Modern Mixture Designs

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Machine Learning and DOE

There is ever-increasing interest in the use of big data machine learning methods to build predictive models using DOE data.[1,2,3]

Big data machine learning methods leverage the data's "bigness" in building predictive models.

Many predictive modeling strategies fit or train the model on one subset of the data and use a second subset, which is the validation set, to tune the parameters and select a model.

The prediction errors from the validation set can also be used to define objective functions in building predictive models.

Can we apply machine learning methods to smaller DOE data sets?

Machine Learning and DOE

Why don't we use holdback cross-validation for DOE model selection?

DOEs are carefully constructed data sets that are designed to extract as much information as possible in the smallest number of observations

No portion of a structured experimental design can be held back for validation purposes.

DOE allows very efficient experimentation.

The budget and resources that are required to obtain a validation set consisting of additional trials are rarely available.

What is a Mixture Design?

In a mixture experiment, the experimental factors are components of a formulation or recipe.

The components can be liquids, gases, or solids.

The impact of the mixture components on the responses of interest **depends only on the proportions of the components and not on the amounts.**

If there is a dependency on the total amount of the components, then classical mixture designs are inappropriate.

Because the experimental factors are components of a formulation, there are inherent constraints on the settings of these factors.

What is a Mixture Design?

Factorial experimental designs allow the experimental factors to be set independently – there are no constraints on the joint factor settings.

Mixture experimental designs impose constraints on the settings of the factors because they are components of a formulation.

Mixture factors can not be independently manipulated.

A mixture experimental design with *q* factors requires, at a minimum, the constraints

$$X_1 + X_2 + \ldots + X_q = 1.0 \quad \text{and} \quad 0 \le X_i \le 1.0 \quad \text{for } i=1,\ldots,q$$

Process factors can also be combined with mixture factors to create mixture process experiments.

Machine Learning and DOE

Classical mixture designs are structured to support explanatory goals:

- Hypothesis testing
- Confidence intervals

However, mixture experimentation is inherently focused on prediction.

- The goal is to predict the future performance of mixtures or recipes.

Also, many classical designs are boundary point designs.

Modern mixture situations tend to exhibit complex interaction structures.

These situations cannot be fit with classical designs and classical models (such as Scheffe polynomials).

Machine Learning and DOE

To address the inherent complexity of today's processes, we suggest the use of space-filling designs (SFDs).

Space-filling designs:

- Cover the mixture design region better than classical designs
- Enable smaller designs than would classical designs
- Result in more accurate and useful predictive models

But how can we use space-filling experimental designs to model the more complex nature of the underlying physical phenomena?

Auto-Validation

Gotwalt and Ramsey proposed a method of validation, referred to as auto-validation or self-validation.[4]

The original data set is used for both training and validation.

The original data is the training set and a copy of the original data is an *auto-validation* set.

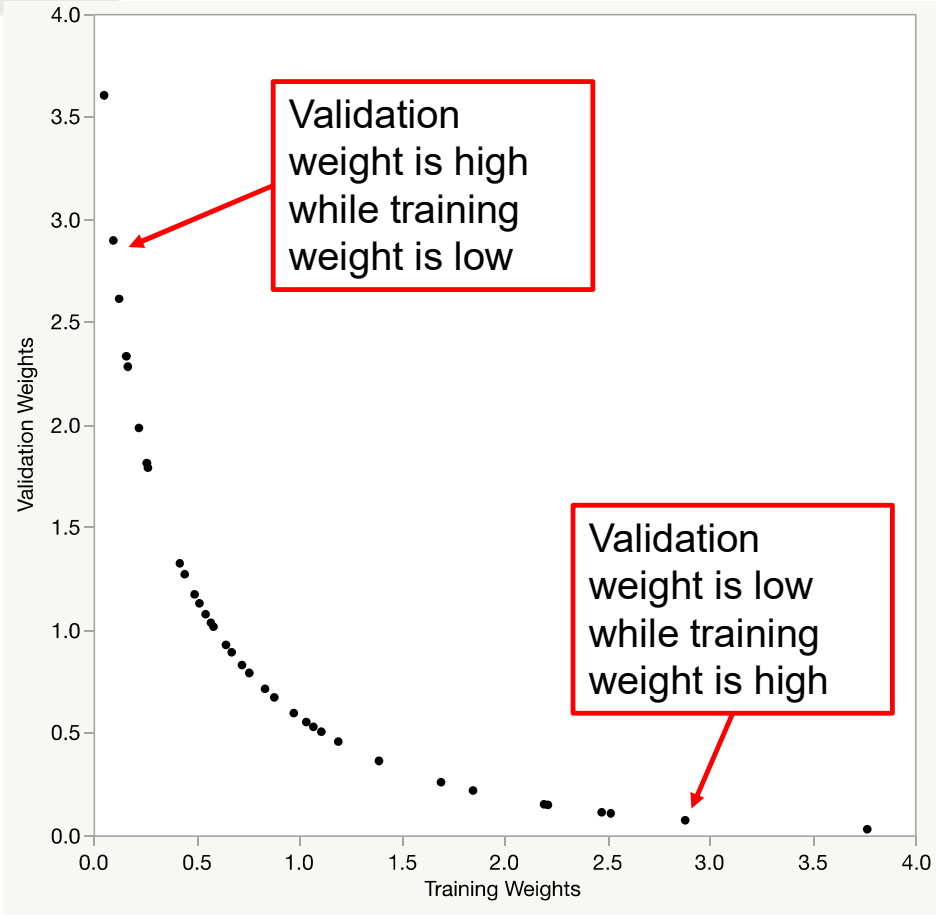
Each observation in the training set has a twin in the auto-validation set.

