Outline

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Simple Example

Consider two coupled 3D Harmonic Oscillators offset in energy.

$$H = -\nabla^2 + \begin{bmatrix} r^2 & z \\ z & 1 + r^2 \end{bmatrix}$$

Take a trial wavefunction of the form:

$$\Psi_T = \begin{bmatrix} \exp(-r^2/2) \\ 0.4\ z\ \exp(-r^2/2) \end{bmatrix}$$

Note: wrong (higher-energy) sign for the asymmetric component.

VMC algorithm

- Use Metropolis to sample points from $\langle \Psi_T^\dagger \Psi_T \rangle = (1 + 0.4^2 z^2) \exp(-r^2)$
- For each point set relative amplitudes in state 1 and 2 to $\phi(\mathbf{R}) = (\exp(-r^2/2), 0.4z \exp(-r^2/2))$
- Calculate the local kinetic energy:

$$\langle T \rangle = \frac{(\exp(-r^2/2) \quad 0.4z \exp(-r^2/2)) \begin{pmatrix} -\nabla^2 & 0 \\ 0 & -\nabla^2 \end{pmatrix} \begin{pmatrix} \exp(-r^2/2) \\ 0.4z \exp(-r^2/2) \end{pmatrix}}{(1 + 0.4^2 z^2) \exp[-r^2]}$$

Local Potential Energy

The local potential energy is:

$$\langle V \rangle = \frac{\begin{pmatrix} \exp(-r^2/2) & 0.4z\exp(-r^2) \end{pmatrix} \begin{pmatrix} r^2 & z \\ z & 1+r^2 \end{pmatrix} \begin{pmatrix} \exp(-r^2/2) \\ 0.4z\exp(-r^2/2) \end{pmatrix}}{(1+0.4^2z^2)\exp[-r^2]}$$

- Average local kinetic and potential energies over all points

DMC Algorithm: No Importance Sampling

1. Start with configurations from VMC (w/ amplitudes from Ψ_T on left and right.
2. Call right-hand wvfn as $\Psi(\tau = 0)$, Left hand wvfn is Ψ_T.
3. For each configuration diffuse to a new point $\mathbf{R}'$ with gaussian.
4. Operate by $1 - V\delta\tau$ on the right hand wvfn $\Psi(\tau)$ to get $\Psi(\tau + \delta\tau)$:

$$1 - V\delta\tau = \begin{bmatrix} 1 - \delta\tau r^2 & -\delta\tau z \\ -\delta\tau z & 1 - \delta\tau(1 + r^2) \end{bmatrix}$$

5. Calculate overlap of $\Psi_T(\mathbf{R}')$ and $\Psi(\tau + \delta\tau)$
6. Calculate new weight from new overlap divided by old overlap
7. proceed as in 'normal' DMC with branching and evaluating local energy

DMC Algorithm: Importance Sampling w/ drift

This is only an example

1. Assume the guiding function is simple (one or a few channels) and has a (simple) real overlap with Ψ_T
2. Otherwise choose a positive real function of this overlap for the guiding function
3. Start with configurations from VMC but drawn from $\langle \Psi_G^\dagger(\mathbf{R})\Psi(\mathbf{R}\rangle^{1/2}$
4. For each configuration diffuse to a new point $\mathbf{R}'$ with a shifted gaussian determined by the overlap of Ψ_G with $\Psi(\tau)$.
5. Operate by $1 - V\delta\tau$ on the wvfn $\Psi(\tau)$ to get $\Psi(\tau + \delta\tau)$:
6. Calculate overlap of $\langle \Psi_G(\mathbf{R}')|\Psi_T(\mathbf{R}'\rangle$ and $\langle \Psi_G(\mathbf{R})|\Psi_T(\mathbf{R}\rangle$
7. Calculate new weight from the ratio of these two overlaps
8. Proceed as in 'normal' DMC with branching and evaluating local energy

Local energy with importance sampling

- The local energy is now given by:

$$\langle H \rangle = \frac{\frac{\langle \Psi_T | H | \Psi(\tau) \rangle}{\langle \Psi_G | \Psi(\tau) \rangle}}{\frac{\langle \Psi_T | \Psi(\tau) \rangle}{\langle \Psi_G | \Psi(\tau) \rangle}}$$

Alternative (plus/minus) importance sampling

The above still requires you to calculate the gradient of the overlap of the guiding wave function and $|\Psi(\tau)\rangle$.

To avoid this, go back to the no importance sampling case.

