Connecting models with data: inverse problems, their well-posedness and computational techniques

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PDEs model real world systems and build the basis of many downstream applications in optimization, control or uncertainty quantification. To ensure alignment, non-observable model parameters are identified that reconstruct observed data from the real system. The quality of this model fitting procedure depends highly on a-priori knowledge and the quality of data. In this talk we look at how these interact, and present three results in this realm and an outlook on ongoing work.

A theoretical study exhibits identifiability of the turning coefficient in a run-and-tumble model for bacterial chemotaxis. Reconstructing this microscopic quantity from experiments that only see the macroscopic bacteria density poses a challenge that we overcome by a delicate construction of an experimental data collection strategy.

Second, we propose a new perspective and methodology for experimental design when no such construction is available. Relaxing the search from an optimal to a sufficient design allows us to down-sample experiments according to their sensitivity, an idea borrowed from randomized linear algebra. This keeps the parameter identifiable with high probability.

Third, we reconciliate two formulations of gradient-based model fitting for the Fokker–Planck equation, arising from the PDE and particle formulation. Discretization yields gradient estimators that converge at the same rate in the number of particles.

We conclude with work in progress on particle-based sampling methods and on uncertainty quantification for equations learned from data.