Zero Temperature QMC

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Given a stoquastic Hamiltonian on n-qubits H, we define the operator W via

$$W = CI - H \tag{1}$$

where C is larger than than the diagonal element of H with the largest amplitude so that W has non-negative matrix elements. W is then interpreted as the transfer matrix of a classical spin chain on $n * L$ spins with partition function:

$$Z = \mathrm{Tr}[W^L] \tag{2}$$

and weight of configuration $\vec{s} = (s^1, ..., s^L)$ given by

$$w(\vec{s}) = \prod_{i=1}^{L} \langle s^i | W | s^{i+1} \rangle \tag{3}$$

The value of Z is approximately the largest eigenvalue of W raised to the power L. To see this expand W in it's eigenbasis $W = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$, where λ_i then:

$$\begin{aligned} W^L &= \sum_i \lambda_i^L |\lambda_i\rangle\langle\lambda_i| = \lambda_1^L \left(|\lambda_1\rangle\langle\lambda_1| + \sum_i \left(\frac{\lambda_i}{\lambda_1}\right)^L |\lambda_i\rangle\langle\lambda_i| \right) \\ &= \lambda_1^L |\lambda_1\rangle\langle\lambda_1| + O\left(\left(\frac{\lambda_2}{\lambda_1}\right)^L \right) \end{aligned} \tag{4}$$

Thus $\mathrm{Tr}[W^L] = \lambda_1^L + O\left(\left(\frac{\lambda_2}{\lambda_1}\right)^L\right)$. More importantly, as the eigenvectors of H and W are the same, with $|\lambda_1\rangle$ corresponding to the ground state of H, we can relate the probability of one of the copies in the classical system being in a certain configuration to the amplitude of the groundstate of H in that basis element.

$$\begin{aligned} \mathbf{P}(s^1 = \mu) &= \frac{\langle \mu | W^L | \mu \rangle}{\mathrm{Tr}[W^L]} \\ &= \frac{\lambda_1^L |\langle \mu | \lambda_1 \rangle|^2 + O\left(\left(\frac{\lambda_2}{\lambda_1}\right)^L\right)}{\lambda_1^L + O\left(\left(\frac{\lambda_2}{\lambda_1}\right)^L\right)} \\ &\approx |\langle \mu | \lambda_1 \rangle|^2 \end{aligned} \tag{5}$$

We will now describe a Markov chain that targets the steady state of the classical chain that is derived from the a Hamiltonian given by:

$$H = H_c + \Gamma \sum_i X_i \tag{6}$$

where H_c is a diagonal in the computational basis. Later we will also consider H_c as a map from a computational configuration s to the reals via:

$$H_c(s) = \langle s|H_c|s\rangle. \tag{7}$$

A standard Metropolis chain that selects a spin at random and flips it with probability given by Metropolis weights will be inefficient as any configuration that has neighboring replicas which differ in more than one coordinate has zero weight. Thus we will use a modified proposal distribution that only suggests moves that lead to non-zero weight configurations. Some care needs to be taken when formulation the Metropolis weights as this modified proposal distribution is non-symmetric.

To begin the analysis we state the general off diagonal Metropolis transition matrix for a non-symmetric proposal distribution M:

$$P(x, y) = \min\left\{1, \frac{\pi(y)M(y,x)}{\pi(x)M(x,y)}\right\} M(x, y) \tag{8}$$

The proposal distribution will pick a replica to update and then pick a spin to flip uniformly from the collection of spins that by flipping will lead to an allowed configuration. To illustrate two cases of this let's consider we picked a replica i to update. If the configuration of replica i, s^i is exactly the same as both of its neighbors s^{i-1} and s^{i+1}, then any spin can be flipped and the result will be an allowed configuration. Thus the full proposal distribution probability is

$$M(x, y) = \frac{1}{nL} \tag{9}$$

where $x = (s^1, ..., s^i, ..., s^L)$ and $y = (s^1, ..., s^{i\prime}, ..., s^L)$.

Now consider the case where $s^{i-1} = s^{i+1}$ and s^i differs in one coordinate, say q, from both of it's neighbors. Note that this is the type of configuration the previous transition leads to. With this in mind we will denote it as configuration y. Now flipping any spin but q would lead to a zero weight configuration, thus we can only flip spin q, which leads us back to the previous configuration x. This leads to the proposal distribution probability:

$$M(y, x) = \frac{1}{L} \tag{10}$$

Now to complete the computation of the stochastic matrix we need compute the steady state ratios $\pi(x)/\pi(y)$ and $\pi(y)/\pi(x)$. For diagonal elements we have $\langle s|W|s\rangle = C - H_c(s)$. For off diagonal elements s, s' differing in one coordinate we have $\langle s|W|s'\rangle = \Gamma$. Since the configurations x, y only differ in one replica the numerator and denominator of their ratios will only include products at most two matrix elements, namely the ones that connect configuration i to it's neighbors. Both of these elements will be Γ for configuration y and both will be $C - H_c(s^i)$ for the x configuration. Thus we have:

$$\frac{\pi(y)}{\pi(x)} = \frac{\Gamma^2}{(C - H_c(s^i))^2} \tag{11}$$

with $\pi(x)/\pi(y)$ the inverse of the above.

Plugging this into (8) we get

$$P(x, y) = \frac{1}{nL} \min\left\{1, \frac{n\Gamma^2}{(C - H_c(s^i))^2}\right\} \tag{12}$$

and

$$P(y, x) = \frac{1}{L} \min\left\{1, \frac{(C - H_c(s^i))^2}{n\Gamma^2}\right\} \tag{13}$$

Another class of transitions to consider is between x where $s^{i-1} = s^i \neq s^{i+1}$ and y where $s^{i-1} \neq s^{i\prime} = s^{i+1}$ where the disagreeing configurations disagree in coordinate q. In this case in either configuration we can only flip spin q so we do not need to consider the asymmetric Metropolis modifications and we straightforwardly get:

$$P(x, y) = \frac{1}{L} \min\left\{1, \frac{C - H_c(s^{i+1})}{C - H_c(s^{i-1})}\right\} \tag{14}$$

and

$$P(y, x) = \frac{1}{L} \min\left\{1, \frac{C - H_c(s^{i-1})}{C - H_c(s^{i+1})}\right\} \tag{15}$$

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The last case is given when $s^{i-1} \neq s^i \neq s^{i+1}$ and $s^{i-1} \neq s^{i+1}$. In this case the only available move is to flip both of spins in which s^i disagrees with its neighbors. This leads to a similar configuration with an identical weight and thus does not require Metropolis modifications and we have

$$P(x, y) = P(y, x) = \frac{1}{L} \tag{16}$$