ON THE CONVERGENCE OF AN IMPROVED DISCRETE SIMULATED ANNEALING VIA LANDSCAPE MODIFICATION

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ABSTRACT. In this paper, we propose new Metropolis-Hastings and simulated annealing algorithms on finite state space via modifying the energy landscape. The core idea of landscape modification relies on introducing a parameter $c$, in which the landscape is modified once the algorithm is above this threshold parameter. We illustrate the power and benefits of landscape modification by investigating its effect on the classical Curie-Weiss model with Glauber dynamics and external magnetic field in the subcritical regime. This leads to a landscape-modified mean-field equation, and with appropriate choice of $c$ the free energy landscape can be transformed from a double-well into a single-well, while the location of the global minimum is preserved on the modified landscape. Consequently, running algorithms on the modified landscape can improve the convergence to the ground-state in the Curie-Weiss model. In the setting of simulated annealing, we demonstrate that landscape modification can yield improved mean tunneling time between global minima, and give convergence guarantee using an improved logarithmic cooling schedule with reduced critical height. Finally, we discuss connections between landscape modification and other acceleration techniques such as Catoni’s energy transformation algorithm, preconditioning, importance sampling and quantum annealing. We stress that the technique developed in this paper is applicable to any difference-based discrete optimization algorithm.

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1. INTRODUCTION

This paper can be considered as a sequel to an earlier work by the author Choi (2020). The original motivation is from Fang et al. (1997), who propose a variant of overdamped Langevin diffusion with state-dependent diffusion coefficient. In Choi (2020), we cast this idea of state-dependent noise via landscape modification in the setting of kinetic simulated annealing and develop an improved kinetic simulated annealing algorithm with convergence guarantee. In this paper, we apply the idea of landscape modification to the finite state space setting in Metropolis-Hastings (MH) and simulated annealing, and investigate the benefits and speedups that this technique can bring in particular to the analysis of Curie-Weiss (CW) model and stochastic optimization. While the technique developed in Choi (2020) can be readily applied to gradient-based continuous optimization algorithms, we emphasize that the landscape modification technique proposed in this paper can be analogously implemented in difference-based discrete optimization algorithms.

In Section 2, we begin our paper by first defining a new MH algorithm using a modified Hamiltonian function. The modification or the transformation is based on the introduction of two parameters, namely $f$ and $c$, which increases the acceptance-rejection probability whenever the algorithm is above the threshold $c$. The corresponding acceptance-rejection probability in the modified MH in general has an integral form, but we show that this integral can be readily calculated upon specializing into various choices of $f$ such as linear, quadratic or square root $f$. We wrap up this section by detailing an example on using landscape modification in the Ehrenfest urn with a linear Hamiltonian, where we prove an upper bound on the spectral gap with polynomial dependence on the dimension, whereas the same technique yields an exponential dependence on the dimension for the classical MH.

In Section 3, we investigate the effect of landscape modification on the CW model. We first consider the CW model under a fixed external magnetic field in the subcritical regime, where the free energy landscape, as a function of the magnetization, has two local minima. Using a Glauber dynamics with landscape modification, we introduce a new mean-field equation, and with appropriate choice of $c$, the free energy landscape is transformed from a double-well into a single-well while preserving the location of the global minimum on the modified landscape. As a result running algorithms on the modified landscape can accelerate the convergence towards the ground-state. We prove a subexponential mean tunneling time in such setting and discuss related metastability results. Similar results are then extended to the random field CW model.

In Section 4, we consider the simulated annealing setting by driving the temperature down to zero. We define a clipped critical height $c^*$ (that depends on the threshold parameter $c$) associated with the landscape modified simulated annealing, and prove tight spectral gap asymptotics based on this quantity. Consequently, this leads to similar asymptotic results concerning the total variation mixing time and the
mean tunneling time in the low-temperature regime. Utilizing existing results concerning simulated annealing with time-dependent target function, we prove convergence guarantee of the landscape modified simulated annealing on finite state space with an improved logarithmic cooling schedule.

In the final section of the paper, Section 5, we elaborate on the similarities and differences between landscape modification and other acceleration techniques in Markov chain Monte Carlo literature such as Catoni’s energy transformation algorithm (Catoni, 1996, 1998), preconditioning of the Hamiltonian, importance sampling and quantum annealing.

1.1. Notations. Throughout this paper, we adapt the following notations. For $x, y \in \mathbb{R}$, we write $x_+ = \max\{x, 0\}$ to denote the non-negative part of $x$, and $x \wedge y = \min\{x, y\}$. For two functions $g_1, g_2 : \mathbb{R} \to \mathbb{R}$, we say that $g_1 = O(g_2)$ if there exists a constant $C > 0$ such that for sufficiently large $x$, we have $|g_1(x)| \leq Cg_2(x)$. We write $g_1 = o(g_2)$ if $\lim_{x \to \infty} g_1(x)/g_2(x) = 0$, and denote $g_1 \sim g_2$ if $\lim_{x \to \infty} g_1(x)/g_2(x) = 1$. We say that $g_1(x)$ is a subexponential function if $\lim_{x \to \infty} \frac{1}{x} g_1(x) = 0$.

2. Metropolis-Hastings with landscape modification

Let $\mathcal{X}$ be a finite state space under consideration, $Q = (Q(x, y))_{x, y \in \mathcal{X}}$ be the transition matrix of a reversible proposal chain with respect to the probability measure $\mu = (\mu(x))_{x \in \mathcal{X}}$, and $\mathcal{H} : \mathcal{X} \to \mathbb{R}$ be the target Hamiltonian function. Denote by $M^0 = (M^0(x, y))_{x, y \in \mathcal{X}}$ to be the infinitesimal generator of the continuized classical Metropolis-Hastings chain $X^0 = (X^0(t))_{t \geq 0}$, with proposal chain $Q$ and target distribution being the Gibbs distribution $\pi^0(x) \propto e^{-\beta \mathcal{H}(x)}/\mu(x)$ at inverse temperature $\beta > 0$. Recall that its dynamics is given by

$$M^0(x, y) = M^0_e(Q, \pi^0)(x, y) := \begin{cases} Q(x, y) \min\{1, e^{\beta(\mathcal{H}(x) - \mathcal{H}(y))}\} = Q(x, y)e^{-\beta(\mathcal{H}(y) - \mathcal{H}(x))}, & \text{if } x \neq y; \\ - \sum_{z : z \neq x} M^0(x, z), & \text{if } x = y. \end{cases}$$

We shall explain the upper script of 0 in both $M^0$ and $\pi^0$ in Definition 2.1 below.

Let us denote the ground-state energy level or the global minimum value of $\mathcal{H}$ to be $\mathcal{H}_{min} := \min_{x \in \mathcal{X}} \mathcal{H}(x)$. Instead of targeting directly the Hamiltonian $\mathcal{H}$ in the Gibbs distribution, we instead target the following modified or transformed function $\mathcal{H}_{\epsilon, c}$ at temperature $\epsilon = 1/\beta$:

$$\mathcal{H}_{\epsilon}(x) = \mathcal{H}_{\epsilon, c}(x) := \int_{\mathcal{H}_{min}}^{\mathcal{H}(x)} \frac{1}{f((u - c)_+) + \epsilon} \, du,$$

where the function $f$ and the parameter $c$ are chosen to satisfy the following assumptions:

**Assumption 2.1.**

1. The function $f : \mathbb{R}^+ \to \mathbb{R}^+$ is differentiable, non-negative and non-decreasing. Furthermore, $f$ satisfies

$$f(0) = f'(0) = 0.$$

2. The parameter $c$ is picked so that $c \geq \mathcal{H}_{min}$.

While it is impossible to calculate $\mathcal{H}_{\epsilon, c}$ without knowing $\mathcal{H}_{min}$ a priori, in Metropolis-Hastings what matters is the difference of the energy function, for $x, y \in \mathcal{X}$,

$$\mathcal{H}_{\epsilon, c}(y) - \mathcal{H}_{\epsilon, c}(x) = \int_{\mathcal{H}(x)}^{\mathcal{H}(y)} \frac{1}{f((u - c)_+) + \epsilon} \, du.$$

In the special case when we choose $f = 0$, the above equation reduces to $\mathcal{H}_{\epsilon, c}(y) - \mathcal{H}_{\epsilon, c}(x) = \beta(\mathcal{H}(y) - \mathcal{H}(x))$. On the other hand, in the case where $c < \mathcal{H}(x) < \mathcal{H}(y)$ and $f$ is chosen such that $f(x) > 0$.
whenever \( x > 0 \), then we have
\[
\mathcal{H}_{\epsilon,c}(y) - \mathcal{H}_{\epsilon,c}(x) \leq \frac{1}{f(H(x) - c)}(\mathcal{H}(y) - \mathcal{H}(x)) < \beta(\mathcal{H}(y) - \mathcal{H}(x)).
\]

Since \( f \) is assumed to be non-decreasing in Assumption 2.1, the greater the difference between \( \mathcal{H}(x) \) and \( c \), the smaller the upper bound in the first inequality in the above equation, the smaller it is we would expect for \( \mathcal{H}_{\epsilon,c}(y) - \mathcal{H}_{\epsilon,c}(x) \), the higher the transition rate \( Q(x,y) \exp\{-\mathcal{H}_{\epsilon,c}(y) - \mathcal{H}_{\epsilon,c}(x)\} \), and the landscape is modified in this sense. With these ideas and notations in mind, we are now ready to introduce the Metropolis-Hastings chain with landscape modification:

**Definition 2.1** (Metropolis-Hastings with landscape modification). Let \( \mathcal{H} \) be the target Hamiltonian function, and \( \mathcal{H}_{\epsilon,c} \) be the landscape-modified function at temperature \( \epsilon = 1/\beta \) introduced in (2.1), where \( f \) and \( c \) satisfy Assumption 2.1. The continuized Metropolis-Hastings chain with landscape modification \( X^f_{\epsilon,c} = (X^f_{\epsilon,c}(t))_{t \geq 0} \) has target distribution \( \pi^f(x) = \pi^f_{\epsilon,c}(x) \propto e^{-\mathcal{H}_{\epsilon,c}(x)} \mu(x) \), proposal chain \( Q \), and its infinitesimal generator \( M^f = (M^f(x,y))_{x,y \in \mathcal{X}} \) is given by
\[
M^f(x,y) = M^f_{\epsilon,c}(Q,\pi^f)(x,y) := \begin{cases} Q(x,y)e^{-(\mathcal{H}_{\epsilon,c}(y) - \mathcal{H}_{\epsilon,c}(x))} & \text{if } x \neq y; \\ -\sum_{z:z \neq x} M^f(x,z), & \text{if } x = y. \end{cases}
\]

Note that when \( f = 0 \), the above dynamics reduce to the classical Metropolis-Hastings \( X^0 \).

We now fix a few notations and recall some important concepts and results that will be used in the upcoming sections, such as the spectral gap and the critical height. We endow the Hilbert space \( \ell^2(\pi_{\epsilon,c}) \) with the usual inner product weighted by the invariant measure \( \pi_{\epsilon,c}^f \): for \( g_1, g_2 \in \ell^2(\pi_{\epsilon,c}^f) \),
\[
\langle g_1, g_2 \rangle_{\pi_{\epsilon,c}^f} := \sum_{x \in \mathcal{X}} g_1(x)g_2(x)\pi_{\epsilon,c}^f(x),
\]
and for \( p > 1 \) we denote the \( p \)-norm by \( \|\cdot\|_{\ell^p(\pi_{\epsilon,c})} \). We write \( \lambda_2(-M^f_{\epsilon,c}) \) to be the spectral gap of \( M^f_{\epsilon,c} \), that is,
\[
\lambda_2(-M^f_{\epsilon,c}) := \inf_{l \in \ell^2(\pi_{\epsilon,c}^f):\pi_{\epsilon,c}^f(l) = 0} \frac{\langle -M^f_{\epsilon,c}l,l \rangle_{\pi_{\epsilon,c}^f}}{\langle l,l \rangle_{\pi_{\epsilon,c}^f}}.
\]

Analogously, we write \( \lambda_2(-M^0_{\epsilon,c}) \) to denote the spectral gap of \( M^0_{\epsilon,c} \).

