Statistical Aspects of the Quantum Supremacy Demonstration

Yosef Rinott
The Hebrew University of Jerusalem
Federmann Center for the Study of Rationality
and Department of Statistics

Tomer Shoham
The Hebrew University of Jerusalem
Federmann Center for the Study of Rationality
and Department of Statistics

Gil Kalai
The Hebrew University of Jerusalem
Einstein Institute of Mathematics and
Efi Arazy School of Computer Science, IDC, Herzliya.∗

Abstract

The notable claim of quantum supremacy presented by Google’s team in 2019 consists of demonstrating the ability of a quantum circuit to generate, albeit with considerable noise, bitstrings from a distribution that is considered hard to simulate on classical computers. Verifying that the generated data is indeed from the claimed distribution and assessing the circuit’s noise level and its fidelity is a purely statistical undertaking. The objective of this paper is to explain the relations between quantum computing and some of the statistical aspects involved in demonstrating quantum supremacy in terms that are accessible to statisticians, computer scientists, and mathematicians. Starting with the statistical analysis in Google’s demonstration, which we explain, we study various estimators of the fidelity, and different approaches to testing the distributions generated by the quantum computer. We propose different noise models, and discuss their implications. A preliminary study of the Google data, focusing mostly on circuits of 12 and 14 qubits is discussed throughout the paper.

KEY WORDS: Random distributions, Estimation of sampling weights, Google’s quantum computer.

∗Federmann Center for the Study of Rationality, and Quantum Information Science Center at HUJI, FACT center at IDC. Supported by ERC advanced grant 834735.
1 Introduction

Google’s announcement of quantum supremacy [2] was compared by various writers to landmark achievements such as the Wright brothers’ invention of a motor-operated airplane, Fermi’s demonstration of a nuclear chain reaction, and Sputnik. It was also met with some skepticism, which is partly due to the fact that Google’s quantum computer cannot at this point perform any practical task such as factoring large integers. Instead, it performs a sampling task; that is, it generates random bitstrings, with considerable noise, from a discrete distribution supported on $M$ values, with probabilities whose computations are far beyond the reach of classical computers for large $M$. (Therefore, classical computers cannot carry out this sampling task.) A quantum computer suitably adjusted is capable of sampling from such a distribution without having to compute the probabilities explicitly, thus claiming its supremacy.

Verifying that the generated data indeed have the claimed distribution in spite of the noise is a statistical problem, which we explain and generalize, offering some new statistical aspects. Aiming for a general mathematical audience, we briefly review some basic relevant statistical ideas and some of the basics of quantum computing, and therefore some parts of the paper have an expository nature. Also, our notation is a compromise between Google’s notation [2] and more standard statistical notation. We start with the main statistical models and problems; background on quantum computing is given in Section 2.

1.1 The main model and statistical problem

A quantum computer (or circuit) consists of $n$ qubits, which are its basic memory units. When read/measured, each qubit takes the value 0 or 1 and thus the whole system yields an $n$-vector of 0’s and 1’s to which we refer as bitstring. Before the system is measured it exists in a superposition of all $2^n$ $n$-vectors. When the circuit is set, it determines a set of $2^n$ probabilities $\{w_{x(i)} : x^{(i)} \in \{0, 1\}^n\}$ such that when the system is measured, it will yield the vector $x^{(i)}$ with probability $w_{x(i)}$ for $i = 1, \ldots, 2^n$, provided it runs without errors. (We may denote $w_{x(i)}$ by $w_i$, and $x^{(i)}$ by $x_i$.) If we run the system $N$ times and measure it, we get $N$ such $n$-vectors, and denoting the probability of no error (aka fidelity) by $\phi$, our sample will consist of $N$ iid vectors, where $x^{(i)}$ is sampled with probability $\phi w_i + (1-\phi)/2^n$; that is, if an error occurs, the vector is chosen uniformly. This describes a sampling task, which will be discussed later.

We describe the main statistical problems that will be addressed in the analysis of samples from a quantum computer, and some generalizations of these problems. Consider a realization of $M$ iid vectors with nonnegative components $z_i = (z_{i1}, \ldots, z_{ip}), i = 1, \ldots, M$, distributed according to some $p$-dimensional distribution $D$ with marginal distributions $D_k$. For example, the vectors’ components can be independent with $z_{ki} \sim D_k, k = 1, \ldots, p$. Assumptions on the distribution of $z_{ki}$ will appear when needed. The main examples we shall consider in detail are when $z_{ki}$ are either Exp(1) variables (with density $e^{-z}$ for $z > 0$) or they are identically equal to 1; however, only a few moments of the distribution will be taken into account, and our study applies more generally. For $i = 1, \ldots, M$, set

$$w_i = (w_{i1}, \ldots, w_{ip}), \text{ where } w_{ki} = z_{ki}/\sum_{j=1}^M z_{kj}, \text{ so that } \sum_{i=1}^M w_{ki} = 1 \text{ for } k = 1, \ldots, p, \quad (1)$$

and thus for each $k$, the vector $(w_{k1}, \ldots, w_{kM})$ is a random probability vector. Let $M = 2^n$; each vector $w_i$ is associated with a vector $x_{w_i} \equiv x^{(i)} \in \{0, 1\}^n$. The sampling task described next can be expressed both in terms of $w_i$ and $x_{w_i}$; the reason for this seemingly redundant notation will be explained later.
A random sample of size $N$, $x_{\tilde{w}_1}, \ldots, x_{\tilde{w}_N}$, or equivalently $\tilde{w}_1, \ldots, \tilde{w}_N$, is drawn (with replacement) from the above set of $M$ vectors $x_{\tilde{w}_i}$, or equivalently from $w_i$, where draws are independent, and in each draw the probability $\pi(x_{\tilde{w}_i}) \equiv \pi(w_i)$ of drawing $x_{\tilde{w}_i}$ (or $w_i$) is

$$\pi(x_{\tilde{w}_i}) \equiv \pi(w_i) = \phi_1 w_{1i} + \ldots + \phi_p w_{pi}, \; i = 1, \ldots, M,$$

(2)

where $\phi_1, \ldots, \phi_p$ are nonnegative parameters, to be discussed, satisfying $\phi_1 + \ldots + \phi_p = 1$, and so $\sum_{i=1}^M \pi(w_i) = 1$. Note that the components of the sampled $\tilde{w}_j$’s do not have the same distribution as the original components due to the sampling scheme that assigns higher probabilities to vectors with larger components. Therefore, we denote the sample by

$$S = \{\tilde{w}_j\} = \{(\tilde{w}_{1j}, \ldots, \tilde{w}_{pj})\} \text{ where } j = 1, \ldots, N, \text{ and } P(\tilde{w}_j = w_i) = \pi(w_i).$$

(3)

Equivalently, we could set $S = \{x_{\tilde{w}_i}\}$ or simply $S = \{\tilde{x}^{(i)}\}$. Such notation is required because the random sampling is from a finite population that is itself random, and $w_{kj}$ and $\tilde{w}_{kj}$ are both random, with different distributions. This sampling scheme is a mixture of size-biased samplings where in each of $N$ rounds, a coordinate of $w_i$ is chosen, where $\phi_k$ is the probability of the $k$th coordinate, and then $w_i$ is chosen with probability proportional to the size of the chosen coordinate. See Section 3 for more details on size bias.

This model arises from Google’s quantum supremacy demonstration [2]. Google’s sampling model is a special case of (2) when $p = 2$, where $z_{1i} = z_i$ are modeled to have the Exp(1) distribution, $z_{2i} \equiv 1$, $w_i = z_i / \sum_{j=1}^M z_j$, and $0 \leq \phi \leq 1$. Thus, in our notation, Google’s model is the special case of sampling $\tilde{w}_1, \ldots, \tilde{w}_N$ or the associated bitstrings $\tilde{x}^{(1)}, \ldots, \tilde{x}^{(N)}$ with a mixture of $w_i$ and uniform probabilities:

$$\pi(x^{(i)}) = \pi(w_i) = \phi w_i + (1 - \phi)/M.$$ 

(4)

Note that $z_{2i}/M = 1/M$ represents a uniform distribution (over the values $w_i$, or equivalently over bitstrings) and the models in (4) represents a mixture of the probabilities $w_i$ with weight $\phi$ and random uniform noise. The quantity $\phi$ is known as the fidelity.

We add some more details on the connection of the statistical models described above to quantum physics and the Google experiment. (Section 2 gives a detailed explanation.) The (ideal) quantum state of a quantum computer with $n$ qubits is represented by a unit vector $u = (u_1, u_2, \ldots, u_M)$ in an $M$-dimensional complex vector space, $M = 2^n$. The coordinates of $u$ are referred to as amplitudes. We cannot probe these amplitudes directly (this follows from Heisenberg’s uncertainty principle), but we can measure the state, and this yield a single sample from a discrete probability distribution with probabilities $w_1 = |u_1|^2, w_2 = |u_2|^2, \ldots, w_M = |u_M|^2$.

Next, come random circuits: when the collection of gates is chosen at random then the vector $u$ behaves like a random unit vector and this implies, when $M$ is large, that the random probabilities $w_1, \ldots, w_M$ are modeled to arise from exponential $z_i$’s normalized by their sum as above. To see this note first that a uniformly distributed $M$-dimensional vector on a sphere of radius 1 can be generated by taking $M$ iid N(0,1) variables, and normalizing the length to 1, which is obtained approximately (for large $M$) by dividing by $\sqrt{M}$. Therefore, if we consider $u$ as a unit vector in a real $2M$-dimensional space, the coordinates over the reals of $u$ behave like iid Gaussian variables, and therefore each squared absolute value of a complex coordinate behaves like the sum of squares of two iid Gaussians, which has an exponential distribution. (The sum of squares of $k$ iid Gaussian is distributed as $\chi^2(k)$; that is,
the $\chi^2$-distribution with $k$ degrees of freedom. Thus the sum of square of two Gaussians and the $\chi^2(2)$ distribution which coincides with Exp(1).)

The quantum computer samples $N$ of these $w_j$’s independently according to (4); the uniform part of (4) is due to errors in the computation process (noise). We denote the $N$ sampled values by $\tilde{w}_j$, and in fact it is the associated sample $\{x_{\tilde{w}_j}\} = \{\tilde{x}^{(j)}\}$ that is observed. This is the sampling task. Given a quantum circuit, the computation of the linked probabilities $w_i$ (even a single one of them) can only be done with exponentially increasing efforts by classical computers if $n < 40$ or so, and it becomes a practically impossible task if $n > 50$, say $40$ (Google’s ultimate experiment is with $n = 53$.) As classical computers cannot compute these probabilities for large $n$, they cannot produce samples according to them. The quantum computer does not compute these probabilities, and its supremacy is in its ability to perform the sampling task nevertheless, and produce a sample of bitstrings $S = \{\tilde{x}_j\}$ according to theses unknown probabilities (mixed with uniform probabilities); see [2]. Verifying that the quantum computer indeed performed its task of sampling from the right distribution, requires to compute this distribution by a classical computer, which it cannot for $n = 53$. Therefore, the proof of quantum supremacy for large $n$ requires various extrapolation arguments based on smaller values of $n$, in addition to statistical reasoning.

In [2] it is assumed that the $\phi$’s are known approximately from an independent source, and part of the supremacy proof consists of showing that the sample is indeed generated as described, which requires to estimate $\phi$. We shall assume that for each sampled $\tilde{x}^{(j)}$ the associated $\tilde{w}_j$ is known and so the sample given by (5) is known. This is required for the computation of any estimator of $\phi$, both Google’s and ours. However, we emphasize that this requires classical computation and is possible only when $n < 40$ or so.

The assumption that $z_i \sim \text{iid Exp}(1)$ implies that the random vector in the $M$-simplex $w = (w_1, \ldots, w_M)$, whose components are $w_i = z_i / \sum_{j=1}^{M} z_j$, has the Dirichlet distribution with parameter $\alpha$ which is an $M$-vector whose components are all equal to 1. All we need here are the facts:

$$E w_i = 1/M, \quad E w_i^2 = 2/M(M + 1), \quad E w_i^k = k!/[M \cdots (M + k - 1)];$$

see, e.g., [10].

In [2] the sample size is denoted by $N_s$ which we abbreviate to $N$, $M = 2^n$, where $n$ is the number of qubits in the quantum computer (see Section 2). Google’s notation for the fidelity is $F$, which we denote by $\phi$, and their notation for the random probabilities is $P(x^{(i)}) := w_i$, known as the Porter–Thomas distribution. We often use the notation $P_C(x^{(i)})$ in order to emphasize the dependence on the (random) circuit $C$.