Auto-Validation

Random fractional gamma weights are applied to each observation in both of the data sets.

If a row in the training set is assigned a large weight, its twin in the auto-validation set is assigned a small weight, and vice versa.

This strategy imposes anti-correlation between the two sets.



Auto-Validation

	X1	X2	X3	Y	Paired FWB Weights	Validation
1	0	1	1	4.03	1.4131	Training
2	0	-1	-1	-1.48	1.3495	Training
3	1	0	-1	-0.38	0.3532	Training
4	-1	0	1	-1.82	0.3498	Training
5	1	-1	0	1.57	5.5015	Training
6	-1	1	0	1.89	0.2364	Training
7	0	0	0	1.21	0.3505	Training
8	0	1	1	4.03	0.2789	Validation
9	0	-1	-1	-1.48	0.3002	Validation
10	1	0	-1	-0.38	1.2122	Validation
11	-1	0	1	-1.82	1.2201	Validation
12	1	-1	0	1.57	0.0041	Validation
13	-1	1	0	1.89	1.5582	Validation
14	0	0	0	1.21	1.2185	Validation

- This is an example of fractional gamma weights applied to a small design.
- The training and auto-validation weights are paired such that a design condition with a high weight in one set has a low weight in the other set.
- In other words, the weights, in pairs, are close to being uncorrelated.
- For example, compare rows 5 and 12, and rows 13 and 6.
- Because of how weights are paired, the auto-validation set is close to being “independent” of the training set.

Self-Validating Ensemble Modeling (SVEM) Methodology

Fractionally weighted bootstrapping (FWB) randomly assigns new gamma weights to the training and auto-validation data sets for each iteration of a modeling procedure.

The combination of auto-validation using FWB and ensemble modeling is called *self-validating ensemble modeling* or *SVEM*.

SVEM has been shown to be a powerful modeling technique for designed experiments.[5,6]

We proceed to describe SVEM modeling.

Self-Validating Ensemble Modeling (SVEM) Methodology

A modeling algorithm is selected (neural network, forward selection, etc.).

Based on that algorithm, SVEM does the following:

- Generates a fractionally weighted bootstrap sample of the original training and auto-validation sets for each of many iterations.
- On each FWB iteration, estimates and saves the prediction model obtained using the selected algorithm.
- Forms an average (or weighted average) of the estimated prediction models to obtain an ensemble prediction model.

SVEM Demonstration

This is an experiment with the goal of optimizing a solution for a cleansing agent.

Water, **Alcohol**, and **Urea** are the three components of interest.

