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Author: John Eason Selen Cremaschi

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Adaptive sequential sampling for surrogate model generation with artificial neural

networks

John Eason, Selen Cremaschi*

Department of Chemical Engineering, The University of Tulsa, 800 South Tucker Drive, Tulsa,

Oklahoma 74104, USA

Surrogate models - simple functional approximations of complex models - can facilitate

engineering analysis of complicated systems by greatly reducing computational expense. The

construction of a surrogate model requires evaluation of the original model to gather the data

necessary for building the surrogate. Sequential sampling procedures are proposed for

determining and minimizing the required number of samples for efficient global surrogate

construction. In this paper, two new adaptive sampling algorithms – one purely adaptive and one

combining adaptive and space-filling characteristics – are proposed and compared to a purely

space-filling approach. Our analysis suggests a mixed adaptive sampling approach for

constructing surrogates for systems where the behavior of the underlying model is unknown.

Results of the case study, optimization of carbon dioxide capture process with aqueous amines,

revealed that the mixed adaptive sampling algorithm may reduce the required sample size by up

to 40% compared to a purely space-filling design.

Keywords: adaptive sampling, space-filling design, artificial neural networks, surrogate models

*Corresponding author: Tel.: +1-918-631-3422; Fax: +1-918-631-3268.

E-mail address: selen-cremaschi@utulsa.edu

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