Returning to the general model of (2), we study the following statistical problem: having observed the sampled vectors $\tilde{w}_1, \ldots, \tilde{w}_N$, one goal is to estimate the coefficients $\phi_1, \ldots, \phi_k$, which together with $w_j$ determine the sampling scheme (2). Furthermore, we want to test the hypothesis that the sample is indeed generated according to the model (2), and also that the $w_j$’s are generated according to the given model, which is Dirichlet distribution in Google’s model (4). The Dirichlet model is also our main example. In particular, in Google’s model, proving that $\phi > 0$ significantly suggests that the data are indeed generated with relation to the given probabilities $w_i$ and are not pure uniform choice of these probabilities, that is, random noise. More specifically, $\phi = 0$ in (4) is tantamount to sampling bitstrings

\[1\] Here we refer to the most complicated circuits in the Google experiment. There are various simplified circuits for which computing the linked probabilities is feasible.
uniformly, a trivial task. We describe and explain the methods proposed in [2], and some variations on estimators and testing methods, which we study theoretically, and using both simulated data and Google’s data.

When the \( w \)'s are non-random, this can be seen as sampling from a discrete (finite) population. However, recalling that the \( w \)'s are generated randomly from a given distribution, we say that the sample is generated from a random discrete distribution in the sense of Kingman [9]. See Section 3 for further details. The estimation takes advantage of both this generating process, and the special nature of the sampling scheme.

We consider two kinds of analyses of estimators. First, we condition on \( \{w_i\}_{i=1}^M := \{w_i\}_{i=1,...,M} \), which amounts to considering a particular quantum circuit, and sampling from the fixed set \( \{w_i\}_{i=1}^M \). We study conditional properties of different estimators, such as their bias and variance. Second, assuming that the \( w_i \)'s are random and satisfy some moment conditions (that hold when \( z_i \sim \text{Exp}(1) \)), we study average properties of estimators when averaging is also over the randomness of \( \{w_i\}_{i=1}^M \). We compare the two analyses and discuss them in Section 4.

Google’s estimator for the fidelity is quite simple and given by

\[
\tilde{\phi} = 2^n \frac{1}{N} \sum_{j=1}^{N} \mathcal{P}_C(\tilde{x}^{(j)}) - 1.  \tag{6}
\]

This estimator, which we later denote by \( U \), is an unbiased estimator when both the sample and the realization of \( \mathcal{P}_C \) are random and expectation is taken over both. This corresponds to an experiment in which several circuits with the same parameters, and a common \( \phi \), are considered (see Section 2). From each circuit a sample is taken and \( \tilde{\phi} \) is computed and then averaged over all circuits in the experiment.

As mentioned above, a somewhat different statistical question, which is perhaps more relevant to the Google supremacy experiment, is to estimate the fidelity \( \phi \) (or the values of \( \phi_1, \phi_2, \ldots \), in the general setting) when the realization \( \{w_i\}_{i=1}^M \) is fixed. For a specific realization (or a specific circuit \( C \)), \( \tilde{\phi} \) is biased. In Sections 4.2 and 4.3 we discuss an unbiased version \( V \) of \( \tilde{\phi} \), and the maximum likelihood estimator (MLE), which is nearly unbiased. Both turn out to be superior to the above \( \tilde{\phi} \) in terms of variance and bias for both types of experiments, that is, sampling repeatedly from a single circuit, and averaging over several circuits. This superiority decreases when \( \phi \) is small and \( M \) is large. It thus matters for relatively small-scale circuit demonstrations (which are relevant for extrapolation arguments to larger circuits) but less so for large-scale ones.

The difference between sampling from a single circuit and averaging over several circuits can perhaps be examined by the following extreme analogy. Suppose we claim to be able to produce perfectly balanced coins. We then label the sides of our coins by 0 or 1 at random, and demonstrate our claim that the coins are balanced by choosing and tossing one coin at a time, and verifying the \( 1/2 - 1/2 \) statistics. However, this test is useless since the result would be the same if our coins were unbalanced with any probabilities, which can vary between coins. On the other hand, testing repeatedly one or some of our coins will yield a valid test of our claim.

This setup brings to mind super-population models, see, e.g., [16] Ch. 14.5 or [12], where a population \( \mathcal{P} \) of size \( M \) of \( p \)-vectors, say vectors of measurements on humans or some species in a given region, is considered to be a realization from a continuous or discrete distribution known as a super-population model, and then a sample of size \( N \) is taken from \( \mathcal{P} \), using a known sampling scheme. A standard goal in this case is to make inference on parameters of the population \( \mathcal{P} \) using the sample. However, in our
case the sampling scheme (2) is unknown and our goal is different; instead of estimating the population
parameters, we want to estimate the parameters $\phi_k$, which are part of the sampling scheme.

1.2 An individual choice model

We briefly describe a simple application unrelated to quantum computing, which is a variation on
problems in individual choice models in economics; see, e.g., [7] for a simple introduction. It provides
another perspective on the models we discuss, and suggests other potential applications. Consider $M$
items, say refrigerators (fridges), in a store (they need not be all different). Each fridge is characterized
by $p$ attributes like size, price per given size, energy per size, etc., which for fridge $i$ are $w_{1i}, \ldots, w_{pi}$.
Each of $N$ customers chooses one fridge and it is assumed that the probability of choosing fridge $i$
is given by (2), that is, a convex combination of the $w$’s that characterize this fridge with the $\phi$’s as
coefficients. Thus, the vector of $\phi$’s characterizes the population from which we have a sample of $N$.
The parameter $\phi_k$ quantifies the weight the population attaches to attribute $k$ in making a choice,
and this is a quantity the seller or the producer would like to know. This paper proposes various ways of
estimating the $\phi$’s from the sample. The information consists of the $N$ chosen fridges and their attributes,
but the customers do not reveal their selection process, and they may not be it.

A useful interpretation of the linear combination in (2) is the following: each customer chooses an at-
tribute at random with probabilities according to the $\phi$’s, and then if attribute $k$ was chosen, the customer
chooses fridge $i$ with a probability proportional to $w_{ki}$, and hence it is a size-biased selection. (See for
example [3], where size-biased observations with respect to one variable out of several are considered.
See also Section 3.) Equivalently, a proportion $\phi_k$ of the population chooses in proportion to the value
of the $k$th attribute. In either interpretation, $\phi_k$ represents the importance of attribute $k$, thus quantifying
the relative importance of attributes like size, price, energy consumption, etc., in the item selection.

1.3 Paper outline

Some background on quantum computing is given in Section 2. In Section 3 we discuss size-biased
distribution and random discrete distributions. In Section 4 we concentrate on the case of $p = 2$ and
compare various statistical methods for estimating the parameters. More precisely, we analyze Google’s
estimator $U$, as well as two unbiased estimators: $V$, which is a variant of $U$ that is unbiased for any given
realization $\{w_i\}_1^M$, and the maximum likelihood estimator, denoted by $MLE$. The results are demon-
strated briefly by simulated data, and by Google’s data. In Section 5 we consider estimation in the case
of general $p$. In Section 6 we propose more detailed noise models for the Google sample based on the
analysis of readout errors, and analyze statistical estimators based on our readout noise models. Confi-
dence intervals for estimated parameters are discussed in Section 7. In Section 8 we briefly address the
question of testing the fit of various empirical distributions to the theoretical expectation. A preliminary
study of Google’s data on small circuits, supporting our findings regarding the fidelity estimators and
the relevance of our readout noise model, is presented in Sections 4 and 6. Yet, neither Google’s basic
noise model nor our refined readout errors model fit the observed data (Section 8). Section 9 concludes
the paper, apart from two proofs given in the Appendix.
2 Quantum computers and Google’s quantum supremacy experiment

2.1 Quantum computers

In this section we provide some background on quantum computing, sampling algorithms and Google’s experiment. The reader is referred to [13] and [19] for further information. The latter reference provides more math and physics details, and an updated summary of quantum information and computation, including various potential statistical applications.

Quantum computers are physical devices that are believed to have the potential for solving certain computational tasks that are well beyond the ability of classical computers. Shor’s famous algorithm shows that suitable quantum computers can factor $n$-digit integers efficiently in roughly $n^2$ computational steps! The best known classical algorithms require an exponential number of steps in $n^{1/3}$. This ability for efficient factoring would allow quantum computers to break the majority of current cryptosystems.

A sampling task is one where the computer (either quantum or classical) produces samples from a certain probability distribution $\pi$. In the main example of Google’s experiment paper [2] each sample is a 0-1 vector of length 53, where $\pi$ is a probability distribution on such vectors. Quantum algorithms allow sampling from probability distributions well beyond the capabilities of classical computers.

Quantum systems are inherently noisy; we cannot accurately control them, and any interaction with them introduces further noise. A noisy quantum computer has the property that at every computational step (applying a gate, measuring a qubit) the computer makes an error with a certain small probability. Noisy intermediate-scale quantum (NISQ) computers, are quantum computers where the number of qubits is in the tens or at most in the hundreds. Over the past decade researchers conjectured that the huge computational advantage of sampling with quantum computers can be realized by NISQ computers that only approximate the target probability distribution. They predict that quantum computational supremacy (for sampling tasks) could be achieved for NISQ computers. NISQ computers are also crucial to the task of creating good-quality quantum error-correction, which is a necessary ingredient for larger-scale quantum computers.

An important feature of NISQ systems – especially for the tasks of quantum supremacy – is the fact that a single error in the computation sequence has a devastating effect on the outcome. In the NISQ regime, the engineering challenge is to keep the computation error-free. We shall refer to the probability that not even a single error occurs as the fidelity. Many companies and research groups worldwide are investing in attempts to implement quantum computations via NISQ computers (as well as by other means). We note that statistical tools from [2] (and this paper) are relevant to the study of fidelity and models for noise of NISQ circuits that goes beyond Google’s current experiment.

2.2 The Google supremacy claim

The Google experiment is based on the building of a quantum computer (circuit) $C$ with $n$ qubits that perform $m$ cycles of computations. Let $M = 2^n$. The computation is carried out by 1-qubit and 2-qubit gates, and each cycle consists of 2-qubit gates acting on non-overlapping pairs of qubits and on 1-qubit gates acting on all qubits. The state of the computer is described by a unit vector $u = (u_1, \ldots, u_M)$ in an $M$-dimensional complex Hilbert space $H$ and every computer cycle represents a unitary operator acting on $H$. At the end of the computation the qubits are measured, leading to a sample from a probability distribution $\mathcal{P}_C$ on 0–1 vectors $x$ of length $n$. This process is repeated $N$ times (for the same circuit $C$)
to produce a sample of size $N$. For the ultimate experiment ($n = 53$, $m = 20$, with 1113 1-qubit gates, and 530 2-qubit gates) the quantum computer produced a sample of several million 0–1 vectors of length 53.

The specific circuit $C$ used for the computation is itself a random circuit. For every experiment, specific gates are chosen, once and for all, at random (by a classical computer). In ideal situations, namely, without noise, the quantum computer would produce samples from a certain probability distribution $\mathcal{P}_C$ that depends on the specific circuit $C$. When the circuit $C$ is chosen at random, the probability distribution $\mathcal{P}_C$ looks like an instance of the random distribution (a Porter–Thomas distribution) that we described in the introduction.

Google’s quantum computers are “noisy,” so what the computer is actually producing are not samples from $\mathcal{P}_C$ but rather a noisy version that could roughly be described as follows: a fraction $\phi$ of the samples are from $\mathcal{P}_C$ and a fraction $(1 - \phi)$ of the samples are from a uniform distribution, and $\phi$ is referred to as the fidelity. This corresponds to (4).

Google’s paper made two crucial claims regarding the ultimate 53-qubit samples.

A) The fidelity $\phi$ of their sample is above $1/1000$.

B) Producing a sample with similar fidelity would require 10,000 years on a supercomputer.

As it was only possible to give indirect evidence for both these claims, we shall now describe the logic of Google’s quantum supremacy argument.

For claim A) regarding the value of $\phi$, the paper describes a statistical estimator for $\phi$ and the argument relies on a bold extrapolation argument that has two ingredients. One ingredient is a few hundred experiments in the classically tractable regime: the regime where the probability distribution $\mathcal{P}_C$ can be computed by a classical computer and the performance of the quantum computer can be tested directly. The other ingredient is a theoretical formula for computing the fidelity. According to the Supplement to Google’s paper [2], the fidelity of entire circuits closely agrees with the prediction of the simple mathematical formula (Formula (77) in the Supplement to [2], Equation (7) below). There are around 200 reported experiments in the classically tractable regime. These experiments support the claim that the prediction given by Formula (77) for the fidelity is indeed very robust and therefore applies also to the 53-qubit circuit in the supremacy regime. To test whether the quantum computer produced a sample with the hoped-for properties we need to be able to simulate the quantum computer on a classical supercomputer. This is beyond reach for 53 qubits and therefore the samples for the 53-qubit experiments demonstrating “supremacy” are archived, but it is not possible to test them in any direct way.

