Diffusion Monte Carlo Notes for Boulder Summer School 2010

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Diffusion Monte Carlo

The big idea: VMC is a useful technique, but often we want to sample observables of the true ground state Ψ_0 and not observables of the trial function Ψ_T. DMC is a method that allows us to accomplish this exactly for bosons and approximately for fermions.

We know that we can write

$$\Psi_0 = \lim_{\beta\to\infty} \exp[-\beta(H - E_0)]\Psi_T$$

If we could simply produce the matrix $\exp[-\tau H]$ and apply it M times on some vector Ψ_T we would decay to the true ground state. This is typically called the power method. Unfortunately, in many body systems, the matrix we would need to create is significantly too large. Instead we will stochastically apply this matrix. We have previously learned how to sample from the distribution Ψ_T (or Ψ_T^2). Schematically we will sample Ψ_0 by starting a bunch of "walkers" distributed from the distribution Ψ_T and then moving these walkers stochastically according to the "probability distribution" $\exp[-\tau H]$. After M steps (such that $\tau M = \beta$), the "new" distributions of the walkers will be distributed according to Ψ_0.

Once we have learned how to sample such distributions, we will then learn how to compute observables by computing integrals over these sampled distributions. Because there is a subtelty in DMC in computing properties that don't commute with the Hamiltonian, we will focus specifically on the energy in this lecture. Moreover, early on we will focus on computing properties of bosons. Later on in the lectures we will learn how to simulate fermionic systems approximately by disallowing certain configurations of the walkers. .

Let us start on our two tasks then:

1. Building algorithms to sample Ψ_0
2. Figuring out how to compute observables given that we've sampled Ψ_0

DMC Sampling I

Let's look at a specific example. Suppose we want to sample from Ψ_0 with a particle in a periodic 1d box with

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + h.c.$$

. We want to sample configurations c_{M+1} with probability sampled from the ground state $\Psi_0(c_{M+1})$. Our trial wave function guess from the ground state is $\Psi_T(c_0) = \frac{1}{N}\cos^2(c_0)$. Recalling that we wish to sample c_{M+1} with

$$Pr(c_{M+1}) = \langle \Psi_T | \exp(-\beta H) | c_{M+1} \rangle$$

we can rewrite our probability distribution as

$$Pr(c_{M+1}) = \left[\int \Psi_T(c_0) \langle c_0 | \exp[-\tau H] | c_1 \rangle ... \langle c_M | \exp[-\tau H] | c_{M+1} \rangle \prod_{i=}^{M} dc_i \right] / Z$$

where $Z = \left[\int \Psi_T(c_0) \langle c | \exp[-\tau H] | c_1 \rangle ... \langle c_M | \exp[-\tau H] | c_{M+1} \rangle \left(\prod_{i=}^{M} dc_i \right) dc_{M+1} \right]$
.

We will start this program by constructing a stochastic process that samples from this distribution. More generically let's write the distribution we want to sample from as

$$S(c_{M+1}) = \left(P(c_0) \int \prod_{i=0}^{N} P(c_i, c_{i+1}) dc_i \right) / Z$$

where we assume all the P are normalized probability distributions. In our case we let

$$P(c_i, c_{i+1}) \propto \langle c_i | (1 - \tau H) | c_{i+1} \rangle.$$

(In lattice systems we will often use the approximation $\exp[-\tau H] \approx (1 - \tau H)$.)

Notice that this probability distribution is very similar to the type of probability distributions we sample with Markov Chain Monte Carlo (but we will be using a different technique here).

Stocahstic Process to sample from S:

- Sample a walker at location c_0 with probability $P(c_0)$
- Have the walker hop from c_i to c_{i+1} with probability $P(c_i, c_{i+1})$.
- Continue to do this for M steps and then return the "location" of the walker.

The walker will be at "location" c_{M+1} with probability $S(c_{M+1})$. In practice, we should really think of starting 10,000 walkers in this way. At the end of the run, these 10,000 walkers will be distributed according to the distribution Ψ_0. Of course, one can simulate this stochastic process computationally.

A quick comment about what we mean by a "location": Although the locations c_1, c_2, c_3.. could consist of the location of a single particle (as in our example of a particle in a box), they could also of many particles, for example $c_1 = (x_1, x_2)$. Then we can think of our walker moving in a $3N$ dimensional space instead of a 3 dimensional space.