- For each walker, calculate two new (+/-) possible positions:

$$\begin{aligned} \mathbf{R}'_1 &= \mathbf{R} + \delta\mathbf{R}, \\ \mathbf{R}'_2 &= \mathbf{R} - \delta\mathbf{R} \end{aligned}$$

- $\delta\mathbf{R}$ is chosen from the gaussian as normal, but is the same in the two cases (up to a sign).
- Calculate the new wave functions and overlaps at the two new possible points: $W_{1,2} = \langle \Psi_G(\mathbf{R}'_{\mathbf{1,2}}) | \Psi(\tau + \delta\tau)_{1,2} \rangle$
- Choose between point one with probability $W_1/(W_1 + W_2)$, otherwise choose point two.
- Assign a weight based on the ratio of the average of the two new points to the old point: $(W_1 + W_2)/(2\langle \Psi_G(\mathbf{R})\Psi(\tau) \rangle$
- Calculate observables as before with importance functions

Convergence of Toy Problem

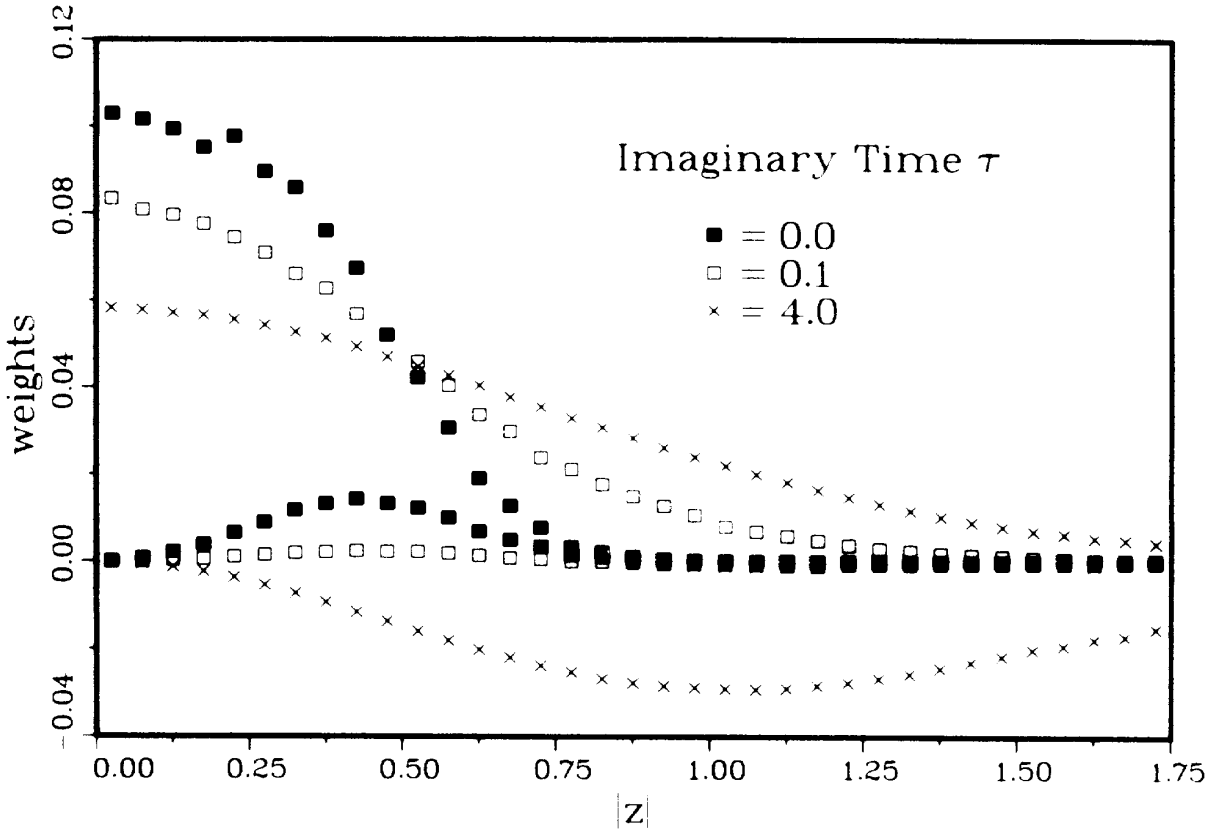

TABLE I. Coupled harmonic oscillators.

τ	Energy	Weight (1)	Weight (2)
0.0	3.101±0.005	0.990	+0.001
0.1	3.044±0.006	1.022	−0.022
0.2	2.972±0.006	1.039	−0.039
4.0	2.830±0.009	1.075	−0.075
Exact	2.829		

Alpha Particle with Minnesota Interaction

The same as the simple example but with bigger matrices. The kinetic energy is still diagonal.

