On physics-inspired methods for combinatorial optimization

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***Abstract*—We survey state-of-the-art approaches to combinatorial optimization (CO) and outline promising directions for future research. By mapping connections between annealing, optimal control, and probabilistic machine learning, we show how thermodynamic principles underpin many exact and approximate optimization methods. This perspective highlights deep similarities between probabilistic computing frameworks, clarifying their shared structure and limitations. The paper is self-contained and includes numerical simulations to demonstrate key concepts in practice, bridging conceptual gaps across the operations research, machine learning, and physics literatures.**

***Index Terms*—Combinatorial optimization, statistical mechanics, probabilistic machine learning, computational complexity**

I. Introduction

CO problems balance choices among sets of discrete variables, typically with constraints. They represent many applications across scheduling/logisitics, finance, machine learning, and have fundamental connections to number theory and physics. A well-studied class of CO problem is the unconstrained binary quadratic program (UBQP[1])

$$\min_{\mathbf{x}\in\{0,1\}^N} f(\mathbf{x}) = \mathbf{x}^\top \mathbf{Q}\mathbf{x} \tag{1}$$

with N variables and symmetric $\mathbf{Q} \in \mathbb{R}^{N\times N}$. The sign of eigenvalues characterize the computational hardness, which becomes NP-hard when $\mathbf{Q}$ is non-convex (indefinite). The convex (positive definite) instances can be solved in polynomial-time (Karmarkar, 1984) with classical integer programming (IP) techniques like branch-and-bound, interior-point relaxations, cutting planes, and dual methods. These typically linearize (1) by introducing constrained auxiliary variables and relax the binary constraint to work with continuous variables. For small instances, exact methods can guarantee optimality with proven resource bounds while large instances require approximations that trade-off quality and runtime.

Modern solvers usually augment these techniques with heuristics, including greedy local search, evolutionary/genetic algorithms, and population-based methods (Glover et al., 2002) (Kochenberger et al., 2014). Although these techniques can be effective, their performance is often sensitive to hyperparameters, initialization, problem structure, and offer limited theoretical guidance for principled design. Relaxation and penalty methods partially address constraints by gradually enforcing integrality or feasibility, but still operate within a paradigm that treats discreteness as a complication rather than a fundamental feature (Ichikawa, 2024).

In parallel, recent advances in machine learning, namely diffusion models, have renewed interest in stochastic approaches to high-dimensional optimization. These methods interpret optimization as inference over a probability distribution and use controlled noise to navigate complex landscapes. While data-driven models can learn effective heuristics for certain CO problems, they often suffer from poor generalization and raise open questions about how continuous-space gradient methods should be adapted to intrinsically discrete settings (Ichikawa, 2024).

We emphasize that physics-based methods provide a unifying framework to bridge operations research, machine learning, and statistical physics. The bitter lesson (Sutton, 2019) seems to imply we should just treat variables as particles with local fields derived from the problem structure. As originally articulated by (Feynman, 1982), this notion of natural computing suggests that new solvers may arise not from increasingly elaborate relaxations or handcrafted heuristics, but from principled agnostic stochastic dynamics with tailored noise geometry and (ir)reversibility. This viewpoint is particularly natural for CO problems, which are inherently graph-structured and closely resemble physical systems exhibiting collective behavior and critical phenomena.

II. Physics-Inspired Optimization

The core idea is to recast the CO problem as probabilistic inference on a Markov random field. Interpreting f as an energy potential defines a statistical ensemble whose equilibrium distribution concentrates on optimal states. In this view, the discrete optimization corresponds to maximum a posteriori (MAP) inference in the zero-temperature limit. At finite temperature, sampling explores the ensemble according to thermodynamic stability, while time-dependent or spatially varying control parameters intentionally drive the system out of equilibrium to enhance exploration. This perspective provides a principled thermodynamic framework for designing inference dynamics.

