Designing Mixture Experiments

Part 2

JMP STATISTICAL DISCOVERY FROM SAS

Objectives

Part 2

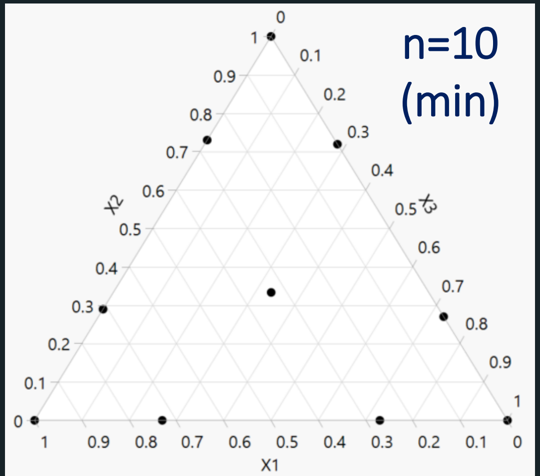
- Generate awareness of new approaches
- Introduce Mixture-Process Designs
- Address open questions from Part 1

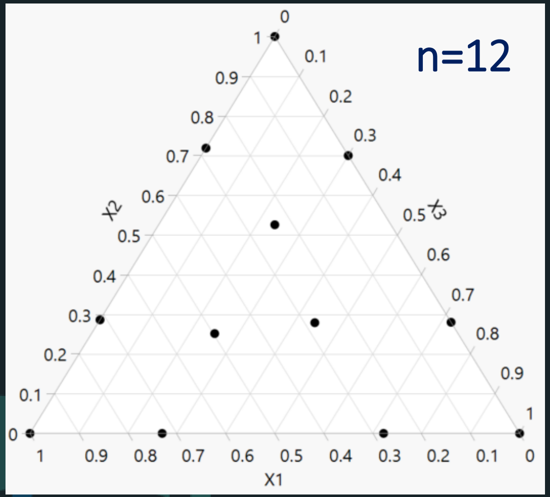
Agenda

- Comparison of designs – Optimal vs Classical vs. Modern
- Mixture-Process Designs
  - Bread Case Study
- Open questions from Part 1
  - Optimality
  - Ternary Plot with 3+ mixture components
- Recommended Continued Learning

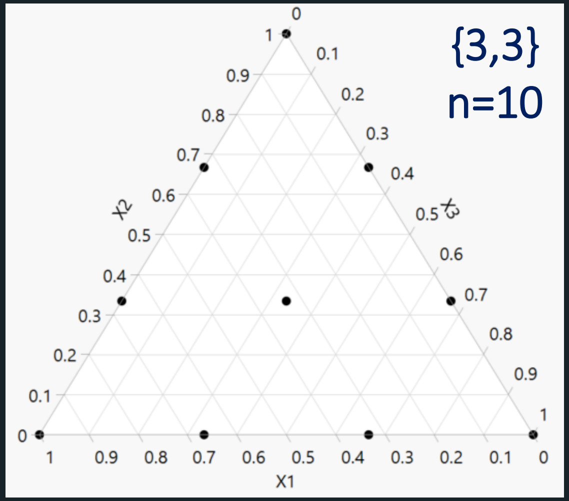
Mixture Designs – Comparison of Coverage

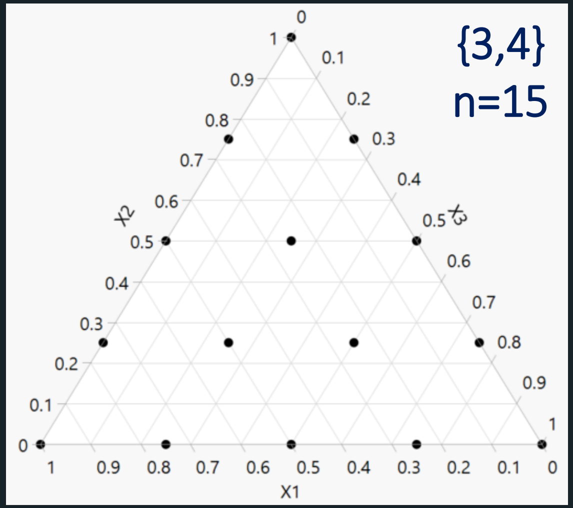
Scheffe Cubic (Optimal)