In the upcoming sections, we shall investigate and compare the total variation mixing time between Metropolis-Hastings chain with and without landscape modification. For any probability measure \( \nu_1, \nu_2 \) with support on \( \mathcal{X} \), the total variation distance between \( \nu_1 \) and \( \nu_2 \) is
\[
\|\nu_1 - \nu_2\|_{TV} := \sup_{A \subset \mathcal{X}} |\nu_1(A) - \nu_2(A)| = \frac{1}{2} \sum_{x \in \mathcal{X}} |\nu_1(x) - \nu_2(x)|.
\]

The worst-case total variation mixing time is defined to be
\[
t_{mix}(M^f_{\epsilon,c},1/4) := \inf \left\{ t; \sup_{x} \| P_t^f(x,\cdot) - \pi_{\epsilon,c}^f \|_{TV} < 1/4 \right\},
\]
where \( (P_t^f = e^{M^f_{\epsilon,c}t})_{t \geq 0} \) is the transition semigroup of \( X^f_{\epsilon,c} \).

Apart from mixing time, we will also be interested in various hitting times of the Metropolis-Hastings chain. These variables naturally appear when we discuss metastability results in the Curie-Weiss model in Section 3 or in discrete simulated annealing in Section 4. For any \( A \subset \mathcal{X} \), we denote \( \tau_A^f := \inf\{ t \geq 0 \mid P_t^f(A) \geq 1 - \epsilon \} \).
Analogously, we write \( x \) of points starting from \( \tau \).

For \( M(2.3) \) and the lowest possible highest elevation along path(s) from \( x \), \( y \), and elements of \( \chi^{x,y} \) are denoted by \( \gamma = (\gamma_i)_{i=0}^{n} \). The highest value of the Hamiltonian function \( H_{\epsilon,c}^{\ell} \) along a path \( \gamma \in \chi^{x,y} \), known as the elevation, is defined to be

\[
\text{Elev}_{\epsilon,c}^{\ell}(\gamma) := \max\{H_{\epsilon,c}^{\ell}(\gamma_i); \ \gamma_i \in \gamma\},
\]

and the lowest possible highest elevation along path(s) from \( x \) to \( y \) is

\[
G_{\epsilon,c}^{\ell}(x, y) := \min\{\text{Elev}_{\epsilon,c}^{\ell}(\gamma); \ \gamma \in \chi^{x,y}\}.
\]

Analogously, we write

\[
\text{Elev}^{0}(\gamma) = \max\{H(\gamma_i); \ \gamma_i \in \gamma\},
\]

\[
G^{0}(x, y) = \min\{\text{Elev}(\gamma); \ \gamma \in \chi^{x,y}\}.
\]

For \( M_{\epsilon,c}^{\ell} \), the associated critical height is defined to be

\[
H_{\epsilon,c}^{\ell} := \max_{x,y \in \mathcal{X}} \{G_{\epsilon,c}^{\ell}(x, y) - H_{\epsilon,c}^{\ell}(x) - H_{\epsilon,c}^{\ell}(y)\}.
\]

Similarly, for \( M_{\epsilon}^{0} \) its critical height is

\[
H^{0} := \max_{x,y \in \mathcal{X}} \{G^{0}(x, y) - H(x) - \inf_{x \in \mathcal{X}} H(y)\}.
\]

To simulate \( X_{\epsilon,c}^{\ell} \) practically, we would need to evaluate the acceptance-rejection probability, which amounts to the following integration:

\[
\exp\left( -(H_{\epsilon,c}^{\ell}(y) - H_{\epsilon,c}^{\ell}(x))_+ \right) = \begin{cases} 1, & \text{if } H(y) \leq H(x); \\ \exp\left( -\beta(H(y) - H(x)) \right), & \text{if } c \geq H(y) > H(x); \\ \exp\left( -\beta(c - H(x)) - \int_{c}^{\infty} \frac{1}{f(u-c)+\epsilon} \, du \right), & \text{if } H(y) > c \geq H(x); \\ \exp\left( -\int_{H(x)}^{H(y)} \frac{1}{f(u-c)+\epsilon} \, du \right), & \text{if } H(y) > H(x) > c. \end{cases}
\]

In the following three subsections, we evaluate the above integrals (2.6) where we choose \( f \) to be linear, quadratic or cubic function respectively.

### 2.1. Linear \( f \): Metropolis-Hastings with logarithmic Hamiltonian and Catoni’s energy transformation method.

In this subsection, we specialize into \( f(u) = u \). It turns out we can understand the landscape modification as if the Hamiltonian is on a logarithmic scale whenever \( H(x) > c \).

For \( x, y \in \{H(y) > H(x) \geq c\} \), since

\[
\int_{H(x)}^{H(y)} \frac{1}{u-c+\epsilon} \, du = \ln \left( \frac{H(y) - c + \epsilon}{H(x) - c + \epsilon} \right).
\]
putting the expression back into (2.6) gives
\[ \exp \left( -\left( \mathcal{H}^f_{c,c}(y) - \mathcal{H}^f_{c,c}(x) \right) \right) = \begin{cases} 1, & \text{if } \mathcal{H}(y) \leq \mathcal{H}(x); \\ \exp \left( -\beta(\mathcal{H}(y) - \mathcal{H}(x)) \right), & \text{if } c \geq \mathcal{H}(y) > \mathcal{H}(x); \\ \exp \left( -\beta(c - \mathcal{H}(x)) \right) \frac{\mathcal{H}(y) - c + \epsilon}{\mathcal{H}(y) - c + \epsilon}, & \text{if } \mathcal{H}(y) > c \geq \mathcal{H}(x); \\ \frac{\mathcal{H}(x) - c + \epsilon}{\mathcal{H}(y) - c + \epsilon}, & \text{if } \mathcal{H}(y) > \mathcal{H}(x) > c. \end{cases} \]

This resulting dynamics \( M^f \) coincides with the energy transformation method introduced by Catoni (1996, 1998) on \( \{ \mathcal{H}(y) > \mathcal{H}(x) > c \} \), which is based on logarithmic Hamiltonian. We refer readers to Section 5 for a more detailed account on the connection between landscape modification and Catoni’s energy transformation.

### 2.2. Quadratic \( f \): Metropolis-Hastings with arctan Hamiltonian

In this subsection, we take \( f(u) = u^2 \). In this case, the effect of landscape modification gives an inverse-tangent-transformed Hamiltonian whenever \( \mathcal{H}(x) > c \).

For \( x, y \in \{ \mathcal{H}(y) > \mathcal{H}(x) \geq c \} \), using the inverse tangent difference formula we obtain
\[
\int_{\mathcal{H}(x)}^{\mathcal{H}(y)} \frac{1}{(u - c)^2 + \epsilon} \, du = \sqrt{\beta} \left( \arctan \left( \sqrt{\beta} (\mathcal{H}(y) - c) \right) - \arctan \left( \sqrt{\beta} (\mathcal{H}(x) - c) \right) \right),
\]
and substituting the above expression back into (2.6) gives
\[
\exp \left( -\left( \mathcal{H}^f_{c,c}(y) - \mathcal{H}^f_{c,c}(x) \right) \right) = \begin{cases} 1, & \text{if } \mathcal{H}(y) \leq \mathcal{H}(x); \\ \exp \left( -\beta(\mathcal{H}(y) - \mathcal{H}(x)) \right), & \text{if } c \geq \mathcal{H}(y) > \mathcal{H}(x); \\ \exp \left( -\beta(c - \mathcal{H}(x)) - \sqrt{\beta} \arctan \left( \sqrt{\beta} (\mathcal{H}(y) - c) \right) \right), & \text{if } \mathcal{H}(y) > c \geq \mathcal{H}(x); \\ \exp \left( \sqrt{\beta} \arctan \left( \sqrt{\beta} (\mathcal{H}(x) - c) \right) - \arctan \left( \sqrt{\beta} (\mathcal{H}(y) - c) \right) \right), & \text{if } \mathcal{H}(y) > \mathcal{H}(x) > c. \end{cases}
\]

### 2.3. Square root \( f \): Metropolis-Hastings with sum of square root and logarithmic Hamiltonian

In the final example, we let \( f(u) = \sqrt{u} \) for \( u \geq 0 \). Note that this choice of \( f \) does not satisfy \( f'(0) = 0 \) as in Assumption 2.1. For \( x, y \in \{ \mathcal{H}(y) > \mathcal{H}(x) \geq c \} \), consider the integral
\[
\int_{\mathcal{H}(x)}^{\mathcal{H}(y)} \frac{1}{\sqrt{u} - c + \epsilon} \, du = 2 \left( \sqrt{\frac{\mathcal{H}(y) - c}{\mathcal{H}(x) - c}} - \epsilon \ln \frac{\sqrt{\mathcal{H}(y) - c + \epsilon}}{\sqrt{\mathcal{H}(x) - c + \epsilon}} \right),
\]
putting the expression back into (2.6) gives
\[
\exp \left( -\left( \mathcal{H}^f_{c,c}(y) - \mathcal{H}^f_{c,c}(x) \right) \right) = \begin{cases} 1, & \text{if } \mathcal{H}(y) \leq \mathcal{H}(x); \\ \exp \left( -\beta(\mathcal{H}(y) - \mathcal{H}(x)) \right), & \text{if } c \geq \mathcal{H}(y) > \mathcal{H}(x); \\ \exp \left( -\beta(c - \mathcal{H}(x)) - 2\sqrt{\mathcal{H}(y) - c} \right) \left( \frac{\sqrt{\mathcal{H}(y) - c + \epsilon}}{\epsilon} \right)^{2\epsilon}, & \text{if } \mathcal{H}(y) > c \geq \mathcal{H}(x); \\ \exp \left( 2\sqrt{\mathcal{H}(x) - c} - 2\sqrt{\mathcal{H}(y) - c} \right) \left( \frac{\sqrt{\mathcal{H}(y) - c + \epsilon}}{\sqrt{\mathcal{H}(x) - c + \epsilon}} \right)^{2\epsilon}, & \text{if } \mathcal{H}(y) > \mathcal{H}(x) > c. \end{cases}
\]
2.4. Use of landscape modification for sampling. This paper focuses on investigating the acceleration effect of landscape modification in stochastic optimization and simulated annealing. Nonetheless, the technique of landscape modification can also be applied to sampling from multimodal distributions. In an ongoing work with Jing Zhang Zhang and Choi (2021), we analyze the use of landscape modification for sampling. We now briefly describe the setting therein. Suppose that we are interested in sampling from a multimodal distribution that we denote by \( \nu(x) \propto e^{-\mathcal{H}(x)} \). Applying the idea of landscape modification, we then construct a Metropolis-Hastings chain with the following transformed Hamiltonian function

\[
\mathcal{H}_{1,c,\alpha}(x) = \int_{\mathcal{H}_{min}}^{\mathcal{H}(x)} \frac{1}{\alpha f((u-c)_+ + 1)} \, du
\]

so that its stationary distribution is given by \( \nu_{1,c,\alpha}^t(x) \propto e^{-\mathcal{H}_{1,c,\alpha}(x)} \). We note that the parameter \( \alpha \geq 0 \) is introduced in (2.7), which controls the bias between the distribution \( \nu \) and its landscape-modified counterpart \( \nu_{1,c,\alpha}^t \). If we anneal this parameter by sending \( \alpha_t \to 0 \) as \( t \to \infty \), then \( \nu_{1,c,\alpha}^t(x) \) converges weakly to the target distribution \( \nu \). As a result, we construct a non-homogeneous Metropolis-Hastings chain that converges to \( \nu \) in the long run while enjoying the benefits of landscape modification.

