Unfolding quantum computer readout noise

Benjamin Nachman, Miroslav Urbanek, Wibe A. de Jong and Christian W. Bauer

In the current era of noisy intermediate-scale quantum computers, noisy qubits can result in biased results for early quantum algorithm applications. This is a significant challenge for interpreting results from quantum computer simulations for quantum chemistry, nuclear physics, high energy physics (HEP), and other emerging scientific applications. An important class of qubit errors are readout errors. The most basic method to correct readout errors is matrix inversion, using a response matrix built from simple operations to probe the rate of transitions from known initial quantum states to readout outcomes. One challenge with inverting matrices with large off-diagonal components is that the results are sensitive to statistical fluctuations. This challenge is familiar to HEP, where prior-independent regularized matrix inversion techniques (“unfolding”) have been developed for years to correct for acceptance and detector effects, when performing differential cross section measurements. We study one such method, known as iterative Bayesian unfolding, as a potential tool for correcting readout errors from universal gate-based quantum computers. This method is shown to avoid pathologies from commonly used matrix inversion and least squares methods.

INTRODUCTION

While quantum algorithms are promising techniques for a variety of scientific and industrial applications, current challenges limit their immediate applicability. One significant limitation is the rate of errors and decoherence in noisy intermediate-scale quantum (NISQ) computers. Mitigating errors is hard in general because quantum bits (“qubits”) cannot be copied. An important family of errors are readout errors. They typically arise from two sources: (1) measurement times are significant in comparison to decoherence times, and thus a qubit in the |1⟩ state can decay to the |0⟩ state during a measurement, and (2) probability distributions of measured physical quantities that correspond to the |0⟩ and |1⟩ states have overlapping support, and there is a small probability of measuring the opposite value. The goal of this paper is to investigate methods for correcting these readout errors. This is complementary to efforts for gate error corrections. One strategy for mitigating such errors is to build in error correcting components into quantum circuits. Quantum error correction is a significant challenge because qubits cannot be cloned. This generates a significant overhead in the additional number of qubits and gates required to detect or correct errors. Partial error detection/correction has been demonstrated for simple quantum circuits, but complete error correction is infeasible for current qubit counts and moderately deep circuits. As a result, many studies with NISQ devices use the alternative zero noise extrapolation strategy, whereby circuit noise is systematically increased and then extrapolated to zero. Ultimately, both gate and readout errors must be corrected for a complete measurement and a combination of strategies may be required.

Correcting measured histograms for the effects of a detector has a rich history in image processing, astronomy, high energy physics (HEP), and beyond. In the latter, the histograms represent binned differential cross sections and the correction is called unfolding. Many unfolding algorithms have been proposed and are currently in use by experimental high energy physicists (see, e.g., refs. 36–38 for reviews). One of the goals of this paper is to introduce these methods and connect them with current algorithms used by the quantum information science (QIS) community.

Quantum readout error correction can be represented as histogram unfolding, where each bin corresponds to one of the possible 2^n_qubits configurations, where n_qubits is the number of qubits (Fig. 1). Correcting readout noise is a classical problem (though there has been a proposal to do it with quantum annealing), but relies on calibrations or simulations from quantum hardware. Even though discussions of readout errors appear in many papers (see, e.g., refs. 24,30–32), we are not aware of any dedicated study comparing unfolding methods for QIS applications. Furthermore, current QIS methods have pathologies that can be avoided with techniques from HEP. In particular, the most popular quantum simulators PyQuil (by Rigetti), Cirq (by Google), and XACC36–38 implement a version of matrix inversion, and the other popular simulator Qiskit by IBM39,40 uses a least squares method (see also refs. 41,42) that is the same as the matrix inversion solution when the the latter is nonnegative. Challenges with methods based on matrix inversion will be discussed in more detail below.