For claim B) regarding the difficulty of classical computers to compute the sampling distribution described by a given quantum circuit, the Google team mainly relies on extrapolation from the running time of a specific algorithm they use. They also rely on results and conjectures from computational complexity that support the assertion that the task at hand requires, for a classical computer, an exponential number (in $n$) of computational steps. We note that a team from IBM [14] managed to find a classical algorithm that would require only several days of computation on a classical supercomputer (which is less than 10,000 years and more than the running time of the quantum computer of 200 seconds).

---

2 The IBM algorithm, like the Google algorithm, computes the entire $M$ probabilities $\mathcal{P}_C(x)$ described by the circuit. It is not known if the task of precise sampling according to these probabilities or the task of producing a sample with fidelity $> 1/1000$ admit an even quicker classical algorithm.
2.3 Estimating the fidelity

The Google argument relies crucially on the following simple formula (Formula (77) in the Supplement to [2]) for estimating the fidelity $\phi$ of their experiments.

$$\phi \approx \prod_{g \in \mathcal{G}_1} (1 - e_g) \prod_{g \in \mathcal{G}_2} (1 - e_g) \prod_{q \in \mathcal{Q}} (1 - e_q).$$  \hspace{1cm} (7)

Here $\mathcal{G}_1$ is the set of 1-gates (gates operating on a single qubit), $\mathcal{G}_2$ is the set of 2-gates (gates operating on a two qubits), and $\mathcal{Q}$ is the set of qubits. For a gate $g$, the term $e_g$ in the formula refers to the probability of error of the individual gate $g$. For a qubit $q$, $e_q$ is the probability of a readout error when we measure the qubit $q$. (Those individual probabilities of errors for gates and qubits are also referred to as fidelities.)

An important aspect of (7) is that it is assumed that the fidelity $\phi$ is common to circuits with common numbers of qubits and gates (and the same individual gate and qubit fidelities) even if the realizations $\mathcal{P}_C$ vary. This allows estimation of the common $\phi$ by averaging over different circuits with the same parameters.

The rationale for Equation (7) is simple: as long as there are no errors in the performance of all the gates and all the measurements of the qubits, then we get a sample from the correct distribution. A single error in one of these components leads to an irrelevant sample. The Google paper reports that for a large number of experiments the actual fidelity estimated by Equation (7) agrees with the statistical estimator of the fidelity up to 10%–20%.

A simpler form of (7) is obtained by replacing the detailed individual values of the fidelities by their average value, leading to

$$\phi' \approx (1 - 0.0016)^{|\mathcal{G}_1|} (1 - 0.0062)^{|\mathcal{G}_2|} (1 - 0.038)^n$$  \hspace{1cm} (8)

The Google team reports that $\phi'$ (more precisely, a slight variant, based on a combined estimate for 2-gate and 1-gate errors) differs from $\phi$ by a few percent (in most cases).

We remark that the excellent predictive power of Equation (7) is, on its own, a major scientific discovery as well as engineering achievement of the Google experiment. Concerns regarding the statistical assumptions behind the strong predictive power of Equation (7) were raised by Kalai [8]. In particular, Formula (7) is based on the assumption of independence of the errors, which is often considered unrealistic in the field of system reliability theory (see, e.g., [17] for a general discussion, and [5] for a convenient specific discussion of potential causes for dependence of errors in quantum systems).

2.4 Google’s Porter–Thomas probability distributions and fidelity estimation

In the introduction we described the Porter–Thomas distributions, a random probability distribution on a finite space $\mathcal{X}$ defined by $\mathcal{P}(x) = z_x / \sum_x z_x$. The values $z_x$ for $x \in \mathcal{X}$ are random nonnegative iid Exp(1) variables. In the case of Google’s experiment $\mathcal{X} = \{0, 1\}^n$ (the set of all 0–1 vectors of length $n$). As already mentioned, the state of a quantum circuit $\mathcal{C}$ is described by a unit vector in an $M$-dimensional complex vector spaces, and whose coordinates are complex numbers $u_x : x \in \{0, 1\}^n$. We cannot probe this complex vector directly, but once we measure the state, this leads to a sample from

---

3The same paper, like several earlier papers, explains Kalai’s skeptical views regarding the entire endeavor of quantum computers. Those views, however, are not related to the present work.
the probability distribution $P_C$ that assigns to a vector $x \in \{0, 1\}^n$ the probability $P_C(x) = \|u_x\|^2$. The crucial fact is that when $C$ is a random circuit, $P_C$ behaves like a realization of a Porter–Thomas distribution.

Once the quantum computer produces $N$ samples $\tilde{x}^{(i)}, \ldots, \tilde{x}^{(N)}$, the Google estimator of $\phi$,

$$\tilde{\phi} = 2^n \frac{1}{N} \sum_{j=1}^N P_C(\tilde{x}^{(j)}) - 1,$$

proposed in [2], can be computed provided $P_C(\tilde{x}^{(j)})$ are known.

This estimator is referred to in [2] as “XEB,” an abbreviation for “cross-entropy benchmarking.” A crucial aspect of this estimator and of Google’s statistical approach as a whole is that relatively small samples (of size $N \sim 10^6$) give powerful confirmation of the fidelity being significantly non-zero for samples from a huge probability space (of size $M$ that can be as large as $10^{12}$–$10^{16}$).

We reiterate that computing the Google estimator (9) requires the computation of the probabilities $P_C(x^{(j)}), j = 1, \ldots, N$. Moreover, computing $P_C(x)$, even for a single value of $x$, is a difficult computational task that is beyond reach in the ultimate experiments involving 53 qubits, and requires heavy computations on (classical) supercomputers for $n$ approaching 40.

We note that for all our purposes we can regard the state obtained by a random circuit $C$ as a random vector in the Hilbert space and, therefore, $P_C$ as a realization of the Porter–Thomas distribution. However, it is not fully random; rather it is a pseudo-random distribution with properties very similar to those of a truly random distribution. Here, by “pseudo-random” we mean values drawn by a computer program that behave “like” random values. Here the computer program used to generate the pseudo-random distribution is a quantum computer program. The assumption behind the claims of quantum supremacy is that computing this pseudo-random distribution is a very hard problem for a classical computer, yet sampling from this distribution can easily be carried out by a quantum computer.

2.5 A little more on quantum computers

We give now a brief overview of quantum computers. A qubit is a piece of quantum memory. The state of a qubit can be described by a unit vector in a two-dimensional complex Hilbert space $H$. For example, a basis for $H$ can correspond to two energy levels of the hydrogen atom, or to horizontal and vertical polarizations of a photon. Quantum mechanics allows the qubit to be in a superposition of the basis vectors, described by an arbitrary unit vector in $H$. The memory of a quantum computer (quantum circuit), denoted by $C$, consists of $n$ qubits. Let $H_k$ be the two-dimensional Hilbert space associated with the $k$th qubit. The state of the entire memory of $n$ qubits is described by a unit vector in the tensor product $H_1 \otimes H_2 \otimes \cdots \otimes H_n$. We can put one or two qubits through gates representing unitary transformations acting on the corresponding two- or four-dimensional Hilbert spaces, and as for classical computers, there is a small list of gates sufficient for universal quantum computing. Applying a gate consists of applying a unitary transformation on the large $2^n$-dimensional Hilbert space: namely, a certain unitary operator on the two- or four-dimensional space that corresponds to the qubits involved in the gate, tensored with the identity transformation on all other qubits. (Each cycle of the Google

---

As a matter of fact, computing the individual probabilities $P(x^{(i)})$ is computationally hard even for a quantum computer. (Sampling according to the probability distribution $P$ is easy for a quantum computer but not computing or estimating individual probabilities.)
experiment consists of applying in parallel single-qubit gates on all qubits or two-qubit gates on non overlapping pairs of qubits.) The final state of the quantum computer is a unit vector $u = (u_1, \ldots, u_M)$ in $\mathbb{C}^M$, where the $M$ indexes correspond to all 0-1 vectors of length $n$. As already mentioned, at the end of the computation process, the state of the entire computer is measured, giving a sample from the probability distribution $P_C$ on 0-1 vectors of length $n$.

Figure 1. The (conjectured) view of some main computational complexity classes. The red ellipse represents efficient quantum algorithms. Note the position of three important computational tasks: factoring, quantum sampling, and computing the probabilities for quantum sampling.

A few words on the connection between the mathematical model of quantum circuits and quantum physics: in quantum physics, states and their evolutions (the way they change in time) are governed by the Schrödinger equation. A solution of the Schrödinger equation can be described as a unitary process on a Hilbert space and quantum computing processes as we just described form a large class of such quantum evolutions. An interesting question is what precisely gives quantum computers their superior computing power. The state of the quantum computer can be a huge superposition that requires an exponential number of “amplitudes,” and therefore, quantum computers allow for specific algorithmic tasks with massive parallelism. Another related fact is that quantum probabilities (unlike classical probabilities) can be both positive and negative, allowing massive cancellations.

Figure 1 illustrates the (conjectural) computational complexity classes and the computational advantages of quantum computers. On the one hand, some computational tasks that quantum computers can perform extend beyond the entire “polynomial hierarchy” and, on the other hand, it is conjectured that quantum computers cannot solve NP-complete problems.
2.6 Randomness and quantumness in computational complexity

Quantum systems, such as the famous “two slits” experiment, are capable of producing truly random sequences. Classical computers produce pseudo-random bits only. In the context of this paper this advantage of quantum computers does not play a role. In our discussion of the computational power of a classical computer, we take for granted that the computer is able to choose at random 0 and 1 with probability 1/2 each. (Indeed, we take it for granted in Fig. [1].) There are good theoretical and practical reasons for why semblances of truly random sequences that a classical computer can produce are as good for classical computation as truly random sequences. (In particular, we will not be able to distinguish them from truly random sequences by statistical tests.)

On the other hand, there are good theoretical reasons to think that classical computers cannot produce semblances of probability distributions that can be achieved by quantum computers and those distributions can lead to a huge computational advantage for certain algorithmic tasks.\footnote{Another distinction between classical and quantum systems arises from the important notion of entanglement, which is a quantum analog of correlation. (Entanglement is related to the famous violation of “Bell’s inequalities” for quantum systems.) A demonstration of entangled quantum systems is not, by itself, an example of quantum computational supremacy, but quantum computational supremacy does rely on the ability to create complicated forms of entanglement for systems with many qubits.}

3 Background on size bias and random discrete distributions

Some background on size-biased distributions will be useful in explaining the nature of the sampling schemes described above. For a recent broad survey with applications see [1]. Let \( p(x) \) be a probability function on a finite space \( \mathcal{X} \subseteq \mathbb{R}_+ \) or a continuous density on \( \mathbb{R}_+ \), and let \( x \) be a nonnegative random variable distributed according to \( p(x) \). We say that the random variable \( x^* \) has the \( p(x) \)-size-biased distribution if \( P(x^* = x) = xp(x)/a \) in the discrete case, and \( x^* \) has density \( xp(x)/a \) in the continuous case, where \( a = \text{Ex} \) is the normalizing constant. If \( p(x) = e^{-x} \) for \( x > 0 \), the density of the \( \text{Exp}(1) \) distribution, then the \( p \)-size-biased density is \( xe^{-x} \), corresponding to the Gamma(2, 1) distribution.

Consider a distribution \( D \) on \( \mathbb{R}_+ \) with expectation =1, and a vector \((z_1, \ldots, z_M)\) whose components are iid-distributed by \( D \), so that \( Ez_i = 1 \). We normalize the vector by setting \( w_i = z_i/\sum_{j=1}^M z_j \), and denote the normalized vector by \( w = (w_1, \ldots, w_M) \). Since \( \sum_{j=1}^M z_j/M \to 1 \) with probability 1, we have \( w_i \approx z_i/M \) for large \( M \). The vector \( w \) defines a probability distribution on a finite set of size \( M \). When \( D \) is the Gamma distribution, the vector \( w \) has the Dirichlet distribution; see, e.g., [9]. The special case where the \( D = \text{Exp}(1) = \text{Gamma}(1, 1) \) with density \( e^{-x} \) for \( x > 0 \) arose in quantum physics; see Porter and Thomas [15]. This case plays an important role in the Google experiment.

More generally, one can assume that \( w \) is a realization of some distribution on the \( M \)-simplex, that is, a random vector of nonnegative components summing to one; this structure is known as a random discrete distribution; see Kingman [9].