We first formulate CO as inference of energy-based models, realize this through probabilistic computing, and review diffusion and annealing as the mechanisms that control exploration and convergence. We also highlight the connections to quantum computing.

[1]This is equivalent to finding groundstate(s) of the Ising model (Lucas, 2014)

A. Energy-Based Models

The energy-based approach defines the target posterior distribution

$$p(\mathbf{x}) = \frac{\exp(-H(\mathbf{x})/\tau)}{Z} \tag{2}$$

for an energy function (Hamiltonian) $H : \mathcal{X} \to \mathbb{R}$ and temperature parameter $\tau \in \mathbb{R}$. The normalization constant $Z = \sum_{\mathbf{x}\in\mathcal{X}} \exp(-H(\mathbf{x})/\tau)$ is generally intractable, so inference typically relies on the unnormalized density. This Boltzmann distribution characterizes equilibrium ensembles using a probability measure over microscopic states weighted by their energy. For CO problems, it is natural to set $H(x) = f(x) + g(x)$ where $g(x)$ can impose penalties for any violated constraints. Designing effective penalty terms is problem-specific and plays a central role in shaping the energy landscape. The MAP objective is therefore

$$\arg\min_{\mathbf{x}} H(\mathbf{x}) = \arg\max_{\mathbf{x}} \log p(\mathbf{x}) \tag{3}$$

which can be achieved with iterative gradient ascent on the log-likelihood, which avoids the intractable partition function.

As $\tau \to 0$, the distribution concentrates on low-energy samples, making the optimization equivalent to sampling from the zero-temperature limit. However, if exact sampling were generally tractable, it would imply NP = RP, which is widely believed to be false. This motivates approximate sampling to sidestep the computational hardness, while still providing good solutions in practice.

Markov Chain Monte Carlo (MCMC) methods are commonly used to construct an approximate distribution q that tracks the target equilibrium as the temperature is gradually lowered. Both theory and empirical evidence suggest that annealing toward low temperature is often more effective than sampling directly at low temperature (Guilmeau et al., 2021). It is a natural question of how temperature should be controlled. This highlights an equilivance between optimal annealing and optimal control of non-equilibrium systems.

B. Probabilistic Computing

It is natural to represent $\mathbf{x}$ as stochastic variables, connecting optimization with the classical theory of energy-based models such as Boltzmann machines (Hinton, 2012), which learn by matching equilibrium statistics via contrastive divergence. Building on this mature framework, we consider a general network of probabilistic bits (Kaiser et al., 2021) $x_i \in \{-1, +1\}$ over $i = 1 \dots N$ updated according to a stochastic threshold rule

$$x_i = \text{sign}(\tanh(v_i/\tau)) - u) \tag{4}$$

$$v_i = \sum_{j,j=i} Q_{ij} x_j \tag{5}$$

for an input $v_i \in \mathbb{R}$ and uniform random variable $u \sim [-1, 1]$. These update equations define a discrete-time Markov process over the configuration space $\{-1, +1\}^N$ (a boolean hypercube). In general, no structure is imposed on $\mathbf{Q}$, which could be symmetric or asymmetric. For a fixed (deterministic or random) update order, iterating these equations reaches the equilibrium distribution given by the eigenvector (with eigenvalue +1) of the corresponding Markov transition matrix. This iterative procedure is equivalent to Gibbs sampling when updates are performed one variable at a time. When $\mathbf{Q}$ is symmetric, the dynamics satisfy detailed balance and the resulting distribution is the equilibrium ensemble in (2). This can be understood as Bayesian inference in an undirected graphical model, with Gibbs sampling implementing local posterior updates defined by the underlying graph structure. Variational inference replaces stochastic sampling of the equilibrium ensemble with deterministic free-energy minimization over a restricted family of distributions, trading expressive exploration for computational tractability (Maasch et al., 2025). Recently, (Abdelrahman et al., 2025) proposed a variational framework that learns annealing schedules by parameterizing local transition matrices, and shows that annealing subgraphs with different temperatures can be discovered through black-box optimization. Prior work on annealing suggests that strongly coupled or high-degree variables benefit from slower annealing to avoid getting stuck too early (Guilmeau et al., 2021).