Thinking about the stochastic process induced by our example again, it should be noted that $P(c_i, c_{i+1})$ is really just a big matrix with non-zero "hopping" elements that either hops to the right, left or stays in the same location. In the long term limit, then, the particle will end up distributed uniformly at random in our periodic box. This is the ground statef for a single (bosonic) particles in a periodic 1d box.

DMC Sampling II

Suppose instead we wish to sample Ψ_0 from the hubbard model

$$H_2 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow} + h.c.$$

Suppose, we just model after what we had done before and write

$$P(c_i, c_{i+1}) = \langle x^i_1, x^i_2 | (1 - \tau H_2) | x^{i+1}_1, x^{i+1}_2 \rangle$$

There are a number of basic issues that we run into in this situation. To begin with, probabilities always have to be positive. The quantity $1 - \tau H_2$ could be negative though for sufficiently large values of U. We saw this in SSE as well and were able to treat it as a "easy" sign problem to remove by replacing $1 - \tau H \rightarrow \Lambda - \tau H$ where we choose a sufficiently large value of Λ that this is always positive. The second basic problem we have is that we need to be careful about the normalization. To care for this in an explicit way let's write

$$G(c_i, c_{i+1}) = \langle x^i_1, x^i_2 | (\Lambda - \tau H_2) | x^{i+1}_1, x^{i+1}_2 \rangle$$

and

$$w(c_i) = \sum_{c'} G(c_i, c'_{i+1})$$

where the sum is over all configurations c'_{i+1} that can be reached from configurations c_i with non-zero matrix elements. Then we can write

$$P(c_i, c_{i+1}) = G(c_i, c_{i+1}) / w(c_i)$$

This has the benefit of explicitly ensuring that P is a proper probability distribution. It does not come without a cost though. We wish to sample configuration

c_{M+1} with probability

$$Pr(c_{M+1}) = \left(P(c_0) \int \prod_{i=0}^{N} G(c_i, c_{i+1}) dc_i \right) /Z$$

which we should now rewrite as

$$Pr(c_{M+1}) = \left(P(c_0) \int \prod_{i=0}^{N} w(c_i) P(c_i, c_{i+1}) dc_i \right) /Z$$

The contributions of these additional weights w make our previous stochastic process no longer effective. Let us instead modify our previous process so that it can simulate with the new appropriate probabilities.

Stochastic Process including weights w

1. Sample 10,000 walkers at 10,000 locations selected from $P(c_0)$.
2. Assign walker α a weight $w_\alpha = 1$
3. Have each of the walkers hop M times according to the probability distribution $P(c_i, c_{i+1})$ and update their weight $w^\alpha \leftarrow w^\alpha w(c_i)$.
4. Return walkers sampled with probability $\frac{|w_\alpha|}{\sum_\alpha |w_\alpha|}$ (with replacement so you might sample the same walker multiple times and some walkers no times.)

Q. Why does this work?

The probability that we select a walker at position c_{M+1} is the probability that the walker is at configuration c_{M+1} times the probability that we choose it given that it is at configuration c_{M+1}. The former is essentially the product of the P's and the latter is the (properly normalized) products of the weights.

Notice, that this stochastic process introduces a slight bias. In the limit where the number of walkers are 1, the weights are ignored entirely. In the limit of an infinite number of walkers $Pr(c_{M+1})$ is sampled exactly. When computing integrals/observables with these samples there is a reasonably simple procedure to correct for this bias. In practice the bias is sufficiently small that the correction is rarely used and we will not discuss it more here.

We also shift $G(c, c)$ by a fixed constant to ensure the weights stay roughly constaint. i.e we let

$$G(c_i, c_{i+1}) = \langle .. | \Lambda - \tau(H - c) | ... \rangle$$

where we set $c = E_0$ (Because we don't know E_0 before the simulation, we choose an arbitrary c and then self consistently update it so as to converge on the value E_0.

Quantum Monte Carlo in your head

Let's just think about some simple example:

Imagine having a single particle with open boundary conditions but with large potential barriers that make it look like it is in a finite box. In other words, we are going to solve the particle in a box problem without telling the stochastic process explicitly that it is working with a particle in a box.