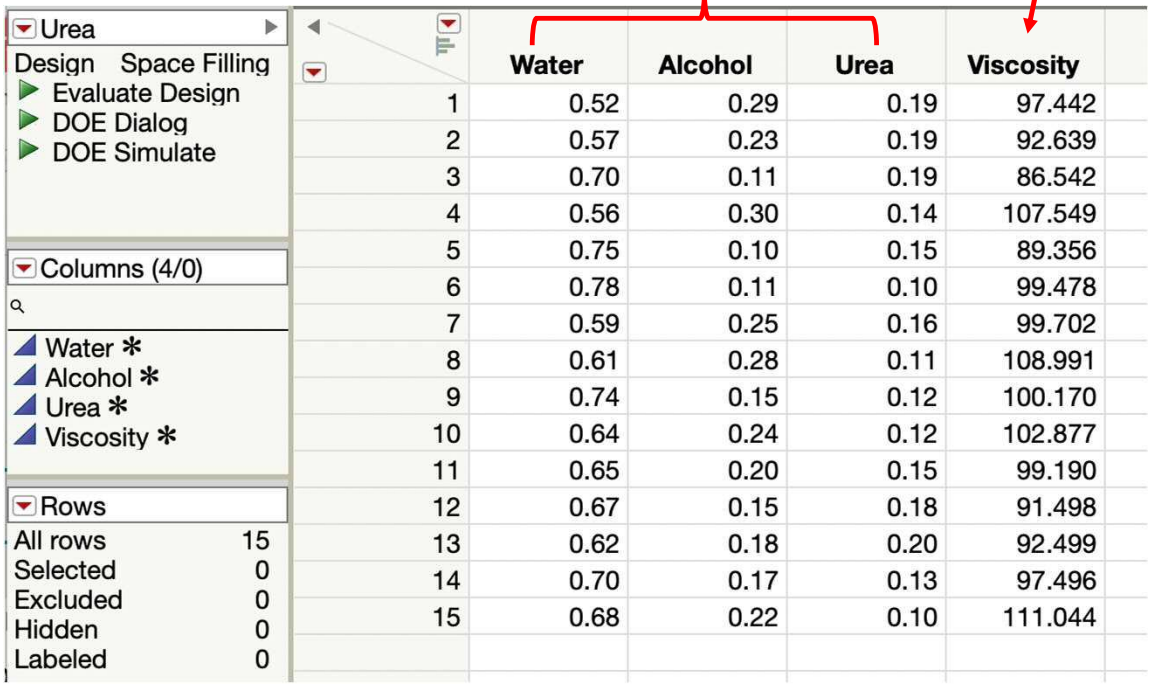
There are bounds on these components.

A three-factor space-filling design was created in JMP.

