

NUMERICAL ANALYSIS AND SCIENTIFIC COMPUTING SEMINAR

Rigorous computations for linear response and sampling

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Abstract: In this talk, we discuss new algorithms for two distinct computational problems, that of linear response and sampling. Linear response refers to the smooth change in the statistics of an observable in a dynamical system in response to a smooth parameter change in the dynamics. The computation of linear response in chaotic systems has been a challenge, despite work pioneered by Ruelle giving a rigorous formula in Anosov systems (mathematically idea chaotic systems). This is because typical linear perturbation-based methods are not applicable due to their instability in chaotic systems. Here, we give a new differentiable splitting of the parameter perturbation vector field, which leaves the resulting split Ruelle’s formula amenable to efficient computation. A key ingredient of the overall algorithm, called space-split sensitivity, is a new recursive method to differentiate quantities along the unstable manifold. Of particular importance is the score – gradient of log density – of the conditional density of the physical measure, which we are differentiating, along the unstable manifold. This fast algorithm for the conditional scores motivates our attack of another longstanding computational challenge in high-dimensional statistics – sampling from complex probability distributions, which we discuss in the second half of the talk.

We present Score Operator Newton (SCONE) transport – a novel approach to sample from a target probability distribution given its score. Transport maps are transformations between the sample space of a source (which is generally easy to sample) and a target (typically non-Gaussian) probability distribution. Our SCONE transport map is a constructive solution of an infinite-dimensional generalization of a Newton method to find the zero of a ”score operator”. We define such a score operator that gives the difference of the score of a transported distribution from the target score. The Newton iteration enjoys fast convergence under smoothness assumptions and does not make a parametric ansatz on the transport map.

Friday, November 17, 2023, 11:00 am
Mathematics and Science Center: MSC W301

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