In this example, in the limit of a large box and large potential barriers $E_0 \approx -2t$. If we want to choose Λ to keep values always positive, then we should take $\Lambda = \tau V + 2\tau t$. There are four possible scenarios:

- Inside the box with all hopping inside the box. Then
  $Pr(hop\,left) \propto \tau t$
  $Pr(hop\,right) \propto \tau t$
  $Pr(not\,move) \propto \Lambda + \tau E_0 - \tau(0) = \Lambda + \tau E_0 = \tau V$
  $w = 2\tau t + \Lambda + \tau E_0 = \tau V + 2\tau t$

- Outside the box with all hopping outside the box: Then
  $Pr(hop\,left) \propto \tau t$
  $Pr(hop\,right) \propto \tau t$
  $Pr(not\,move) \propto \Lambda + \tau E_0 - \tau(V) = \Lambda + \tau(E_0 - V) = \tau V + 2t\tau + \tau(-2t - V) = 0$
  $w = 2\tau t$

- Inside the box with one hop possibly outside
  $Pr(hop\,left) \propto \tau t$
  $Pr(hop\,right) \propto \tau t$
  $Pr(not\,move) \propto \Lambda + \tau E_0 - \tau(V) = \Lambda + \tau E_0$
  $w = 2\tau t + \Lambda + \tau E_0$

- Outside the box with one hop possibly outside
  $Pr(hop\,left) \propto \tau t$
  $Pr(hop\,right) \propto \tau t$
  $Pr(not\,move) \propto \Lambda + \tau E_0 - \tau(V) = \Lambda + \tau(E_0 - V)$
  $w = 2\tau t + \Lambda + \tau(E_0 - V)$

Notice what's going on here. First let us look at the probabilities of moving around. No matter where you are there is an equal probability of moving left or right and some fixed probability of staying where you are. The probability of staying where you are depends if you are inside or outside the box. If you are outside the box it is much less likely to stay in the same place then if you are inside the box. Now, let's look at the weights. There is a weight that you are accumulating if you are inside the box and a weight that you are accumulating if you are outside the box. Since V is taken to be large (and the weights are only defined up to an arbitrary multiplicative factor), any weight that you are accumulating while outside the box is much smaller (let's call it nearly 0). Therefore, in this example, we are essentially measuring the following process:

Particles hop around. If they leave the box then they are no longer counted. What is the stationary distribution for this configuration?

A comment on Branching

It turns out that carrying around these weights causes some trouble. We resolve this problem in a simple way. At each step we take a walker of weight w and split the walker up into w walkers each of weight 1. (in the case where part of the weight is a fraction f we keep this walker with probability f and destroy it with probability $(1-f)$.

Observables:

Now we'd like to learn how to compute the energy E_0 of our system. We start by assuming that we now have effective methods to sample configurations c with probability $\Psi_0(c)$. Therefore we would like to phrase our energy as

$$\frac{\int \Psi_0(c) O(c;\Psi_T)\, dc}{\int \Psi_0(c)\, dc}$$

We need to do a little work to massage the integral into this form. We start by writing

$$\langle E\rangle = \frac{\langle \Psi_T| \exp[-\beta H/2] H \exp[-\beta H/2] |\Psi_T\rangle}{\langle \Psi_T| \exp[-\beta H/2] \exp[-\beta H/2] |\Psi_T\rangle}$$

Because the Hamiltonian commutes with $\exp[-\beta H]$ we can rewrite this as

$$\langle E\rangle = \frac{\int \Psi_0(c)\Psi_T(c) \frac{[H\Psi_T](c)}{\Psi_T(c)}\, dc}{\int \Psi_T(c)\Psi_0(c)\, dc}$$

Note, that to massage this integral into the form we need it we write,

$$\begin{aligned} A &= \frac{\int \Psi_0(c)\Psi_T(c) E_L(c)\, dc}{\int \Psi_0(c)\, dc} \\ B &= \frac{\int \Psi_0(c)\Psi_T(c)\, dc}{\int \Psi_0(c)\, dc} \\ A/B &= E_0 \end{aligned}$$

Now, A and B can be computed through the describe process by taking the average of $\langle \Psi_T(c) E_L(c)\rangle$ and $\langle \Psi_T(c)\rangle$ respectively.

