Simulation Bifurcation

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Combinatorial problems, such as Ising problems, are important while hard to solve. Here in this note I tried to review and summarize a heuristic solver called SB (Simulation Bifurcation). It is inspired by adiabatic evolution in quantum computing, but relies on a classical analog.

1 Quantum Harmonic Oscillator

The quantum harmonic oscillator, analogous to the classical harmonic oscillator, serves as a very important model in quantum mechanics. In this section I aim to briefly review its basics. Most of the contents below are from [6].

Given a Hamiltonian $H = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2$ of the system, define its energy eigenstates $\{|n\rangle\}$ as

$$H|n\rangle = E_n|n\rangle . \tag{1}$$

This tells us that $\{|n\rangle\}_{n=0}^{\infty}$ form an orthogonal basis.

Developed by Paul Dirac, the annihilation operator a and the creation operator $a^\dagger$ are defined as

$$\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle , \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle . \end{aligned} \tag{2}$$

Additionally they admit

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{\imath}{m\omega}\hat{p}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{\imath}{m\omega}\hat{p}\right), \tag{3}$$

where $\omega = \sqrt{k/m}$ is the angular frequency. One can represent the position and momentum using a and $a^\dagger$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a), \quad \hat{p} = \imath\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a). \tag{4}$$

It is worth noting that $a|0\rangle = 0 = 0|0\rangle$, indicating the state is completely annihilated. Thus the vacuum state $|0\rangle$ is defined to be the state with the lowest possible energy.

Firstly we need to discuss the eigenvalues of the annihilation/creation operator. Take $|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$, if it is an eigenvector of $a^\dagger$ with eigenvalue k,

$$a^\dagger|\psi\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n+1}\,|n+1\rangle = \sum_{n=1}^{\infty} c_{n-1}\sqrt{n}\,|n\rangle = \sum_{n=0}^{\infty} kc_n|n\rangle . \tag{5}$$

It is clear that $k \neq 0$. For other cases, $c_0 = 0$, and $c_{n-1}\sqrt{n} = kc_n$. This makes $a^\dagger$ has no eigenstates.

If $|\psi\rangle$ is an eigenstate of a,

$$a|\psi\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}\,|n\rangle = \sum_{n=0}^{\infty} kc_n|n\rangle . \tag{6}$$

This leads to $k = \frac{c_{n+1}\sqrt{n+1}}{c_n}$. We then take $c_n = \frac{k^n}{\sqrt{n!}}$. To normalize, one can apply the inverse of the following:

$$\sqrt{\sum_{n=0}^{\infty} \frac{(|k|^2)^n}{n!}} = e^{|k|^2/2}. \tag{7}$$

We then thus define the coherent states

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\alpha\rangle . \tag{8}$$

as the eigenvectors of the annihilation operator, i.e.

$$a |\alpha\rangle = \alpha |\alpha\rangle . \tag{9}$$

It is worth noting that $\{|\alpha\rangle\}$ also form a (overcomplete) basis.

We can also define the number operator $N := a^\dagger a$, which is positive semi-definite. Simple computation yields

$$N |n\rangle = a^\dagger a |n\rangle = \sqrt{n} a^\dagger |n-1\rangle = n |n\rangle . \tag{10}$$

2 Simulation Bifurcation and the Classical Mechanics

Example 1 (Hamiltonian from [1])**.** *Consider a Hamiltonian*

$$H = \hbar \frac{K}{2} (a^\dagger)^2 a^2 - \hbar \frac{p}{2} (a^2 + (a^\dagger)^2), \tag{11}$$

where a and $a^\dagger$ are the annihilation and creation operators for quanta of the oscillator, K and p are constants, its ground state are the coherent states $|\pm\sqrt{p/K}\rangle$.

Proof. An important observation [2] is that, in the sense of ignoring some constants.

$$H = \frac{\hbar K}{2} \left((a^\dagger)^2 - \frac{p}{K} \right) \left(a^2 - \frac{p}{K} \right). \tag{12}$$

It can be further observed that H is positive semi-definite, since $\left(a^2 - \frac{p}{K}\right)^\dagger = \left((a^\dagger)^2 - \frac{p}{K}\right)$. Take the coherent state $|\sqrt{p/K}\rangle$ or $|-\sqrt{p/K}\rangle$, we have

$$H |\pm\sqrt{p/K}\rangle = 0. \tag{13}$$

Thus $|\pm\sqrt{p/K}\rangle$ is the ground state of H. □

Example 2. *For Hamiltonian*

$$H = \hbar \Delta a^\dagger a + \hbar \frac{K}{2} (a^\dagger)^2 a^2 - \hbar \frac{p}{2} (a^2 + (a^\dagger)^2), \tag{14}$$