RESULTS

Unfolded quantum readout

For the results presented here, we simulate a quantum computer using qiskit-terra 0.9.0, qiskit-aer 0.2.3, and qiskit-ignis 0.1.139. Note that multi-qubit readout errors are not supported in all versions of qiskit-aer and qiskit-ignis. This work uses a custom measure function to implement the response matrices. We choose a Gaussian distribution as the true distribution, as this is ubiquitous in quantum mechanics as the ground state of the harmonic oscillator. An alternative distribution that is mostly zero with a small number of spikes is presented in Supplementary Fig. 5. This system has been recently studied in the context quantum field theory as a benchmark 0 + 1-dimensional noninteracting scalar field theory43–50. In practice, all of the qubits of a system would be entangled to achieve the...
A schematic diagram illustrating the connection between binned differential cross section measurements in high energy physics (left) and interpreting the output of repeated measurements from quantum computers (right). Given this connection, techniques used to mitigate detector effects for measurements in high energy physics can be studied for readout errors in quantum computing.

![Fig. 1](image)

The measurement of a Gaussian distribution (ground state of harmonic oscillator) using the pathological response matrix.

One million total shots are used both to sample from $m$ and to construct $R$. The IBU method uses ten iterations.

![Fig. 2](image)

The measurement of a Gaussian distribution using the response matrix from the IBM Q Johannesburg machine. One million total shots are used to construct $R$ and $10^4$ are used for $t$ and $m$. The IBU method uses 100 iterations. The significant deviations on the far left and right of the distributions are due in part to large statistical fluctuations, where the counts are low. The uncertainty band in the ratio is the statistical uncertainty on $t$.

![Fig. 3](image)

The measurement of a Gaussian distribution using the response matrix from the IBM Q Johannesburg machine.
Regularization and uncertainties

One feature of any regularization method is the choice of regularization parameters. For the IBU method, these parameters are the prior and number of iterations. Figure 5 shows the average bias from statistical and systematic sources in the measurement from the Gaussian example shown in Fig. 2, as a function of the number of iterations. With a growing number of iterations, \( \hat{t}_{\text{IBU}} \) approaches the oscillatory \( \hat{t}_{\text{ignis}} \). The optimal number of iterations from the point of view of the bias is three. However, the number of iterations cannot be chosen based on the actual bias because the true answer is not known a priori. In HEP, the number of iterations is often chosen before unblinding the data by minimizing the total expected uncertainty. In general, there are three sources of uncertainty: statistical uncertainty on \( m \), statistical and systematic uncertainties on \( R \), and non-closure uncertainties from the unfolding method. Formulae for the statistical uncertainty on \( m \) are presented in ref. 52 and can also be estimated by bootstrapping\(^3\) the measured counts. Similarly, the statistical uncertainty on \( R \) can be estimated by bootstrapping and then repeating the unfolding for each calibration pseudo-dataset. The sources of statistical uncertainty are shown as dot-dashed and dashed lines in Fig. 6. Adding more iterations enhances statistical fluctuations and so these sources of uncertainty increase monotonically, with the number of iterations.

The systematic uncertainty on \( R \) and the method non-closure uncertainty are not unique and require careful consideration. In HEP applications, \( R \) is usually determined from simulation, so the systematic uncertainties are simulation variations that try to capture potential sources of mis-modeling. These simulation variations are often estimated from auxiliary measurements with data. There are additional uncertainties related to the modeling of background processes, as well as related to events that fall into or out of the measurement volume. These are not relevant for QIS. In the QIS context, \( R \) is determined directly from the data, so the only uncertainty is on the impurity of the calibration circuits. In particular, the calibration circuits are constructed from a series of single-qubit X gates. Due to gate imperfections and thermal noise, there is a chance that the application of an X gate will have a different effect on the state than intended. In principle, one can try to correct for such potential sources of bias by an extrapolation method. In such methods, the noise is increased in a controlled fashion and then extrapolated to zero noise\(^{20-24}\). This method may have a residual bias and the uncertainty on the method

Fig. 4 The distribution of the difference between true and predicted counts from a Gaussian distribution using the response matrix from the IBM Q Johannesburg machine. The simulation is repeated 1000 times. For each of the 1000 pseudo-experiments, a discretized Gaussian state is prepared with no gate errors and it is measured 104 times. The bin counts without readout errors are the “true” values. The measured distribution with readout errors is unfolded and the resulting counts are the “predicted” values. Each of the 2^2 states over all 1000 pseudo-experiments contribute one entry to the above histogram. The standard deviations of the distributions are given in the legend. The IBU method uses 100 iterations.

Fig. 5 The difference between \( \hat{t}_{\text{IBU}} \) and \( \hat{t} \) as a function of the number of iterations for the example presented in Fig. 2. By definition, the \( \hat{t}_{\text{ignis}} \) method does not depend on the number of iterations.