Importance Sampling

We should notice that the variance of these quantities is unfortunately large even in the limit where $\Psi_T = \Psi_0$. The quantities A and B have (large) sample

by sample fluctuations. Imagine instead, though, that we were able to sample from the distribution

$$\Psi_T \Psi_0$$

instead of just the distribution Ψ_0. If we could do this, then our integral

$$\langle E \rangle = \frac{\int \Psi_0(c)\Psi_T(c)\frac{[H\Psi_T](c)}{\Psi_T(c)}\,dc}{\int \Psi_T(c)\Psi_0(c)\,dc}$$

could be computed by just averaging $\langle E_L \rangle$. Recall that the variance of E_L is 0 in the limit where $\Psi_0 = \Psi_T$. This would therefore give us a much more effecient algorithm. To accomplish this, let's write our distribution as

$$\langle \Psi_T | \exp(-\beta H) | c_{M+1} \rangle \langle \Psi_T | c_{M+1} \rangle$$

which we can expand as

$$\begin{array}{c} \langle \Psi_T | c_0 \rangle \langle c_0 | \exp[-\tau H] | c_1 \rangle ... \langle c_M | \exp[-\tau H] | c_{M+1} \rangle \quad \times \\ \langle \Psi_T | c_0 \rangle \frac{\langle \Psi_T | c_1 \rangle}{\langle \Psi_T | c_0 \rangle} \frac{\langle \Psi_T | c_2 \rangle}{\langle \Psi_T | c_1 \rangle} ... \frac{\langle \Psi_T | c_{M+1} \rangle}{\langle \Psi_T | c_M \rangle} \end{array}$$

We note that in order to change our stochastic process to accomplish this, we need to change two things:

- Instead of sampling c_0 with the probability $\Psi_T(c_0)$, sample c_0 with probability $|\Psi_T(c_0)|^2$.
- Change the values of $G(c_i, c_{i+1})$ to be

$$G(c_i, c_{i+1}) = \langle c_i | (1 - \tau H) | c_{i+1} \rangle \frac{\Psi_T(c_{i+1})}{\Psi_T(c_i)}$$

We can also show that this new distribution helps us spend time sampling more important areas of our wave function. Examine how our modification of g changes the hopping matrix of our walker in our "particle in a finite box" example. If we happen to have chosen $\Psi_T = \Psi_0$ then the probability that the walker hops outside our box is proporitional to $\Psi(outside)/\Psi_0(inside) \approx 0$. Therefore, we don't waste our time evaluating anything outside the box.

Sign Problem

So far we have mainly talked about simulating bosons. Instead suppose we wanted to simulate fermions. To begin with, we should recall that we are working in first quantized notation, so the Hamiltonian for both the bosons and fermions are identical. Consequently, our formula,

$$\langle \Psi_T | \exp(-\beta H) \rangle$$

will always give us the bosonic ground state assuming Ψ_T has some overlap with this ground state. Notice, though, if we choose a fermionic Ψ_T then it will be antisymmetric. An antisymmetric function will not have any overlap with the symmetric bosonic ground state and therefore will decay to the lowest antisymmetric ground state: i.e. the fermionic answer. This tells us that we have to choose a fermionic Ψ_T as our trial wave function.

Recall though that our stochastic process involved sampling with a probability proportional

$$\propto \frac{\Psi_T(c')}{\Psi_T(c)}\langle c|H|c'\rangle$$

This means that any two elements in the hamiltonian that connect pieces of the wave-function of different signs is going to cause problems (because we can't sample a negative probability). Notice that these configurations are on the node of the wave-function.

Let us define a node to be a configuration such that

$$\Psi_T(c) \equiv \Psi_T(r_1, r_2 ... r_n) = 0$$

. We note that in any fermionic wave function, there must be nodes. We can see this because as we swap two electrons by moving them around each other the wave function $\Psi_T \rightarrow -\Psi_T$. Since the sign of the wavefunction changes, this means that at some point during the move of the electrons, the value of $\Psi_T = 0$.