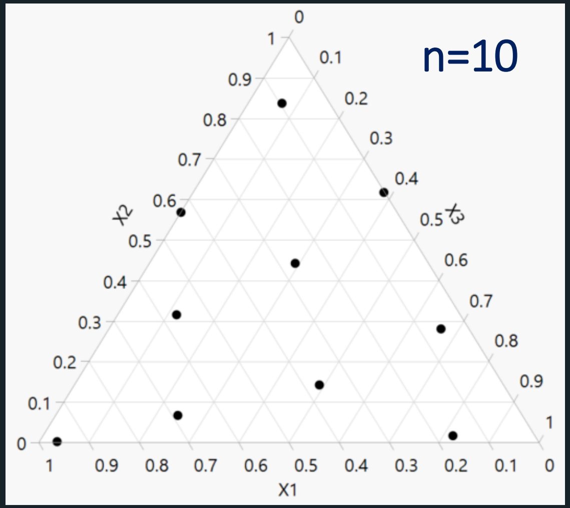


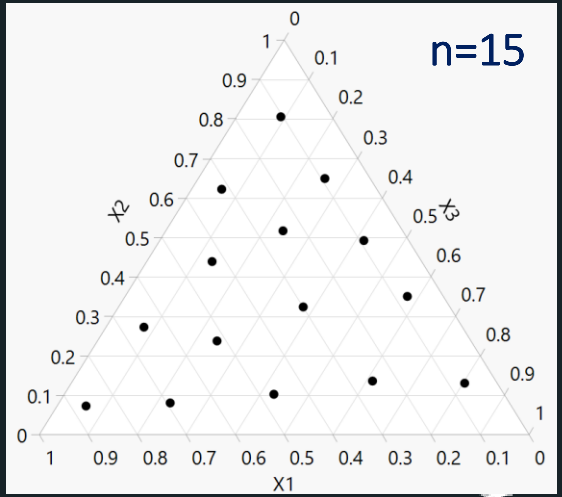
Simplex Lattice (Classical)