2.5. A Metropolised Ehrenfest urn with landscape modification. This section serves as a warm-up example before we discuss the more complicated Curie-Weiss model in Section 3, and our exposition follows closely as that in (Deuschel and Mazza, 1994, Section 5.1.2). Let us first briefly fix the setting. We consider the state space \( \mathcal{X} = \{0, 1, \ldots, d\}^d \) with \( d \in \mathbb{N} \) and take a linear Hamiltonian \( \mathcal{H}(x) = x \), where \( \mathcal{H}_{min} = 0 \). The proposal birth-death chain has generator \( Q \) given by \( Q(x,x+1) = 1 - x/d, \) \( Q(x,x-1) = x/d, Q(x,x) = -1 \) and zero otherwise, and we note that the stationary measure of \( Q \) is \( \mu(x) \propto 2^{-d(x)} \). With these choices, the classical Metropolised dynamics is \( M_\epsilon^0(x,x+1) = Q(x,x+1)e^{-\beta}, M_\epsilon^0(x,x-1) = Q(x,x-1) \) and \( \pi^0(x) \propto e^{-\beta x\mu(x)} \). It is shown in (Deuschel and Mazza, 1994, equation (5.1.1)) that

\[
\lambda_2(-M_\epsilon^0) \leq \lambda_2(-Q) \frac{1}{\sum_{x=0}^{d} e^{-\beta x \mu(x)}} = \frac{d}{2} \frac{2^d}{(1 + e^{-\beta})^d}.
\]

At a fixed inverse temperature \( \beta \), we note that the upper bound in (2.8) is exponential in \( d \).

Now, we consider the landscape modified Metropolis-Hastings with \( f(x) = x \) and \( c = 1 \). With these parameters, we compute

\[
\mathcal{H}(x) = \int_0^x \frac{1}{(u-1)_+ + \epsilon} \, du = \beta \ln \left( \frac{(x-1)_+ + \epsilon}{\epsilon} \right).
\]

Using (Deuschel and Mazza, 1994, equation (5.1.1)) leads to

\[
\lambda_2(-M_{\epsilon,c=1}^f) \leq \lambda_2(-Q) \frac{1}{\sum_{x=0}^{d} e^{-\mathcal{H}(x) \mu(x)}} = \frac{d}{2} \frac{2^d e^\beta}{e^{-\epsilon}(d/2)^{d/2}} \sim d^3 \beta e^\beta,
\]

where we use the Stirling’s formula that gives for large enough \( d \),

\[
\left( \frac{d}{[d/2]} \right) \sim \frac{2^d}{\sqrt{\pi [d/2]}}.
\]

As a result, the upper bound in (2.9) gives a polynomial dependency on \( d \), at the tradeoff of an exponential dependency on \( \beta \). In retrospect this result is not surprising, since we are working with a logarithmic Hamiltonian and hence the asymptotics is in the polynomial of \( d \) instead of \( 2^d \).


3. THE CURIE-WEISS MODEL WITH LANDSCAPE MODIFICATION

In this section, we demonstrate the power of landscape modification by revisiting the Curie-Weiss (CW) model. With appropriate choice of parameters, the landscape of the CW free energy is modified and the local minimum is eliminated while the global minimum is preserved on the transformed function. As a result, landscape modification convexifies the free energy from a double-well to a single-well as a function of the magnetization.

Let us first recall the setting of the CW model of a ferromagnet with external field \( h \in \mathbb{R} \) and fix a few notations. We shall follow the setting as in (Bovier and den Hollander, 2015, Chapter 13, 14). Let \( \mathcal{X} = \{-1, 1\}^N \) be the set of possible configurations of the CW model with \( N \in \mathbb{N} \). The CW Hamiltonian is given by, for \( \sigma = (\sigma_i)_{i=1}^N \in \mathcal{X} \),

\[
H_N(\sigma) := -\frac{1}{2N} \sum_{i,j=1}^N \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i = -\frac{N}{2} m_N(\sigma)^2 - h N m_N(\sigma) =: \beta \mathbb{E}(m_N(\sigma)),
\]

where \( m_N(\sigma) = (1/N) \sum_{i=1}^N \sigma_i \) is the empirical magnetization. Consider the continuized Glauber dynamics by picking a node uniformly at random and flipping the sign of the selected spin, while targeting the Gibbs distribution with the CW Hamiltonian \( H_N \) at inverse temperature \( \beta \). The resulting Metropolis dynamics is given by

\[
P_{\epsilon,N}(\sigma, \sigma') = \begin{cases} 
(1/N)e^{-\beta(H_N(\sigma') - H_N(\sigma))}, & \text{if } ||\sigma - \sigma'||_1 = 2; \\
-\sum_{\eta,\eta\neq\sigma} P_{\epsilon,N}(\sigma, \eta), & \text{if } \sigma = \sigma'; \\
0, & \text{otherwise},
\end{cases}
\]

where \( ||\cdot||_1 \) is the \( l^1 \) norm on \( \mathcal{X} \).

The dynamics of the empirical magnetization \( \langle m^0(t) \rangle_{t \geq 0} \) can be described by lumping the Glauber dynamics to give

\[
M^0_N(m, m') = M^0_{\epsilon,N}(m, m') = \begin{cases} 
\frac{1-m}{2} e^{-\beta N(\mathbb{E}(m') - \mathbb{E}(m))}, & \text{if } m' = m + 2N^{-1}; \\
\frac{1+m}{2} e^{-\beta N(\mathbb{E}(m') - \mathbb{E}(m))}, & \text{if } m' = m - 2N^{-1}; \\
-\sum_{m':m'\neq m} M^0_{\epsilon,N}(m, m'), & \text{if } m = m'; \\
0, & \text{otherwise}.
\end{cases}
\]

on the state space \( \Gamma_N := \{-1, -1 + 2N^{-1}, \ldots, 1 - 2N^{-1}, 1\} \) with the image Gibbs distribution

\[
\pi^0_N(m) = \pi^0_{\epsilon,N}(m) \propto e^{-\beta N \mathbb{E}(m)} \left( \frac{N}{1+m/2N} \right) 2^{-N}, \quad m \in \Gamma_N,
\]

as the stationary distribution. Note that the dependency on \( \epsilon \) is suppressed in the notations of \( M^0_N \) and \( \pi^0_N \). Denote by

\[
\begin{align*}
I_N(m) &:= -\frac{1}{N} \ln \left( \left( \frac{N}{1+m/2N} \right) 2^{-N} \right), \\
I(m) &:= \frac{1}{2} (1+m) \ln(1+m) + \frac{1}{2} (1-m) \ln(1-m), \\
g_{\epsilon,N}(m) &:= \mathbb{E}(m) + \epsilon I_N(m),
\end{align*}
\]
where \( I(m) \) is the Cramér rate function for coin tossing. As a result, the image Gibbs distribution can be written as

\[
\pi_0^{\epsilon,N}(m) \propto e^{-\beta Ng_{\epsilon,N}(m)},
\]

\[
\lim_{N \to \infty} I_N(m) = I(m),
\]

\[
g_{\epsilon}(m) := \lim_{N \to \infty} g_{\epsilon,N}(m) = E(m) + \epsilon I(m).
\]

\( g_{\epsilon} \) is called the free energy of the CW model. The stationary point(s) of \( g_{\epsilon} \) satisfies the classical mean-field equation

\[
m = \tanh(\beta(m + h)).
\]

(3.1)

To seek the ground state(s) of the free energy, we consider modifying the landscape of the CW Hamiltonian from \( H_N \) to

\[
E_{\epsilon,c}^f(m) := \int_d^{E(m)} \frac{1}{f((u-c)_+)} du,
\]

(3.2)

\[
H_{\epsilon,c,N}^f(\sigma) := NE_{\epsilon,c}^f(m(\sigma)),
\]

(3.3)

where \( d \in \mathbb{R} \) can be chosen arbitrarily since we are only interested in the difference of \( E_{\epsilon,c}^f \). The infinitesimal generator of the magnetization \( (m^f(t))_{t \geq 0} \) is

\[
M_{\epsilon,c,N}(m, m') = \begin{cases} 
\frac{1-m}{2} e^{-N(E_{\epsilon,c}(m') - E_{\epsilon,c}(m))_+}, & \text{if } m' = m + 2N^{-1}; \\
\frac{1+m}{2} e^{-N(E_{\epsilon,c}(m') - E_{\epsilon,c}(m))_+}, & \text{if } m' = m - 2N^{-1}; \\
- \sum_{m': m' \neq m} M_{\epsilon,c,N}(m, m'), & \text{if } m = m'; \\
0, & \text{otherwise},
\end{cases}
\]

with stationary distribution

\[
\pi_{\epsilon,c,N}^f(m) \propto e^{-NE_{\epsilon,c,N}^f(m)} \left( \frac{N}{1+m} \right)^{2N} = e^{-Ng_{\epsilon,c,N}(m)}, \quad m \in \Gamma_N,
\]

where

\[
g_{\epsilon,c,N}^f(m) := E_{\epsilon,c}^f(m) + I_N(m).
\]

By taking the limit \( N \to \infty \), the free energy in the landscape-modified CW model is therefore

\[
g_{\epsilon,c}^f(m) := E_{\epsilon,c}^f(m) + I(m).
\]

Setting the derivative of \( g_{\epsilon,c}^f \) equals to zero gives the \textbf{landscape-modified mean-field equation}:

\[
m = \tanh \left( \frac{m + h}{f((E(m) - c)_+) + \epsilon} \right).
\]

(3.4)

Observe that if we take \( f = 0 \), then (3.4) reduces to the classical mean-field equation in (3.1).
3.1. **Main results.** Without loss of generality, assume the external magnetic field is \( h < 0 \). In the subcritical regime where \( \beta > 1 \), it is known that there are two local minima of \( g_c \). We denote the global minimum of \( g_c \) by \( m_-^* < 0 \) and the other local minimum by \( m_+^* > 0 \), where \( \vert m_-^* \vert > m_+^* \), and let \( z^* \) be the saddle point between \( m_-^* \) and \( m_+^* \). We also write \( m_-^*(N) \) (resp. \( m_+^*(N) \)) to be the closest point in Euclidean distance on \( \Gamma_N \) to \( m_-^* \) (resp. \( m_+^* \)).

**Theorem 3.1** (Landscape modification in the subcritical regime). Suppose \( \beta > 1 \), \( h < 0 \) and \( f, c \) are chosen as in Assumption 2.1.