Proposition 3.1. Let \( z_1, z_2, \ldots \) be nonnegative, iid-distributed by \( D \), with expectation =1, and for each \( M \) define \( w^{(M)}_i = z_i/\sum_{j=1}^M z_j \). Let \( x^*_M \) denote a value drawn at random from \( \{z_1, \ldots, z_M\} \), where \( P(x^*_M = z_i) = w^{(M)}_i \), \( i = 1, \ldots, M \). Then with probability =1 (over sequences \( z_1, z_2, \ldots \)) we have that \( x^*_M \) converges in distribution to the \( D \)-size-biased distribution as \( M \to \infty \).
Proof: We give a slightly informal proof. If we denote a draw \( z_i \) by \( x^* \), taking one of the values \( z_1, \ldots, z_M \), then for large \( M \) we have \( P(x^* = z_i) \approx z_i/M \) (this is the part stated informally), which means that the distribution of \( x^* \) converges to the size-biased version of the empirical distribution function \( F_n \) of \( z_1, \ldots, z_M \) (which assigns probability \( 1/M \) to each \( z_i \)). Since \( F_n \) converges in distribution to \( D \), the \( F_n \)-size-biased distribution converges in distribution to the \( D \)-size-biased distribution by Theorem 2.3 in [1].

In the sampling scheme of (4), \( N \) values of \( w_i \) are sampled from the set \( \{w_i\}^M \), where with probability \( \phi \) the value \( w_i \) is drawn with the probability \( w_i^{(M)} \) above. The corresponding values \( z_i \) are asymptotically distributed according to a mixture of \( D \)-size-biased values with weight \( \phi \), and the original \( D \) with weight \( 1 - \phi \). Obviously, relative to the distribution \( D \), large values of \( z_i \) or \( w_i \) are overrepresented under this sampling, and the distribution of the sample is tilted to the right.

When \( D \) is \( \text{Exp}(1) \), that is, the original \( z \)'s have the \( \text{Exp}(1) \) distribution, the distribution of the sampled \( z_i \) is a mixture of approximately \( \text{Gamma}(2,1) \) (with density function \( xe^{-x} \)) with probability \( \phi \) and the original \( D \) (with density \( e^{-x} \)) with probability \( 1 - \phi \).

4 Estimation of the fidelity \( \phi \) for \( p = 2 \)

For given \( w_1, \ldots, w_M \) we observe a sample \( \tilde{w}_1, \ldots, \tilde{w}_N \) of vectors drawn independently according to (2) (equivalently we observe the associated vectors \( x_{\tilde{w}_1}, \ldots, x_{\tilde{w}_N} \)). Our goal is to estimate \( \phi_1, \ldots, \phi_p \). We start with Google’s case of \( p = 2 \); a (random) quantum circuit determines a set of values \( w_1, \ldots, w_M \) from which it samples \( \tilde{w}_1, \ldots, \tilde{w}_N \) according to (4).

We study two types of analyses and consider biases, variances, etc.: the first type is conditioned on the \( w \)'s, and the second is with expectation taken over the random \( w \)'s. We compare these analyses and their implications for different estimators, and for different parameters of the problem. In particular, we compare Google’s estimator with the maximum likelihood estimator (MLE).

Google’s estimator \( \tilde{\phi} \) of (6), which we henceforth denote by \( U \), defined again in (12) below, and the MLE, see (22), are statistics (i.e., functions of observed data) if we assume that the sample (3) is observed, that is, \( U \) and the MLE depend only on the sampled \( \tilde{w}_1, \ldots, \tilde{w}_N \). Another estimator considered below in (14). \( V \), is not a statistic in the sense that computing it requires the knowledge of \( w^{(2)} = \sum_{i=1}^M w_i^2 \). We mention again that a quantum circuit produces a sample of bitstrings \( x_{\tilde{w}_1}, \ldots, x_{\tilde{w}_N} \); however, calculating the associated \( \tilde{w}_1, \ldots, \tilde{w}_N \) is done by classical computers only, and for limited values of \( M = 2^n \). For \( n < 40 \), a classical supercomputer can compute all \( w_i \) and hence \( V \) can also be computed. For \( n > 50 \) or so, computing even a single \( w_i \) is practically impossible, and hence the statistics presented in [2] and here cannot be computed. Therefore, Google’s supremacy claim with \( n = 53 \) is based on skillful extrapolation.

Google’s estimator \( U \) turns out to be biased for each given circuit. Averaged over sufficiently many different circuits, or in expectation over the random probabilities \( w_x = P_C(x) \), it becomes unbiased, and hence consistent as a function of the number of circuits, as we show below. The bias for each circuit entails a large variance between circuits; this variance diminishes along with the bias as \( \phi \) becomes small or \( M \) large.
4.1 Moment estimators

Google’s estimator (see \((6)\) or \((9)\), which we denote by \(U\) in \((12)\) below, is basically a moment estimator, a notion we briefly review. The method of moments (see, e.g., [6] Chapter 18) can be described as follows: let \(x_i\) be \(N\) iid observations taking values in some space \(\mathcal{X}\) and assume \(x_i \sim F_\theta\) where \(\theta \in \Theta \subseteq \mathbb{R}^p\). Let \(\varphi : \mathcal{X} \rightarrow \mathbb{R}^p\) and assume \(E_\theta \varphi(x_i) = g(\theta)\), where \(g : \Theta \rightarrow \mathbb{R}^p\) is one-to-one. The moment estimator of \(\theta\) is defined by

\[
T_N = g^{-1} \left( \frac{1}{N} \sum_{i=1}^{N} \varphi(x_i) \right). \tag{10}
\]

With standard assumptions, the law of large numbers implies that \(\frac{1}{N} \sum_{i=1}^{N} \varphi(x_i) \rightarrow E_\theta \varphi(x_i)\), and further standard smoothness assumptions imply that \(T_N\) is consistent; that is, \(T_N\) converges to \(\theta\) in probability. Moreover, \(\sqrt{N}(T_N - \theta) \rightarrow N(0, \Sigma)\) in distribution, where the asymptotic covariance matrix \(\Sigma\) depends on the variance of the variables \(x_i\), the functions \(\varphi\) and \(g\), and their derivatives. In this case we say that \(T_N\) is root-\(N\) consistent and asymptotically normal.

In Section 4.3 we will discuss the maximum likelihood estimator (MLE). The MLE is known to be asymptotically efficient, that is, asymptotically normal with the smallest asymptotic variance among asymptotically normal estimators, under certain regularity conditions (see, e.g., Theorem 3.10, Chapter 6 in [11]). Theorems 4.3 and 5.3 of Chapter 6 in [11] show that one Newton–Raphson iteration (toward the MLE) starting from any root-\(N\) consistent estimator is asymptotically efficient, which means that like the MLE it has the smallest asymptotic variance.

4.2 Google’s estimator \(U\) of the fidelity and its unbiased variant \(V\)

We denote the set \(\{w_i\}_{i=1}^{M} \) by \(\{w_i\}_{1}^{M}\), and \(\{\tilde{w}_j\}_{1}^{N}\) is defined similarly. Expectation of \(\{\tilde{w}_j\}_{1}^{N}\) conditional on \(\{w_i\}_{1}^{M}\), with respect to the sampling of \(4\), which is repeated in \((11)\) below, will be denoted by \(E^w\). Expectation over the randomness of \(\{w_i\}_{1}^{M}\) is denoted by \(E\). Thus \(Eg(\tilde{w}_j) = EE^w g(\tilde{w}_j)\) denotes expectation over both the sampling of \(\tilde{w}_j\) and the randomness of the random probabilities \(w_i\). Similarly \(Var^w\) denotes variance conditioned on \(\{w_i\}_{1}^{M}\).

In this section we consider the case where \(p = 2\), and discuss Google’s estimator of \(\phi\) for the sampling distribution of \(4\). Consider \(w_1, \ldots, w_M\) defined as before by \(w_i = z_i / \sum_{j=1}^{M} z_j\) with iid \(z_i \sim \text{Exp}(1)\). Let \(\tilde{w}_1, \ldots, \tilde{w}_N\) be a sample (with replacement) of \(N\) values of \(w_i\) that are sampled according to the mixture probabilities

\[
\pi(w_i) = \phi w_i + (1 - \phi)/M. \tag{11}
\]

Google’s estimator \(\tilde{\phi}\) of \(\phi\) becomes in our notation

\[
U = \frac{1}{N} \sum_{j=1}^{N} M \tilde{w}_j - 1. \tag{12}
\]

We now compute its expectation and variance conditioned on \((w_1, \ldots, w_M)\). The latter vector has the Dirichlet distribution; however, the calculations that follow require only condition on moments up to order 4. Put \(w^{(k)} = \sum_{i=1}^{M} w_i^k\) and note that by \((5)\) we have \(Ew^{(k)} = k!/(M + 1) \cdots (M + k - 1)\) and in particular \(Ew^{(2)} = 2/(M + 1)\).
With expectations being conditional on \( w \) we have, using \( \sum_{i=1}^{M} w_i = 1 \),

\[
E^w M \bar{w}_i = \sum_{i=1}^{M} M w_i [\phi w_i + (1 - \phi)/M] = \phi (M w^{(2)} - 1) + 1
\]

and therefore

\[
E^w U = \phi (M w^{(2)} - 1). \tag{13}
\]

Thus we see that for a given set \( \{w_i\}_1^M \), that is, a given circuit, Google’s estimator \( U \) is biased. Clearly the bias diminishes when \( \phi \to 0 \) and also as \( M \to \infty \); see below. However, the bias does not depend on the sample size \( N \), and therefore as \( N \to \infty \) the estimator \( U \) does not converge to \( \phi \); that is, it is inconsistent.

Google’s estimator \( U \) can be improved and become consistent in \( N \) by adjusting it to be unbiased. Define

\[
V = U/(M w^{(2)} - 1). \tag{14}
\]

An averaged version of \( V \) (that is still biased and hence not consistent) appears in Equation (21) in the Supplement to [2]. We shall see that the unbiased estimator \( V \) has smaller variance than that of \( U \), and thus it is an improvement over \( U \). This estimator requires access to all \( \{w_i\}_1^M \) so that we can compute \( w^{(2)} \) and hence it is not a statistic relative to the sample \( \tilde{w}_1, \ldots, \tilde{w}_N \). Using \( E w^{(2)} = 2/(M + 1) \) and therefore \( E[(M w^{(2)} - 1)] = (M-1)/(M+1) \) we see that the advantage of \( V \) diminishes with \( M \).

Taking expectation over \( \{w_i\}_1^M \) we have

\[
EU = E E^w U = E[\phi (M w^{(2)} - 1)] = \phi \left( \frac{M-1}{M+1} \right) \approx \phi. \tag{15}
\]

Thus, \( U \) is nearly unbiased for large \( M \) when considered over the randomness of \( \{w_i\}_1^M \). If \( U \) is computed from samples taken from different independent sets of \( \{w_i\}_1^M \) (that is, different independent circuits) and the results are averaged, then the resulting average is nearly unbiased for large \( M \); however, as we shall see, the bias of \( U \) for each realization \( \{w_i\}_1^M \) makes its variance larger than that of \( V \).

To obtain the variance we compute \( E^w M^2 \bar{w}_i^2 = M^2 \sum_{i=1}^{M} w_i^2 [\phi w_i + (1 - \phi)/M] = \phi (M^2 w^{(3)} - M w^{(2)}) + M w^{(2)} \). Therefore,

\[
Var^w U = \frac{1}{N} Var^w (M \bar{w}_i) \\
= \frac{1}{N} \left[ \phi (M^2 w^{(3)} - M w^{(2)}) + M w^{(2)} - (\phi (M w^{(2)} - 1) + 1)^2 \right] \\
= \frac{1}{N} \left[ \phi (M^2 w^{(3)} - 3M w^{(2)} + 2) - \phi^2 (M w^{(2)} - 1)^2 + M w^{(2)} - 1 \right]. \tag{16}
\]

Taking the denominator \( (M w^{(2)} - 1) \) of (14) into account we obtain

\[
Var^w (V) \\
= \frac{1}{N(M w^{(2)} - 1)^2} \left[ \phi (M^2 w^{(3)} - 3M w^{(2)} + 2) - \phi^2 (M w^{(2)} - 1)^2 + M w^{(2)} - 1 \right]. \tag{17}
\]

Given all \( \{w_i\}_1^M \) of a given circuit, or just \( w^{(2)} \) and \( w^{(3)} \), the quantities of (16) and (17) can be computed.
Under the moment conditions of (5) we have $w^{(2)} \approx 2/M$ and $w^{(3)} \approx 6/M^2$ (where the approximation is in the sense that the ratio of the two sides converges to 1 as $M \to \infty$), and therefore

$$Var^w(U) \approx Var^w(V) \approx \frac{1}{N}(2\phi - \phi^2 + 1). \quad (18)$$

The difference between the two estimators $U$ and $V$ is that $V$ is unbiased and $U$ is not, and the overall (unconditional) variance of $U$ depends also on $Var(E^wU)$, which we discuss next.