Fig. 6 Sources of uncertainty for \( \hat{t}_{\text{IBU}} \) as a function of the number of iterations for the example presented in Fig. 2. Each uncertainty is averaged over all states. The total uncertainty is the sum in quadrature of all the individual sources of uncertainty, except gate noise (which is not used in the measurement simulation, but would be present in practice).
would then become the systematic uncertainty on \( R \). A likely conservative alternative to this approach is to modify \( R \) by adding in gate noise, and taking the difference between the nominal result and one with additional gate noise, simulated using the \texttt{thermal_relaxation_error} functionality of \texttt{qiskit}. This is the choice made in Fig. 6, where the gate noise is shown as a dotted-dashed line. In this particular example, the systematic uncertainty on \( R \) increases monotonically with the number of iterations, just like the sources of statistical uncertainty.

The non-closure uncertainty is used to estimate the potential bias from the unfolding method. One possibility is to compare multiple unfolding methods and take the spread in predictions as an uncertainty. Another method advocated in ref. 34 and widely used in HEP is to perform a data-driven reweighting. The idea is to reweight the \( \bar{t}^2 \) so that when folded with \( R \), the induced \( m^0 \) is close to the measurement \( m \). Then, this reweighted \( m^0 \) is unfolded with the nominal response matrix and compared with the reweighted \( \bar{t}^2 \). The difference between these two is an estimate of the non-closure uncertainty. The reweighting function is not unique, but should be chosen so that the reweighted \( \bar{t}^2 \) is a reasonable prior for the data. For Fig. 6, the reweighting is performed using the nominal unfolded result itself. In practice, this can be performed in a way that is blinded from the actual values of \( f_{\text{true}} \) so that the experimenter is not biased, when choosing the number of iterations.

Altogether, the sources of uncertainty presented in Fig. 6 show that the optimal choice for the number of iterations is 2. In fact, the difference in the uncertainty between two and three iterations is <1\% and so consistent with the results from Fig. 5. Similar plots for the measurement in Fig. 3 can be found in Supplementary Figs. 3 and 4.

**DISCUSSION**

This work has introduced a suite of readout error correction algorithms developed in HEP for binned differential cross section measurements. These unfolding techniques are well-suited for quantum computer readout errors, which are naturally binned and without acceptance effects (counts are not lost or gained during readout). In particular, the iterative Bayesian method has been described in detail, and shown to be robust to a failure mode of the matrix inversion and \texttt{ignis} techniques. When readout errors are sufficiently small, all the methods perform well, with a preference for the \texttt{ignis} and Bayesian methods that produce nonnegative results. The \texttt{ignis} method is a special case of the \texttt{TUnfold} algorithm, where the latter uses the covariance matrix to improve precision and incorporates regularization to be robust to the failure modes of matrix inversion. It may be desirable to augment the \texttt{ignis} method with these features or provide the iterative method as an alternative approach. In either case, Fig. 3 showed that even with a realistic response matrix, readout error corrections can be significant and must be accounted for in any measurement on near-term hardware.

An important challenge facing any readout error correction method is the exponential resources required to construct the full \( R \) matrix (see the “Methods” section). While \( R \) must be constructed only once per hardware setup and operating condition, it could become prohibitive when the number of qubits is large. On hardware with few connections between qubits, per-qubit transition probabilities may be sufficient for accurate results. When that is not the case, one may be able to achieve the desired precision with polynomially many measurements. These ideas are left to future studies.

Another challenge is optimizing the unfolding regularization. The numerical examples presented in the “Results” section considered various sources of uncertainty, and studied how they depend on the number of iterations in the IBU method. The full measurement is performed for all 2^{t_{\text{max}}} states and the studies in the “Results” section collapsed the uncertainty across all bins into a single number by averaging across bins. This way of choosing a regularization parameter is common in HEP, but is not a unique approach. Ultimately, a single number is required for optimization, but it may be that other metrics are more important for specific applications, such as the uncertainty for a particular expectation value, or the maximum or most probable uncertainty across states. Such requirements are application specific, but should be carefully considered prior to the measurement.