1. [Convexification of the free energy \( g_c \) and subexponential mean crossover time] If we choose \( c \in [E(m_-^*), E(m_+^*)] \), \( c < h^2/2 \), \( -h - \sqrt{h^2 - 2c} \leq z^* \) and for \( m \in [-h - \sqrt{h^2 - 2c}, -h + \sqrt{h^2 - 2c}] \),

\[
m > \tanh \left( \frac{m + h}{f((E(m) - c)_+) + \epsilon} \right),
\]

then \( m_-^* \) is the only stationary point of the modified free energy \( g_{\epsilon,c}^f \), which is a global minimum. Consequently,

\[
(3.5) \quad \lim_{N \to \infty} \frac{1}{N} \log \mathbb{E}_{m_-^*(N)} \left( \tau_{m_-^*(N)}^f \right) = 0.
\]

2. Assume in addition that \( f \) is twice differentiable and satisfies \( f'(0) = f''(0) = 0 \). If we choose \( c \in [E(m_+^*), E(z^*)] \), then there exists \( z^* = \arg \max_{m_-^* \leq m \leq m_+^*} g_{\epsilon,c}^f(m) \) and as \( N \to \infty \),

\[
\mathbb{E}_{m_-^*(N)} \left( \tau_{m_-^*(N)}^f \right) = \exp \left( N(g_{\epsilon,c}^f(z^*) - g_{\epsilon,c}^f(m_+^*)) \right) \times 
\frac{2}{1 - |z^*| \sqrt{\frac{1 - z^*^2}{1 - m_+^2}} \left( -g_{\epsilon,c}^{f''}(z^*) \right) g_{\epsilon,c}^{f''}(m_+^*)} \left( 1 + o(1) \right).
\]

Consequently,

\[
\lim_{N \to \infty} \frac{1}{N} \log \mathbb{E}_{m_-^*(N)} \left( \tau_{m_-^*(N)}^f \right) = g_{\epsilon,c}^f(z^*) - g_{\epsilon,c}^f(m_+^*)
\]

\[
= \beta(c - E(m_+^*)) + \int_c^{E(z^*)} \frac{1}{f((u - c)_+) + \epsilon} \, du + (I(z^*) - I(m_+^*))
\]

\[
\leq \beta(g_c(z^*) - g_c(m_+^*)) = \lim_{N \to \infty} \frac{1}{N} \log \mathbb{E}_{m_-^*(N)} \left( \tau_{m_-^*(N)} \right).
\]

**Remark 3.1** (Landscape modification for minimizing the sum of two functions). In fact, the proof strategy employed in the above Curie-Weiss model can be generalized to minimizing the sum of two functions. Suppose that we are interested in minimizing

\[
T(x) := H(x) + G(x),
\]

where \( T, H, G : \mathbb{R}^d \to \mathbb{R} \) are differentiable. Assume that \( T \) has finite number of critical points with an unique global minimum at \( x^* \), and denote the set of critical points of \( T \) to be \( \mathcal{C} \). We also assume that \( H \) has non-vanishing gradient in the sense that \( \nabla H(x) \neq 0 \) for all \( x \in \mathbb{R}^d \). Instead of minimizing \( T \) directly, we instead minimize

\[
T_{\epsilon,c}^f(x) := \epsilon H_{\epsilon,c}^f(x) + G(x),
\]
\[ H_{\epsilon,c}^f(x) := \frac{1}{\int_{H(x^*)}^{H(x)} \frac{1}{f((u-c)_+)} + \epsilon \, du}. \]

We also impose the following assumption on \( H \), in the sense that \( c \) can be chosen such that \( c \in [H(x^*), H(x_2^*)] \), where \( x_2^* := \arg \min_{x \in C \setminus \{x^*, x_1^* \}} H(x) \). Let \( 0 < \delta < H(x_2^*) - c \). For \( x \in \{ H(x) \leq c + \delta \} \),

\[ \nabla T_{\epsilon,c}^f(x) = \nabla T(x), \]

and \( x^* \) is the only critical point of \( T \) or \( T_{\epsilon,c}^f \) on this set. On the other hand, for \( x \in C \cap \{ H(x) > c + \delta \} \), we compute that

\[ \nabla T_{\epsilon,c}^f(x) = \nabla H_{\epsilon,c}^f(x) + \nabla G(x) = \nabla H(x) \left( \frac{\epsilon}{f(H(x) - c) + \epsilon} - 1 \right). \]

If we choose \( f \) so that \( f(\delta) > 0 \), then \( T_{\epsilon,c}^f \) has no critical point in this region, since if otherwise \( 1 = f(H(x) - c)/\epsilon + 1 > 1 \), which is impossible. Writing \( C' \) to be the complement of \( C \) and \( v_i \) for the \( i \)-th element of the vector \( v \), consider \( x \in C' \cap \{ H(x) > c + \delta \} \). Since \( x \in C' \), first we suppose there exists \( i \) such that \( (\nabla H(x))_i > -(\nabla G(x))_i \). If \( (\nabla G(x))_i > 0 \), and if we choose \( \epsilon \) small enough, this gives

\[ (\nabla T_{\epsilon,c}^f(x))_i \geq (\nabla G(x))_i \left( 1 - \frac{\epsilon}{f(H(x) - c) + \epsilon} \right) > 0. \]

If \( (\nabla G(x))_i < 0 \), then \( (\nabla H(x))_i > 0 \). If \( x \) is a critical point of \( T_{\epsilon,c}^f \), then

\[ \frac{\epsilon}{f(H(x) - c) + \epsilon} = \frac{-(\nabla G(x))_i}{(\nabla H(x))_i}, \]

which cannot be true since the left hand side goes to 0 as \( \epsilon \to 0 \) while the right hand side is independent of \( \epsilon \) and is positive. Similar argument holds for the second case if we have \( (\nabla H(x))_i < -(\nabla G(x))_i \).

In summary, we show that with appropriate choice of \( f, c \) and \( \epsilon \), one can possibly eliminate all local minima except the global minimum by minimizing \( T_{\epsilon,c}^f \) instead of \( T \).

Before we present the proof, we interpret the results in Theorem 3.1 intuitively: in item (1), on one hand we would like to choose \( c \) small enough such that the mapping

\[ m \mapsto \tanh \left( \frac{m + h}{f(E(m) - c)_+ + \epsilon} \right) \]

is flattened and only intersects with the straight line \( m \mapsto m \) at the global minimum \( m^* \). In this way the landscape of \( g_{\epsilon,c}^f \) is transformed from a double-well to a single-well, while the location of the global minimum at \( m^* \) is preserved as that in the original landscape \( g_\epsilon \). This is illustrated in Figure 1 and Figure 2. On the other hand, we cannot choose \( c \) to be too small if we are interested in seeking the ground state of \( g_\epsilon \), since otherwise if \( c < E(m^*_\epsilon) \) then \( m^*_\epsilon \) may no longer be the global minimum in the transformed free energy \( g_{\epsilon,c}^f \). In Theorem 3.1 item (2), we choose a larger value of \( c \) compared with that in item (1).

Although the transformed free energy \( g_{\epsilon,c}^f \) is not a convex function, it has a smaller critical height than the original free energy \( g_\epsilon \).

The power of landscape modification or energy transformation lies in tuning the parameter \( c \) appropriately. One way to tune \( c \) is to use the running minimum generated by the algorithm on the original free energy \( g_\epsilon \). Suppose we start in the well containing the local minimum \( m^*_\epsilon \), and setting \( c \) to be the running minimum eventually gives \( c = E(m^*_\epsilon) \), and hence Theorem 3.1 item (2) can be applied and the critical height on the modified landscape is reduced.
We illustrate Theorem 3.1 with a concrete numerical example in Figure 1 and Figure 2, where we take $h = -0.05$ and $f(x) = x$ at inverse temperature $\beta = 1.5$. We numerically compute that $m^* = -0.8863$, $m^* = 0.8188$ and $z^* = 0.1524$. As a result we have $E(m^*) = -0.4371$, $E(m^*) = -0.2943$ and $E(z^*) = -0.004$. In the leftmost plot of Figure 1 and Figure 2, we choose $c = -0.4 \in \{E(m^*), E(z^*)\}$. We numerically check that the conditions in Theorem 3.1 item (1) are satisfied, and we see that the blue curve and the orange curve share the same location of the global minimum. In the rightmost plot of Figure 1 and Figure 2, we choose $c = -0.2 \in \{E(m^*), E(z^*)\}$. We see that the blue curve and the red curve share the same locations of the two local minima, while the critical height is smaller than that in the original landscape $g_c$.

\[ \text{Figure 1. Plots of the free energy } g_c \text{ and the modified free energy } g^f_{c,c} + E_{\min} \text{ with } h = -0.05 \text{ and } f(x) = x \text{ at inverse temperature } \beta = 1.5, \text{ where } E_{\min} = \min_{m \in [-1,1]} E(m). \text{ We shift the modified free energy by } E_{\min} \text{ so that it is on the same scale as the original free energy } g_c. \]

\[ \text{Figure 2. Plots of the mean-field equation (3.1) and the modified mean-field equation (3.4) with } h = -0.05 \text{ and } f(x) = x \text{ at inverse temperature } \beta = 1.5. \]

3.2. Proof of Theorem 3.1. Before we give the proof, we first recall the concept of critical height. In Section 2, we define the critical height of the Hamiltonian function. However here in the CW model with landscape modification we are interested in the free energy $g^f_{c,c,N}$. As a result we define the analogous concepts by inserting a subscript of $N$. The highest value of the free energy $g^f_{c,c,N}$ along a path $\gamma \in \chi^{x,y}$,
known as the elevation, is defined to be
\[
\text{Elev}_{\epsilon,c,N}^f(\gamma) = \max \{ g_{\epsilon,c,N}^f(\gamma_i); \; \gamma_i \in \gamma \},
\]
and the lowest possible highest elevation along path(s) from \(x\) to \(y\) is
\[
G_{\epsilon,c,N}^f(x,y) := \min \{ \text{Elev}_{\epsilon,c,N}^f(\gamma); \; \gamma \in \chi^{xy} \}.
\]
For \(M_{\epsilon,c,N}^f\), the associated critical height is defined to be
\[
H_{\epsilon,c,N}^f := \max_{x,y \in \Gamma_N} \{ G_{\epsilon,c,N}^f(x,y) - g_{\epsilon,c,N}^f(x) - g_{\epsilon,c,N}^f(y) + \min_{x \in \Gamma_N} g_{\epsilon,c,N}^f(x) \}.
\]
Similarly, for \(M_{\epsilon,c,N}^0\) its critical height is
\[
H_{\epsilon,c,N}^0 := \max_{x,y \in \Gamma_N} \{ G_{\epsilon,c,N}^0(x,y) - g_{\epsilon,N}(x) - g_{\epsilon,N}(y) + \min_{x \in \Gamma_N} g_{\epsilon,N}(x) \}.
\]

**Proof of Theorem 3.1.** First, we prove item (1). We observe that \(\{E(m) \geq c\} = \{m \in [-h - \sqrt{h^2 - 2c}, -h + \sqrt{h^2 - 2c}]\} \), On this interval,
\[
\frac{d}{dm} g_{\epsilon,c,N}^f(m) = \text{arctanh}(m) - \frac{m + h}{f((E(m) - c)_+)} + \epsilon > 0,
\]
and hence the modified free energy is strictly increasing on this interval. On the interval \(\{m > -h + \sqrt{h^2 - 2c}\}, \frac{d}{dm} g_{\epsilon,c,N}^f(m) = \frac{d}{dm} g_{\epsilon}(m) > 0\) as the original free energy is strictly increasing. On the interval \(\{m < -h - \sqrt{h^2 - 2c}\}\), we also have \(\frac{d}{dm} g_{\epsilon,c,N}^f(m) = \frac{d}{dm} g_{\epsilon}(m)\). Thus, with these parameter choices, the only stationary point of \(g_{\epsilon,c,N}^f\) is \(m^*_\epsilon\), which is the global minimum.

