 1	X	X	X		
Response 2		X	X	X	
Response 3	X		X		X
Response 4	X			X	

Results & Future Research



Wilmina (Billie) Marget
margetw@Augsburg.edu

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