With active research and development across a variety of application domains, there are many promising applications of quantum algorithms in both science and industry on NISQ hardware. Readout errors are an important source of noise that can be corrected to improve measurement fidelity. HEP experimentalists have been studying readout error correction techniques for many years under the term unfolding. These tools are now available to the QIS community and will render the correction procedure more robust to resolution effects, in order to enable near-term breakthroughs.

**METHODS**

The unfolding challenge

Let \( t \) be a vector that represents the true bin counts before the distortions from detector effects (HEP) or readout noise (QIS). The corresponding measured bin counts are denoted by \( m \). These vectors are related by a response matrix \( R \) as \( m = R t \), where \( R_{ij} = \text{Pr}(m_i = t_j) \). In HEP, the matrix \( R \) is usually estimated from detailed detector simulations, while in QIS, \( R \) is constructed from measurements of computational basis states. The response matrix construction is discussed in more detail below.

The most naive unfolding procedure would be to simply invert the matrix \( R: f_{\text{true}} = R^{-1} m \). However, simple matrix inversion has many known issues. Two main problems are that \( f_{\text{true}} \) can have unphysical entries, and that statistical uncertainties in \( R \) can be amplified and can result in oscillatory behavior. For example, consider the case

\[
R = \begin{pmatrix}
1 - \epsilon & \epsilon \\
\epsilon & 1 - \epsilon
\end{pmatrix},
\]

where \( 0 < \epsilon < 1/2 \). Then, \( \text{Var}(f_{\text{true}}) = 1/\det(R) = 1/(1 - 2\epsilon) \rightarrow \infty \) as \( \epsilon \rightarrow 1/2 \). As a generalization of this example to more bins (from ref. 55), consider a response matrix with a symmetric probability of migrating one bin up or down,

\[
R = \begin{pmatrix}
1 - \epsilon & \epsilon & 0 & \cdots \\
\epsilon & 1 - 2\epsilon & \epsilon & \cdots \\
0 & \epsilon & 1 - 2\epsilon & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

Unfolding with the above response matrix and \( \epsilon \approx 25\% \) is presented in Fig. 7. The true bin counts have the Gaussian distribution with a mean of zero and a standard deviation of 3. The values are discretized with 21 uniform unit width bins spanning the interval \([-10, 10] \). The leftmost bin correspond to the first index in \( m \) and \( t \). The indices are monotonically incremented with increasing bin number. The first and last bins include underflow and overflow values, respectively. Due to the symmetry of the migrations, the true and measured distributions are nearly the same. For this reason, the measured spectrum happens to align with the true distribution; the optimal unfolding procedure should be the identity. The significant off-diagonal components result in an oscillatory behavior and the statistical uncertainties are also amplified by the limited size of the simulation dataset used to derive the response matrix.

Even though it is simple, matrix inversion is an important benchmark for comparing with the methods described below because it is widely used in quantum computing, as introduced at the end of the “Introduction” section. Many of these implementations are even simpler than full matrix inversion by assuming that errors are uncorrelated across qubits. In some cases, additional mitigation strategies are used to make the matrix inversion corrections smaller. This is demonstrated in ref. 55 (see also ref. 56), where a symmetrization step is first applied with \( X \) gates prior to matrix inversion. A minimal modification to matrix inversion is to ensure that the counts are nonnegative. One such approach is to use a least
IBU calls for the repeated application of Bayes widely used IBU method, which avoids further regularization requirements in order to avoid pathologies from matrix inversion. The focus of this paper will be on the matrix inversion. The SVD approach applies some regularization directly on entries. This is the method implemented in the optimization problem

\[ \text{arg min}_{x} \left\| R x - y \right\|_1, \quad \text{subject to} \quad \left\| x \right\|_1 = 1 \]

where \( x \) is the true and measured probability mass functions, respectively. Simple matrix inversion is represented by \( \mathbf{R}^\dagger \mathbf{m} \) whereas \( \mathbf{R}^\dagger \mathbf{y} \) and \( \mathbf{R}^\dagger \mathbf{m} \) are represented by \( \mathbf{R}^\dagger \mathbf{m} \) and \( \mathbf{R}^\dagger \mathbf{m} \) respectively. Simple matrix inversion is represented by \( \mathbf{R}^\dagger \mathbf{m} \) and \( \mathbf{R}^\dagger \mathbf{m} \). The IBU method uses ten iterations and a uniform prior (other iterations choices are studied in Supplementary Fig. 1).