We consequently know that we must change our stochastic process so that we are again sampling positive probabilities. The following modifications need to be made:

- Let $g(c_i, c_{i+1}) = \left|\langle c_i|H|c_{i+1}\rangle \frac{\Psi_T(c_{i+1})}{\Psi_T(c_i)}\right|$
- For each walker, have not only a weight w^α but also a sign s^α which is initialized to the sign of the starting configuration of each walker: $sign(\Psi_T(c_0))$. Whenever a walker is moving from $c_i \rightarrow c_{i+1}$ update the sign of the walker

$$s^\alpha \leftarrow s^\alpha sign\left(\langle c_i|H|c_{i+1}\rangle \frac{\Psi_T(c_{i+1})}{\Psi_T(c_i)}\right)$$

- When computing integrals over the walkers, ensure that the observable O is multiplied by the sign of the walker s^α. (i.e, the average energy would be

$$\sum_{\alpha \in Walkers} \frac{s^\alpha [H\Psi_T](c^\alpha_{M+1})}{\Psi_T(c^\alpha_{M+1})}$$

We can see how this would introduce a sign problem that would cause the variance of your energy to become exponentially large with system size. Notice the fundamental problem here is that there exist configurations c and c' that one hops between for which $s(c, c')$ is negative. For $s(c, c')$ to be negative we have to hop over a node. Therefore, it is the hopping from one node to another that causes the sign problem in this algorithm.

Fixed Node

Because the sign problem prevents us from simulating large systems in a reasonable period of time, we want to make an additional approximation to our fermionic systems that gives us (approximate) answers that scale well. The big picture is the following. The nodes of the true ground state partition the system into a series of nodal bubbles. If we know exactly where the nodes are then we can solve the problem inside each of these bubbles. Inside each of these bubbles there are no nodes. Consequently, we are essentially solving a bosonic problem inside the bubble. But we have good algorithms (DMC) to solve bosonic problems. (Pretend for example that we have a new Hamiltonian that has an infinite potential barrier at the location of the nodes). Of course, we don't happen to know the actual nodal surface. Therefore, we will make a guess for the nodal surface and then get the best answer we can with respect to this guess. One way we can think about this is that we've separated the hard part of doing fermions (getting the nodes) from the easy part of doing fermions (everything else).

Q: Is this just another variational approach?

Yes and no. It's variational with respect to the nodes. But, we should note that it's possible to simulate systems whose wave functions don't have a compact representation. This is pretty remarkable. Our intuition, coming from say DMRG and PEPS and VMC, is that systems with wave functions that are compactly representable are easier to simulate then those that don't have such representations. But fixed node challenges this intuition.

Fixed Node on a Lattice

We will now formally specify how we implement the above idea in a lattice as well as prove some important properties of this.

Let us call a pair of configurations $[c, c']$ sign-violating (sv) if

$$\Psi_T(c)\,\Psi_T^*(c')\,\langle c|H|c'\rangle > 0$$

Recall that having sign violating configurations are those that induce a sign problem (i.e. hop over a node). This was because we are sampling with a probability proportional to $-\tau\langle c|H|c'\rangle\frac{\Psi_T(c)}{\Psi_T(c')}$ and will have to tack on this sign to the weight of the configuration.

We will define a new Hamiltonian (which is a function of Ψ_T) as

$$\langle c|H_{eff}|c'\rangle = \begin{cases} 0 & if\ \Psi_T(c)\Psi_T(c')\langle c|H|c'\rangle < 0 \\ \langle c|H|c'\rangle & otherwise \end{cases}$$

$$\langle c|H_{eff}|c\rangle = \langle c|H|c\rangle + \sum_{c'\,s.t.[c,c']\in s.v.} \langle c|H|c'\rangle\frac{\Psi_T(c')}{\Psi_T(c)}$$

Now we we wish to argue four things:

1. Simulating this Hamiltonian has no sign problem
   This is easy to see. By construction none of the off-diagonal terms are positive. We never hop over a node! All hops from configurations $c \rightarrow c'$ give a positive value.

2. This Hamiltonian gives a higher energy in the case when $\Psi_T \neq \Psi_0$.
   Although not strictly required, this is a desirable feature.

