Ising Spin Glass

- Ising spin glasses are prototypical models for disordered systems.
- Ising spin glasses are also challenging class of optimization problems:
  - Fast growth of the number of local optima.
  - High-quality solutions divided by a barrier of low-quality solutions.
  - High-order interactions.
  - Cannot be factored into subproblems of bounded order on a single level (and 3D is NP-complete).

Purpose of this work

- Use cluster exact approximation method as a fast polynomial solver capable of reaching high-quality local optima efficiently by changing large parts of solutions.
- Use hierarchical BOA and other evolutionary algorithm to supply starting points for CEA.
- Compare the resulting hybrids on large sets of spin glass instances in 2D and 3D.

Energy of a spin glass

\[ E(C) = \sum_{(i,j)} s_i J_{ij} s_j \]

Optimization problem: Find ground state

- Given all coupling constants \( J_{ij} \).
- Find values of spins so that energy is minimized.

Cluster Exact Approximation (Hartmann, 1996)

- Basic principle:
  - Find largest nonfrustrated subcluster, defined as the largest subset of spins that can be arranged optimally with respect to each other without conflicting constraints (greedy).
  - Subclusters usually contain majority of spins.
  - Consider the problem of setting only spins in the nonfrustrated cluster given that all remaining spins remain fixed.
  - Convert the problem into maximum flow.
  - Use polynomial maximum flow algorithm to set all subcluster spins optimally.
  - Assuming that all remaining spins remain fixed; we know we have reached optimality with respect to the selected cluster.
  - However, unless we could select all the spins or we got lucky that the remaining spins are set as in some ground state configuration, we cannot guarantee global optimum...

- Advantages
  - Speed (polynomial performance).
  - Power (changes large subsets of spins optimally).

- How do we use CEA?
  - Use CEA to improve every solution we reach with an evolutionary algorithm.
  - Repeat CEA updates until many failures to improve.
  - Number of failures set to grow with spin glass size.

Experiments

- Compared evolutionary algorithms
  - Estimation of distribution algorithms (EDAs):
    - Hierarchical Bayesian optimization algorithm (hBOA) (Pelikan & Goldberg).
    - Univariate marginal distribution algorithm (UMDA).
  - Simple genetic algorithm (one-point crossover).
- Compared hybrids
  - Use deterministic 1-bit-flip hill climber (DHC).
  - Use cluster exact approximation (CEA).

Comparison of hBOA+DHC, GA+DHC and UMDA+DHC

Comparison of hBOA+CEA and GA+CEA

Conclusions

- hBOA outperforms others in all settings.
- Hybrids prove important in solving large problems.
- CEA works great.
  - CEA allows all algorithms to solve much bigger problems.
  - Proves the utility of hybridization in solving complex problems.
- Bad news
  - CEA hurts asymptotic growth of time complexity.
  - So for extremely large problems, simple DHC will outperform CEA...
  - But in currently feasible applications, CEA remains the winner.
- Ideas for future work
  - How to improve CEA by enabling it to select good subclusters?
  - How to maximize performance by dividing the labor between hBOA and CEA more carefully?

Acknowledgments

- NSF
- NSF CAREER grant ECS-0547013 (at UMSL)
- ITR grant DMR-03-25939 (at Materials Computation Center, UIUC)
- Air Force
  - Air Force Materiel Command, USAF, under grant FA9550-06-1-0096 (UIUC, partly UMSL)
- University of Missouri
  - High Performance Computing Collaboratory sponsored by Information Technology Services
  - Research Award
  - Research Board