Classical shadows with general probability distribution

Charles Hadfield

July 2020

Consider an observable $O = \sum_Q \alpha_Q Q$ where the summation is over n-qubit Pauli operators $Q \in \{I, X, Y, Z\}^{\otimes n}$. For such a Pauli operator Q and for a given qubit $i \in \{1, 2, \ldots, n\}$ we shall write Q_i for the i^{th} single-qubit Pauli operator so that $Q = \otimes_i Q_i$. We denote the support of such an operator $\operatorname{supp}(Q) = \{i | Q_i \neq I\}$ and its weight $\operatorname{wt}(Q) = |\operatorname{supp}(Q)|$. An n-qubit Pauli operator Q is said to be full-weight if $\operatorname{wt}(Q) = n$.

Given a full-weight Pauli operator P, we let $\mu(P, i) \in \{\pm 1\}$ denote the eigenvalue measurement when qubit i is measured in the P_i basis. For a subset $A \subseteq \{1, 2, \ldots, n\}$ declare $\mu(P, A) = \prod_{i \in A} \mu(P, i)$ with the convention that $\mu(P, \varnothing) = 1$.

Let β be a probability distribution on full-weight Pauli operators: $\beta : \{X, Y, Z\}^{\otimes n} \to \mathbb{R}^+$ with $\sum_P \beta(P) = 1$. For a Pauli operator Q, define

$$\operatorname{Lift}(Q) = \left\{ P \in \{X, Y, Z\}^{\otimes n} \,|\, P_i = Q_i \text{ for every } i \in \operatorname{supp}(Q) \right\}, \tag{1}$$

$$\zeta(Q, \beta) = \sum_{P \in \operatorname{Lift}(Q)} \beta(P). \tag{2}$$

We shall also use the characteristic function χ where $\chi_\Omega(x)$ returns 1 if $x \in \Omega$ and 0 if $x \notin \Omega$.

Algorithm 1 Classical shadows with general probability distribution

Prepare ρ;
Randomly pick $P \in \{X, Y, Z\}^{\otimes n}$ from β-distribution;
for qubit $i \in \{1, 2, \ldots, n\}$ **do**
  Measure qubit i in P_i basis providing evalue measurement $\mu(P, i) \in \{\pm 1\}$;
Estimate observable expectation

$$\nu = \sum_Q \alpha_Q \cdot \frac{\chi_{\operatorname{Lift}(Q)}(P)}{\zeta(Q, \beta)} \cdot \mu(P, \operatorname{supp}(Q))$$

return ν.

Lemma 1. *The estimator ν from Algorithm 1 satisfies*

$$\mathbb{E}(\nu) = \sum_Q \alpha_Q \operatorname{tr}(\rho Q). \tag{3}$$

Proof. Let $\mathbb{E}_P$ denote the expected value over the distribution $\beta(P)$. Let $\mathbb{E}_{\mu(P)}$ denote the expected value over the measurement outcomes for a fixed Pauli basis P. By definition, the expected value in Eq. (3) is a composition of the expected values over a Pauli basis P and over the measurement outcomes $\mu(P)$, that is, $\mathbb{E} = \mathbb{E}_P \mathbb{E}_{\mu(P)}$.

Consider $Q \in \{I, X, Y, Z\}^{\otimes n}$. Whenever $P \in \operatorname{Lift}(Q)$, we observe $\mathbb{E}_{\mu(P)} \mu(P, \operatorname{supp}(Q)) = \operatorname{tr}(\rho Q)$.

Combining these observations implies

$$\begin{aligned}
\mathbb{E}(\nu) &= \mathbb{E}_P \mathbb{E}_{\mu(P)} \nu && (4)\\
&= \sum_Q \alpha_Q \frac{1}{\zeta(Q, \beta)} \mathbb{E}_P \chi_{\operatorname{Lift}(Q)}(P) \mathbb{E}_{\mu(P)} \mu(P, \operatorname{supp}(Q)) && (5)\\
&= \sum_Q \alpha_Q \frac{1}{\zeta(Q, \beta)} \sum_{P \in \operatorname{Lift}(Q)} \beta(P) \cdot \operatorname{tr}(\rho Q) && (6)\\
&= \sum_Q \alpha_Q \operatorname{tr}(\rho Q). && (7)
\end{aligned}$$

□

For Pauli operators Q, R, define

$$g(Q,R,\beta) = \frac{1}{\zeta(Q,\beta)}\frac{1}{\zeta(R,\beta)}\sum_{P\in \mathrm{Lift}(Q)\cap \mathrm{Lift}(R)} \beta(P) \tag{8}$$

This function simplifies greatly when β is a product distribution. Specifically, if $\beta = \prod_{i=1}^n \beta_i$ with $\beta_i : \{X,Y,Z\} \to \mathbb{R}^+$, then $g(Q,R,\beta)$ is non-zero only when Q, R agree with each-other on $A = \mathrm{supp}(Q)\cap \mathrm{supp}(R)$ and in which case $g(Q,R,\beta) = \left(\prod_{i\in A}\beta_i(Q_i)\right)^{-1}$.

Lemma 2. *The estimator ν from Algorithm 1 satisfies*

$$\mathbb{E}(\nu^2) = \sum_{Q,R} \alpha_Q\alpha_R g(Q,R,\beta)\,\mathrm{tr}(\rho Q R) \tag{9}$$

Proof. We use the same notation as in the preceding lemma. Consider $Q, R \in \{I,X,Y,Z\}^{\otimes n}$. As operators, we obtain the identity

$$\mathbb{E}_P \frac{\chi_{\mathrm{Lift}(Q)}(P)}{\zeta(Q,\beta)}\frac{\chi_{\mathrm{Lift}(R)}(P)}{\zeta(R,\beta)} = g(Q,R,\beta) \tag{10}$$

and, whenever $P \in \mathrm{Lift}(Q)\cap\mathrm{Lift}(R)$,

$$\mathbb{E}_{\mu(P)}\mu(P,\mathrm{supp}(Q))\mu(P,\mathrm{supp}(R)) = \mathrm{tr}(\rho P Q). \tag{11}$$

To get the last equality, observe that $\mu(P,A)\mu(P,A') = \mu(P, A\oplus A')$ for any subsets of qubits A, A', where $A\oplus A'$ is the symmetric difference of A and A'. The assumption that P is in the lift of both Q and R implies that $\mathrm{supp}(Q)\oplus\mathrm{supp}(R) = \mathrm{supp}(QR)$.

Combining these observations implies

$$\begin{aligned}
\mathbb{E}(\nu^2) &= \mathbb{E}_P\mathbb{E}_{\mu(P)}\nu^2 &(12)\\
&= \sum_{Q,R}\alpha_Q\alpha_R\mathbb{E}_P\frac{\chi_{\mathrm{Lift}(Q)}(P)}{\zeta(Q,\beta)}\frac{\chi_{\mathrm{Lift}(R)}(P)}{\zeta(R,\beta)}\mathbb{E}_{\mu(P)}\mu(P,\mathrm{supp}(Q))\mu(P,\mathrm{supp}(R)) &(13)\\
&= \sum_{Q,R}\alpha_Q\alpha_R g(Q,R,\beta)\,\mathrm{tr}(\rho QR) &(14)
\end{aligned}$$

□