Restricted-Randomization Optimal Design of Experiments Combining Mixture and Non-Mixture Factors

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Hank Anderson – prime mover

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A mathematician is a device for turning coffee into theorems.

--Alfréd Rényi
Probability Theorist

Office Coffee Experiment

Motivation of Martin and Hank :

- Current coffee in the office is disgusting* and unacceptable.
  ** Like "The Bitter Tonic" depicted by Antwerp artist Adriaen Brouwer.*
- Want to see if there is a better blend of coffee that we can use.
- Need to answer the following questions via experimentation:
  - ✓ What coffee to use?
  - ✓ How much coffee to use?
  - ✓ How to grind the coffee?
- The new coffee, on average, should be judged better than the current blend on average by the core group of 5 drinkers and no one should hate it.

Overview of Combined Designs

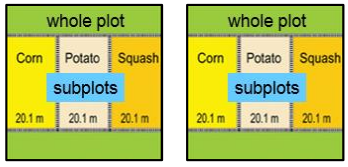
- Incorporate both mixture components and process factors, e.g.,
  - Bread doughs baked at different times and temperatures.
  - Fertilizers laid down in various amounts.
  - Metals rods soaked in a chemical bath (mixture 1), heated, and then sprayed with a coating (mixture 2).
- Mixture components $x_1, x_2, \ldots, x_q$ must sum to a fixed total, e.g. 100 weight percent.
- Process factors $z_1, z_2, \ldots, z_k$ can be numeric or categorical variables--they are not inherently restricted.

Randomized Combined Designs

- Classical randomized designs require independence from run to run.
- In a design that combines mixture and process factors, this means that:
  - an independent mixture must be prepared for every run,
  - and the process factors must be reset each time.
- Sometimes it is not practical, or even possible, to perform an experiment in this way, e.g. making cookies with various recipes by mixing one batch at a time and then baking it all by itself.

The Solution: Split-Plot Designs

- Often factors cannot easily be randomized, e.g., temperature.
- Split plots conveniently group runs by factor difficulty:
  - Hard-to-change (HTC) into "whole plots"
  - Easy-to-change (ETC) within "subplots"



- Building and analyzing these designs (versus one that is completely randomized) was extremely challenging.

Split plots are easy using DOE software! ☺

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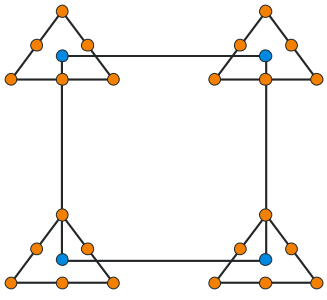
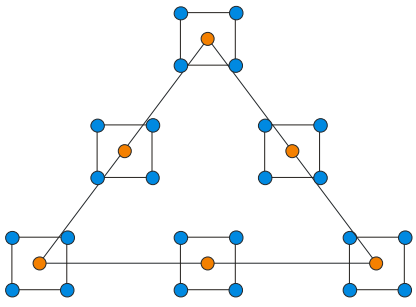
Two Ways to Split Up a Combined Design

Process Factors HTC
e.g.; powder-coat parts, then bake a bunch at time vs temp



Mixture Components HTC
e.g.; blend coffee beans, then grind & brew at varying conditions



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Office Coffee Experiment

- Mixture portion blended three coffee roasts:
  a. Light
  b. Medium
  c. Dark
- The beans were then processed by these varying factors:
  D. Grind setting: Fine, Medium, Coarse (3 level categoric)
  E. Amount of coffee: 2.5 to 4.0 oz. (continuous numeric)

Factors held constant: water temperature, amount of water, brew time, and filter type.

Practical Considerations

- Coffee is roasted and mixed in batches. It's not practical to purchase freshly roasted coffee beans for each run.
- Amount of coffee and grinder setting easily changed from run to run.
- Must not waste coffee for fear of incurring wrath of 'caffiends'.
- Preparation and tasting of coffee takes up valuable time and considerable distraction from work, so keep runs to a minimum.
- To avoid overdosing staff, best not do more than 4 to 6 runs per day.

Experimental Design

Set up a D-optimal combined design to fit a full quadratic model. Martin specified 16 groups to keep the number of subplot runs at 4 to 6.

Select	Group	Run	Comments	Compon... a:Light	Compon... b:Med	Compon... c:Dark	Factor 4 D:Amount	Factor 5 E:Grind ...	Respon... Mean	Respon... Min
	1	1		0	0	1	4	Cuis 3	6.4	5
	1	2		0	0	1	2.5	Cuis 12	5.2	4
	1	3		0	0	1	3.25	Krups 9	5.2	3
	1	4		0	0	1	2.5	Cuis 3	5	4
	2	5		0.5	0.5	0	4	Krups 9	4.2	3
	2	6		0.5	0.5	0	3.25	Cuis 3	5.6	5
	2	7		0.5	0.5	0	4	Cuis 12	5.4	4
	2	8		0.5	0.5	0	2.5	Krups 9	5.2	3
	3	9		0.5	0	0.5	3.18	Krups 9	5.4	4

He also added 6 runs of standard SE coffee at random as controls.

Taste Testing

- Hank prepared all 80 runs of coffee (74 designed + 6 control).
- Testing was done blindly by 5 tasters.
- They rated several attributes—aroma, acidity, body & flavor—on a scale of ☹1 – 9☺ —most importantly the overall likeability (OL).
- Same group of 5 taste-testers led to distillation of 2 responses:
  - ✓ Average OL rating.
  - ✓ Minimum OL rating.