Next, we proceed to prove (3.5). According to \((\text{Löwe, 1996, Theorem 2.1})\), for \(\xi_1(N)\) a polynomial function in \(N\), we have
\[
\frac{1}{\lambda_2(-M_{\epsilon,c,N}^f)} \leq \xi_1(N)e^{NH_{\epsilon,c,N}^f}.
\]
Now, using the random target lemma \((\text{Levin and Peres, 2017, Lemma 12.17})\) and the above inequality lead to
\[
\pi_{\epsilon,c,N}^f(m^*_-(N))\mathbb{E}_{m^*_+(N)}(\tau_{m^*_-(N)}^f) \leq \sum_{y \in \Gamma_N} \pi_{\epsilon,c,N}^f(y)\mathbb{E}_{m^*_+(N)}(\tau_y^f) \leq (|\Gamma_N| - 1)\frac{1}{\lambda_2(-M_{\epsilon,c,N}^f)} \leq N\xi_1(N)e^{NH_{\epsilon,c,N}^f}.
\]
Now, let \(\overline{m}(N) := \arg \min g_{\epsilon,c,N}^f(m)\) and compute
\[
g_{\epsilon,c,N}^f(m^*_-(N)) - g_{\epsilon,c,N}^f(\overline{m}(N)) = E_{\epsilon,c}^f(m^*_-(N)) - E_{\epsilon,c}^f(\overline{m}(N)) + I_N(m^*_-(N)) - I_N(\overline{m}(N))
\]
\[
= E_{\epsilon,c}^f(m^*_-(N)) - E_{\epsilon,c}^f(\overline{m}(N)) + I_N(m^*_-(N)) - I_N(\overline{m}(N))
\]
\[
= E_{\epsilon,c}^f(m^*_-(N)) - E_{\epsilon,c}^f(\overline{m}(N)) + [1 + o(1)] \frac{1}{2N} \ln \left( \frac{\pi N (1 - m^*_-(N))^2}{2} \right)
\]
\[
+ I(m^*_-(N)) - I(\overline{m}(N))
\]
Now, for equation (3.1) is continuous in $m$, the landscape modified mean-field equation (3.4) has at least two solutions as $N \to \infty$. Together with (3.6) yields
\begin{equation}
\lim_{N \to \infty} \frac{1}{\pi(N)} \ln \left( \pi(N) (1 - \bar{m}(N)^2) \right) \to 0 \quad \text{as } N \to \infty,
\end{equation}
where we use (Bovier and den Hollander, 2015, equation (13.2.5)) in the third equality, and $m^*_+(N), \bar{m}(N) \to m^*_+$ as $N \to \infty$. Together with (3.6) yields
\begin{equation}
\lim_{N \to \infty} \sup E_{m^*_+}(N) \left( \tau_{m^*_-}^f(N) \right) \leq \lim_{N \to \infty} H_{f, c, N}^f = 0.
\end{equation}

On the other hand, as the magnetization $(m^f(t))_{t \geq 0}$ is a birth-death process, using (Bovier and den Hollander, 2015, equation (13.2.2)) the mean hitting time can be calculated explicitly as
\begin{align*}
E_{m^*_+}(N) \left( \tau_{m^*_-}^f(N) \right) &= \sum_{m, m' \in \Gamma_N, m \leq m'} \frac{\pi_{f, c, N}(m')}{\pi_{f, c, N}(m)} \frac{1}{M_{f, c, N}^f(m, m - 2N^{-1})} \\
&\geq \frac{1}{M_{f, c, N}^f(m^*_+(N), m^*_+(N) - 2N^{-1})} = \frac{2}{1 + m^*_+(N)} e^{N(E_{f, c}^f(m^*_+(N) - 2N^{-1}) - E_{f, c}^f(m))_+} \\
&\geq \frac{2}{1 + m^*_+(N)}.
\end{align*}
As a result, as $m^*_+(N) \to m^*_+$ we have
\begin{equation}
\lim_{N \to \infty} \inf E_{m^*_+}(N) \left( \tau_{m^*_-}^f(N) \right) \geq 0.
\end{equation}
Using both (3.8) and (3.7) gives (3.5).

Next, we prove item (2), which follow closely with the proof of (Bovier and den Hollander, 2015, Theorem 13.1). Since we choose $c \in [E(m^*_+), E(z^*)]$, then we have $E(m^*_+) - c < E(m^*_+) - c \leq 0$, and hence the landscape modified mean-field equation (3.4) has at least two solutions $m^*_+$ and $m^*_-$, which are exactly the same as the original mean-field equation (3.1). As the landscape modified mean-field equation is continuous in $m$, there exists $z^* = \arg \max_{m \leq m^*_+} g_{f, c}^f(m)$ which also satisfies (3.4). Now, for $m \in \Gamma_N$ we consider
\begin{align*}
N \left( E_{f, c}^f(m - 2N^{-1}) - E_{f, c}^f(m) \right) &= N \int_{E(m)}^{E(m) + 2N^{-1}(m + h - N^{-1})} \frac{1}{f((u - c)_+ + \epsilon)} du \\
&\to \frac{2(m + h)}{f((E(m) - c)_+ + \epsilon)} \quad \text{as } N \to \infty.
\end{align*}
If we take $N \to \infty$ and $m \to z^*$, we obtain
\begin{equation}
\frac{1}{M_{f, c, N}^f(m, m - 2N^{-1})} \to \frac{2}{1 + z^*} \exp \left( \frac{2(z^* + h)_+}{f((E(z^*) - c)_+ + \epsilon)} \right) = \frac{2}{1 - |z^*|},
\end{equation}
since if $z^* > 0$, then $z^* + h > 0$ and satisfies the mean-field equation (3.4). Using the mean hitting time formula again leads to, for any $\delta > 0$,
\begin{align*}
E_{m^*_+}(N) \left( \tau_{m^*_-}^f(N) \right) &= \sum_{m, m' \in \Gamma_N, m \leq m'} \frac{\pi_{f, c, N}(m')}{\pi_{f, c, N}(m)} \frac{1}{M_{f, c, N}^f(m, m - 2N^{-1})} \\
&= \frac{1}{1 + m^*_+} e^{N(E_{f, c}^f(m^*_+(N) - 2N^{-1}) - E_{f, c}^f(m))_+} \\
&\geq \frac{1}{1 + m^*_+} e^{N(E_{f, c}^f(m^*_+(N) - 2N^{-1}) - E_{f, c}^f(m))_+} \\
&\geq \frac{2}{1 + m^*_+}.
\end{align*}
We proceed to use a Laplace method argument to handle the sum in (3.10). Note that as $f$ followed by substitution to (3.9) gives applying the third-order Taylor expansion gives be twice-differentiable with $f$ since $g$ (the setting as in Mathieu and Picco (1998). Let free energy in such setting. Let us begin by first recalling the random field CW model. We shall adapt field CW model with landscape modification, and discuss related metastability results and its ground state with landscape modification under 3.3.

Extension to the random field Curie-Weiss. In Section 3.1, we discuss the classical CW model with landscape modification under fixed magnetic field. In this section, we aim at considering the random field CW model with landscape modification, and discuss related metastability results and its ground state free energy in such setting. Let us begin by first recalling the random field CW model. We shall adapt the setting as in Mathieu and Picco (1998). Let $(h_i)_{i \in \mathbb{N}}$ be a sequence of i.i.d. random variables with $\mathbb{P}(h_i = 1) = \mathbb{P}(h_i = -1) = 1/2$. We consider the random Hamiltonian function given by, for a fixed $\theta > 0$ and $\sigma \in \{-1, 1\}^N$,

$$H_N(\sigma) = H_N(\sigma, \omega) := -\frac{N}{2} \mathbf{m}_N(\sigma)^2 - \theta \sum_{i=1}^N h_i(\omega)\sigma_i = -\frac{N}{2}(\mathbf{m}_N^+(\sigma) + \mathbf{m}_N^-(\sigma))^2 - \theta N(\mathbf{m}_N^+(\sigma) - \mathbf{m}_N^-(\sigma)),$$
where \( m_N(\sigma) := (1/N) \sum_{i=1}^N \sigma_i \), \( m_N^+(\sigma) := (1/N) \sum_{i=1; \, h_i = +1}^N \sigma_i \) and \( m_N^-(\sigma) := (1/N) \sum_{i=1; \, h_i = -1}^N \sigma_i \).

In the sequel, we shall suppress the dependency on \( \omega \). Denote the Gibbs distribution at inverse temperature \( \beta \) on \( \{-1, 1\}^N \) by

\[
\nu_N(\sigma) \propto \exp\{-\beta H_N(\sigma)\}.
\]

Let \( N^+ := \{|i; \, h_i = +1|\}, \, N^- := \{|i; \, h_i = -1|\} \) and define the random set

\[
\Gamma_N := \left( -\frac{N^+}{N}, -\frac{N^+}{N} + \frac{2}{N}, \ldots, \frac{N^+}{N} \right) \times \left( -\frac{N^-}{N}, -\frac{N^-}{N} + \frac{2}{N}, \ldots, \frac{N^-}{N} \right).
\]

For \( m = (m^+, m^-) \in \Gamma_N \), with slight abuse of notation we write

\[
H_N(m) = -\frac{N}{2}(m^+ + m^-)^2 - \theta N(m^+ - m^-) =: NE(m).
\]

Let \( \pi^{0}_{\epsilon,N} \) denote the image Gibbs distribution of \( \nu_N \) by \( \Gamma_N \), where

\[
\pi^{0}_{\epsilon,N}(m) \propto \exp\{-\beta Ng_{\epsilon,N}(m)\},
\]

\[
g_{\epsilon,N}(m) := -\frac{1}{2}(m^+ + m^-)^2 - \theta (m^+ - m^-) - \frac{1}{\beta N} \log \left( \frac{N^+}{N^+ + \frac{N N^-}{2}} \right) \left( \frac{N^-}{N^+ + \frac{N N^-}{2}} \right).
\]

As \( N \to \infty \), by the strong law of large number \( g_{\epsilon,N} \) converges almost surely to the free energy given by

\[
g_{\epsilon}(m) := -\frac{1}{2}(m^+ + m^-)^2 - \theta (m^+ - m^-) + \frac{1}{2\beta} \left( I(2m^+) + I(2m^-) \right),
\]

where \( I(m) \) is the Cramér rate function as introduced in Section 3. The critical points of \( g_{\epsilon} \) satisfy

\[
m^+ = \frac{1}{2} \tanh(\beta(m^+ + m^- + \theta)),
\]

\[
m^- = \frac{1}{2} \tanh(\beta(m^+ + m^- - \theta)).
\]

In this section, we shall only consider the subcritical regime where \( \beta > \cosh^2(\beta \theta) \). It can be shown (see e.g. Mathieu and Picco (1998)) that there are exactly three critical points. Let \( m_* > 0 \) be the unique positive solution to the mean-field equation

\[
m_* = \frac{1}{2} \left( \tanh(\beta(m_* + \theta)) + \tanh(\beta(m_* - \theta)) \right).
\]

The three critical points of \( g_{\epsilon} \) are given by

\[
m_0 = \left( \frac{1}{2} \tanh(\beta \theta), -\frac{1}{2} \tanh(\beta \theta) \right),
\]

\[
m_1 = \left( \frac{1}{2} \tanh(\beta m_* + \beta \theta), \frac{1}{2} \tanh(\beta m_* - \beta \theta) \right),
\]

\[
m_2 = \left( \frac{1}{2} \tanh(-\beta m_* + \beta \theta), -\frac{1}{2} \tanh(\beta m_* + \beta \theta) \right),
\]

where \( m_0 \) is the saddle point and \( m_1, m_2 \) are the two global minima. Consider the continuized Glauber dynamics \( (\sigma_N(t))_{t \geq 0} \) by picking a node uniformly at random and changing the sign of the selected spin, while targeting the Gibbs distribution \( \pi_N \) at inverse temperature \( \beta \). Denote by \( m_N(t) := m_N(\sigma_N(t)) \) be the induced dynamics on the magnetization, and its infinitesimal generator by \( M^0_{\epsilon,N} \). This is proven to be a Markov chain in Mathieu and Picco (1998), with stationary measure \( \pi^{0}_{\epsilon,N} \).
Now, let us consider the landscape modified Hamiltonian on $\Gamma_N$:

\begin{align}
E_{\epsilon,c}^f(m) &:= \int_d^{E(m)} \frac{1}{f((u - c)_+) + \epsilon} \, du, \\
H_{\epsilon,c,N}^f(m) &:= NE_{\epsilon,c}^f(m),
\end{align}

(3.15)  (3.16)

where $d \in \mathbb{R}$ can be chosen arbitrarily since we are only interested in the difference of $E_{\epsilon,c}^f$. The transformed image Gibbs distribution is therefore

\[
\pi_{\epsilon,c,N}^f(m) \propto \exp\{-Ng_{\epsilon,c,N}^f(m)\},
\]

\[
g_{\epsilon,c,N}^f(m) := E_{\epsilon,c}^f(m) - \frac{1}{N} \log \left( \frac{N^+}{N^+ + m^+ N^-} + \frac{N^-}{N^- + m^- N^+} \right).
\]

The strong law of large number yields that as $N \to \infty$, $g_{\epsilon,c,N}^f$ converges almost surely to the transformed free energy

\[
g_{\epsilon,c}^f(m) := E_{\epsilon,c}^f(m) + \frac{1}{2} \left( I(2m^+) + I(2m^-) \right).
\]

The critical points of $g_{\epsilon,c}^f$ satisfy the following landscape modified mean-field equations:

\begin{align}
m^+ &:= \frac{1}{2} \tanh \left( \frac{m^+ + m^- + \theta}{f(E(m) - c)_+ + \epsilon} \right), \\
m^- &:= \frac{1}{2} \tanh \left( \frac{m^+ + m^- - \theta}{f(E(m) - c)_+ + \epsilon} \right).
\end{align}

(3.17)  (3.18)

Note that (3.17) and (3.18) reduce to the classical case (3.13) and (3.14) if we take $f = 0$. Consider the continuized Glauber dynamics $(\sigma_N^f(t))_{t \geq 0}$ by picking a node uniformly at random and changing the sign of the selected spin, while targeting the Gibbs distribution with Hamiltonian $H_{\epsilon,c,N}^f$ at inverse temperature $1$. Denote by $m_N^f(t) := m_N^f(\sigma_N^f(t))$ be the induced dynamics on the magnetization, and its infinitesimal generator by $M_{\epsilon,c,N}^f$, which is a Markov chain with stationary measure $\pi_{\epsilon,c,N}^f$.