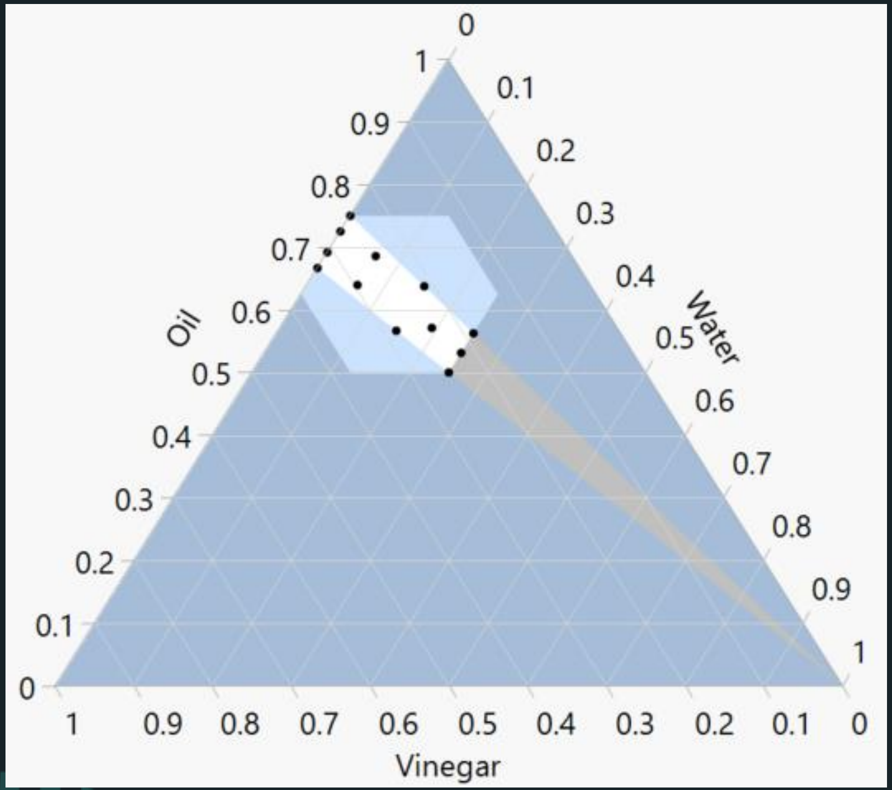
Space Filling (Modern)*



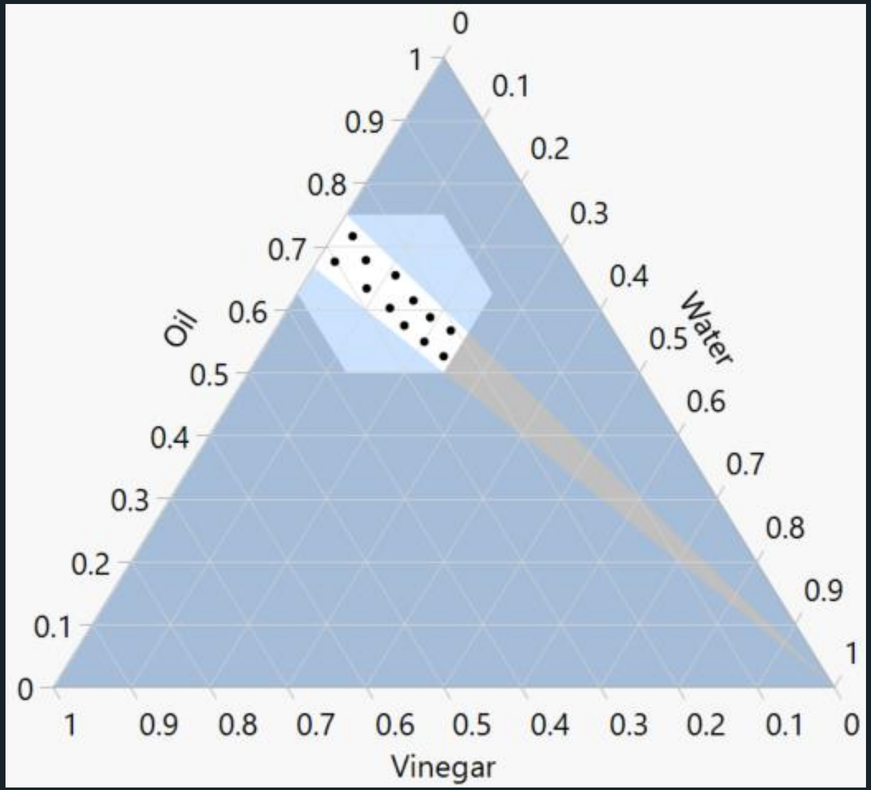


Salad Dressing DOE Design

Scheffe Special Cubic
n=12



Space Filling Design
n=12



Mixture Designs

Optimal

- I-Optimal recommended (binary, Scheffe Special Cubic, Scheffe Cubic)
- User specifies model (runs ≥ # of model terms)
- Boundary-focused designs
- Large designs if you want interior points
- JMP: DOE > Custom

Classical

- Simplex Lattice, Simplex Centroid, Aug. Simplex Centroid
- User specifies the number of levels or proportions
- Boundary-focused designs
- Large designs if you want interior points
- JMP: DOE > Classical > Mixture

Modern

- Space Filling
- User specifies run budget
- Interior focused designs
- Designs based on budget
- JMP 17: DOE > Special Purpose > Space Filling Design*

*In JMP 16: DOE > Classical > Mixture > Space Filling Design; but no ability to add mixture process/amount factors
Special Purpose SFD unable to support constraints currently

