Day 3 (Poster D)

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Title: Rejection-free MCMC for QUBO Optimization and Boltzmann Sampling

Abstract:
Markov chain Monte Carlo (MCMC) algorithms have become extremely popular in statistical applications and have led to a tremendous amount of research activity on sampling and optimization. One problem with a standard MCMC algorithm, such as the Metropolis algorithm, is that it might reject many proposals, leading to inefficiencies in its convergence. Recent technological advances have allowed for specialized digital hardware for optimization, which examines all possible proposals in parallel and reduces the frequency of rejection. In [1], an approximate rejection-free operation has been achieved with low computational overhead by applying an energy offset to each parallelized Metropolis trial. The usability of this scheme is greatly improved when we implement an ideal rejection-free operation [2] that does not require energy offset adjustment. Also, using the multiplicity as a weighting allows for correct sampling. This paper presents how the rejection-free MCMC works combined with Parallel Tempering, a standard method to improve convergence and usability of MCMC. We show the effectiveness of the rejection-free method for optimization and sampling, which can be implemented in future generations of Fujitsu's Digital Annealer optimization service.

[1] M. Aramon, et al., Front. Phys. 7, 48 (2019).
[2] J.S. Rosenthal, et al., Comp. Stats. (2021).