In the following, we shall consider the case where $c \in \{E(m_1), E(m_0)\}$. It can be seen that the two global minima of $g_{\epsilon,c}^f$ remain to be $m_1, m_2$ with this choice of $c$. For any path $\gamma_{m_1,m_0}$ connecting $m_1$ and $m_0$, we define

\[
m_3(\gamma_{m_1,m_0}) := \arg \max \{g_{\epsilon,c}^f(\gamma_i) ; \gamma_i \in \gamma_{m_1,m_0}\},
\]

\[
\Delta g_{\epsilon,c}^f := \min_{\gamma_{m_1,m_0}} m_3(\gamma_{m_1,m_0}) - g_{\epsilon,c}^f(m_1) = \min_{\gamma_{m_1,m_0}} m_3(\gamma_{m_1,m_0}) - g_{\epsilon,c}^f(m_0),
\]

where $\Delta g_{\epsilon,c}^f$ is the critical height on the modified landscape. We also write $\Delta g_\epsilon$ to denote the critical height on the original landscape. Suppose that $\Delta g_\epsilon$ is attained at $m_4$ so that $\Delta g_\epsilon = g_\epsilon(m_4) - g_\epsilon(m_0)$, and we deduce

\[
\Delta g_{\epsilon,c}^f \leq g_{\epsilon,c}^f(m_4) - g_{\epsilon,c}^f(m_0) = \int_{E(m_0)}^{E(m_4)} \frac{1}{f((u - c)_+) + \epsilon} \, du \\
+ \frac{1}{2} \left( I(2m_4^+) + I(2m_4^-) \right) - \frac{1}{2} \left( I(2m_0^+) + I(2m_0^-) \right) \\
\leq \beta (g_\epsilon(m_4) - g_\epsilon(m_0)) = \beta \Delta g_\epsilon.
\]

In other words, the critical height of the free energy in the modified landscape is bounded above by $\beta$ times the critical height of the free energy in the original landscape.
A direct application of (Mathieu and Picco, 1998, Theorem 2.7) yields the following result on the asymptotics of the spectral gap:

**Theorem 3.2** (Asymptotics of the spectral gap). Suppose $\theta > 0$, $\beta > \cosh^2(\beta \theta)$ are fixed, and $m_0$ is the saddle point while $m_1, m_2$ are the two global minima on the original free energy landscape $g_c$. For $c \in [E(m_1), E(m_0)]$, we have

$$
\lim_{N \to \infty} \frac{1}{N} \log \lambda_2(-M_{c,N}^f) = -\Delta g_{c,N}^f \geq -\beta \Delta g_c = \lim_{N \to \infty} \frac{1}{N} \log \lambda_2(-M_0^N).
$$

In essence, the relaxation time in the mean-field limit of the transformed generator $M_{c,N}^f$ is asymptotically less than or equal to that of the original generator $M_0^N$.

4. DISCRETE SIMULATED ANNEALING WITH LANDSCAPE MODIFICATION

In previous sections of this paper, the temperature parameter is fixed. In this section, we consider the non-homogeneous Metropolis-Hastings with landscape modification where the temperature schedule $(\epsilon_t)_{t \geq 0}$ is time-dependent, non-increasing and goes to zero as $t \to \infty$.

We first introduce the notion of clipped critical height $c^*$. Recall that in (2.4) we introduce $H_{c,t}^f$ and $H_0$ as the critical height for $M_{c,t}^f$ and $M_0^0$ respectively. It turns out that these critical heights are closely related to $c^*$:

$$
c^* := \max_{x,y \in \mathcal{X}} \left\{ G^0(x, y) \wedge c - H(x) \wedge c - H(y) \wedge c + \min \mathcal{H} \right\},
$$

where $G^0(x, y)$, the lowest possible maximum elevation between $x$ and $y$, is defined in (2.3). One can understand $c^*$ as if the Hamiltonian function is $H \wedge c$.

Our first result gives the asymptotic order of the spectral gap $\lambda_2(-M_{c,N}^f)$ in terms of $c^*$ in the low temperature regime, which will be proven to be essential in obtaining convergence result for simulated annealing:

**Theorem 4.1.** Assume that $f$ and $\min \mathcal{H} \leq c \leq \max \mathcal{H}$ satisfy Assumption 2.1, and in addition for small enough $x > 0$ we have $f(x) \geq x$. There exists positive constants $C_2, C_3, C_4$ that depend on the state space $\mathcal{X}$ and the proposal generator $Q$ but not on the temperature $\epsilon$, and subexponential function

$$
C_1(\beta) := \begin{cases} 
\frac{1}{C_2} \left(1 + \beta(\max \mathcal{H} - c)\right) \exp \left\{ \frac{1}{f(\delta)} (\max \mathcal{H} - \min \mathcal{H}) \right\}, & \text{if } c < \max \mathcal{H}; \\
\frac{1}{C_2}, & \text{if } c = \max \mathcal{H},
\end{cases}
$$

where $\delta := \min_{x \in \mathcal{X} \setminus \mathcal{H}_0} \{ \mathcal{H}(x) - c \}$, such that

$$
C_1^{-1}(\beta) e^{-\beta c^*} \leq C_2 e^{-H_{c,t}^f} \leq \lambda_2(-M_{c,t}^f) \leq C_3 e^{-H_{c,t}^f} \leq C_4 e^{-\beta c^*},
$$

where $H_{c,t}^f$ is introduced in (2.4) and $c^*$ is defined in (4.1). Consequently, this leads to

$$
\lim_{\beta \to \infty} \frac{1}{\beta} \log \lambda_2(-M_{c,t}^f) = -c^*.
$$

As a corollary of the above result Theorem 4.1, using the asymptotics of the spectral gap we derive similar asymptotics of the mixing time and tunneling time:

**Corollary 4.1** (Asymptotics of mixing and tunneling times in the low-temperature regime). Assume the same setting as in Theorem 4.1. Let $S_{min} = \arg \min \mathcal{H}(x)$ be the set of global minima of $\mathcal{H}$, $\eta \in S_{min}$, and $\sigma, \eta$ attain $H^0$ such that $H^0 = G^0(\sigma, \eta) - \mathcal{H}(\sigma)$. Then the following statements hold:
\[ \lim_{\beta \to \infty} \frac{1}{\beta} \log t_{\text{mix}}(M_{\epsilon,c}, 1/4) = c^{*}. \]

\[ \lim_{\beta \to \infty} \frac{1}{\beta} \log E_{\sigma}(\tau_{\eta}^{f}) = c^{*} \leq H^{0} = \lim_{\beta \to \infty} \frac{1}{\beta} \log E_{\sigma}(\tau_{\eta}^{0}). \]

In particular, when \( c = \mathcal{H}_{\text{min}} \), we have subexponential tunneling time as \( \lim_{\beta \to \infty} \frac{1}{\beta} \log E_{\sigma}(\tau_{\eta}^{f}) = 0 = c^{*} \).

Note that in the case where both \( \sigma, \eta \in S_{\text{min}} \) with initial state \( \sigma \), it is a reasonable choice to pick the parameter \( c = \mathcal{H}(X_{f}(0)) = \mathcal{H}(\sigma) = \mathcal{H}_{\text{min}} \), and in this setting we have subexponential tunneling time on the modified landscape. For example, in the Widom-Rowlinson model with \( m \in \mathbb{N} \) particle types, \( S_{\text{min}} \) is precisely the set of configurations in which all sites are occupied by particles of the same type. We refer interested readers to Nardi and Zocca (2019); Zocca (2018) for recent work on the energy landscape analysis of various statistical physics models in this direction.

To prove convergence result for simulated annealing with landscape modification, as our target function \( \mathcal{H}_{f, c} \) depends on time through the cooling schedule, we are in the setting of simulated annealing with time-dependent energy function as in Löwe (1996). We first present the following auxiliary lemma, where we verify various assumptions in Löwe (1996) in our setting. We also decide to put it in this section rather than in the proof since it will help to better understand the convergence result in Theorem 4.2 below.

**Lemma 4.1.** Assume the same setting as in Theorem 4.1. Let \( M := \max \mathcal{H} - \min \mathcal{H} \), and the cooling schedule is, for small enough \( \epsilon \) such that \( M + \max \mathcal{H} - c > \epsilon > 0 \) and \( t \geq 0 \),

\[ \epsilon_{t} = \frac{c^{*} + \epsilon}{\ln(t + 1)}. \]

We have

1. For all \( x \in \mathcal{X} \) and all \( t \geq 0 \),
\[ 0 \leq \epsilon_{t} \mathcal{H}_{t, c}^{f}(x) \leq M. \]

2. For all \( x \in \mathcal{X} \),
\[ \left| \frac{\partial}{\partial t} \epsilon_{t_{t,c}}^{f}(x) \right| \leq \frac{2M}{(\ln(1 + t))(1 + t)}. \]

3. Let \( R_{t} := \sup_{x} \frac{\partial}{\partial t} \epsilon_{t}^{f}(x) \) and \( B := 6M/(c^{*} + \epsilon) \). For all \( t \geq 0 \),
\[ \beta_{t} M + \beta_{t} R_{t} \leq \frac{3M}{(c^{*} + \epsilon)(1 + t)} = \frac{B}{2(1 + t)}. \]

4. Let
\[ p := \frac{2M}{M + \max \mathcal{H} - c - \epsilon} > 2, \]

and
\[
A := \left\{ \begin{array}{ll}
\frac{1}{C_{2}(\min_{x} \mu(x))^{(p-2)/p}} \exp \left\{ \frac{1}{f(\delta)} (\max \mathcal{H} - \min \mathcal{H}) \right\}, & \text{if } c < \max \mathcal{H}, \\
\frac{1}{C_{2}(\min_{x} \mu(x))^{(p-2)/p}}, & \text{if } c = \max \mathcal{H},
\end{array} \right.
\]
where $C_2, \delta$ are as in Theorem 4.1 and we recall that $\mu$ is the stationary measure of the proposal generator $Q$. For $g \in \ell^p(\pi_{t,e,c})$, we have

$$\|g - \pi_{t,e,c}^f(g)\|_{\ell^p(\pi_{t,e,c})}^2 \leq A(1 + t)\langle -M_{t,e,c}^f, g \rangle_{\pi_{t,e,c}}.$$ 

With the above Lemma and the notations introduced there, we are ready to give one of the main results of this paper concerning the large-time convergence of discrete simulated annealing with landscape modification. In a nutshell, we can operate a faster logarithmic cooling schedule with clipped critical height $c^*$, while in classical simulated annealing the critical height is $H^0$. This result is analogous to the result that we have obtained in Choi (2020) for improved kinetic simulated annealing.