The simulation used in this plot is based on standard Python functions and does not use a quantum computer simulator (see instead Fig. 3).

The IBU does not suffer from rapid oscillations and like the ignis approaches discussed in the previous section, Fig. 7 shows the IBU result with \( \mathbf{R} \) and \( \mathbf{m} \) for all possible states. Note that this matrix depends on the calibration quality, so while it is representative, it is not precisely the version valid for all measurements made on this hardware.

\[
\mathbf{R}_n = \sum_{i} \mathbf{R}_{ni},
\]

where \( n \) is the iteration number and one iterates a total of \( N \) times. The advantage of Eq. (5) over simple matrix inversion is that the result is a probability (nonnegative and unit measure) when \( m \geq 0 \). In HEP applications, \( m \) can have negative entries resulting from background subtraction. In this case, the unfolded result can also have negative entries. The parameters \( R^\dagger \mathbf{m} \) and \( N \) must be specified ahead of time. A common choice for \( R^\dagger \mathbf{m} \) is the uniform distribution. The number of iterations needed to converge depends on the desired precision, how close \( R^\dagger \mathbf{m} \) is to the final distribution, and the importance of off-diagonal components in \( R \). In practice, it may be desirable to choose a relatively small \( N \) prior to convergence to regularize the result. Typically, \( \leq O(10) \) iterations are needed.

In addition to the \( R^\dagger \mathbf{m} \) and \( R^\dagger \mathbf{m} \) approaches discussed in the previous section, Fig. 7 shows the IBU result with \( N = 10 \). Unlike the \( R^\dagger \mathbf{m} \) and \( R^\dagger \mathbf{m} \) results, the \( R^\dagger \mathbf{m} \) does not suffer from rapid oscillations and like \( R^\dagger \mathbf{m} \) is nonnegative. Analogous results for quantum computer simulations are presented in the “Results” section.

Constructing the response matrix

In practice, the \( R \) matrix is not known exactly, and must be measured for each quantum computer and set of operating conditions. One way to suppress amplified statistical fluctuations.

Fig. 7 A comparison of unfolding techniques for a Gaussian example and the \( R \) matrix from Eq. (3). The symbols \( t \) and \( m \) denote the true and measured probability mass functions, respectively. Simple matrix inversion is represented by \( \mathbf{R}^\dagger \mathbf{m} \). The \( \mathbf{R}^\dagger \mathbf{m} \) and \( \mathbf{R}^\dagger \mathbf{m} \) methods are represented by \( \mathbf{R}^\dagger \mathbf{m} \) and \( \mathbf{R}^\dagger \mathbf{m} \) respectively. Simple matrix inversion is represented by \( \mathbf{R}^\dagger \mathbf{m} \) and \( \mathbf{R}^\dagger \mathbf{m} \). The IBU method uses ten iterations and a uniform prior (other iterations choices are studied in Supplementary Fig. 1).

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measure $R$ is to construct a set of $2^{\text{qubit}}$ calibration circuits as shown in Fig. 8. Simple $X$ gates are used to prepare all of the possible qubit configurations and then they are immediately measured.

Figure 9 shows the $R$ matrix from five qubits of the IBM Q Johannesburg machine. As expected, there is a significant diagonal component that corresponds to cases, when the measured and true states are the same. However, there are significant off-diagonal components, which are larger toward the right when more configurations start in the one state. The diagonal stripes with transition probabilities of $\sim 7\%$ are the result of the same qubit flipping from 0 $\rightarrow$ 1. This matrix is hardware dependent and its elements can change over time due to calibration drift. Machines with higher connectivity have been observed to have more readout noise.

Figure 10 explores the universality of qubit migrations across $R$. If every qubit was identical, and there were no effects from the orientation and connectivity of the computer, then one may expect that $R$ can actually be described by just two numbers $p_{0 \rightarrow 1}$ and $p_{1 \rightarrow 0}$ assuming an equal rate of readout errors for each qubit. Big filled markers represent a fit with independent values for each qubit. Small semitransparent open markers show the $2^{\text{qubit}}$ transition probabilities for each qubit, when the other $n_{\text{qubit}} - 1$ qubits are unchanged between truth and measured states.

The code for the work presented here can be found at https://github.com/bnachman/QSUnfolding.

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