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Bayesian Optimization as Design of Experiments: The Entropy Connection

Bayesian optimization (BO) and classical design of experiments (DOE) are rarely taught together. DOE courses cover factorial designs, response surface methodology, and optimality criteria like D and I-optimality. BO courses cover Gaussian processes and acquisition functions like expected improvement. The two communities use different notation, different software, and publish in different journals. Yet both address a closely related problem: how to allocate a limited experimental budget to learn what matters most.

This talk grew out of the Experimental Design course in the Master of Statistics and Data Science at KU Leuven. It starts from a classical DOE lecture and extends it with modern Bayesian optimization material, showing how both fit within a common experimental-design framework. The key message is that every experimental design involves three choices: a model for the response, an objective that defines what “good” means, and a rule for choosing additional runs. In familiar DOE settings, that rule may produce an initial design and then augment it to improve parameter estimation or prediction, often using polynomial models and criteria such as D- and I-optimality. BO makes different choices within the same template: a Gaussian process prior instead of a polynomial model, an objective focused on the optimum rather than all coefficients, and an adaptive rule for adding runs as data are collected.

The bridge between the two is entropy. D-optimality maximizes $\log \det(\mathbf{X}^\top \mathbf{X})$, which for Gaussian linear models is equivalent to maximizing the information gained about the regression coefficients. Information-theoretic BO acquisition functions such as Max-value Entropy Search do the same, but for the location or value of the optimum rather than for the model parameters. The principle is shared; what changes is what we want information *about*.

This perspective has practical value for teaching and consulting. It gives a DOE-trained audience a principled way to understand what is new in BO and what is not: the surrogate model, the objective, and the rule used to augment the design change, but the underlying logic of designing informative experiments remains. Framing BO in this way helps students and practitioners extend familiar DOE ideas to modern model-based optimization, rather than treating BO as a separate black-box machine-learning technique.

Special/ Invited session

Classification

Mainly methodology

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