**Theorem 4.2.** Assume the same setting as in Theorem 4.1. Let $A, B, p$ be the quantities as introduced in Lemma 4.1. Define

$$\tilde{\epsilon} := \frac{p - 2}{p}, \quad K := \frac{4(1 + 2AB)}{1 - \exp\{-\frac{1}{2A} - B\}}, \quad S_{\min} := \arg \min_{H} \mathcal{H}, \quad d := \min_{x : \mathcal{H}(x) \neq \mathcal{H}_{\min}} \mathcal{H}(x).$$

Under the cooling schedule of the form, for any $\epsilon > 0$ as in Lemma 4.1,

$$\epsilon_t = \frac{c^* + \epsilon}{\ln(t + 1)},$$

we then have, for any $x \in \mathcal{X}\setminus S_{\min}$ and $t \geq e^{1/\epsilon} - 1$,

$$\mathbb{P}_x \left( \tau_{S_{\min}}^f > t \right) \leq (1 + K\tilde{\epsilon})\sqrt{\pi_{t,e,c}^f(\mathcal{X}\setminus S_{\min}) + \pi_{t,e,c}^f(\mathcal{X}\setminus S_{\min})} \to 0 \quad \text{as } t \to \infty.$$ 

Note that

$$\pi_{t,e,c}^f(\mathcal{X}\setminus S_{\min}) \leq \begin{cases} \frac{1}{\mu(S_{\min})} e^{-\beta_t(d - \mathcal{H}_{\min})}, & \text{if } c \geq d; \\ \frac{1}{\mu(S_{\min})} \exp \left\{ - \int_c^d \frac{1}{f(u - c) + \epsilon_t} du \right\}, & \text{if } \mathcal{H}_{\min} \leq c < d. \end{cases}$$

**Remark 4.1 (On tuning the parameter $c$).** There are various ways to tune the parameter $c$ for improved convergence. In Choi (2020), we propose to use the running minimum generated by the algorithm to tune $c$, while in Section 4.1 below, we study another method to tune $c$ by using the Hamiltonian function value of the proposed move. Note that for the Curie-Weiss model, in the second paragraph below Theorem 3.1 we have already explained how one can tune the parameter $c$ in that setting.

**4.1. Numerical illustrations.** Before we proceed to discuss the proofs of the main results above, we illustrate and compare the convergence performance of simulated annealing with landscape modification, that we call improved simulated annealing (ISA), against the classical simulated annealing algorithm (SA) on the famous travelling salesman problem (TSP). We first state the parameters that we used to generate the numerical results:

**TSP and its objective function.** 50 nodes are uniformly random on the grid $[0, 100] \times [0, 100]$. The objective is to find a configuration that minimize the total Euclidean distance with the same starting and ending point. Each node can only be visited once.

**Initial configuration.** Both ISA and SA have the same initialization. They are initialized using the output of the nearest-neighbour algorithm: a node is randomly chosen as the starting point, which is then connected to the closest unvisited node. It repeats until every node has been visited, and subsequently the last node is connected back to the starting node.
**Proposal chain.** Both ISA and SA share the same proposal chain: at each step, a proposal move is generated using the 2-OPT algorithm Croes (1958).

**Acceptance-rejection mechanism.** In SA, the proposed move is accepted with probability \( \min \{1, e^{\beta(H(x) - H(y))}\} \), while in ISA, the acceptance probability is computed as in Section 2.1. In other words, we use a linear \( f \) in ISA. Both SA and ISA share the same source of randomness.

**Cooling schedule.** Both ISA and SA use the same logarithmic cooling schedule of the form

\[
\epsilon_t = \frac{\sqrt{50}}{\ln(t + 1)}.
\]

**Choice of \( c \) in ISA.** In Choi (2020), we propose to tune the threshold parameter \( c \) by using the running minimum of the algorithm. In this paper, if we denote the proposal configuration at time \( t \) to be \( y_t \), we set \( c = c_t \) to be

\[
c_t = H(y_t) - 5.
\]

**Number of iterations.** We run both ISA and SA for 100,000 iterations.

We generate 1000 random TSP instances. For each instance we compute what we call the improvement percentage \( (IP) \) of ISA over SA, defined by

\[
IP := 100 \frac{\min_{t \in [0,100\,000]} H(X^0(t)) - \min_{t \in [0,100\,000]} H(X^f_{c_t}\epsilon t, c_t(t))}{\min_{t \in [0,100\,000]} H(X^0(t))}.
\]

The summary statistics of \( IP \) are provided in Table 1, while its histogram over these 1000 instances can be found in Figure 3. The code for reproducing these results can be found in https://github.com/mchchoi/Improved-discrete-simulated-annealing.

The summary statistics in Table 1 and the histogram in Figure 3 offer strong empirical evidence in using ISA over SA: out of the 1000 TSP instances, there are 798 instances in which the improvement percentage \( IP \) is non-negative. The sample mean of \( IP \) is approximately 1.87\% while its sample median is 1.47\%.

Next, we look into a particular instance and investigate the difference between SA and ISA in Figure 4. We see that SA (blue curve) is stuck at a local minimum, while ISA (orange curve) is able to escape the local minimum, owing to the increased acceptance probability compared with SA, and it reaches regions where the objective value is smaller than that of SA.

| Sample mean | 1.87\% |
|-------------|--------|
| Sample median | 1.47\% |
| Sample maximum | 11.35\% |
| Sample minimum | -9.21\% |
| Numbers of \( IP \geq 0 \) | 798 |
| Numbers of \( IP < 0 \) | 202 |

**Table 1.** Summary statistics of \( IP \) on 1000 random TSP instances
Figure 3. Histogram of improvement percentage of ISA over SA on 1000 randomly generated TSP instances

Figure 4. TSP objective value against iteration of ISA and SA

The rest of this section is devoted to the proofs of Theorem 4.1, Corollary 4.1, Lemma 4.1 and Theorem 4.2.
4.2. **Proof of Theorem 4.1.** First, using the classical result by Holley and Stroock (1988), it is immediate that

\[ C_2 e^{-\mathcal{H}_{\epsilon,c}^f} \leq \lambda_2(-M_{\epsilon,c}^f) \leq C_3 e^{-\mathcal{H}_{\epsilon,c}^f}. \]

For any arbitrary \(x_1, x_2 \in \{H(x_1) \geq H(x_2)\}\), we deduce the following upper bound:

\[
\mathcal{H}_{\epsilon,c}^f(x_1) - \mathcal{H}_{\epsilon,c}^f(x_2) = \int_{\mathcal{H}(x_1)}^\mathcal{H}(x_2) \frac{1}{f((u - c)_+ + \epsilon)} du = \begin{cases} \\
\beta(\mathcal{H}(x_1) - \mathcal{H}(x_2)), & \text{if } c \geq \mathcal{H}(x_1) > \mathcal{H}(x_2); \\
\beta(c - \mathcal{H}(x_2)) + \int_c^{\mathcal{H}(x_1)} \frac{1}{f(u - c)_+ + \epsilon} du, & \text{if } \mathcal{H}(x_1) > c \geq \mathcal{H}(x_2); \\
\int_{\mathcal{H}(x_2)}^\mathcal{H}(x_1) \frac{1}{f(u - c)_+ + \epsilon} du, & \text{if } \mathcal{H}(x_1) > \mathcal{H}(x_2) > c.
\end{cases}
\]

As a result, \(C_2^{-1} e^{\mathcal{H}_{\epsilon,c}^f} \leq e^{\beta c^*} C_1(\beta)\). On the other hand, we have the following lower bound:

\[
\mathcal{H}_{\epsilon,c}^f(x_1) - \mathcal{H}_{\epsilon,c}^f(x_2) \geq \begin{cases} \\
\beta(\mathcal{H}(x_1) \wedge c - \mathcal{H}(x_2) \wedge c), & \text{if } c \geq \mathcal{H}(x_1) > \mathcal{H}(x_2); \\
\beta(\mathcal{H}(x_1) \wedge c - \mathcal{H}(x_2) \wedge c), & \text{if } \mathcal{H}(x_1) > c \geq \mathcal{H}(x_2); \\
\frac{1}{\mathcal{H}(x_1) - c} (\mathcal{H}(x_1) - \mathcal{H}(x_2)), & \text{if } \mathcal{H}(x_1) > \mathcal{H}(x_2) > c,
\end{cases}
\]

and hence \(e^{\mathcal{H}_{\epsilon,c}^f} \geq e^{\beta c^*} C_4^{-1}\).

4.3. **Proof of Corollary 4.1.** We first prove item (1). For continuous-time reversible Markov chain, by (Levin and Peres, 2017, Theorem 12.5, 20.6) we bound the total variation mixing time by relaxation time via

\[
\frac{1}{\lambda_2(-M_{\epsilon,c}^f)} \log 2 \leq t_{\text{mix}}(M_{\epsilon,c}^f, 1/4) \leq \frac{1}{\lambda_2(-M_{\epsilon,c}^f)} \log \left( \frac{4}{\pi_{\text{min}}} \right),
\]

where \(\pi_{\text{min}} := \min_x \pi_{\epsilon,c}^f(x) = \frac{\mu(x^*)}{Z_{\epsilon,c}^f}\), for some \(x^* \in S_{\text{min}}\) and \(Z_{\epsilon,c}^f := \sum_{x \in X} e^{-\mathcal{H}_{\epsilon,c}^f(x)} \mu(x)\) is the normalization constant. Note that since \(\ln Z_{\epsilon,c}^f \to \ln \mu(S_{\text{min}})\) and so

\[
\lim_{\beta \to \infty} \frac{\ln Z_{\epsilon,c}^f}{\beta} = 0.
\]

Item (1) follows by collecting the above results together with Theorem 4.1.

Next, we prove item (2). First, using the random target lemma (Levin and Peres, 2017, Lemma 12.17), we have

\[
\pi_{\epsilon,c}(\eta) \mathbb{E}_\sigma(\tau_{\eta}^f) \leq \sum_{x \in X} \pi_{\epsilon,c}^f(x) \mathbb{E}_\sigma(\tau_{x}^f) \leq (|X| - 1) \frac{1}{\lambda_2(-M_{\epsilon,c}^f)}.
\]

Since \(\mathcal{H}(\eta) = 0\) and \(Z_{\epsilon,c}^f \leq 1\), upon rearranging and using Theorem 4.1 yields

\[
\lim_{\beta \to \infty} \frac{1}{\beta} \log \mathbb{E}_\sigma(\tau_{\eta}^f) \leq \lim_{\beta \to \infty} \frac{1}{\beta} \log \frac{1}{\lambda_2(-M_{\epsilon,c}^f)} = c^*.
\]
Define the equilibrium potential and capacity of the pair \((\sigma, \eta)\) as in (Bovier and den Hollander, 2015, Chapter 7.2) to be respectively
\[
h^f_{\sigma, \eta}(x) := P^x_{\tau_f^\sigma < \tau_f^\eta},
\]
\[
cap^{M_{\epsilon,c}}(\sigma, \eta) := \inf_{f : |A = 1, f|_B = 0} \langle -M_{\epsilon,c}f, f \rangle_{\pi_{\epsilon,c}^f} = \langle -M_{\epsilon,c}h^f_{\sigma, \eta}, h^f_{\sigma, \eta} \rangle_{\pi_{\epsilon,c}^f}.
\]
If we prove that
\[
(4.2) \quad \cap^{M_{\epsilon,c}}(\sigma, \eta) \leq \frac{1}{Z_{\epsilon,c}} \left( \sum_{x, y} \mu(x)Q(x, y) \right) e^{-\beta G^0(\sigma, \eta)},
\]
then together the mean hitting time formula with equilibrium potential and capacity leads to
\[
\mathbb{E}_\sigma(\tau_f^\eta) = 1 \cap^{M_{\epsilon,c}}(\sigma, \eta) \sum_{y \in X} \pi_{\epsilon,c}^f(y) h^f_{\sigma, \eta}(y) \geq \frac{1}{\cap^{M_{\epsilon,c}}(\sigma, \eta)} \sum_{y \in X} \pi_{\epsilon,c}^f(\sigma) h^f_{\sigma, \eta}(\sigma) \geq \frac{\mu(\sigma)}{\sum_{x, y} \mu(x)Q(x, y)} e^{\beta c^*},
\]
and the desired result follows since
\[
\liminf_{\beta \to \infty} \frac{1}{\beta} \log \mathbb{E}_\sigma(\tau_f^\eta) \geq c^*.
\]