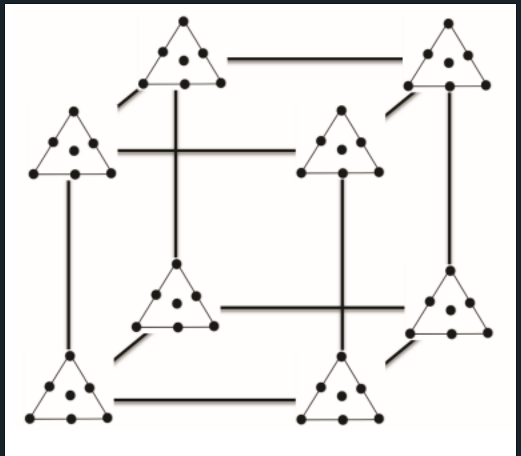
demo

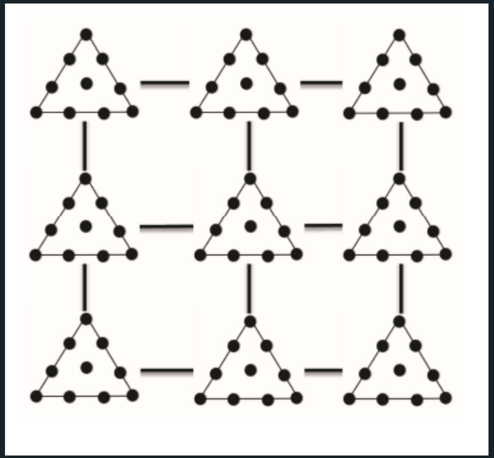
JMP Menus for Mixtures

STATISTICAL DISCOVERY FROM SAS

Mixture-Process Experiments

- Addition of non-mixture factors to experiment
  - Process factors (e.g., mixing time, temperature, pressure)
  - Amount
  - Material type
- Tend to be cost-prohibitive with optimal and classical designs
  - Multiply mixture model with process model





Bread Experiment

Mixture-Process Example

- Goal: Identify mixture proportions and process settings that will make bread that is "tall"

- Mixture ingredients: Flour 1, Flour 2, Flour 3
  - Flour 1: 25 – 100%
  - Flour 2: 0 – 75%
  - Flour 3: 0 – 75%
- Process: Proofing Time (30, 60 min)

demo Bread Experiment

- Design & Visualize
  - ✓ Optimal Design
  - ✓ Space Filling Design
- Analyze

Mixture Analysis

Optimal, Classical

- Based on model specified in design
- Standard Least Squares
- JMP: Analyze > Fit Model

