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A Comparison of DOE and BO in the In Silico Optimization of Lipid Nanoparticles (LNPs)

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Carefully designing experiments is crucial for gaining a deeper understanding of process behaviour. Design of Experiments (DOE) is a well-established active learning methodology with an extensive track record of solid contributions to research and industry in various areas, including screening, modelling, optimisation, specification matching, and robust design. Based on a reduced set of assumptions regarding process behaviour, DOE proposes an experimentation plan for estimating a parametric model, upon which follow-up experiments may be suggested in a sequential and iterative manner until the intended goal is achieved.
More recently, other methodologies have emerged and are being increasingly tested and explored, primarily focusing on optimization for a specific goal. Among these, Bayesian Optimisation (BO) stands out, gaining recognition and interest for its simplicity and effectiveness in certain test scenarios. Unlike DOE, where modelling and optimisation are treated sequentially as distinct tasks, BO aims to enhance sampling efficiency for optimisation, relaxing the need for an explicit modelling process[1]. Linear least squares models are central to DOE, which creates challenges and awkwardness to avoid design matrix singularities. These problems largely disappear in BO with mixture and constrained effects because the model is based on spatial correlations rather than design matrices. The question that practitioners face now is which methodology to adopt when the goal is optimisation. Despite the numerous papers published, the vast majority address small toy examples. Although these examples are interesting and useful for elucidating the properties of the methodologies, they hardly provide a suitable basis for inference in real systems. In summary, there is currently a scarcity of comprehensive studies and practical case studies that compare these two approaches and assess their relative efficiency in realistic and challenging scenarios.
To promote discussion and gain further insights into their relative merits, we have adopted a realistic simulated scenario as a test bed to compare the two approaches for active learning (DOE vs BO). The system regards the synthesis of lipid nanoparticles (LNPs)[2], which is currently an important process for the development of modern drug delivery systems. Both approaches were applied and comparably tested for their efficiency in achieving optimal values for the examined responses (“potency”and average “size”of LNPs).

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