Notice that $[a, a^\dagger] = 1$ and ignoring some constants, it can be re-written as

$$\begin{aligned} H &\simeq \frac{\hbar K}{2} \left((a^\dagger)^2 - \frac{p-\Delta}{K} \right) \left(a^2 - \frac{p-\Delta}{K} \right) + \hbar \Delta a^\dagger a - \frac{\hbar \Delta}{2} (a^2 + (a^\dagger)^2) \\ &= \frac{\hbar K}{2} \left((a^\dagger)^2 - \frac{p-\Delta}{K} \right) \left(a^2 - \frac{p-\Delta}{K} \right) - \frac{\hbar \Delta}{2} (a^2 - 2a^\dagger a + (a^\dagger)^2) \\ &\simeq \frac{\hbar K}{2} \left((a^\dagger)^2 - \frac{p-\Delta}{K} \right) \left(a^2 - \frac{p-\Delta}{K} \right) - \frac{\hbar \Delta}{2} (a^2 - a^\dagger a - a a^\dagger + (a^\dagger)^2) \\ &= \frac{\hbar K}{2} \left((a^\dagger)^2 - \frac{p-\Delta}{K} \right) \left(a^2 - \frac{p-\Delta}{K} \right) - \frac{\hbar \Delta}{2} (a - (a^\dagger))^2. \end{aligned} \tag{15}$$

Notice that $(a - a^\dagger)$ is anti-Hermitian, indicating its eigenvalues are all imaginary. Thus $(a - a^\dagger)^2$ is negative semi-definite. Treat the detuning term $\hbar\Delta a^\dagger a$ as a perturbation [2], the ground state is $|\pm\sqrt{\frac{p-\Delta}{K}}\rangle$.

To understand the Hamiltonian in Equation 14 better, let us consider its classical analog. Set the expectation of a as $x + \imath y$, where x and y should be understood as location and momentum, we have

$$H^{\text{classical}} = \hbar\Delta(x^2 + y^2) + \frac{\hbar K}{2}(x^2 + y^2)^2 - (\hbar p)(x^2 - y^2), \tag{16}$$

and the dynamics follows

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{\partial H^{\text{classical}}}{\partial y} = 2\hbar\Delta y + 2\hbar K(x^2 + y^2)y + 2\hbar p y \simeq y(\Delta + p + K(x^2 + y^2)), \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= -\frac{\partial H^{\text{classical}}}{\partial x} = -2\hbar\Delta x + -2\hbar K(x^2 + y^2)x + 2\hbar p x \simeq x(-\Delta + p - K(x^2 + y^2)). \end{aligned} \tag{17}$$

When $p < \Delta$, the dynamics above only admits one equilibrium, i.e. $x = y = 0$. When $p \geq \Delta$, the stable fixed points are now $x = \pm\sqrt{(p - \Delta)/K}, y = 0$. This inspires us to leverage the bifurcation signs of x for combinatorial problems.

3 Simulation Bifurcation for Combinatorial Optimization

The Ising problem, formulated as minimizing the following energy:

$$E_{\text{Ising}} = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} J_{i,j} s_i s_j, \tag{18}$$

where the spins $\{s_i\}$ take ± 1.

Take the Hamiltonians $\{H_i\}$ as in Equation 14 and introduce a new parameter ξ_0, we can couple them as

$$\widetilde{H} = \sum_{i=1}^{N} H_i - \hbar\xi_0 \sum_{i=1}^{N}\sum_{j=1}^{N} J_{i,j}(a_i^\dagger a_j). \tag{19}$$

The parameter ξ_0 is set such that $\widetilde{H}$ is positive semi-definite, making the vacuum state still serve as the ground state when $p = 0$.

Denote $\alpha_S = \sqrt{(p - \Delta)/K}$, Example 2 tells us by increasing p slowly we finally will get state $|s\rangle = |s_1\alpha_S\rangle \cdots |s_N\alpha_S\rangle$, where $s_i = \pm 1$. And the corresponding energy is

$$\langle s|\, \widetilde{H} \,|s\rangle = \text{const} - \hbar\xi_0\alpha_S^2 \sum_{i,j=1}^{N} J_{i,j} s_i s_j. \tag{20}$$

Thus we expect the solution to the Ising problem is carried by the signs of the coherent states.