Modern Designs

- Self Validating Ensemble Modeling (SVEM)
- JMP Pro 17: Fit Model > Gen Reg > SVEM
- SVEM Neural Network (Add-In)

Recommended Continued Learning

Courses

- Design of Experiments for Mixtures Using Machine Learning Course by Predictum, a JMP Partner
- Design and Analysis of Mixture Experiments Course by Adsurgo, a JMP Partner

Discovery Presentations

- Accelerating Innovation with Space Filling Mixture Designs, Neural Networks and SVEM (2021 JMP Discovery Presentation)
- JMP Pro 17 Remedies for Practical Struggles with Mixture Experiments (2022 JMP Discovery Presentation)

Book

Strategies for Formulations Development, A Step-by-Step Guide in JMP (Snee and Hoerl, 2016)

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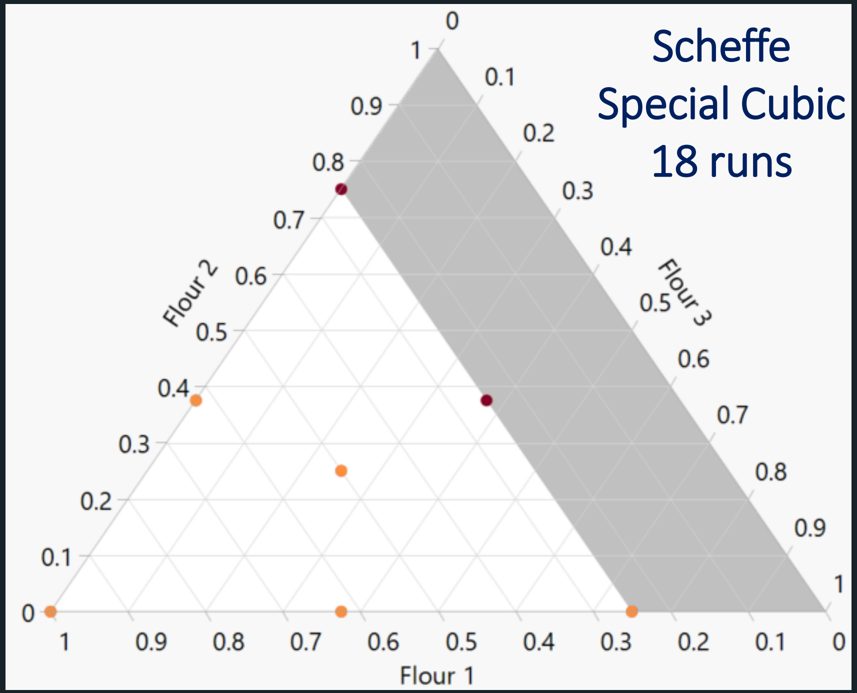
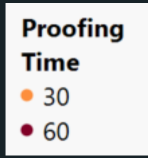
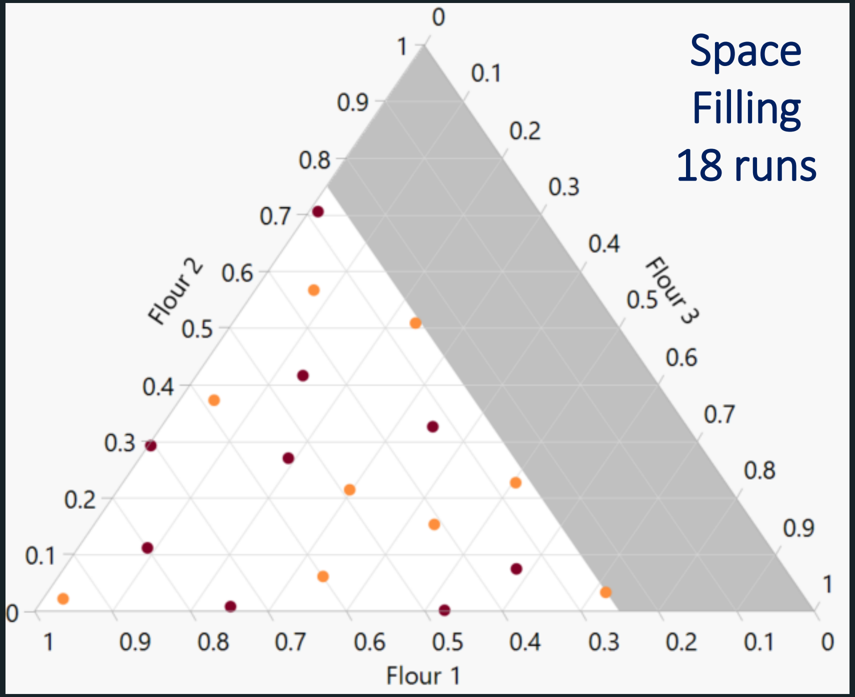
Visualizing Mixture Design Spaces with >3 Components

