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Global Optimization: For Some Problems, There's HOPE

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We present a new method for solving unconstrained minimization problems—
Homotopy Optimization with Perturbations and Ensembles (HOPE). HOPE is
a homotopy optimization method that finds a sequence of minimizers of a homo-
topy function mapping a template function to the target function, the objective
function of our minimization problem. To increase the likelihood of finding a
global minimizer, points in the sequence are perturbed and used as starting
points to find other minimizers. Points in the resulting ensemble of minimizers
are used as starting points to find minimizers of the homotopy function as it
deforms the template function into the target function.

We show that certain choices of the parameters used in HOPE lead to in-
stances of existing methods: probability-one homotopy methods, stochastic
search methods, and simulated annealing. We use these relations and further
analysis to demonstrate the convergence properties of HOPE.

The development of HOPE was motivated by the protein folding problem, the
problem of predicting the structure of a protein as it exists in nature, given its
amino acid sequence. However, we demonstrate that HOPE is also successful
as a general purpose minimization method for nonconvex functions.

Numerical experiments performed to test HOPE include solving several stan-
dard test problems and the protein folding problem using two different protein
models. In most of these experiments, standard homotopy functions are used in
HOPE. Additionally, several new homotopy functions are introduced for solving
the protein folding problems to demonstrate how HOPE can be used to exploit
the properties or structure of particular problems.

Results of experiments demonstrate that HOPE outperforms several methods
often used for solving unconstrained minimization problems—a quasi-Newton
method with BFGS Hessian update, a globally convergent variant of Newton's
method, and ensemble-based simulated annealing.