3. This Hamiltonian gives the correct energy in the case when $\Psi_T = \Psi_0$

4. What are the minimum requirements for our Hamiltonian so as to get the correct energy.

We start by showing (2)

To do this we will take the difference between

$$\begin{aligned}
\Delta E_0 &= \langle\Psi|[H_{eff} - H|\Psi\rangle \\
&= \sum_c \Psi^*(c) \left[\sum_{c' s.t. [c,c'] \in s.v.} \langle c|H|c'\rangle \frac{\Psi_T(c')}{\Psi_T(c)} \Psi(c) - \sum_{c' s.t. [c,c'] \in s.v.} \Psi(c') \langle c|H|c'\rangle \right] \\
&= \sum_{[c,c'] \in s.v.} \langle c|H|c'\rangle \left[|\Psi(c)|^2 \frac{\Psi_T(c')}{\Psi_T(c)} + |\Psi(c')|^2 \frac{\Psi_T(c)}{\Psi_T(c')} - \Psi^*(c)\Psi(c') - \Psi^*(c')\Psi(c) \right] \\
&= \sum_{[c,c] \in s.v.} |\langle c|H|c'\rangle| \left| \Psi(c) \sqrt{\left| \frac{\Psi_T(c')}{\Psi_T(c)} \right|} - s(c,c')\Psi(c') \sqrt{\left| \frac{\Psi_T(c)}{\Psi_T(c')} \right|} \right|^2 \\
&\geq 0
\end{aligned}$$

Now, let us look at the situation where $\Psi_T = \Psi_0$.

Then we have that $\Delta E = \sum_{[c,c] \in s.v.} |\langle c|H|c'\rangle| \left| \Psi_0(c) \sqrt{\left| \frac{\Psi_0(c')}{\Psi_0(c)} \right|} - s(c,c')\Psi_0(c') \sqrt{\left| \frac{\Psi_0(c)}{\Psi_0(c')} \right|} \right|^2$.
We notice that this is equal to 0 as long as $s(c,c')\Psi_0(c')\Psi_0(c) > 0$ for all sign violating configurations. But this is the definition for a configuration to be sign violating. Therefore we have verified that in the limit where we have the correct wave function, we are guaranteed to get the correct energy.

Finally, let us try to figure out what are the minimum requirements for $\Delta E = 0$ for any configuration c. This means that for any sign violating configuration,

$$\Psi(c) \sqrt{\left| \frac{\Psi_T(c')}{\Psi_T(c)} \right|} - s(c,c')\Psi(c') \sqrt{\left| \frac{\Psi_T(c)}{\Psi_T(c')} \right|} = 0$$

or equivalently for any sign violating configuration

$$\frac{\Psi(c)}{\Psi(c')} = s(c,c') \left| \frac{\Psi_T(c)}{\Psi_T(c')} \right|$$

Moreover note for sign violating configurations that the two cases below

- $s(c,c') > 0$ and $sign(\Psi_T(c)) = sign(\Psi_T(c'))$ so that $\left|\frac{\Psi_T(c)}{\Psi_T(c')}\right| s(c,c') = \frac{\Psi_T(c)}{\Psi_T(c')}$
- $s(c,c') < 0$ and $sign(\Psi_T(c)) \neq sign(\Psi_T(c'))$. Then $\left|\frac{\Psi_T(c)}{\Psi_T(c')}\right| s(c,c') = \frac{\Psi_T(c)}{\Psi_T(c')}$

imply that

$$\left|\frac{\Psi_T(c)}{\Psi_T(c')}\right| = \frac{\Psi_T(c)}{\Psi_T(c')}$$

One can then see that the requirement for any wave function to get the correct energy is that:

- For any sign violating configurations, $\Psi_T(c)/\Psi_T(c') = \Psi_0(c)/\Psi_0(c')$

Connection to the continuum

How can we make a connection between this and the continuum situation. Let us consider the case where the off diagonal term of the Hamiltonian is always negative (i.e. the typical kinetic energy). Then, sign violating terms are those where the wave function changes (i.e. you walk over a node). What is actually important then for getting the correct energy:

1. You've determined the sign violating terms. This means that you have the nodes correct (i.e. you know when you go from $c \to c'$ that you have walked over a node.
2. On the sign violating terms, you get the magnitudes correct. This means that if you are essentially sitting right on the edge of a node, you get the magnitudes correct. Essentially this means that you are doing a linear extrapolation to identify the location of the node. In the continuum, this latter case is not relevant. Since the paths on which you are hopping are formally continuous, there is never a situation where you cross a node in a single hop.