appendix

Bread Designs



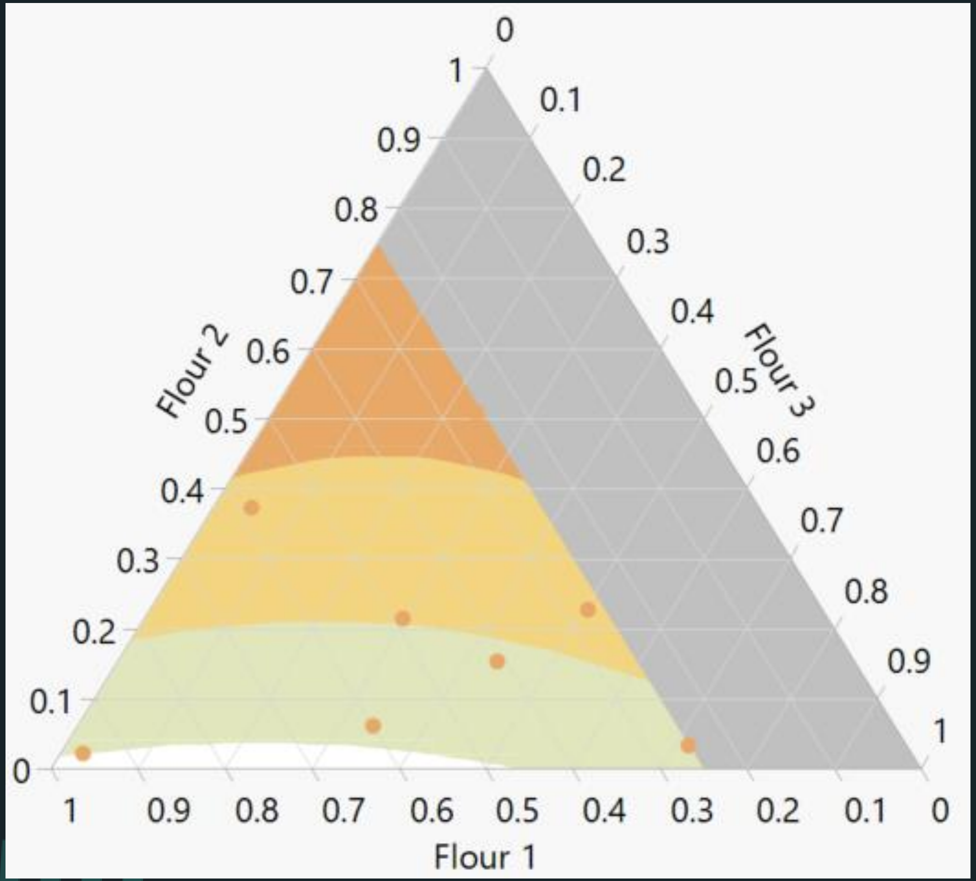




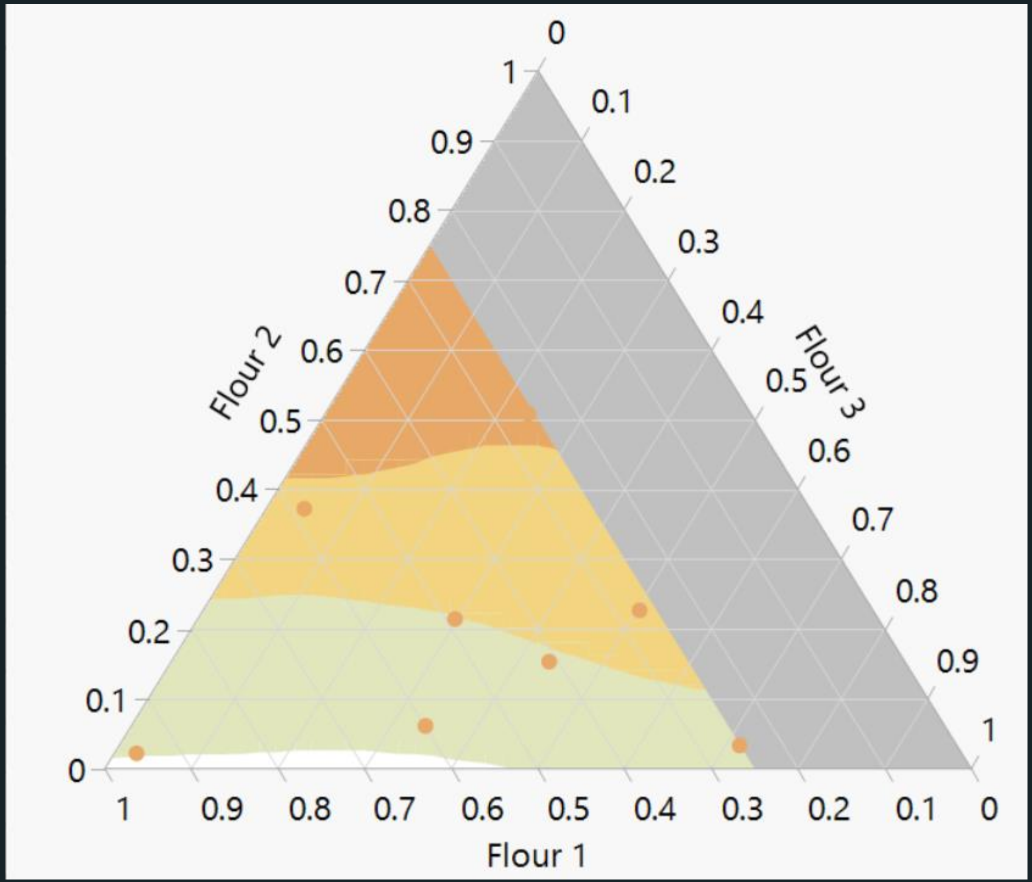
Standard Least Squares vs. SVEM NN

