Optimizing Household Cleaners with INForm

Household cleaners are complex formulations, frequently involving a combination of surfactants. Customers look for properties like the lather that is formed, the amount of soil that the product will dissolve, the foam height and how long the product lasts. Formulating cleaners to meet customer requirements is demanding – Heinsman and Montgomery, writing in Quality Engineering, 7(3) 583-600 (1995) estimate that at least two months of effort are involved by a trial-and-error process, although this can be reduced by modelling.

Traditionally, statistical methods have been employed to generate models, with response surfaces used to try to determine optimum formulations. This is the approach adopted by Heinsman and Montgomery. However, using statistics often means that the problem is over-simplified in order to render it tractable, and statistical expertise is generally needed to use the method.

A powerful alternative, **INForm**, has now been developed by Intelligensys. **INForm** integrates neural network modelling with efficient optimization routines based on Genetic Algorithms. **INForm** lets the user bypass many "what if" questions typically required to find an acceptable formulation, and tells the user directly how to achieve certain properties with minimum effort.

To use **INForm**, you carry out some initial experiments, and feed these into the neural network directly from your spreadsheet package. Once your model is developed, you can then specify the values of the properties you want, and the relative importance of any conflicting properties. The optimization process will tell you what conditions are required to obtain them. Cost can even be included as a factor if you wish, and the optimum solution is obtained in seconds, saving you valuable time.

Here, we used the data published by Heinsman (of the Dial Corporation) and Montgomery (Arizona State University) in our study.

Data and Models for Household Cleaners

Heinsman and Montgomery looked at a mixture of two non-ionic surfactants (labelled A and B) with an anionic surfactant and a zwitterionic surfactant. They designed an experiment in which the total amount of material needed to sum to a constant value of 1, with constraints

- Non-ionic A $1 \geq x_1 \geq 0.5$
- Anionic $0.5 \geq x_2 \geq 0$
- Non-ionic B $0.5 \geq x_3 \geq 0$
- Zwitterionic $0.05 \geq x_4 \geq 0$

20 different experiments were performed, varying the amounts of each ingredient and measuring four properties

- lather (a measure of the life of the product)
- number of soil pellets dissolved (a measure of the amount of grease the cleaner can remove)
- foam height
- total amount of foam produced

Lather is the most important property, since it is the one used by consumers to judge the product. The final three properties are measured using the beater foam test, in which soil pellets are added to a dilute solution of the product while it is beaten by a mixer.

The 20 experiments were copied into **INForm's** "enter/edit data" spreadsheet. 18 of the records were used to develop the models, while the other 2 were used for validation to ensure that the models were predictive. A separate model was developed for each of the properties. The models gave a good fit to the training data, with R^2 values from ANOVA statistics of 96.4% for lather, 99.9% for pellets, 92.0% for foam height and 75.0% for total foam. This last value is relatively low, indicating that an unmeasured variable may be affecting this output.

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Optimizing for Customer Satisfaction

According to Heinsman and Montgomery, customers judge the cleaner primarily on the number of lather units obtained. Therefore, this property is the most important, and it should be maximized. The other properties should also be maximized (insofar as practical) but they are of lesser importance. Heinsman and Montgomery carried out consumer tests for potential products, and determined that the objectives should be

Pellets ≥ 19
Foam Height ≥ 82
Total foam ≥ 1000

Heinsman and Montgomery found that a formulation in which there were 0.7666 units of non-ionic surfactant A, 0.1941 units of anionic surfactant, and 0.0393 units of zwitterionic surfactant gave an optimum, with properties of lather 5.056, pellets 19.17, foam height 82 and total foam 1000. Using our models, and the same values for the ingredient amounts, we predict that this formulation will have lather value of 5.47, pellets 20.0, foam height 81.67 and total foam 910.7. (Recall that the model for total foam indicated that perhaps other variables were important, but were not included in the model.) Although they say they were aiming to maximize the lather, the value of 5.056 from the Heinsman-Montgomery optimum is relatively low since the largest value in the training set used to develop the model is 7.17. In fact, they found in later consumer tests that lather was less important than first expected – the amount of foam was more significant to consumers.

Genetic algorithms, based on 'survival of the fittest solutions' are used in **INForm** for optimization. **INForm** can handle conflicting objectives, allowing the user to weight each of the properties so that the most important is emphasized. In addition, the optimization can be constrained so that the sum of ingredients is 1 – a necessary requirement for this mixture. Weighting the lather at 10, and all other properties at 5, gave a formulation with

Non-ionic surfactant A	0.8838
Anionic surfactant	0.0638
Non-ionic surfactant B	0.0025
Zwitterionic surfactant	0.0

and predicted properties

Lather	6.75
Pellets	19.39
Foam Height	72.47
Total Foam	857

These do not meet the consumer requirements for Foam Height and Total Foam, though. Consequently, new optimizations were performed, weighting these properties at various levels on a scale of 1-10. Lather remained weighted at 10. These results showed clearly that achieving high values of lather was only possible when the values for total foam lay below the required value of 1000.

Like the study by Heinsman and Montgomery, our results showed that Non-ionic surfactant B was unnecessary for the formulation, thereby simplifying the production process and potentially reducing the cost of the formulation.

Conclusions

If a high value for lather units is achieved, this is generally at the expense of the values for foam height and total foam. To achieve the consumer requirements of foam height greater than 82, and total foam greater than 1000, high values of lather must be sacrificed.

The neural network in **INForm** developed models of similar quality to the statistical models reported by Heinsman and Montgomery.

Optimization using conflicting objectives was straightforward with **INForm**. The different consumer requirements could be assigned weights according to their importance. Constraints on the ingredient sum could be imposed easily.

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