Equation (18) provides $Var^w(U)$, the conditional variance of $U$ of (12). Recalling the Pythagorean formula, aka as the law of total variance, we have (for any $U$)

$$Var(U) = EVar^w(U) + Var(E^w(U)), \quad (19)$$

and given the fact that $V$ is conditionally unbiased, that is, $E^w(V) = \phi$ we conclude by (18) that

$$Var(V) = EVar^w(V) \approx \frac{1}{N}(2\phi - \phi^2 + 1). \quad (20)$$

The situation with $U$ is different and in view of (19) we have to compute $Var(E^wU)$. We have by (5) $Var(w_i^2) = Ew_i^4 - (Ew_i^2)^2 \approx 4M^4 - (2M^2)^2 = 12M^4$. By (13) we have $Var(E^wU) = Var[\phi(Mw^{(2)} - 1)] \approx 12\phi^2/M$. From (19) and (18) we conclude that the overall variance of $U$ is

$$Var(U) \approx \frac{1}{N}(2\phi - \phi^2 + 1) + 12\phi^2/M. \quad (21)$$

This variance does not decrease to zero when the sample size $N \to \infty$, and hence $U$ as a function of $N$ is not a consistent sequence of estimators. If $M$ and $N$ are of similar order, the term $12\phi^2/M$ may matter and $U$ will be inferior to $V$ (and to the MLE as shown later). This may happen if one extrapolates from relatively small circuits, that is, small $M$. When $n = 53$, the number of qubits in Google’s ultimate quantum computer, and when $N$ is of order $10^6$, a typical sample size in Google’s experiment, that term is unlikely to matter.

The variances of $V$ and $U$ given in (20) and (21) are approximations to the respective expected variances when $\{w_i\}_{i=1}^M$ are considered random with the first four moments corresponding to the Dirichlet distribution. Suppose we have $L$ estimators $V_1, \ldots, V_L$ arising from different circuits having a common fidelity $\phi$. Then for $V = \frac{1}{L} \sum_{\ell=1}^LV_\ell$ we have $EV = \phi$ and by (20) $Var(V) \approx \frac{1}{LN}(2\phi - \phi^2 + 1)$. A similar result holds for $U, \text{ where from (15) we obtain for } U = \frac{1}{L} \sum_{\ell=1}^LU_\ell \text{ that } EU = \phi$ and by (21) $Var(U) \approx \frac{1}{LN}(2\phi - \phi^2 + 1) + \frac{12}{LM}\phi^2$. These results will be used in Section 7 for constructing approximate confidence intervals.

4.3 Maximum likelihood estimation of $\phi$

The likelihood function of the sample $\tilde{w}_1, \ldots, \tilde{w}_N$ is given by the product $\prod_{i=1}^N(\phi\tilde{w}_i + (1 - \phi)/M)$ and the MLE of $\phi$ is obtained by maximizing it with respect to $\phi$. It is easy to see that this can be done by equating the derivative of the log-likelihood to zero; that is, the MLE is the solution in $\phi$ to the equation

$$f(\phi) := \frac{\partial}{\partial \phi} \sum_{i=1}^N \log(\phi\tilde{w}_i + (1 - \phi)/M) = \sum_{i=1}^N \frac{\tilde{w}_i - 1/M}{\phi\tilde{w}_i + (1 - \phi)/M} = 0. \quad (22)$$
An algorithm for the solution will be given below. The MLE for several different circuits together is considered in the Supplement to [2] (20).

We now discuss the variance of the MLE. Under the present conditions, it is well known that the asymptotic (in \(N\)) variance of the MLE is given by \(1/J(\phi)\), where \(J(\phi)\) is the Fisher information, which is the expectation, conditioned on \(\{w_i\}_1^M\), of the second derivative of the log-likelihood function with a negative sign. See, e.g., [11] Chapter 6, Theorem 3.10. We have

\[
J(\phi) = \sum_{i=1}^N \frac{(\tilde{w}_i - 1/M)^2}{(\phi\tilde{w}_i + (1 - \phi)/M)^2}.
\]

In view of (19) we need to consider the unconditional variance, is the same as in (24). We have,

\[
Var^w(MLE) = \frac{1}{N \int_0^\infty \frac{(z-1)^2}{\phi z + 1 - \phi} e^{-z} dz}.
\]

In view of (19) we need to consider \(Var[\hat{E}^w(MLE)]\). In our case the variables, the log-likelihood, and its derivatives are all bounded and therefore \(\hat{E}^w[(MLE) - \phi] = O(1/N)\) (see, e.g., [4] Section 9.2) and therefore its variance is of order \(O(1/N^2)\), which we neglect, and our approximation for \(Var(MLE)\), the unconditional variance, is the same as in (24).

If we have \(L\) different independent MLE estimators, denoted by MLE\(_\ell\), arising either from the same or from several circuits assuming they have a common \(\phi\), we can define \(\bar{MLE} = \frac{1}{L} \sum_{\ell=1}^L MLE\(_\ell\). We then have

\[
Var(MLE) \approx \frac{1}{LN \int_0^\infty \frac{(z-1)^2}{\phi z + 1 - \phi} e^{-z} dz}.
\]

We next provide explicit formulas for the Newton–Raphson algorithm for computing the MLE. This requires computations of

\[
J(\phi) = \sum_{i=1}^N \frac{\log(\phi\tilde{w}_i + (1 - \phi)/M)}{(\phi\tilde{w}_i + (1 - \phi)/M)^2}.
\]

With \(f(\phi)\) of (22) the Newton–Raphson iterations are given by

\[
\phi_{k+1} = \phi_k - f(\phi_k)/J(\phi_k).
\]

To see the relation between the MLE and Google’s estimator \(U\) of (12) we write a first order Taylor expansion of the function \(f(\phi)\) of (22) at \(\phi = 0\) to obtain

\[
f(\phi) \approx \sum_{i=1}^N \frac{\tilde{w}_i - 1/M}{\phi\tilde{w}_i + (1 - \phi)/M} = M \sum_{i=1}^N (\tilde{w}_i - 1/M) - \phi M^2 \sum_{i=1}^N (\tilde{w}_i - 1/M)^2.
\]
By (11) we have

\[ M^2 \frac{1}{N} \sum_{i=1}^{N} (\tilde{w}_i - 1/M)^2 \approx M^2 E(\tilde{w}_i - 1/M)^2 = M^2 \sum_{i=1}^{M} (w_i - 1/M)^2 \left( \phi w_i + (1 - \phi)/M \right), \]

and for \( \phi = 0 \) the latter expression equals \( M w(2) - 1 \approx 1 \) for large \( M \) under the assumptions that lead to (5). Setting \( f(\phi) = 0 \) in the above Taylor expansion and solving for \( \phi \), we obtain that the solution is approximately equal to \( \frac{1}{N} \sum_{i=1}^{N} M \tilde{w}_i - 1 \), which is Google’s estimator \( U \). Thus, \( U \) is an approximation to the MLE for small values of \( \phi \) and large \( M \).

4.4 Estimator comparisons

We compare the unconditional variances of the estimators \( U \), \( V \), and MLE for \( N = 500,000 \), \( M = 2^{12} - 2^{28} \), and \( 0 \leq \phi \leq 1/2 \) according to the formulas

\[ \text{Var}(U) \approx \frac{1}{N} (2\phi - \phi^2 + 1) + \frac{12\phi^2}{M}, \quad \text{Var}(V) \approx \frac{1}{N} (2\phi - \phi^2 + 1), \]

\[ \text{Var}(\text{MLE}) \approx \frac{1}{N} \int_{0}^{\infty} \frac{(z-1)^2}{\phi z+1-\phi} e^{-z} dz. \]

The variance are given as a function of \( \phi \) in Figure 2. Note that the units in the y-axes change between plots. Consider the following numerical example: for \( M = 2^{18} \), and \( \phi = 0.15 \) we have that \( \text{Var}(V) \) based on \( N = 356,000 \) equals \( \text{Var}(U) \) based on \( N = 500,000 \), and so \( V \) entails a reduction by more than 30% in the required sample size to achieve the same variance or confidence interval width.

In Figure 3 we generated files \( \{w_i\}_1^M \) with \( M = 2^{12}, 2^{14}, \) and \( 2^{16} \), from the Dirichlet distribution, and sampled from them using (4) with \( \phi = 0.3862, 0.3320, \) and \( 0.2828 \), respectively (indicated by orange dashed lines), and \( N = 500,000 \). The above values of \( \phi \) correspond to values computed in [2] for similar data sets. We averaged the estimator over 10 files for each \( M \), as done in [2]. This was repeated 500 times. We know that the MLE and \( V \) are unbiased even without averaging, whereas \( U \) is biased. The boxplots below show that the average value of \( U \) over 10 files has a small bias, but its variance is larger than that of the other two estimators.

We next present comparisons of MLE, \( U \), and \( V \) conditional on \( \{w_i\}_1^M \), that is, for given circuits. This is demonstrated on Google’s data sets. In Figure 4 we took 10 files \( \{w_i\}_1^M \) of size \( M = 2^n = 2^{14} \) which we computed from Google’s data as follows. Google provided samples of size \( N = 500,000 \) for each of 10 circuits of \( n \) qubits, for various values of \( n \). For \( n = 12 \) and 14 this allowed us to reconstruct the whole sets \( \{w_i\}_1^M \) associated with these circuits. These reconstructed files will be used several times below. As before, we sampled \( N = 500,000 \) values from \( \{w_i\}_1^M \) according to (4) with \( \phi = 0.3320 \) (indicated by the dashed orange line) from each of the 10 files with \( n = 14 \). This was repeated 100 times for each of the 10 files. The dotted green line represents Google’s estimate \( U \) of the fidelity which we computed for each file. The boxplots show the MLE, \( U \), and \( V \) for 100 values each.

We see that if the true fidelity is 0.3320 as suggested by Google, then their estimate is off target in each case, but only by 5% or less. There are at least two possible explanations: first, we know that \( U \) is biased. For some of the files Google’s estimator is within the range of our simulated \( U \)’s, but for others it is not, suggesting that another explanation is needed. A possible explanation is that the theoretical number \( \phi = 0.3320 \) is not exactly the actual \( \phi \) that generated the sample. When we compute Google’s
Figure 2. Variances of MLE, $U$, and $V$ as a function of $\phi$.

$U$ we see that indeed for each of the 10 files it is biased, and as expected the bias can be upward or downward, depending on the particular $\{w_i\}_1^M$. On the other hand, the MLE and $V$ are always right on target, which is no surprise as they are unbiased for each given set $\{w_i\}_1^M$, and $N$ is large.

Figure 5 is similar to Figure 4 where the only difference is that we sampled with the value of the average MLE over the 10 files (indicated by a dashed turquoise line), rather than a theoretical $\phi$. In Figure 6 we calculated the MLE of each of the 10 files separately, and used it as $\phi$ for the simulation based on (4). This is the most accurate way to simulate Google-like experiments based on the full list of probabilities $\{w_i\}_1^M$. Figure 6 suggests that the fidelity varies only slightly between circuits, and that the MLE represents the actual value of $\phi$ for each circuit.

4.5 Further analysis of Google's estimator

Although the MLE is in general better than $U$, it is of interest to consider explicit estimators like $U$. We next show that Google's choice of $U$ is best in the sense of minimizing the variance as $\phi \to 0$ in a class of linear estimators defined below, while for larger values of $\phi$ another estimator, also discussed in [2], is better. Some of these results, which motivated their choice of $U$, are reported in the Supplement to [2]. We have the following somewhat informal proposition:
Figure 3. Boxplots of 500 averages of MLE, $U$ and $V$

Figure 4. Boxplots of 100 value MLE, $U$ and $V$, with $\phi$ as stated in [2]

**Proposition 4.1.** Among all linear unbiased estimators of the form
\[
U_g := \frac{1}{N} \sum_{j=1}^{N} g(\tilde{w}_j) - B/A,
\]
that is, with $A$ and $B$ such that $U_g$ is unbiased, the choice $g(w) = w$ for which $U_g = U$ of (12) minimizes the variance as $\phi \to 0$. For large values of $\phi$ (approximately $\phi > 0.32$) and for $w_i$ obtained as $z_i/\sum_{j=1}^{M} z_j$ with $z_i \sim \text{Exp}(1)$, the choice $g(z) = \log(z)$ yields a better estimator.