The response for our demo is **Viscosity**:
Target = 100
Spec limits = 95 to 105

Components

Response
Target =100

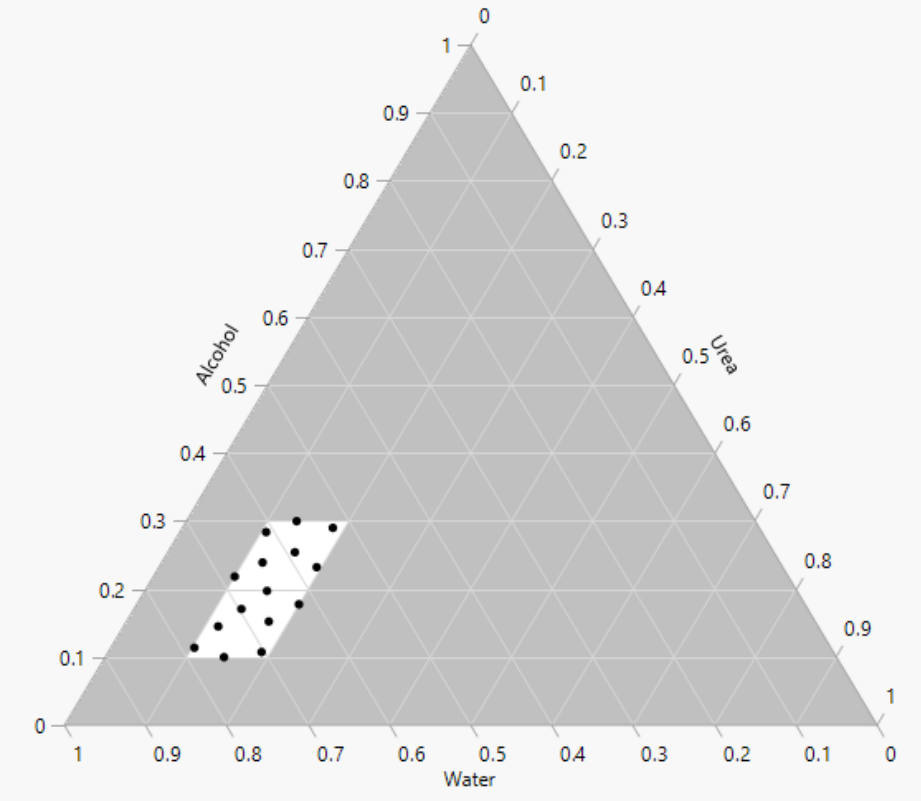


	Water	Alcohol	Urea	Viscosity
1	0.52	0.29	0.19	97.442
2	0.57	0.23	0.19	92.639
3	0.70	0.11	0.19	86.542
4	0.56	0.30	0.14	107.549
5	0.75	0.10	0.15	89.356
6	0.78	0.11	0.10	99.478
7	0.59	0.25	0.16	99.702
8	0.61	0.28	0.11	108.991
9	0.74	0.15	0.12	100.170
10	0.64	0.24	0.12	102.877
11	0.65	0.20	0.15	99.190
12	0.67	0.15	0.18	91.498
13	0.62	0.18	0.20	92.499
14	0.70	0.17	0.13	97.496
15	0.68	0.22	0.10	111.044

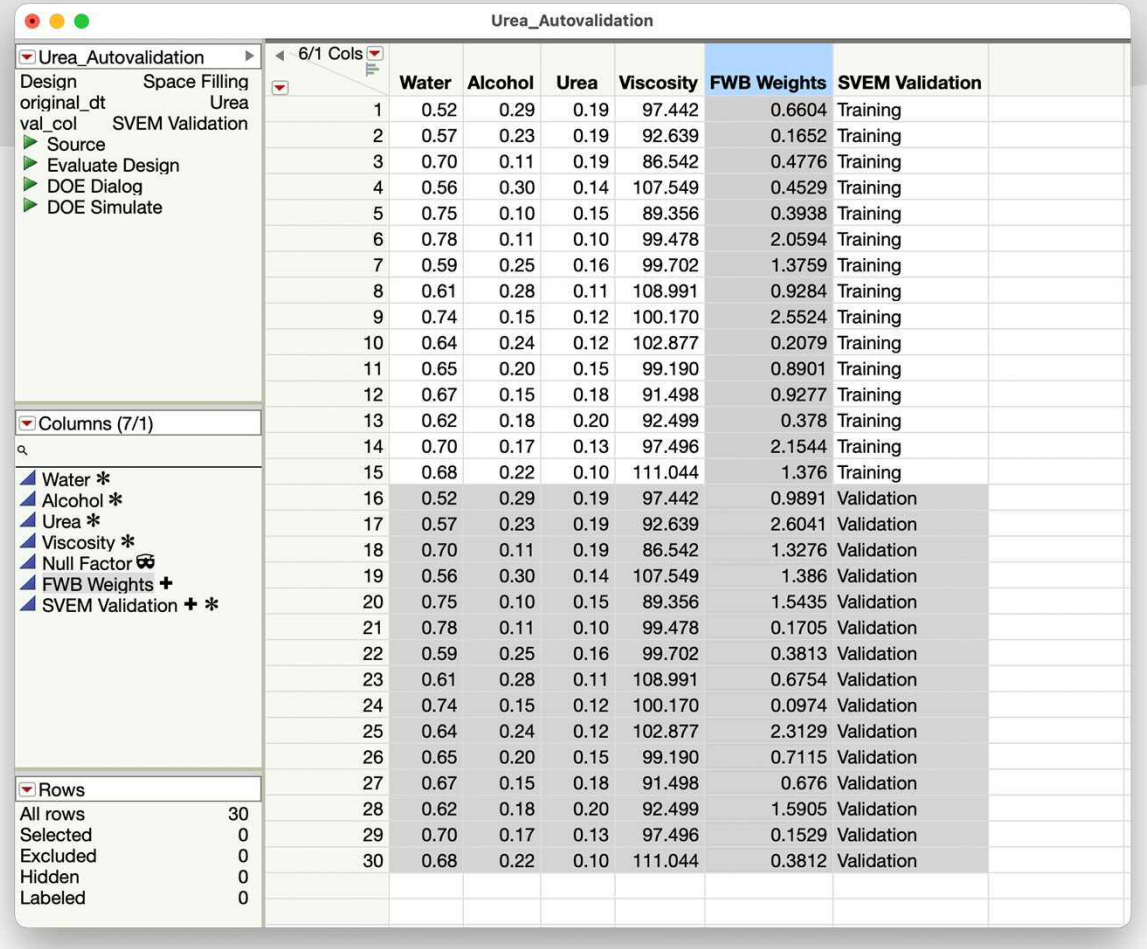
SVEM Demonstration

The ternary plot shows the design space for this experiment.