Proofing Time = 30 min

Standard Least Squares – Special Cubic



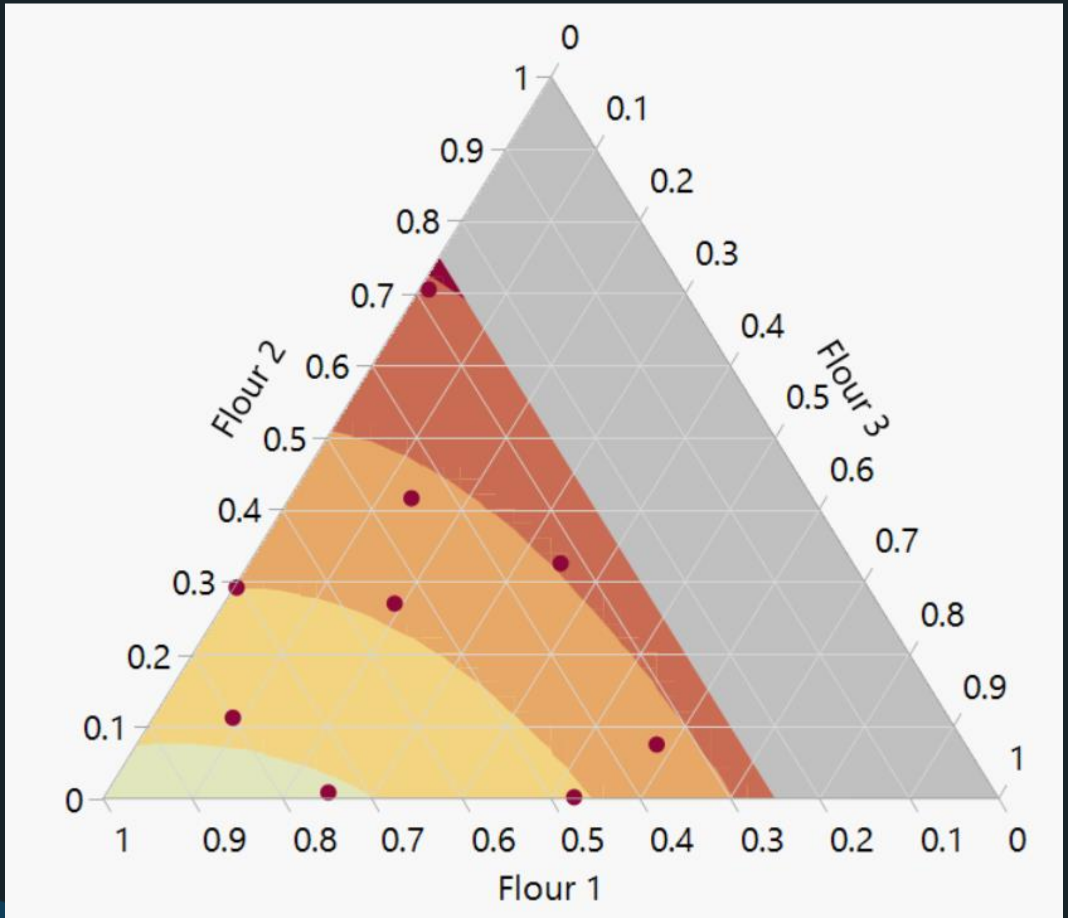
SVEM NN – TanH(5)