Again, if we consider the classical analog of $\widetilde{H}$,

$$\widetilde{H}^{\text{classical}} = \sum_{i=1}^{N} H_i^{\text{classical}} - \hbar\xi_0 \sum_{i,j=1}^{N} J_{i,j}(x_i x_j + y_i y_j). \tag{21}$$

Thus the dynamics is

$$\begin{aligned} \frac{\mathrm{d}x_i}{\mathrm{d}t} &= \frac{\partial \widetilde{H}^{\text{classical}}}{\partial y_i} \simeq y_i(\Delta + p + K(x_i^2 + y_i^2)) - \xi_0 \sum_{j=1}^{N} J_{i,j} y_j, \\ \frac{\mathrm{d}y_i}{\mathrm{d}t} &= -\frac{\partial \widetilde{H}^{\text{classical}}}{\partial x_i} \simeq x_i(-\Delta + p - K(x_i^2 + y_i^2)) + \xi_0 \sum_{j=1}^{N} J_{i,j} x_j. \end{aligned} \tag{22}$$

Remark 3. *If one believes that the dynamics driven by the Hamiltonian $\widetilde{H}^{classical}$ is capable of finding the minima, the signs of x_i provide the solution to the Ising problem.*

In order to get a faster (parallel) implementation, the above Hamiltonian inspires us to design

$$H_{\text{sb}} = \sum_{i=1}^{N} \frac{\Delta}{2} y_i^2 + V(x, t). \tag{23}$$

Here $V(x, t)$ should be designed that it contains the Ising energy and bifurcation.

A possible setting is given in [3]:

$$V(x, t) = \sum_{i=1}^{N} \left(\frac{K}{4} x_i^4 + \frac{\Delta - p(t)}{2} x_i^2 \right) - \frac{\xi_0}{2} \sum_{i,j=1}^{N} J_{i,j} x_i x_j. \tag{24}$$

When $p(t) \leq \Delta$, the first term $\sum_{i=1}^{N} \left(\frac{K}{4} x_i^4 + \frac{\Delta - p(t)}{2} x_i^2 \right)$ admits only one minima at $x_i = 0$. While $p(t) > \Delta$, it gets 2^N minimas at $x_i = \pm\sqrt{\frac{p(t)-\Delta}{K}}$.

Set $\{x_i\}$ and $\{y_i\}$ initially around zero, gradually increase $p(t)$, and the hope is that the dynamics has a high probability to go to the global minima, where the sign of x_i's represent the solution to the Ising problem. The updating rule is

$$\begin{aligned} \frac{\mathrm{d}x_i}{\mathrm{d}t} &= \Delta y_i, \\ \frac{\mathrm{d}y_i}{\mathrm{d}t} &= -x_i(K x_i^2 - p(t) + \Delta) + \xi_0 \sum_{j=1}^{N} J_{i,j} x_j. \end{aligned} \tag{25}$$

4 Improved Design of Potential Functions

To prevent analog errors, it is possible to introduce perfectly inelastic walls at $x_i = \pm 1$ [4]. Define

$$\begin{aligned} V_{\text{bSB}} &:= \sum_{i=1}^{N} \frac{\Delta - p(t)}{2} x_i^2 - \frac{\xi_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{i,j} x_i x_j, \quad \text{when } |x_i| \leq 1, \\ V_{\text{bSB}} &:= \infty, \quad \text{otherwise.} \end{aligned} \tag{26}$$

One can normalize part of the updating rule, introducing V_{dSB} [4]:

$$\begin{aligned} V_{\text{bSB}} &:= \sum_{i=1}^{N} \frac{\Delta - p(t)}{2} x_i^2 - \frac{\xi_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{i,j} x_i \operatorname{sign}(x_j), \quad \text{when } |x_i| \leq 1, \\ V_{\text{bSB}} &:= \infty, \quad \text{otherwise.} \end{aligned} \tag{27}$$

In [5], a thermal fluctuation is added. And the corresponding updating rule is

$$\begin{aligned} \frac{\mathrm{d}x_i}{\mathrm{d}t} &= \Delta y_i, \\ \frac{\mathrm{d}y_i}{\mathrm{d}t} &= -x_i(\Delta - p(t)) + c_0 f_i - \xi y_i, \\ \frac{\mathrm{d}\xi}{\mathrm{d}t} &= \frac{1}{M} \left(\sum_{i=1}^{N} y_i^2 - NT \right). \end{aligned} \tag{28}$$

Here M and $T = \sum_{i=1}^{N} y_i^2 / N$ are constants, and ξ is acting as thermal fluctuation.

References

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