Calculating Expectation Values for Quantum Trajectories

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This note examines the proposition that the total expectation value of an operator is the average of the expectation value of all trajectories and that the total variance is the average of the variance of all trajectories. The proposition holds exactly for the expectation value. For the variance, it holds only under the approximation that the expectation values in each trajectory deviate only negligibly from the mean over all trajectories. An exact formula for the total variance is derived.

I. ASSUMPTIONS

1. When using quantum trajectories, we generate a set of N trajectories $\vert\Psi_i(t)\rangle$, $i \in [1,N]$ by evolving $\vert\Psi(0)\rangle$ using a stochastic differential equation (an "unravelling of the master equation"). The basic assumption is now that for $N \rightarrow \infty$, the system density matrix can be reconstructed as

$$\hat{\rho}_N(t) = \frac{1}{N}\sum_{i=1}^{N} \vert\Psi_i(t)\rangle\langle\Psi_i(t)\vert \tag{1}$$

   In the following, we drop the argument t.

2. We further assume that for an Operator $\hat{\mathsf{A}}$, and for a Hilbert space of dimension n with an orthonormal basis $\{\vert j\rangle\}, j \in [1,n]$, the expectation value of $\hat{\mathsf{A}}$ is calculated as

$$\langle\hat{\mathsf{A}}\rangle_\Psi = \left\langle \Psi \middle\vert \hat{\mathsf{A}} \middle\vert \Psi \right\rangle = \sum_{k=1}^{n} \langle k \,\vert\, \Psi\rangle \left\langle \Psi \middle\vert \hat{\mathsf{A}} \middle\vert k \right\rangle \tag{2a}$$

   in Hilbert space, and as

$$\langle\hat{\mathsf{A}}\rangle_\rho = \operatorname{tr}\left[\hat{\rho}\hat{\mathsf{A}}\right] = \sum_{k=1}^{n} \left\langle k \middle\vert \hat{\rho}\hat{\mathsf{A}} \middle\vert k \right\rangle \tag{2b}$$

   in Liouville space.

3. Lastly, we assume that variances are defined as

$$\operatorname{var}(\hat{\mathsf{A}})_{\Psi,\rho} \equiv \langle\hat{\mathsf{A}}^2\rangle_{\Psi,\rho} - \langle\hat{\mathsf{A}}\rangle^2_{\Psi,\rho}\,. \tag{3}$$

II. CALCULATING EXPECTATION VALUES

Proposition 1. *The total expectation value of an operator $\hat{\mathsf{A}}$ is the average of the expectation values from the individual trajectories.*

$$\langle\hat{\mathsf{A}}\rangle_{\rho_N} = \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i\,; \qquad \langle\hat{\mathsf{A}}\rangle_i \equiv \langle\hat{\mathsf{A}}\rangle_{\Psi_i} \tag{4}$$

Proof. By plugging Eq. (1) into Eq. (2b), we find

$$\begin{aligned}
\langle\hat{\mathsf{A}}\rangle_{\rho_N} &= \sum_{i=1}^{N}\sum_{k=1}^{n}\frac{1}{N}\langle k \,\vert\, \Psi_i\rangle \left\langle \Psi_i \middle\vert \hat{\mathsf{A}} \middle\vert k \right\rangle \\
&= \frac{1}{N}\sum_{i=1}^{N}\left\langle \Psi_i \middle\vert \hat{\mathsf{A}}\left(\sum_{k=1}^{n}\vert k\rangle\langle k\vert\right) \middle\vert \Psi_i \right\rangle \\
&= \frac{1}{N}\sum_{i=1}^{N}\left\langle \Psi_i \middle\vert \hat{\mathsf{A}} \middle\vert \Psi_i \right\rangle \\
&= \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i
\end{aligned} \tag{5}$$

□

III. CALCULATING VARIANCES

Proposition 2. *The total variance of an operator* $\hat{\mathsf{A}}$ *is (approximately) the average of the variance from the individual trajectories.*

$$\mathrm{var}(\hat{\mathsf{A}})_{\rho_N} \approx \frac{1}{N}\sum_{i=1}^{N}\mathrm{var}(\hat{\mathsf{A}})_i\,; \qquad \mathrm{var}(\hat{\mathsf{A}})_i \equiv \mathrm{var}(\hat{\mathsf{A}})_{\Psi_i}\,. \tag{6}$$