**Proof:** Let $W = \frac{1}{N} \sum_j g(\tilde{w}_j)$. We have
\[
E^{w}W = E(W \mid \{w_i\}) = E[g(\tilde{w}_j) \mid \{w_i\}] = \sum_{i=1}^{M} g(w_i)(\phi w_i + (1 - \phi)/M). \tag{25}
\]
Unconditioning, that is, taking expectation in (25) over $w_i$, we have
\[
EW = Eg(\tilde{w}_j) = ME[g(w)(\phi w - 1/M)] + Eg(w) = \phi A + B, \tag{26}
\]
Figure 5. Boxplots of 100 value MLE, $U$ and $V$, with $\phi=$MLE

where $A = ME[g(w)(w - 1/M)]$ and $B = Eg(w)$.

To compute $Var(W) = Var[\frac{1}{N} \sum_i g(\tilde{w}_i)]$, note that conditionally on all the $w$’s, $f(\tilde{w}_i)$ are independent. If $M$ is much larger than $N$ (which holds in the quantum supremacy regime) we can approximately assume that the $f(\tilde{w}_i)$’s are independent. However, a value of $M$ that is not large relative to $N$ results in repetitions in the sampled $\tilde{w}_i$’s, implying positive dependence, and hence assuming independence will lead to underestimation of the variance. More details on the approximation are given at the end of the proof. Assuming $M$ large and hence approximate independence of the sampled $\tilde{w}_i$, we analyze the best approximate choice of $g$ for small $\phi$ first, setting $\phi = 0$. In this case $\tilde{w}_i$ have the same distribution as $w_i$. Using $Var(w) = Ew^2 - (Ew)^2 = 2/M(M + 1) - 1/M^2 = (M - 1)/M^2(M + 1)$ and recalling $A$ from (26) we have for small $\phi$

$$NVar(U_g) \approx \frac{Var[g(w)]}{M^2\{E[g(w)(w - 1/M)]\}^2} \frac{Var[g(w)]Var(w)}{M^2Var(w)\{E[g(w)(w - 1/M)]\}^2} = \frac{(M + 1)}{(M - 1)Corr^2(g(w), w)}.$$  

Thus $Var(U_g)$ is minimized when the correlation takes its maximal value 1, which is equivalent to $g$ being linear.

We now analyze the choice $g(w) = \log(w)$, which is mentioned in [2] and seems natural from the point of view of information and maximum likelihood theory. Using the approximation $w_i = z_i/M$, and assuming $z_i \sim \text{Exp}(1)$ and some calculations given in the Appendix, we have

$$Var(U_{g(w)=\log(w)}) \approx \frac{1}{N}(\pi^2/6 - \phi^2) \approx \frac{1}{N}(1.6449 - \phi^2).$$  (27)

Equation (21) with large $M$ implies

$$Var(U) \approx \frac{1}{N}(2\phi - \phi^2 + 1).$$  (28)
Figure 6. Boxplots of 100 value MLE, $U$ and $V$, $\phi=$average MLE of each file

Note also that the expression in (28) is increasing in $\phi$ and that of (27) is decreasing. They intersect when $\phi = 0.6449/2 = 0.32$. It follows that for small values of $\phi$ Google’s linear estimator of (12), which coincides with $U_9(z)=z$, is better than $U_f(z)=\log(z)$; however, for approximately $\phi > 0.32$ we see that $U_f(z)=\log(z)$ is better in the sense of having a smaller variance.

The results given in (28) and (27) and the comparison between them appear in the Supplement to [2] (without proof and details).

5 The general case of $p$

5.1 Google-type estimator

We now consider sampling according to (2) for a general $p$, that is, $\pi(\tilde{w}_i) = \phi_1\tilde{w}_{i1} + \ldots + \phi_p\tilde{w}_{pi}$. The Google-type estimator is defined by

$$U_k = \frac{1}{N} \sum_{i=1}^{N} (M\tilde{w}_{ki} - 1).$$

Using the fact that $\phi_1 + \ldots + \phi_p = 1$ and $\sum_{i=1}^{M} w_{ki} = 1$, we have

$$E^wU_1 = \sum_{i=1}^{M} (Mw_{1i} - 1)(\phi_1w_{1i} + \ldots + \phi_pw_{pi}) = M\phi_1w_1^{(2)} + M \sum_{k=2}^{p} \sum_{i=1}^{M} \phi_kw_{1i}w_{ki} - 1,$$

where $w_1^{(2)} = \sum_{i=1}^{M} w_{1i}^2$. For small $M$ the estimator is significantly biased and as for $U$ of (12), the bias can be corrected if all $\{w_{ki}\}$ are known (in fact the sum of squares and inner products suffice). For large
we expect $E^wU_1$ to be close to the expectation

$$EU_1 = EE^wU_1 = E[M\phi_1w_1^{(2)} + M\sum_{k=2}^{p} \sum_{i=1}^{M} \phi_kw_{1i}w_{ki}] - 1$$

$$= 2\phi_1M/(M + 1) - \phi_1 = \phi_1 \left(\frac{M - 1}{M + 1}\right),$$

where we assumed that $w_{ki}$ are independent for different $k$'s and satisfy the moment conditions in (5). In fact, it suffices to assume that $Ew_1^{(2)} = 2/(M + 1)$ and $Ew_{ki} = 1/M$. Thus, $U_k$ is asymptotically unbiased in $M$.

5.2 Maximum likelihood estimation

The log likelihood of the sample (ignoring constants) is

$$\ell(\phi) = \sum_{i=1}^{N} \log(\phi_1\tilde{w}_{1i} + \ldots + \phi_p\tilde{w}_{pi}) = \log[\phi_1(\tilde{w}_{1i} - \tilde{w}_{pi}) + \ldots + \phi_{p-1}(\tilde{w}_{(p-1)i} - \tilde{w}_{pi}) + \tilde{w}_{pi}].$$

The maximum likelihood estimator of $\phi = (\phi_1, \ldots, \phi_p)$ such that $\phi_1 + \ldots + \phi_p = 1$ is obtained by computing the gradient $f(\phi)$ (also known as the score) and solving the equation

$$f(\phi) = \left(\frac{\partial}{\partial \phi_1} \ell(\phi), \ldots, \frac{\partial}{\partial \phi_{p-1}} \ell(\phi)\right) = 0,$$

where

$$\frac{\partial}{\partial \phi_k} \ell(\phi) = \sum_{i=1}^{N} \frac{\phi_1(\tilde{w}_{1i} - \tilde{w}_{pi}) + \ldots + \phi_{p-1}(\tilde{w}_{(p-1)i} - \tilde{w}_{pi}) + \tilde{w}_{pi}}{\phi_1(\tilde{w}_{1i} - \tilde{w}_{pi}) + \ldots + \phi_{p-1}(\tilde{w}_{(p-1)i} - \tilde{w}_{pi}) + \tilde{w}_{pi}}. \quad (31)$$

Starting with root-N consistent estimators such as the moment estimators described above, we compute the MLE’s by the Newton–Raphson algorithm. As mentioned before, asymptotically, one iteration suffices. To describe the Newton-Raphson iteration, form the $p-1 \times p-1$ Hessian matrix $J(\phi))$ whose $j,k$th entry is

$$J_{jk}(\phi) = \frac{\partial^2}{\partial \phi_j \partial \phi_k} \sum_{i=1}^{N} \log[\phi_1(\tilde{w}_{1i} - \tilde{w}_{pi}) + \ldots + \phi_{p-1}(\tilde{w}_{(p-1)i} - \tilde{w}_{pi}) + \tilde{w}_{pi}]$$

$$= -\sum_{i=1}^{N} \frac{(\tilde{w}_{ji} - \tilde{z}_{pi})(\tilde{w}_{ki} - \tilde{w}_{pi})}{[\phi_1(\tilde{w}_{1i} - \tilde{w}_{pi}) + \ldots + \phi_{p-1}(\tilde{w}_{(p-1)i} - \tilde{w}_{pi}) + \tilde{w}_{pi}]^2}$$

for $1 \leq j, k \leq p - 1$. The Newton–Raphson iteration can now be written as

$$\phi_1 = \phi_0 - f(\phi_0)J^{-1}(\phi_0).$$
6 Refined noise models and readout errors

Recall that Google’s notation $P(x^{(i)}) = w_i$ is the (random) probability of observing the bitstring $x^{(i)}$ ($i = 1, 2, \ldots, M$) in the noiseless situation, namely, when $\phi = 1$. The actual values $w_i$ depend on the quantum circuit $C$ and they are modeled to behave as independent $\text{Exp}(1)$ random variables normalized by their sum (that is, as a Dirichlet distribution). We write $P_C(x^{(i)})$ instead of $P(x^{(i)})$, to indicate the dependence on the quantum circuit $C$. When the fidelity $\phi < 1$, Google’s basic noise model (4) is

$$\phi P_C(x^{(i)}) + (1 - \phi)/M.$$  

We can expect a refined description of the noise of the form

$$\phi P_C(x) + (1 - \phi)N_C(x),$$  

where $N_C(x)$ is a small fluctuation of the uniform distribution that depends on the circuit $C$. In this section we describe a more detailed noise model for the effect of readout errors when there are no gate errors. This formula will allow us to offer statistical estimators of the probability that no gate errors occur.

6.1 A readout noise model

We consider a refined version of Google’s model that treats carefully the effect of readout errors. (Readout errors are discussed in the Supplement to [2] Section VI.D.) For this study we define the total gate fidelity $\phi_g$ as the probability that no errors occurred in the gate operations. Two crucial ingredients of the Google experiment are the prediction of the fidelity (7) based on the fidelities of the individual components, and the statistical estimator (9) of the fidelity based on the experimental bitstrings. A major discovery of the Google’s experiment is the very close agreement between the predicted fidelity via (7) and the experimental outcomes. The statistical assumptions that allow good predictions of the fidelity also allow prediction of the total gate fidelity $\phi_g$, and a simple extension of the Google estimator allows an estimation of $\phi_g$ from the experimental bitstrings. This is discussed in this section.

We need to consider first how to estimate $\phi_g$ from Equation (7), and then how to estimate $\phi_g$ from the experimental bitstrings. Our first task is easy. Equation (7) (Google’s Formula (77)) gives us an approximate description of the total gate fidelity $\phi_g$ via its relation with the fidelity $\phi$:

$$\phi = \phi_g \cdot \prod_{q \in Q} (1 - e_q).$$  

In this section we use a further simplification based on (8) $\phi = \phi_g (1 - 0.038)^n$, where $n$ is the number of qubits. Let $\phi_{ro} = \phi_g - \phi$ be the probability that there are no gate errors but there are some readout errors.

We now discuss the estimation of $\phi_g$ based on the experimental bitstrings, a task that fits our general framework. As before, the quantum circuit $C$ defines a probability $P_C(x^{(i)}) = w_i$, also denoted by $w_{x^{(i)}}$, $i = 1, \ldots, M = 2^n$, where $x^{(i)} \in \{0, 1\}^n$. The Hamming distance between such strings is relevant to the nature of noise considered in this section. Assuming that in the computation process there are no gate errors, we can observe a bitstring $x$ in two ways:

1. Reading the output without error, and therefore observing $x$ with probability $P_C(x) = w_x$, or
2. Observing $x$ because the true output is $x \oplus y$ for some $y$, an event whose probability is $P_C(x \oplus y)$ (where $\oplus$ denotes the XOR operation, that is, mod-2 addition) and then reading errors occur exactly in the coordinate $i$ in which $y_i = 1$, an event whose probability is $q^{y_i}(1 - q)^{n - |y|}$, where $q$ is the probability of an individual reading error.

We assume independent errors with a common probability $q$, and so the components of $y$ are iid Bernoulli($q$) and the probability of $y$ is defined as $B_q(y) := B_q(|y|) = q^{|y|}(1 - q)^{n - |y|}$. We can take $q = 0.038$; see Equation (8) and [2]. Let $D := P(y \neq 0) = \sum_{|y| \neq 0} B_q(y) = 1 - (1 - q)^n$, and let $N_C^{x}(x)$ denote the probability of observing $x$ due to the second reason, conditioned on the existence of readout errors only (and no gate errors). Then

$$N_C^{x}(x) = \frac{1}{D} \sum_{y \in \{0,1\}^n, y \neq 0} P_C(x \oplus y)B_q(y) = \frac{1}{D} \sum_{y \in \{0,1\}^n, y \neq 0} w_{x \oplus y}B_q(y). \quad (33)$$

We consider the noise model for the quantum circuit $C$ in which a sample of size $N$, $\tilde{x}_1, \ldots \tilde{x}_N$ of $n$-strings is obtained by drawing $x^{(i)}$’s independently $N$ times with probabilities given by (see (2) and (3))

$$\pi(\tilde{x}^{(i)} = x) = \phi P_C(x) + \phi_{ro} N_C^{x}(x) + (1 - \phi_g)/M, \quad i = 1, \ldots, N, \ x \in \{0,1\}^n. \quad (34)$$

This is a refinement of Google’s basic model (4), offering a more detailed description of the sampling probability when there are only readout errors and no gate errors. When there are gate errors, we still assume that the read outcome has the uniform distribution. As explained already in [2] and in the previous sections, such a noise model will not make a difference for estimating $\phi$, but it will give us an opportunity to estimate $\phi_{ro}$.