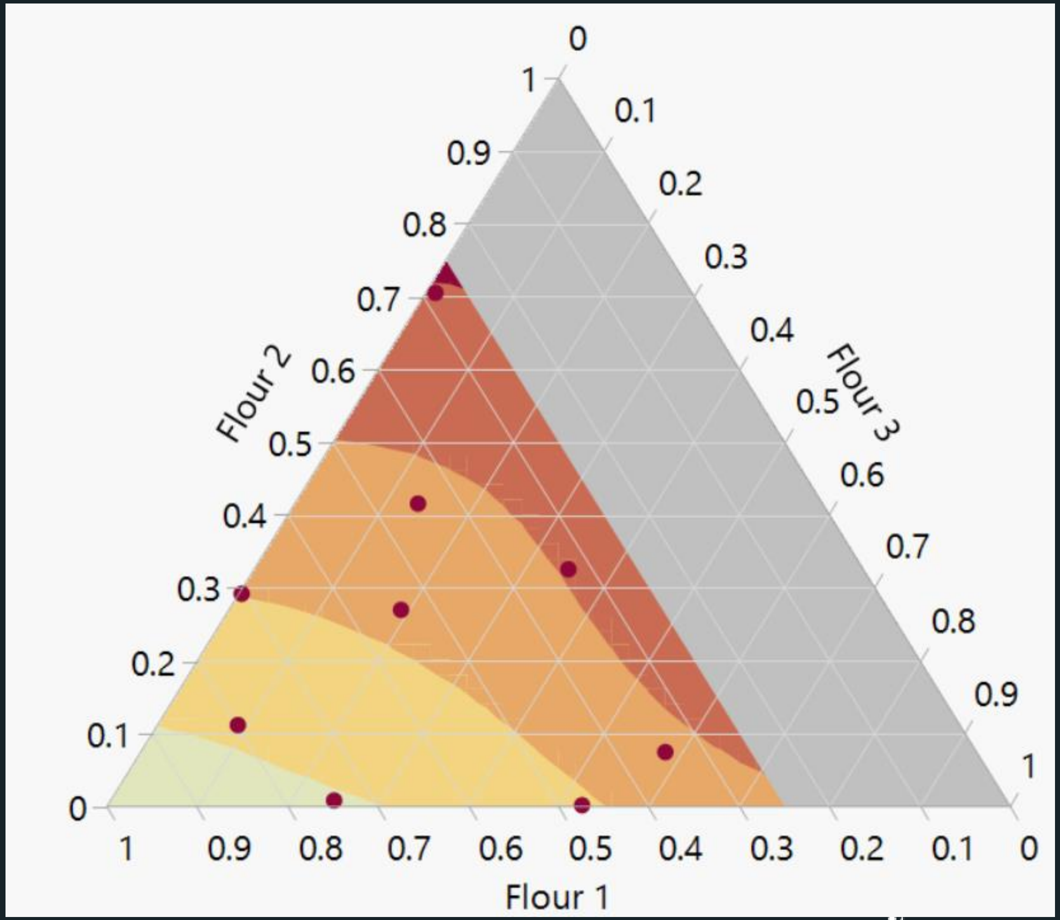
Standard Least Squares vs. SVEM NN

Proofing Time = 60 min

Standard Least Squares – Special Cubic

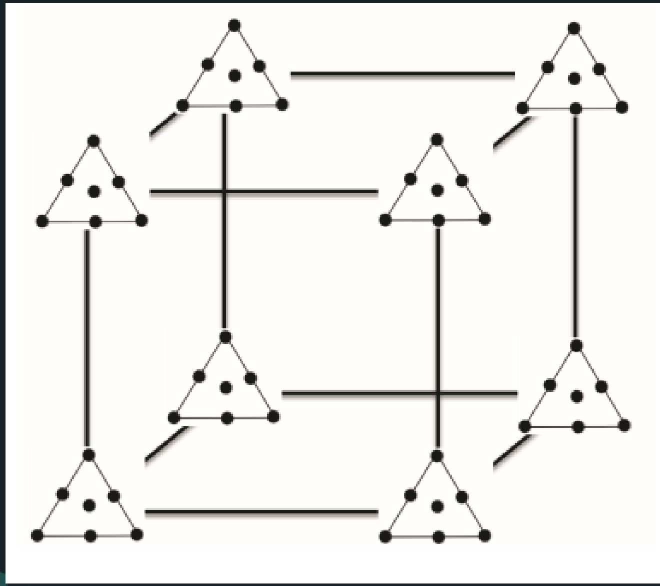


SVEM NN – TanH(5)



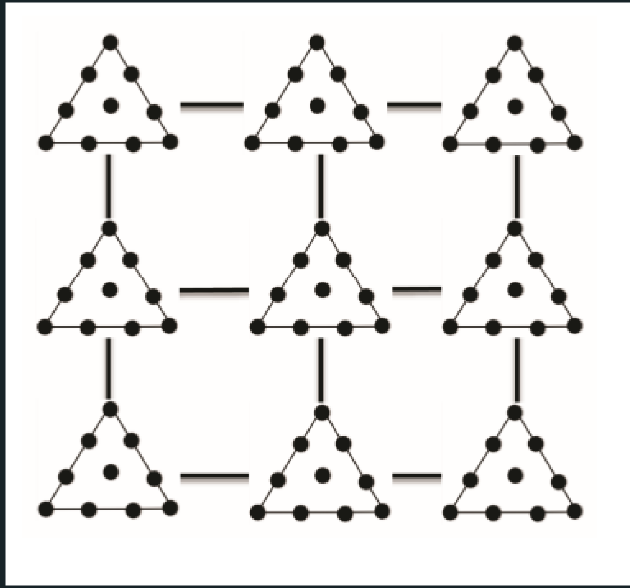
Fish Patty Design

- 3 mixture components: mullet, sheepshead, croaker
- 3 process factors: fry time, oven time, oven temp
- Simplex Centroid Design (7) with a 23 (8) factorial
- 7*8 = 56 runs



Bread Experiment

- 3 mixture components: Tjalve, Folke, Hard Red Spring
- 3 process factors: proofing time, mixing time
- Simplex Lattice Design (10) with a 3^2 (9) factorial
- 10*9 = 90 runs



Reference: Strategies for Formulations Development, A Step-by-Step Guide Using JMP | Snee and Hoerl, 2016