Tickling the Monte Carlo Tail

Introduction to Breit in stone

My want to do

My DF7

Why BMC
\[ \hat{H} = -\frac{1}{2} \nabla^2 \psi + \int \left( V_{\text{coul}}(\mathbf{r}) \right) \psi^* \psi \, d^3 \mathbf{r} + \int V_{\text{ext}}(\mathbf{r}) \psi^* \psi \, d^3 \mathbf{r} \]

To calculate energy:

\[ E = \frac{\int \hat{H} \psi \, d^3 \mathbf{r}}{\int \psi \, d^3 \mathbf{r}} \]

Many-body so use Monte Carlo integral.

But \( \hat{H} \psi / \psi \) not constant so expensive, better to weight samples:

\[ E = \int \frac{\hat{H} \psi}{\psi} \, d^3 \mathbf{r} \quad \text{(Monte Carlo algorithm)} \]

Sample \( \hat{H} \psi / \psi \) carefully:

- If eigenstate constant
  - If not eigenstate \( \psi \to 0 \) but \( \hat{H} \psi \neq 0 \), so diverges

Monte Carlo: average + uncertainty that is \( \sim N^{-1/2} \).
\[ P(E) = \frac{d\alpha}{dE} P(\alpha) \]
\[ E = \alpha^{-1} \]
\[ \alpha = E^{-1} \]
\[ P(\alpha) = x^2 \epsilon^{-2} \]

\[ \frac{d\alpha}{dE} = E^{-2} \]

\[ 0^2 = \int E^{-\beta} E^2 \, dE \]
\[ = \int E^{2-\beta} \, dE \]
\[ = \left[ E^{3-\beta} \right]_0^\infty \rightarrow \text{need } \beta > 3 \]

\[ P(F) = \frac{d\alpha}{dF} P(\alpha) \]
\[ F = x^{-3} \]
\[ \alpha = F^{-\frac{1}{3}} \]
\[ P(\alpha) = x^2 = F^{-1} \]
\[ \frac{dx}{dF} = F^{-\frac{3}{2}} \]

\[ 0^2 = \int F^{-\frac{3}{2}} F^2 \, df \]
\[ = \int F^{-\frac{1}{2}} \, df \]
\[ = \left[ F^{\frac{1}{2}} \right]_0^\infty \rightarrow \text{diverges, so cannot have uncertainty!} \]
Method 1: Low energy softening

\[ E_l \begin{cases} \text{decreased by } 1 \cdot E_l \\ E_l \end{cases} \]

Try

\[ E_l \rightarrow \frac{E_l}{E_l^2/E_l^2 + 1} \quad \text{so } E_l \text{ at small } E_l \text{ and } E_l \sim \frac{E_l^2}{E_l} \text{ at large } E_l \]

- Remover divergences
- Easy to do
- Reinforces average that may be incorrect

\[ E_l - E \frac{E_l - E}{1 + (E_l - E)^2} \]
Method 2:

\[ P(A) \]

Just from o. RH5

![Graph with shaded area and formulas]

\[ \lambda = \frac{1}{M} \sum_{\mu=1}^{M} A^\mu + \sum_{n=0}^{\infty} C_n \int |A-A_c|^{r-n_A} A \ dA \]

As before Analyzed

\[ Y = \frac{1}{M-1} \sum |A^\mu-A_c|^2 \sum_{n=0}^{\infty} C_n \int (A-A_c)^{T-n_A} (A-A_c)^2 \ dA \]

As before Analyzed

Use knowledge of asymptotic form
Study the tail with the aid of the sample quintiles:

\[
\int_{A_0}^{\infty} \alpha(A) dA \approx q_m = \frac{m - \frac{1}{2}}{M}
\]

with

\[
P_B = \sum_{n=0}^{m} \binom{n}{\alpha} |A - A_c|^{-\mu - \eta n}
\]

\[
\sum_{n=0}^{m} \frac{\binom{n}{\alpha}}{\mu + \eta n - 1} |A^m - A_c|^{-\mu - \eta n + 1} = q_m
\]

\[
q_m / |A^m - A_c|^{\mu-1} = \sum_{n=0}^{m} \frac{\binom{n}{\alpha}}{\mu + \eta n - 1} |A^m - A_c|^{-\mu - \eta n + 1}
\]

Try distribution

\[
\frac{\mu \sin \theta}{2\pi} \frac{1}{1 + |A|^\mu}
\]

Normalized

Expectation value of 0

Agg update \( A \)

Summary

\[ \text{Cor} = \text{Cor} \]

Optimization

\[
\text{Minimize } \frac{1}{M - n(\alpha + 1)} \sum_{n=1}^{M} (y_m - y(x_n))^2
\]

All normally distributed