Using the notation $v_i := \sum_{|y| \neq 0} w_{x^{(i)} \oplus y}B_q(y)/D$ we have $\sum_{i=1}^{M} v_i = 1$, and recalling that $P_C(x^{(i)}) = w_{x^{(i)}} = w_i$, it is easy to see that Equation (34) is equivalent to sampling $N$ times (with replacement) with probabilities

$$\pi(x^{(i)}) = \phi w_i + \phi_{ro} v_i + (1 - \phi_g)/M, \quad i = 1, \ldots, M. \quad (35)$$

6.2 Estimating the total gate fidelity

Let $\tilde{x}^{(i)}$ denote an observation, $i = 1, \ldots, N$, corresponding to $(\tilde{z}_i, \tilde{v}_i)$ where $\tilde{v}_i = \sum_{|y| \neq 0} w_{\tilde{x}^{(i)} \oplus y}B_q(y)/D$. To estimate $\phi_g$ or $\phi_{ro}$, define a Google-type estimator

$$W = \frac{M}{N} \sum_{i=1}^{N} \tilde{v}_i - 1, \quad Y = \frac{M}{N} \sum_{i=1}^{N} \tilde{w}_i - 1,$$

Note that $W$ is not a statistic relative to the sampling defined in (34)–(35) since it requires knowledge of all $P_C(x^{(i)}) = w_i$ and not just those in the sample. Taking expectation of $W$ with respect the sampling probabilities of (35) conditioned on $\{w_i\}_{1}^{M}$ and $\{v_i\}_{1}^{M}$ we have using $\phi_g = \phi + \phi_{ro}$

$$E^w W = M \phi \sum_{i=1}^{M} v_i w_i + M \phi_{ro} \sum_{i=1}^{M} v_i^2 - (\phi + \phi_{ro}),$$

$$E^w Y = M \phi \sum_{i=1}^{M} w_i^2 + M \phi_{ro} \sum_{i=1}^{M} w_i v_i - (\phi + \phi_{ro}).$$
For given \( \{w_i\}_1^M \) and \( \{v_i\}_1^M \) it is easy to see that \( W \) and \( Y \) are averages of iid variables, and hence they are consistent estimators of their expectations. The method of moments (see Section 4.1) applied here means replacing \( EW \) by the statistic \( W \) and \( EwY \) by \( Y \) in the above two equations and solving the resulting linear system for \( \phi \) and \( \phi_{ro} \).

We next consider \( EW = EEwW \). Define \( C := [q^2 + (1-q)^2]^n - 2(1-q)^n + 1 \), and recall that \( D = 1 - (1-q)^n \). In the Appendix we explain the approximation for large \( M \)

\[
EW \approx \phi_{ro}[C/D^2 - 1],
\]

and therefore the estimator

\[
\tilde{\phi}_{ro} := \frac{1}{C/D^2 - 1} W
\]

is unbiased for \( \phi_{ro} \) when expectation is taken with respect to the sampling in (35) and also with respect to all \( \{w_i\}_1^M \) and \( \{v_i\}_1^M \), that is, in the same sense that Google’s \( U \) is unbiased.

### 6.3 MLE of \( (\phi, \phi_{ro}) \)

We rewrite the sampling rule (35) as

\[
\pi(x^{(i)}) = \phi(w_i - 1/M) + \phi_{ro}(v_i - 1/M) + 1/M, \quad i = 1, \ldots, M.
\]

The log-likelihood function is

\[
\ell(\phi) = \sum_{i=1}^{N} \log[\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M].
\]

The maximum likelihood estimator of \( \phi = (\phi, \phi_{ro}) \) is obtained by computing the gradient \( f(\phi) \) and solving the equation \( f(\phi) = \left( \frac{\partial}{\partial \phi} \ell(\phi), \frac{\partial}{\partial \phi_{ro}} \ell(\phi) \right) = 0 \), where

\[
\frac{\partial}{\partial \phi} \ell(\phi) = \sum_{i=1}^{N} \frac{(\tilde{w}_i - 1/M)}{\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M}
\]

and

\[
\frac{\partial}{\partial \phi_{ro}} \ell(\phi) = \sum_{i=1}^{N} \frac{(\tilde{v}_i - 1/M)}{\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M}.
\]

Starting with root-N consistent estimators such as the moment estimators described above, we approach the MLE’s by the Newton–Raphson algorithm. As mentioned before, asymptotically, one iteration suffices. To describe the Newton–Raphson iteration, form the \( 2 \times 2 \) Hessian matrix \( J(\phi) \) whose \( jk \)th entry is

\[
J_{jk}(\phi) = -\sum_{i=1}^{N} \frac{(\tilde{w}_i - 1/M)(\tilde{v}_i - 1/M)}{[\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M]^2}
\]

for \( 1 \leq j \neq k \leq 2 \),

\[
J_{11}(\phi) = -\sum_{i=1}^{N} \frac{(\tilde{w}_i - 1/M)^2}{[\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M]^2},
\]

and

\[
J_{22}(\phi) = -\sum_{i=1}^{N} \frac{(\tilde{v}_i - 1/M)^2}{[\phi(\tilde{w}_i - 1/M) + \phi_{ro}(\tilde{v}_i - 1/M) + 1/M]^2}.
\]


The Newton–Raphson iteration can now be written as
\[
\phi_1 = \phi_0 - f(\phi_0) J^{-1}(\phi_0).
\]

We estimated \( \phi \) and \( \phi_{ro} \) under the sampling model (34) - (35) for ten Google files for \( n = 12 \) and sample size \( N = 500,000 \). For these files formula (7) gives \( \phi = 0.3862 \). The average of the MLE estimates of the pair \((\phi, \phi_{ro})\) over the ten files is \((0.3687, 0.1958)\). The average MLE computed as in Section 4.3 with sampling according to (4) came out the same value 0.3687, and individual estimates in the ten files differed slightly in the third and fourth digit after the decimal point when estimated according to the two models.

### 6.4 Related noise models

We remark briefly on other noise models. In (33) the random noises \( \mathcal{N}_C^{ro}(x) \) for different \( x \)'s are dependent, with stronger dependence between \( x \)’s that are close together in the Hamming distance. Since for a fixed \( x \) the summands composing the error \( \mathcal{N}_C^{ro}(x) \) are independent (with weights) it is approximately normal for large \( n \). A Gaussian assumption simplifies the dependence structure across \( x \)’s and allows further calculations. One can also consider replacing the Binomial distribution \( B_y(y) \) in (33) by another, for example, a distribution that is supported only on \( |y| \leq k \), thus considering neighbors of \( x \) having Hamming distance \( \leq k \), with, say, \( k = 1 \) or 2 or so. (This seems a good approximation and will simplify the necessary computations.) In [8] it is suggested that replacing the Binomial distribution with a mixture of Binomial distributions (more specifically, with a Curie–Weiss distribution) could give a good description of the total effect of gate errors for random quantum circuits. (Such a mixture will introduce a strong positive correlation between errors.)

Finally, as it turns out, for the actual readout errors of the Google device the probability \( q_1 \) that 1 is read as 0 is 0.055 and the probability \( q_2 \) that 0 is read as 1 is 0.023. This leads to the following sampling model

\[
\pi(x) = \phi_g \sum_{y \in \{0,1\}^n} \mathcal{P}_C(x \oplus y) q_1^a q_2^b (1 - q_1)^c (1 - q_2)^d + (1 - \phi_g) B_y(x),
\]

where \( q_1 = 0.055, q_2 = 0.023, a = \{|i : y_i = 1 \text{ and } x_i = 0\}|, b = \{|i : y_i = 1 \text{ and } x_i = 1\}|, c = \{|i : y_i = 0 \text{ and } x_i = 1\}|, d = \{|i : y_i = 0 \text{ and } x_i = 0\}|, \) and as before, \( B_y(x) := B_y(|x|) = q^{|x|}(1 - q)^{n-|x|} \), where now \( q = (1 - q_1 + q_2)/2 = 0.484 \).

The first term of (39) represents the distribution conditioned on no gate errors. To see it note, for example, that if \( y_i = 1 \text{ and } x_i = 0 \), then without a reading error \( 1 = 0 \oplus 1 \) appears; it will be read as 0 (the \( i \)th coordinate of \( x \)) if a reading error from 1 to 0 occurs, which happens with probability \( q_1 \) (corresponding to case a). We continue to assume that the effect of gate errors is to replace the desired distribution with a uniform probability but the asymmetric readout errors make a difference also there. If uniformly distributed \( n \)-vectors are read with errors such that 1 is read as 0 with probability \( q_1 = 0.055 \) and 0 is read as 1 with probability \( q_2 = 0.023 \) then their distribution is no longer uniform. Instead, for each coordinate the probability of 1 becomes \((1 - 0.055)/2 + 0.023/2 = 0.484\), and the probability of 0 is 0.516.

When \( n = 12 \) we have from (7) \( \phi = 0.3862 \) and then \( \phi_g = \phi/(1 - 0.038)^{12} = 0.6148 \). Using ten Google samples of size \( N = 500,000 \) with \( n = 12 \) the average MLE of \( \phi_g \) is 0.5880.
We also computed the MLE, regarding \((\phi, q_1, q_2)\) as parameters, and obtained for Google’s file 1 the estimates \((0.5571, 0.0465, 0.0196)\). Thus our estimate of \(\phi\) and the value derived from (7) are all within at most 10% of each other, while our estimates of \(q_i\) differ from Google’s numbers by about 15%.

The chi-square goodness of fit statistics for the different models is discussed in Section 8. It will be interesting to compute the estimators for \(\phi\) for larger values of \(n\), and also to refine our study based on the readout errors for individual qubits.

### 7 Confidence intervals

In this section we compute confidence intervals for \(\phi\) for the three estimators discussed in Section 4. We start with the unbiased estimator defined in (14),

\[
\bar{V} = \left[ \frac{1}{N} \sum_{j=1}^{N} M \tilde{w}_j - 1 \right] / (M w^{(2)} - 1) .
\]

For the computation of \(V\), knowing the sample values \(\{\tilde{w}_i\}_1^N\) is not enough and it requires knowledge of \(w^{(2)}\), which is a function of \(\{w_i\}_1^M\). This differs from computing \(U\) and the MLE, which are functions of \(\{\tilde{w}_i\}_1^N\), and hence statistics. As mentioned before, this distinction is relevant if for some reason only the sample \(\{\tilde{w}_i\}_1^N\) is available, and this holds for some of Google’s data; however, in principle, computing a single \(w_i\) or all of them is of the same order of complexity, and so this distinction boils down to a matter of what data was actually stored. The variance of \(V\) conditional on the realization \(\{w_i\}_1^M\) is given in (17). We denote it now by

\[
\sigma_N^2(V; \phi, w^{(2)}, w^{(3)}) = \frac{1}{N(M w^{(2)} - 1)^2} \left[ \phi(M^2 w^{(3)} - 3M w^{(2)} + 2) - \phi^2(M w^{(2)} - 1)^2 + M w^{(2)} - 1 \right].
\]

We assume that the realization \(\{w_i\}_1^M\) is known, and therefore so are \(w^{(2)}\) and \(w^{(3)}\). If in a simulation \(\phi\) is known, and we study the distribution of the estimator \(V\), then we can use the known \(\phi\) in computing \(\sigma_N^2(V) = \sigma_N^2(V; \phi, w^{(2)}, w^{(3)})\). If \(\phi\) is unknown, it is standard practice to plug in an estimator, such as \(\bar{V}\) itself. Thus we assume that \(\sigma_N(V; \phi, w^{(2)}, w^{(3)})\) is given. Since \(V\) is based on a sum of iid variables it is asymptotically normal, and a standard 95% confidence interval is

\[
\phi \in \bar{V} \pm 1.96 \sigma_N(V; \phi, w^{(2)}, w^{(3)}).
\]

The normal and plug-in approximations suggest rounding 1.96 to 2 in general; we will keep 1.96 only because of its connotation. This is a *conditional* (on the realization \(\{w_i\}_1^M\)) confidence interval.