Proof. We first rewrite the right hand side using Eq. (3) as

$$\begin{aligned}\frac{1}{N}\sum_{i=1}^{N}\mathrm{var}(\hat{\mathsf{A}})_i &= \frac{1}{N}\sum_{i=1}^{N}\left(\langle\hat{\mathsf{A}}^2\rangle_i - \langle\hat{\mathsf{A}}\rangle_i^2\right)\\ &= \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}^2\rangle_i - \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i^2\,.\end{aligned} \tag{7}$$

For the left hand side, by using Eq. (3) and Eq. (5), we find

$$\begin{aligned}\mathrm{var}(\hat{\mathsf{A}})_{\rho_N} &= \langle\hat{\mathsf{A}}^2\rangle_{\rho_N} - \langle\hat{\mathsf{A}}\rangle_{\rho_N}^2\\ &= \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}^2\rangle_i - \left(\frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i\right)^2\,.\end{aligned} \tag{8}$$

The first term in Eq. (8) already matches the first term in Eq. (7). For the second term, we continue

$$\left(\frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i\right)^2 = \left(\frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i\right)\left(\frac{1}{N}\sum_{j=1}^{N}\langle\hat{\mathsf{A}}\rangle_j\right) = \left(\frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i\right)\langle\hat{\mathsf{A}}\rangle_{\rho_N}\,. \tag{9}$$

At this point, we must make the approximation $\langle\hat{\mathsf{A}}\rangle_i \approx \langle\hat{\mathsf{A}}\rangle_{\rho_N}$, that is, the expectation value obtained from any trajectory deviates only slightly from the average expectation value. Under that approximation, we finally find

$$\mathrm{var}(\hat{\mathsf{A}})_{\rho_N} \approx \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}^2\rangle_i - \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathsf{A}}\rangle_i^2 = \frac{1}{N}\sum_{i=1}^{N}\mathrm{var}(\hat{\mathsf{A}})_i\,, \tag{10}$$

Without the approximation, Eq. (8) gives the exact variance. □

IV. UPDATING THE MEAN EXPECTATION VALUE AND VARIANCE

For numerical purposes, it is important to be able to update the mean of the expectation value and the variance with an $N+1$'st new trajectory, without keeping a record of the expectation values and variances of the N old trajectories, but only the mean values $\langle\hat{\mathsf{A}}\rangle_{\rho_N}$ and $\mathrm{var}(\hat{\mathsf{A}})_{\rho_N}$

For the mean expectation value, we can write

$$\langle\hat{\mathsf{A}}\rangle_{\rho_{N+1}} = \frac{1}{N+1}\left(\left(N\langle\hat{\mathsf{A}}\rangle_{\rho_N}\right) + \langle\hat{\mathsf{A}}\rangle_{N+1}\right)\,. \tag{11}$$

If the mean variance is given (approximately) by Eq. (10), it can be updated with a formula equivalent to Eq. (11). If instead the mean variance is calculated exactly according to Eq. (8), we can update it as

$$\mathrm{var}(\hat{\mathsf{A}})_{\rho_{N+1}} = \frac{1}{N+1}\left(N\left(\mathrm{var}(\hat{\mathsf{A}})_{\rho_N} + \langle\hat{\mathsf{A}}\rangle_{\rho_N}^2\right) + \langle\hat{\mathsf{A}}^2\rangle_{N+1}\right) - \left(\frac{1}{N+1}\left(N\langle\hat{\mathsf{A}}\rangle_{\rho_N} + \langle\hat{\mathsf{A}}\rangle_{N+1}\right)\right)^2\,. \tag{12}$$

An alternative – and preferred – approach would be to keep a record of both $\langle\hat{\mathsf{A}}\rangle_{\rho_N}$ and $\langle\hat{\mathsf{A}}^2\rangle_{\rho_N}$, and to calculate the variance on the fly, as

$$\mathrm{var}(\hat{\mathsf{A}})_{\rho_{N+1}} = \langle\hat{\mathsf{A}}^2\rangle_{\rho_{N+1}} - \langle\hat{\mathsf{A}}\rangle_{\rho_{N+1}}^2\,. \tag{13}$$