Note that the space-filling design efficiently covers the experimental region.



SVEM Demonstration



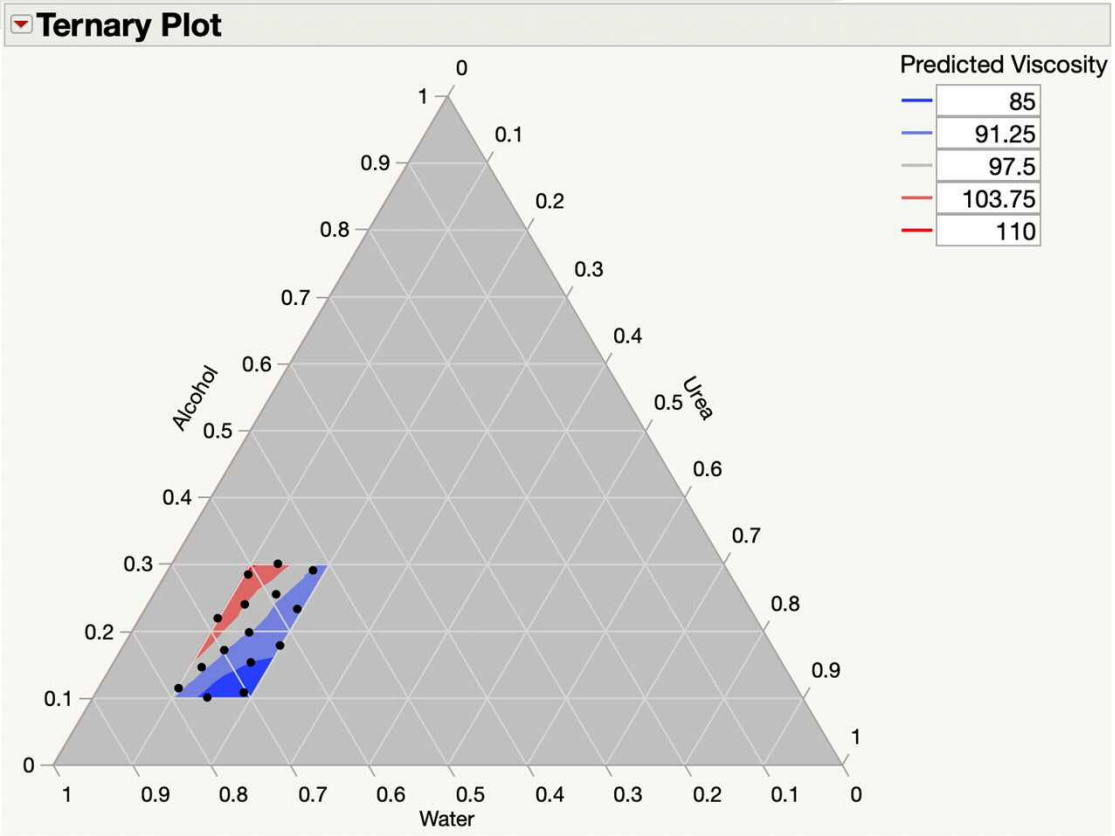
	Water	Alcohol	Urea	Viscosity	FWB Weights	SVEM Validation
1	0.52	0.29	0.19	97.442	0.6604	Training
2	0.57	0.23	0.19	92.639	0.1652	Training
3	0.70	0.11	0.19	86.542	0.4776	Training
4	0.56	0.30	0.14	107.549	0.4529	Training
5	0.75	0.10	0.15	89.356	0.3938	Training
6	0.78	0.11	0.10	99.478	2.0594	Training
7	0.59	0.25	0.16	99.702	1.3759	Training
8	0.61	0.28	0.11	108.991	0.9284	Training
9	0.74	0.15	0.12	100.170	2.5524	Training
10	0.64	0.24	0.12	102.877	0.2079	Training
11	0.65	0.20	0.15	99.190	0.8901	Training
12	0.67	0.15	0.18	91.498	0.9277	Training
13	0.62	0.18	0.20	92.499	0.378	Training
14	0.70	0.17	0.13	97.496	2.1544	Training
15	0.68	0.22	0.10	111.044	1.376	Training
16	0.52	0.29	0.19	97.442	0.9891	Validation
17	0.57	0.23	0.19	92.639	2.6041	Validation
18	0.70	0.11	0.19	86.542	1.3276	Validation
19	0.56	0.30	0.14	107.549	1.386	Validation
20	0.75	0.10	0.15	89.356	1.5435	Validation
21	0.78	0.11	0.10	99.478	0.1705	Validation
22	0.59	0.25	0.16	99.702	0.3813	Validation
23	0.61	0.28	0.11	108.991	0.6754	Validation
24	0.74	0.15	0.12	100.170	0.0974	Validation
25	0.64	0.24	0.12	102.877	2.3129	Validation
26	0.65	0.20	0.15	99.190	0.7115	Validation
27	0.67	0.15	0.18	91.498	0.676	Validation
28	0.62	0.18	0.20	92.499	1.5905	Validation
29	0.70	0.17	0.13	97.496	0.1529	Validation
30	0.68	0.22	0.10	111.044	0.3812	Validation