Video of Experiment

Experimental Results

- Martin applied a number of automatic model selection methods, but all produced very similar predictive models (~15 terms).
- He discovered that most of the variability came from:
  - process factors (grind setting and amount of coffee), and
  - taste testing.
- Batch-to-batch differences were surprisingly small, i.e., the roasts/bean-types were very consistent.

Optimization
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Being very thorough as statistician and programmer; respectively, Martin and Hank considered a number of goals:

- Maximize the average rating for overall liking (OL).
- Maximize the minimum OL, provided it is at least 5, i.e., not settling on a coffee that any one taster dislikes.
- Minimize the amount of coffee used, thus pleasing the SE bean counters.

The solution for these goals is:

- ✓ **50/50 medium/dark blend** (none of the lightly roasted beans).
- ✓ **2.5 oz of coffee** at the **fine grind setting**.

Optimization
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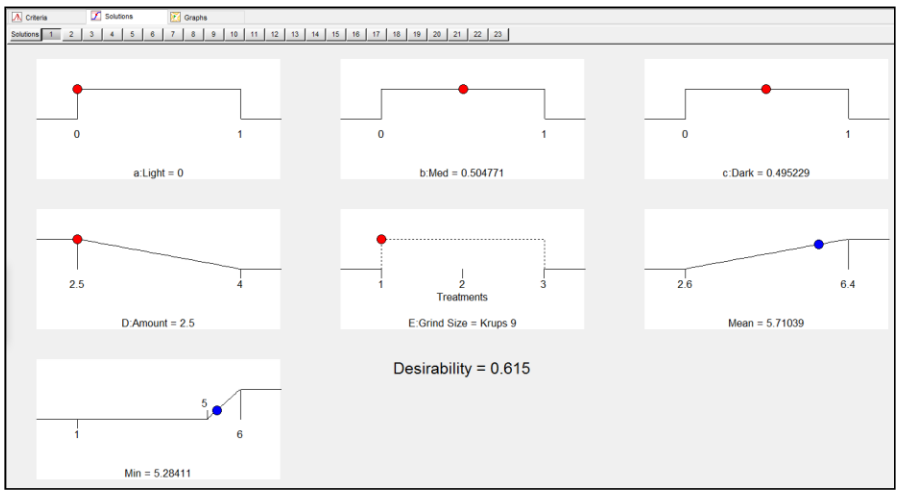

Optimization
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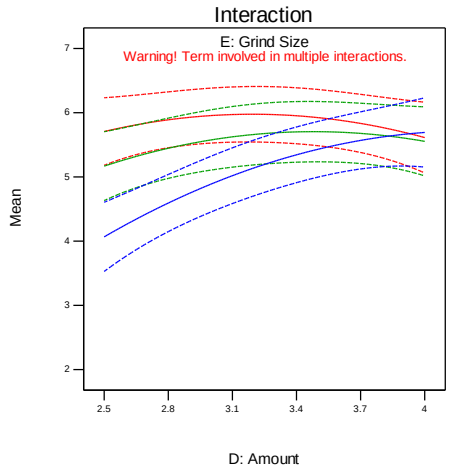
Design-Expert® Software
Component Coding: Actual
Factor Coding: Actual
Mean
---- 95% CI Bands

X1 = D: Amount
X2 = E: Grind Size

Actual Components
a: Light = 0
b: Med = 0.5
c: Dark = 0.5

E1 Krups 9
E2 Cuis 3
E3 Cuis 12



Optimization
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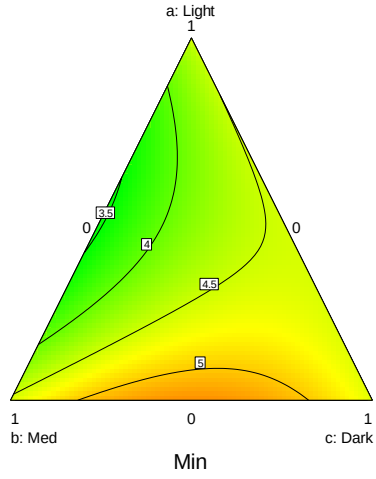
Design-Expert® Software
Component Coding: Actual
Factor Coding: Actual
Min
6
1

X1 = a: Light
X2 = b: Med
X3 = c: Dark

Actual Factors
D: Amount = 2.5
E: Grind Size = Krups 9



Confirmation

To confirm the optimal coffee, 10 follow-up runs were brewed up:

- 4 of the chosen blend.
- 2 of the standard office coffee.
- 4 at various other combinations of beans that were ground in different ways and produced with changing amounts.

Despite all these efforts to fool the 5, by-now expert tasters, they remained true to the predictive model. Thus the results of the experiment were confirmed. ☺

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Future Research on Coffee: Cold Brew

"Drip by drip Cold Bruer's slow hypnotic process unmasks the natural sweetness, and full-bodied origin flavors of any coffee you brew."
www.bruer.com

"The absence of hot water means that the oils, acids, and other compounds dissolve much more slowly. The acids also aren't degraded, making for a much smoother beverage, free of bitterness."
– The Science of Smooth, June 2016, *Consumer Reports,* "Cool Ways to Make Cold Joe" p25.

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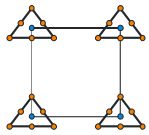
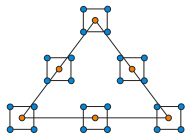
Conclusions





- Split plots provide very accommodating layouts for experiment designs that combine mixture components with process factors, whichever may be hardest to change (HTC).
- Optimal selection of runs facilitates customization of group sizes to make things even more convenient.
- Any combination of variables be they mixture, numeric or categorical can be handled with the tools of DOE software.

Statistics Made Easy®

Best of luck for your experimenting!

Thanks for listening!

-- Pat