For the potential energy we can diagonalize the matrix:

$$V = V^c(r) + V^\sigma(r)\sigma\cdot\sigma + V^\tau(r)\tau\cdot\tau + V^{\sigma\tau}(r)\sigma\cdot\sigma\tau\cdot\tau \qquad (1)$$

Reproject into (S,T) = (0,0), (0,1), (1,0), and (1,1) channels:

$$\begin{aligned} V(S=0,T=0) &= V^c - 3V^\sigma - 3V^\tau + 9V^{\sigma\tau} \\ V(S=0,T=1) &= V^c - 3V^\sigma + 1V^\tau - 3V^{\sigma\tau} \\ V(S=1,T=0) &= V^c + 1V^\sigma - 3V^\tau - 3V^{\sigma\tau} \\ V(S=1,T=1) &= V^c + 1V^\sigma + 1V^\tau + 1V^{\sigma\tau} \end{aligned} \qquad (2)$$

Exponentiate in each channel since the potential is diagonal there.:

Exponentiating the Potential

Rewrite exponentiated potential in operator form using

$$P(S=1) = (3+\sigma\cdot\sigma)/4$$
$$P(S=0) = (1-\sigma\cdot\sigma)/4$$

$$\begin{aligned}
\exp(-V\delta\tau) &= \exp(-V(S=0,T=0)\delta\tau)[1-\sigma\cdot\sigma][1-\tau\cdot\tau]/16 \\
&+ \exp(-V(S=0,T=1)\delta\tau)[1-\sigma\cdot\sigma][3+\tau\cdot\tau]/16 \\
&+ \exp(-V(S=1,T=0)\delta\tau)[3+\sigma\cdot\sigma][1-\tau\cdot\tau]/16 \\
&+ \exp(-V(S=1,T=1)\delta\tau)[3+\sigma\cdot\sigma][3+\tau\cdot\tau]/16
\end{aligned}$$

Note this is only for one pair, we calculate $\exp[-V_{ij}\delta\tau/2]$ for one pair at a time (with random order).

Calculating the propagation

1. Start with a left-hand trial wave function $\Psi_T(\mathbf{R})$, a propagated wave function $\Psi(\tau)(\mathbf{R})$, and a positive definite function used to guide the solution $W_0 = W(\Psi_T, \Psi(\tau))$
2. Compute a new partially propagated wave function by calculating $\Psi' = \exp(-V(\mathbf{R})\delta\tau/2]\Psi(\tau)$
3. Compute two new moves by sampling a gaussian, and taking the minus displacement: $R'_1 = R - \delta R, R'_2 = R + \delta R$.
4. Compute the propagation to the new final states
   $\Psi'_1 = [\exp(-V(\mathbf{R'_1})\delta\tau/2]\Psi'$
   $\Psi'_2 = [\exp(-V(\mathbf{R'_2})\delta\tau/2]\Psi'$

Calculating the propagation, continued

5. Compute the trial function at the new positions $\Psi_T(R_1')$ and $\Psi_T(R_1')$
6. Compute the two possible functions $W_1 = W(\Psi_T(R_1'), \Psi_1')$ and $W_2 = W(\Psi_T(R_2'), \Psi_2')$
7. pick point 1 with probability $W_1/(W_1 + W_2)$ otherwise pick point 2
8. Use the function $W' = (W_1 + W_2)/(2W_0)$ to generate the weight for the new point.
9. Set the new wave function $\Psi(\tau + \delta\tau) = \Psi_1'$ or Ψ_2', respectively, and the new trial function to $\Psi_T(R_1')$ or $\Psi_T(R_2')$.
10. Go to step 2 and repeat, with branching and expectation values.

Contrained path and transient estimation

If we let the propagation go indefinitely, it may have a sign problem.

Constrained Path

We can do a constrained path simulation by:

- for Real overlaps: deleting the walker when the overlap $\langle \Psi_T(\mathbf{R})\Psi(\tau)\rangle \leq 0$ (similar to fixed node).
- for Complex overlaps: project the new $\langle \Psi'(\tau)\rangle$ down to the axis of real overlap with Ψ_T:

$$\Psi'(\tau) \leftarrow \gamma \exp[i\phi]\Psi(\tau)$$
$$Re\ \Psi_T\Psi'(\tau) = Re\ \Psi_T\Psi(\tau)$$
$$Im\ \Psi_T\Psi'(\tau) = 0$$

For a real (scalar) wave functions, this correspond to fixed node.

For a single complex wave function, this correspond to fixed phase.

They are not upper bounds; there are corresponding simulations with auxiliary field. Exact for exact trial function.

Expectation Values

Expectation values of an operator can be estimated from:

$$\langle O \rangle = \frac{\sum_i \langle \Psi_T(\mathbf{R}_i)|O|\Psi(\tau)\rangle / W_i}{\sum_i \langle \Psi_T(\mathbf{R}_i)|\Psi(\tau)\rangle / W_i}$$