Focusing exploration with confidence

Prof. Dr. Andreas Krause
ETH Zürich

Affiliation: *Learning & Adaptive Systems Group*, ETH Zürich, Universitätstrasse 6, CH-8093 Zürich, Switzerland

Email: krausea@ethz.ch – **URL**: http://las.ethz.ch/krausea.html

Abstract: In many applications, ranging from autonomous experimental design to robotic monitoring to system tuning, we wish to gather information about some unknown function. Often, acquiring samples is noisy and expensive. In this talk, I will discuss how Bayesian confidence bounds can play a natural role in focusing exploration: Reducing uncertainty in a structured way to reliably estimate properties of interest such as extremal values, location of critical regions, Pareto-frontiers etc. First, I will show how a simple confidence-guided sampling rule attains near-minimal regret for bandit problems involving objectives modeled via Gaussian process priors. I will further demonstrate how the approach allows to scale up through parallelization, effectively localize level-sets, and address multi-objective tradeoffs. I will illustrate the approach in several real-world applications. Applied to experimental design for protein structure optimization, our approach enabled engineering of active P450 enzymes that are more thermostable than any previously made by chimeragenesis, rational design, or directed evolution.