This is an example of the SVEM data table structure for this experiment.

Notice that:

- Rows 16 – 30 clone the design.
- There is a column containing weights based on the fractionally-weighted bootstrap
- There is a column for the self-validation.

SVEM Demonstration



This is a ternary contour plot for the SVEM model based on 50 iterations.

The contours show the response surface over the design space for the three components.

Using the profiler and the mixture profiler, you can find a range of optimal or near-optimal settings for Viscosity.

SVEM and Space-Filling Designs

One of the motivations for using model averaging is the fact that many model fitting algorithms are inherently unstable.[7]

- Small changes in the data can lead to big changes in predictions
- A single predictive model can be unstable, particularly when multicollinearity is present, resulting in predictions that are artifacts of the noise in the data

Given the multicollinearity that is inherent in mixture experiments, a technique that mitigates collinearity:

- Results in stable and more accurate predictive models
- Together with space-filling designs, which cover the mixture space more thoroughly, provides more confidence in predictive models over that space

The SVEM Add-In and Modern Mixture Design Course

Model Averaging using SVEM is not automated in JMP Standard or JMP Pro.

However, Predictum has a Self-Validating Ensemble Modeling add-in that automates the method for both JMP Standard and JMP Pro users.

More information can be found on the SVEM page[8] on the Predictum website.

For information about the Modern Mixture Design Course, see the Training page[9] on the Predictum website.

Summary

In this talk, we have:

- Seen how building predictive models from DOE data is limited by the infeasibility of conducting validation trials to control overfitting
- Suggested the use of space-filling designs for mixture experiments, and, more generally, DOE situations
- Described SVEM, which is based on auto-validation and fractionally weighted bootstrapping
- Discussed how SVEM enables predictive modeling for DOE data without a separate set of validation runs.
- Demonstrated SVEM using the Urea experiment data

References

1. Arboretti, R., Ceccato, R., Pegoraro, L, Salmaso, L., Housmelerides, C., Spadoni, L., Pierangelo, E., Quaggia, S., Tveit, C, and Vianello, S. "Machine learning and design of experiments with an application to product innovation in the chemical industry" (research paper, Journal of Applied Statistics, 2021).
2. Freiesleben, J., Keim, J., and Grutsch, M. "Machine Learning and Design of Experiments: Alternative approaches or complimentary methodologies for quality improvement?" (discussion paper, Quality and Reliability Engineering International, 2020).
3. Lakshminarayanan, B., Pritzel, A., and Blundell, C.. "Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles" (research paper, 31st Conference on Neural Information Processing Systems, 2017).

References

4. Ramsey, P. and Gotwalt, C. "Model Validation Strategies for Designed Experiments Using Bootstrapping Techniques with Applications to Biopharmaceuticals" (PowerPoint presentation, JMP Discovery Summit Americas, October 25, 2018).

5. Gotwalt, C., Xu, L., Hong, Y., and Meeker, W. Q. "Applications of the Fractional-Random-Weight Bootstrap" (research paper, ResearchGate GmbH, 2018).

6. Lemkus, T., Ramsey, P., Gotwalt, C., and Weese, M. "Self-Validated Ensemble Models for Design of Experiments" (research paper, arXiv.org, Cornell University, 2021).

References

7. Breiman, L. “Heuristics of Instability and Stabilization in Model Selection” (research paper, Project Euclid, Cornell University Library and Duke University Press, 1996).

8. “Self-Validating Ensemble Modeling,” Predictum Inc., accessed August 12, 2021.

9. "Modern Mixture Designs", Predictum Inc.