C. Diffusion

This work focuses on (overdamped) Langevin dynamics as a continuous-time, stochastic ascent on the log-density

$$d\mathbf{x}_t = \nabla \log p(\mathbf{x}_t)dt + \sqrt{2}d\mathbf{B}_t, \tag{6}$$

where $\mathbf{B}_t$ is standard Brownian motion and the drift satisfies $\nabla \log p(\mathbf{x}) = -\frac{1}{\tau}\nabla H(x)$ for the target distribution. At equilibrium, this diffusion is reversible and has p as its stationary distribution under mild regularity conditions, so it can be viewed as gradient flow toward high-probability regions while injecting noise to escape metastable wells. In practice, a numerical scheme is used to discretize (6), which introduces bias and can degrade ergodicity in stiff or multimodal landscapes. A Metropolis-Hastings correction restores exact invariance with respect to p, but at the cost of additional computation and potential random-walk behavior due to rejections. Moreover, while the continuous Langevin diffusion is reversible, many empirically effective samplers deliberately introduce non-reversible components (e.g., skewed drift) to improve mixing and reduce asymptotic variance relative to purely reversible dynamics (Duncan et al., 2016). The Langevin process transports q along a Wasserstein gradient flow that monotonically decreases the KL divergence $D_{\text{KL}}(q \,\|\, p)$. In the zero-temperature limit, this drives q to concentrate around MAP estimates that minimize the energy H. Langevin dynamics is closely related to perturbed gradient ascent, however, always adding noise even when not in local minima seems unnecessary and highlights the importance of clever noise injection. Local optima in the continuous domain typically have a zero gradient under the smoothness condition, but this is often not true in a discrete domain.

D. Annealing

A broad class of simulated annealing and tempering methods can be interpreted as controlling the level, structure, or persistence of noise to improve exploration of complex energy landscapes (Aarts and Korst, 1989). One such approach is lifting, where a Markov chain on the original state space is augmented with auxiliary variables, effectively embedding the dynamics into an expanded space (Bruna and Han, 2025). This construction preserves the target invariant distribution while enabling non-reversible transitions that generate longer trajectories and reduce diffusive behavior, thereby accelerating mixing.

Closely related ideas appear in parallel tempering (Earl et al., 2005), where multiple replicas of the system are simulated at different temperatures and periodically exchanged. Extensions such as multi-dimensional or replica-tiling schemes further interpolate additional parameters, such as constraint or penalty strengths, allowing the sampler to move efficiently between soft and hard regimes without explicitly tuning these parameters. These methods can be viewed as tiling the energy landscape with overlapping ensembles that collectively facilitate transport across barriers. Furthermore, (Delacour et al., 2025) added a second dimension of replicas interpolating the penalty strengths, which improve mixing in heavily constrained replicas and eliminates the need to explicitly tune the penalty strength.

Classical simulated annealing corresponds to a single-replica limit of this broader framework, where the temperature is slowly decreased over time. While asymptotic convergence to the global optimum is guaranteed under logarithmically slow cooling schedules, such guarantees are largely impractical, motivating faster, non-equilibrium variants. Related population-based methods, including population annealing and annealed importance sampling, exploit weighted resampling to concentrate probability near low-energy states while maintaining diversity.

These approaches highlight a fundamental design principle: effective optimization and inference arise from carefully shaping stochastic dynamics through temperature schedules, auxiliary variables, or non-reversible flows rather than enforcing strict equilibrium. This perspective naturally motivates variants of Langevin dynamics, which modify the noise structure and temporal correlations to achieve faster mixing and improved exploration (Feng et al., 2025), (Wang et al., 2025), (Parulekar et al., 2025), (Zhang et al., 2022). Recently, (Guo et al., 2025) provides a non-asymptotic analysis for annealed Langevin dynamics with provable guarantees.

E. Quantum Computing

Quantum computers operate on quantum states $|\psi\rangle \in \mathbb{C}^{2^N}$, which represent superpositions over all binary configurations simultaneously. Their dynamics are governed by unitary transformations that preserve the 2-norm, in contrast to classical Markov dynamics, which preserve probability under the 1-norm. In this setting, the classical energy function H becomes a linear operator acting on a Hilbert space, whose eigenvalues correspond to the energy of all 2^N configurations. This formulation enables quantum dynamics to exploit interference and entanglement that allow transitions in ways unavailable to classical stochastic sampling. Several quantum algorithms leverage this structure to perform ground-state search. The variational quantum eigensolver (VQE) minimizes the expected energy of a parameterized unitary ansatz using classical optimization, analogous to variational inference and free-energy minimization. Imaginary-time evolution (ITE) performs dissipative ground-state filtering by exponentially suppressing excited states. The quantum approximate optimization algorithm (QAOA) discretizes adiabatic quantum evolution into alternating problem and mixing unitaries, mirroring classical simulated annealing and controlled non-equilibrium dynamics. Despite promising advantages in some areas, no general or scalable advantage over classical methods has yet been demonstrated for CO problems.

III. Numerical Experiments

We present a basic simulation of Gibbs sampling to solve small UBQP instances. This is done by iteratively updating (4) and (5) to evolve a network of probabilistic bits. The number of required Gibbs steps can be estimated from the mixing time, which is derived from the spectral gap of the transition matrix. To achieve the best results, the temperature parameter τ would be annealed as described in the main text.

Fig.1 shows the stationary distribution for $N = 10$ with random normal weights $Q_{ij} \sim N(0, 1)$. The configurations that minimize H occur with high probability.

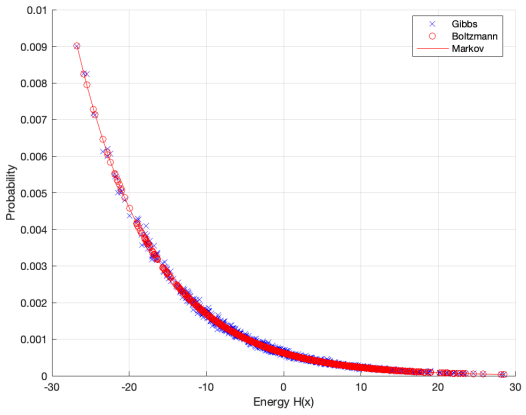

Fig. 1. The stationary distribution with $N = 10$ at fixed $\tau = 10$. The distribution aligns closely with the exact Boltzmann and Markov expectation.

IV. Conclusion and Outlook

We outline modern practice in physics-based approaches to CO problems, which include energy-based models, probabilistic computing, diffusion, and annealing as a unifying framework. Rather than relying on elaborate heuristics, this viewpoint highlights the role of noise, reversibility, and non-equilibrium control in navigating complex optimization landscapes.

A key research direction is developing annealing schedules over multiple parameters for non-equilibrium dynamics, particular for hard and soft constraints. (Barzegar et al., 2024) develops a formalism for optimized annealing schedules over multiple parameters while the system remains near equilibrium. This is naturally similar to (Sivak and Crooks, 2012) and (Rotskoff and Crooks, 2015), which introduced a theory for optimal control of thermodynamic systems, showing how the so-called friction tensor induces a pseudometric whose geodesics minimize dissipation in parameter space. Interestingly, (Chen, 2025) recently showed that an energy function under a heat semigroup on the boolean hypercube exhibits a uniform tail bound that is better than Markov's inequality. More work is needed to connect these ideas to edge of chaos dynamics commonly used in analyzing information flow in neural networks (Yang and Schoenholz, 2017).

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