Convex envelope, primal-dual interior-point algorithm, and modeling atmospheric aerosol state

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The convex envelope f of a non-convex function g is the greatest convex function majorized by g. There are several ways of constructing a convex envelope. A natural idea is to take the convex hull of the epigraph of g; this gives a convex set, which is not an epigraph, but which can be made so by "closing its bottom" via its lower-bound function. An other way, more convenient from the analysis and computational point of view, is to solve the following minimization problem:

$$f(x) = \inf\Big\{ \sum_{j=1}^{\pi} \alpha_j g(x_j) : \alpha_j \geq 0, x_j \in \mathrm{dom}(g), \sum_{j=1}^{\pi} \alpha_j = 1, \sum_{j=1}^{\pi} \alpha_j x_j = x \Big\}. \quad (1)$$

The optimization problem (1) is a subject of active research in global optimization, where the true global solution is found; the compromise is efficiency. The worst-case complexity of global optimization methods grows exponentially with the problem size. Even small problems with a few tens of variables, can take a very long time (e.g., hours or days) to solve.

In the context of modeling atmospheric aerosols, the convex envelope is related to the thermodynamic equilibrium, where the function $g : R^n \mapsto R$ represents the Gibbs free energy of a particle, x_j is the compositions of phase, y_j is the partition fraction of the particle compositions x among phases x_j. The challenge here is twofold: first of all, the problem size n, which is the number of chemical compounds in a particle, can be in the order of hundreds, and secondly, the computing time is critical, since, in the context of 3D simulation of atmospheric aerosol transformation, one would need hundreds of thousand of spatial grid points and integrate over thousands of time steps, thus the optimization problem (1) needs to be solved millions of times.

In this talk, we first introduce some basic concepts in convex analysis, then apply these convex arguments to analyze/reformulate the problem (1) in both primal and dual forms. A geometrical notion of phase simplex related to the convex envelope is introduced to characterize mathematically the phases at equilibrium. A local optimization method, e.g. a primal-dual interior-point algorithm, is our basis for solving efficiently the optimization problem (1). At the end of talk, we present numerical results for the reconstruction of some complex phase diagrams related to atmospheric organic aerosol states.