It therefore remains to prove (4.2). Define
\[
\Phi(\sigma, \eta) := \{ x \in \mathcal{A} ; G^0(x, \sigma) \leq G^0(\sigma, \eta) \}.
\]
Writing \(1_A\) to be the indicator function of the set \(A\), the Dirichlet principle of capacity gives
\[
\cap^{M_{\epsilon,c}}(\sigma, \eta) \leq \langle -M_{\epsilon,c}1_{\Phi(\sigma, \eta)}, 1_{\Phi(\sigma, \eta)} \rangle_{\pi_{\epsilon,c}^f} = \frac{1}{Z_{\epsilon,c}} \sum_{x \in \Phi(\sigma, \eta) \lor H(y) \pi(x, y)} e^{-\beta(H(x) + H(y))} \mu(x)Q(x, y)
\leq \frac{1}{Z_{\epsilon,c}} \left( \sum_{x, y} \mu(x)Q(x, y) \right) e^{-\beta G^0(\sigma, \eta)}.
\]
where in the last inequality we use the fact that \(G^0(\sigma, \eta)\) is the lowest possible highest elevation between \(\sigma\) and \(\eta\).

4.4. Proof of Lemma 4.1. We first prove item (1). The lower bound is immediate, while the upper bound can be deduced via
\[
\epsilon_t \mathcal{H}_{t, \epsilon,c}^f \leq \epsilon_t \int_{\mathcal{H}\min} \frac{1}{\epsilon_t} du \leq M.
\]
Next, we prove item (2). We consider
\[
\frac{\partial}{\partial t} \epsilon_t \mathcal{H}_{t, \epsilon,c}^f(x) = \mathcal{H}_{t, \epsilon,c}^f(x) \left( \frac{\partial}{\partial t} \epsilon_t \right) + \epsilon_t \frac{\partial}{\partial t} \mathcal{H}_{t, \epsilon,c}^f(x)
= \mathcal{H}_{t, \epsilon,c}^f(x) \left( -c^* - \epsilon - \epsilon \frac{1}{(\ln(t+1))^2} - \epsilon \epsilon_t \int_{\mathcal{H}\min} \frac{1}{\epsilon_t} du \right).
\]
This leads to
\[
\left| \frac{\partial}{\partial t} \epsilon_t \mathcal{H}_{t, \epsilon,c}^f(x) \right| \leq \frac{2M}{(\ln(t+1))(t+1)}.
\]
Thirdly, we prove item (3), and using item (2) we calculate that
\[ \beta_t'M + \beta_t R_t \leq \frac{2M}{(c^* + \epsilon)(t + 1)} + \frac{2M}{(c^* + \epsilon)(1 + t)} = \frac{3M}{(c^* + \epsilon)(1 + t)}. \]

Finally, we prove item (4). Following exactly the same calculation as in the proof of (Löwe, 1996, Lemma 3.5), we see that
\[ \|g - \pi^f_{\epsilon t, c}(g)\|_{\ell^2(\pi^f_{\epsilon t, c})} \leq A(1 + \beta_t(\max H - c)) e^{\beta_t(c^* + \frac{p - 2}{p} \max H - c)} \langle -M^f_{\epsilon t, c} g, g \rangle_{\pi^f_{\epsilon t, c}}. \]

The desired result follows if we let
\[ \epsilon = \frac{M(p - 2)}{p} + \max H - c \]
so that
\[ p = \frac{2M}{M + \max H - \epsilon - c}. \]

4.5. **Proof of Theorem 4.2.** We would like to invoke the results in Löwe (1996) for time-dependent target function in simulated annealing. In Lemma 4.1 item (1), (2), (3) and (4), we verify that equation (11), (12) and Assumption (A1), (A2) respectively hold in Löwe (1996). Consequently, if we let
\[ h_t(y) := \mathbb{P}_x(X^f_{\epsilon t, c}(t) = y)/\pi^f_{\epsilon t, c}(y), \]
then according to (Holley and Stroock, 1988, Lemma 1.7), its \( \ell^2 \) norm is bounded by
\[ \|h_t\|_{\ell^2(\pi^f_{\epsilon t, c})} \leq 1 + K \frac{1}{\pi^f_{\epsilon t, c}} \]

for \( t \geq e^{1/\pi} - 1 \). The desired result follows from exactly the same argument as in (Löwe, 1996, Theorem 3.8).

Now, we calculate \( \pi^f_{\epsilon t, c}(X\setminus S_{\min}) \). For \( c \geq d \), we compute that
\[ \pi^f_{\epsilon t, c}(X\setminus S_{\min}) = \frac{\sum_{x \in X \setminus S_{\min}} e^{-\mathcal{H}^f_{\epsilon t, c}(x)} \mu(x)}{\sum_{x \in X} e^{-\mathcal{H}^f_{\epsilon t, c}(x)} \mu(x)} \]
\[ \leq \frac{\sum_{x: \mathcal{H}(x) \geq d} \mu(x)}{\sum_{x: \mathcal{H}(x) \leq d} \exp\{f^d_{\epsilon t} \frac{1}{\epsilon_t} du\} \mu(x)} \]
\[ \leq e^{-\beta_t(d - \mathcal{H}_{\min})} \frac{1}{\mu(S_{\min})}. \]

On the other hand, for \( \mathcal{H}_{\min} \leq c < d \),
\[ \pi^f_{\epsilon t, c}(X\setminus S_{\min}) = \frac{\sum_{x \in X \setminus S_{\min}} e^{-\mathcal{H}^f_{\epsilon t, c}(x)} \mu(x)}{\sum_{x \in X} e^{-\mathcal{H}^f_{\epsilon t, c}(x)} \mu(x)} \]
\[ \leq \frac{1}{\mu(S_{\min})} \exp\left\{ - \int_{\mathcal{H}_{\min}}^{d} \frac{1}{f((u - c)_+) + \epsilon_t} du \right\} \]
\[ \leq \frac{1}{\mu(S_{\min})} \exp\left\{ - \int_{c}^{d} \frac{1}{f(u - c) + \epsilon_t} du \right\}. \]
connections between landscape modification and …

In this section, we outline similarities and differences in idea between Metropolis-Hastings (MH) with landscape modification and other common acceleration techniques in the literature for MH and simulated annealing.

5.1. Catoni’s energy transformation algorithm. Let $\alpha_1 \geq 0, \alpha_2 \geq 0, \alpha_3 > -\mathcal{H}_{\min}$ be three parameters. In Catoni (1996, 1998), the author introduces the energy transformation algorithm by transforming the Hamiltonian $\mathcal{H}$ to

$$ F_{\alpha_1, \alpha_2, \alpha_3}(x) := \alpha_1 \mathcal{H}(x) + \alpha_2 \log (\mathcal{H}(x) + \alpha_3). $$

Recall that in Section 2.1, MH with landscape modification can be considered as a state-dependent version of energy transformation if we take $f(x) = x, \alpha_3 = -c + \epsilon$ and $\alpha_1, \alpha_2$ are chosen in a state-dependent manner:

$$ \alpha_1(x) = 1_{\{\mathcal{H}(x) \leq c\}}, \quad \alpha_2(x) = 1_{\{\mathcal{H}(x) > c\}}. $$

Note that MH with landscape modification can give rise to other kinds of energy transformation by different choices of $f$, see for example the quadratic case or the square root case in Section 2.2 and 2.3 respectively. Another remark is that the idea of mapping the function from $\mathcal{H}$ to $F(\mathcal{H})$ with $F$ being strictly increasing and concave can be dated back to R. Azencott.

5.2. preconditioning of the Hamiltonian. Landscape modification can be understood as a state-dependent preconditioning of the Hamiltonian $\mathcal{H}$. Recall that in (2.6) we compute the acceptance-rejection probability by

$$ \exp \left( \left( \mathcal{H}^f_{\epsilon,c}(y) - \mathcal{H}^f_{\epsilon,c}(x) \right) \right) = \begin{cases} 1, & \text{if } \mathcal{H}(y) \leq \mathcal{H}(x); \\ \exp \left( -\beta (\mathcal{H}(y) - \mathcal{H}(x)) \right), & \text{if } c \geq \mathcal{H}(y) > \mathcal{H}(x); \\ \exp \left( -\beta (\mathcal{H}(y) - \mathcal{H}(x)) - \int_{\epsilon}^{\mathcal{H}(y)} \frac{1}{f(u-c)+\epsilon} \, du \right), & \text{if } \mathcal{H}(y) > c \geq \mathcal{H}(x); \\ \exp \left( -\int_{\mathcal{H}(x)}^{\mathcal{H}(y)} \frac{1}{f(u-c)+\epsilon} \, du \right), & \text{if } \mathcal{H}(y) > \mathcal{H}(x) > c. \end{cases} $$

On the set $\{c \geq \mathcal{H}(y) > \mathcal{H}(x)\}$, the acceptance-rejection probability is the same as the original MH, while on the set $\{\mathcal{H}(y) > c \geq \mathcal{H}(x)\}$ and $\{\mathcal{H}(y) > \mathcal{H}(x) > c\}$, the acceptance-rejection probability is higher than that of the original MH. Therefore, there is a higher chance of moving to other states when the algorithm is above the threshold $c$.

5.3. importance sampling. In importance sampling, the target distribution is altered for possible benefits and speedups such as variance reduction. In landscape modification, the target distribution in MH is altered from the original Gibbs distribution $\pi^0(x) \propto e^{-\beta \mathcal{H}(x)}$ to $\pi^f_{\epsilon,c}(x) \propto e^{-\mathcal{H}^f_{\epsilon,c}(x)}$, while the set of stationary points is preserved in the sense that $\mathcal{H}$ and $\mathcal{H}^f_{\epsilon,c}$ share the same set of stationary points. In importance sampling however, the set of stationary points need not be preserved between the altered function and the original function.

5.4. quantum annealing. In quantum annealing Wang et al. (2016), given a target Hamiltonian $\mathcal{H}$ and an initial Hamiltonian $\mathcal{H}_{\text{init}}$ that is usually easy to optimize, we optimize a time-dependent function $Q_t$ defined by, for $t \in [0,T]$,

$$ Q_t(x) := A(t)\mathcal{H}_{\text{init}}(x) + B(t)\mathcal{H}(x), $$

where $A(t)$ and $B(t)$ are smooth annealing schedules that satisfy $A(T) = B(0) = 0$ and $T$ is the total annealing time. We also choose $A(t)$ to be decreasing and $B(t)$ to be increasing on the interval $[0,T]$. 
In simulated annealing with landscape modification, we also optimize a time-dependent function $H_{t,c}^f$ which shares the same set of stationary points as the target $H$. In quantum annealing, $H_{\text{init}}$ and $H$ do not necessarily share the same set of stationary points. We mention the work Del Moral and Miclo (1999); Frigerio and Grillo (1993); Löwe (1996) for simulated annealing with time-dependent energy function.

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