Suppose now that we have \(L\) independent samples, all taken under the same \(\phi\) according to (4). These samples may arise from a single realization \(\{w_i\}_1^M\) or from several different ones, all known. We now assume that \(\phi\) is unknown. We have estimates \(V_1, \ldots, V_L\), and a natural approach is to first estimate \(\phi\) by \(\bar{V} = \frac{1}{L} \sum_{i=1}^{L} V_i\) and plug it in to obtain variances estimates \(\sigma_{N_1}^2(V_1), \ldots, \sigma_{N_L}^2(V_L)\). We then replace \(\bar{V}\) by the variance-minimizing convex combination of the estimators \(\overline{\bar{V}} = \sum_{i=1}^{L} \frac{V_i}{\sigma_{N_i}^2(V_i)} / \sum_{i=1}^{L} \frac{1}{\sigma_{N_i}^2(V_i)}\), whose variance is \(\frac{1}{\sum_{i=1}^{L} 1/\sigma_{N_i}^2(V_i)}\). This process can be iterated, that is, plug in \(\overline{\bar{V}}\) to reestimate the variances, etc.; however, we will not pursue this. We obtain the conditional confidence interval

\[
\phi \in \overline{\bar{V}} \pm 1.96 \sqrt{\frac{1}{\sum_{i=1}^{L} 1/\sigma_{N_i}^2(V_i)}},
\]

28
where in $\sigma^2_N(V_i) = \sigma^2_{N_i}(V_i; \phi, w^{(2)}_i, w^{(3)}_i)$ we set $\phi = \bar{V}$.

Consider now the maximum likelihood estimator MLE discussed in Section 4.3. To compute the MLE, as well as $U_i$, only the sample values $\{\tilde{w}_i\}_N$ are needed. We can repeat all the above steps and obtain the same kind of confidence intervals as in (40) and (41) by now replacing $V$ by the MLE and $\sigma^2_N(V; \phi, w^{(2)}_i, w^{(3)}_i)$ by

$$
\sigma^2_N(\text{MLE}; \phi, w^{(2)}_i, w^{(3)}_i) = 1/N \sum_{i=1}^M (w_i - 1/M)^2 / [\phi w_i + (1 - \phi)/M].
$$

Since Google’s estimator $U$ is conditionally biased, we cannot apply to it the same procedure to obtain a conditional confidence interval. Unconditional confidence intervals are discussed next.

We can also consider the above estimators when both $\{\tilde{w}_i\}_N$ and $\{w_i\}_N$ are considered random, and we do not condition on them. We refer to intervals as *unconditional*. This seems to be the approach taken by Google [2]. In this case all these estimators are practically unbiased (for large $M$) and their (approximate) variances are given in (20) and (24) (where the approximate conditional and unconditional variances are the same as discussed in Sections 4.2 and 4.3) and in (21), where the variance reflects the conditional bias of $U$.

As above, we consider $L$ samples from $L$ different circuits with the same parameter and the same $\phi$, and $L$ estimators of $\phi$. In this case Google’s approach is to average these estimators and obtain the confidence interval

$$
\phi \in \bar{U} \pm 1.96 \sqrt{1/LN} (2\phi - \phi^2 + 1) + \frac{1}{LM} \phi^2 12,
$$

(42)

where $\bar{U} = \frac{1}{L} \sum_{\ell=1}^L U_\ell$ is the average of the different estimators. For the estimator $V$ we have in the same way

$$
\phi \in \bar{V} \pm 1.96 \sqrt{1/LN} (2\phi - \phi^2 + 1),
$$

(43)

where $\bar{V} = \frac{1}{L} \sum_{\ell=1}^L V_\ell$, and for the MLE, we have by the results of Section 4.3

$$
\phi \in \text{MLE} \pm 1.96 \sqrt{1/LN} \int_0^\infty \frac{1}{\phi z + 1 - \phi} e^{-z} dz.
$$

(44)

Figure 7 shows confidence intervals computed using (42) and (44) with $L = 10$ and $N = 500,000$ for 10 Google files for each $n$. Note that the scale of the $y$-axis changes with $n$. We see that for $n = 12$ and 14 the estimate $\bar{U}$ (the turquoise dot) is not in the confidence interval around the MLE, and the latter confidence interval is much smaller than that round $\bar{U}$. As $n$ increases the estimates and their confidence intervals get closer.

8 Testing the various distributions based on the data

To demonstrate quantum supremacy, a convincing separation of the fidelity estimator from zero is crucial. But there are various reasons to try to understand the actual state of the quantum computer and the actual probability distribution it represents. There are also various ways, some mentioned in [2], to compare the values $P_C(x)$ for bitstrings obtained in an experiment with the size-biased theoretical
distribution, and this goes beyond the estimator of the fidelity. For small values of \( n \), \( N \) is rather large compared to \( M = 2^n \) and we do have a number of measurements allowing us to reconstruct experimental output probabilities and study them.

Given a sample \( \{\tilde{x}^{(j)}\}, j = 1, \ldots, N \) corresponding to the sample \( \{x^{(i)}\} \) with the sampling rule (2), let \( N_i \) denote the number of sampled bitstrings that equal \( x^{(i)} \), that is, \( N_i = |\{j : \tilde{x}^{(j)} = x^{(i)}\}| \), \( i = 1, \ldots, M \). We have \( \sum_{i=1}^{M} N_i = N \). As explained in Section 1, there is an association between the probabilities and bitstrings \( x^{(i)} \) expressed by \( P(x^{(i)}) = w_i = w_{x^{(i)}} \). Assuming all \( \{w_i\}_1^M \) known, set \( p_i = \phi w_i + (1 - \phi)/M \), \( i = 1, \ldots, M \). Pearson’s chi-square test statistic is

\[
\chi^2 = \sum_{i=1}^{M} \frac{(N_i - N p_i)^2}{N p_i},
\]

and its asymptotic distribution is chi-square with \( M - 1 \) degrees of freedom. The asymptotic is valid for fixed \( N \) and large \( M \). If the sample size \( N \) does not suffice, we can merge cells and probabilities, starting with cells with small \( p_i \). The above test is relevant when we wish to verify the sampling for a given realization \( \{w_i\}_1^M \). We looked at the 10 files given in [2] with \( n = 12 \) and sample size \( N = 500,000 \). Since the sample size is much larger than \( M = 2^n \), we can infer all \( \{w_i\}_1^M \)’s from the sample.

Using these \( w_i \)’s and the MLE of the sample for \( \phi \) we determine \( p_i \) and calculate \( \chi^2 \) for Google’s samples. We obtain very large \( \chi^2 \) values, of the order of 40,000. This is extremely significant and the \( p \)-value is practically zero (since the 0.01 and 0.000001 critical values for \( M - 1 = 4095 \) degrees of freedom are 4308 and 4540, respectively). A rough calculation shows that the average deviation of cells’ empirical probabilities from the theoretical \( p_i \) is about 0.25 standard deviations, and that the \( \chi^2 \) statistic is sufficiently large to reject the model with about a tenth of the sample size used here, and so the large \( \chi^2 \) is not only due to the large sample size. We computed the value of \( \phi \) that minimizes the \( \chi^2 \) statistic in the 10 Google files, and find that it closely agrees with the MLE; hence the large \( \chi^2 \) is not due to our choice of \( \phi \) in determining \( p_i \). The \( \chi^2 \) statistics for the different readout models discussed in Section 6 were smaller by only about 10%, and still extremely significant. We intend to explore further models elsewhere.
We also plot $Np_i$ against the corresponding empirical frequencies, and compare to the same plot for a sample from the same file which we generated using (4) with $\phi = 0.3687$, the MLE estimated from the 10 files combined (which practically coincides with the average of the 10 MLE’s); See Figure 8. One can see with the naked eye that Google’s sample is much more variable than a sample obtained according to the theoretical model. The truncation on the left is due to the fact that $Np_i \geq N(1-\phi)/M = 77$ in present case.

We plotted various histograms of Google’s samples (for which the $X^2$ values were huge) and compared them to simulated samples based on the same $\{w_i\}_{i=1}^M$ and the MLE (for which $X^2$ was around 4000 as expected). Histograms involve smoothing and when we eyeballed these histograms, we could not tell them apart in spite of the large difference in the $X^2$ values values. Such histograms, with 200 cells each, are given in Figure 9. The reader is invited to choose which histogram corresponds to Google’s sample, and which to our simulated sample using (4) with a non-significant $X^2$ value⁶. To understand the theoretical distribution of such samples, recall that in Google’s model $w_i = z_i/\sum_{j=1}^M z_j = \frac{z_i}{\sum_{j=1}^M z_j/M} \approx z_i/M$, where the approximation follows from the fact that $z_j \sim \text{Exp}(1)$ with mean = 1, and so the denominator $\to 1$ as $M \to \infty$. If we approximate the sampling model (4) by $\pi(x^{(i)}) = \pi(z_i) = \phi z_i/M + (1-\phi)/M$ then by Proposition 3.1, the resulting sampled $\tilde{z}_{X_i}$ will be approximately from the distribution with density $\phi z e^{-z} + (1-\phi)e^{-z}$, a mixture of Gamma(2,1), which is the size-biased Exp(1), with Exp(1) itself. This approximation is used in [2].

Similarly, samples obtained by (4) from a Dirichlet vector $w_1, \ldots, w_M$ are expected to have a distri-

---

⁶On the right side Google’s data; on the left a simulated sample.
Figure 9. Histogram of a simulated sample \( \{\tilde{w}_i\}^N_1 \) with \( N = 500,000 \) from \( \{w_i\}^N_1 \) of Google’s file 0 (\( n = 12 \)) according to (4) with \( \phi = 0.3862 \), and histogram of Google’s empirical frequencies. The black curves represent the asymptotic density of (45).

bution that is close to the distribution whose density it a mixture of Beta densities given by

\[
\phi M (M - 1)t(1 - t)^{M-2} + (1 - \phi)(M - 1)(1 - t)^{M-2}.
\]  

(45)

To see this note that the marginal distribution of the Dirichlet vector is Beta(1, \( M-1 \)) with density \((M - 1)(1 - t)^{M-2} \) for \( t \in (0, 1) \). Therefore, the size-biased distribution has the Beta density \( M(1 - t)^{M-2} \), and sampling by (4) implies that the distribution of the sample \( \tilde{w}_1, \ldots, \tilde{w}_N \) should be a discrete distribution (taking values from the set \( \{w_i\}^M_1 \) ) that is close to the above mixture by Proposition 3.1. This is a mixture of Beta distributions, with the first part being the size-biased version of the second (see Section 3).

These two types of analysis can be applied to more general noise models. Also here, we can consider size-biased distribution not only with respect to the Dirichlet or exponential distributions. If a proposed noise model has several ingredients, e.g.,

\[
Q(x) = \phi_1 P_C(x) + \phi_2 N_1(x) + \phi_3 N_3(x) + \cdots,
\]

then given a sample \( \tilde{x}^{(1)}, \ldots, \tilde{x}^{(N)} \), the statistical tools of the previous sections can be used to estimate the different \( \phi_i \)'s, and we can test the distribution of the sample as above for a fixed given realization or over different realizations.

It is important to note that both the fidelity estimators and the size-biased distributions, when examined by standard histograms, are robust to various radical changes of the underlying probability distribution. For example, they will not be affected if we exclude from the sample all strings with an odd number of ones. They will also be robust to various different noise models. Such radical changes will greatly affect the empirical distribution and the outcomes of the chi-square test.

9 Conclusion

The purpose of this paper is to describe and analyze central statistical aspects of the Google quantum supremacy experiment: Google’s estimation of the fidelity and their modeling of the samples generated by the quantum computers.
We study various related fidelity estimators. When the realization of the probabilities $\{w_i\}_1^M$ is given, which is arguably relevant for the Google experiment and sampling based on NISQ computers, then Google’s estimator $U$ is biased in a way that depends on the realization. We study two unbiased estimators, $MLE$ and $V$, that are more suitable for relatively small circuits. As a fidelity estimator of an unknown realization, that is, when $\{w_i\}_1^M$ are considered random (with some assumptions, and expectation is also with respect to this randomness), the estimator $U$ is unbiased but has a larger variance compared to $V$ and the MLE. When the number of qubits increases and the fidelity decreases, the gap between these estimators diminishes and thus our results largely confirm the choice of the estimator chosen by the Google team for large-scale circuits.

Based on Google’s readout analysis we considered various readout error models that refine Google’s basic model, and the associated estimators of the fidelity. Preliminary study of the Google data on 12 and 14 qubits suggests that neither Google’s basic noise model nor our refined readout errors model fit the observed data. An extension of the analysis beyond 12 and 14 qubits can shed light on the statistical assumptions behind the Google fidelity predictions and on other aspects of their experiment. We note that there are further statistical aspects of the experiments described in [2], mainly those related to the quality of individual components of the circuit and to the process of “calibration,” that are not considered here.

Finally, we expect that our study can contribute to the understanding of the nature of noise in noisy intermediate-scale quantum computers. