Optimization of a Metallurgical Process with Uncertain Dynamics

Scott Koermer
PhD Candidate in Mining Engineering
Virginia Tech

Aaron Noble
Associate Professor, Mining Engineering
Virginia Tech

1. Background

Integrated laboratory testing and process modeling are often used to optimize metallurgical process operations. While many metallurgical models are available for commercial processes, observations often differ from model predictions by some amount of *bias*. Bias can be related to factors unaccounted for in the model including mineral speciation, and complex chemical dynamics. When the function for describing the biased observations is unknown, polynomial regression can be used to aid in optimization[1]. Polynomial and gradient ascent techniques can get stuck at local optima, and require a large number of tests to ensure convergence on the global optimum[3], making these methods prohibitive for use in the design of laboratory experiments.

2. Research Aims

Optimization through Gaussian Process (GP) regression has established advantages over polynomial regression for finding the global optimum of high dimensional computer simulations, with less simulation tests[3]. The goal of this presentation is to explore the utility of using GP regression in conjunction with Expected Improvement (EI) optimization criteria[4] to find and test the optimum of a noisy chemical process with unknown dynamics.

3. Materials and Methods

Ce recovery from leaching is simulated using the function $f(x_1, x_2) = y_{\text{Shrinking Core}}(x_1, x_2) + b(x_1, x_2) + \epsilon$, where $y_{\text{Shrinking Core}}$ is the shrinking core model[2], b is a bias function, x_1 is the molarity of HCl used in leaching, x_2 is the addition of a leaching additive, and ϵ is random error. An 8 point maximum entropy design[5] is first tested, and a GP is fit to the results. Based on GP predictions and uncertainty of those predictions, an algorithm then finds the point $(x_1^\star, x_2^\star)$ where it is expected there will be the maximum improvement in recovery over the previously tested values.

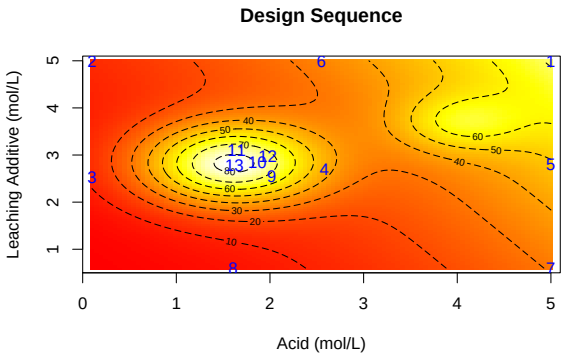

Figure 1: Ce recovery (%) response surface, sans noise, with sequential testing locations

The simulation is then evaluated at $f(x_1^\star, x_2^\star)$, the GP model is refit, and another test point is chosen based on expected improvement criteria. This process is repeated, sequentially adding each data point to the GP regression, until convergence on the optimum. Because of the variability in the data, this procedure was repeated 100 times to observe the mean behavior.

4. Results

The sequential experimental design found and tested the technical optimum in as little as 11 tests. In testing the algorithm 100 times, 55% of the trials found the optimum after only 17 tests. 91% of the trials found the optimum in under 27 simulated lab experiments.

5. Conclusion

This proof of concept shows how sequential experimental design can be used to optimize complex processes, when the process dynamics are not fully understood. In application, this methodology can considerably reduce metallurgical testwork requirements, leading to superior process optimization at a lower development cost.

References

[1] Box, George E. ; Draper, Norman R.: *Response surfaces, mixtures, and ridge analyses*. Bd. 649. John Wiley & Sons, 2007

[2] Gbor, Philip K. ; Jia, Charles Q.: Critical evaluation of coupling particle size distribution with the shrinking core model. In: *Chemical Engineering Science* 59 (2004), Nr. 10, S. 1979–1987

[3] Gramacy, Robert B.: *Surrogates: Gaussian process modeling, design, and optimization for the applied sciences*. CRC Press, 2020

[4] Schonlau, Matthias: Computer experiments and global optimization. (1997)

[5] Shewry, Michael C. ; Wynn, Henry P.: Maximum entropy sampling. In: *Journal of applied statistics* 14 (1987), Nr. 2, S. 165–170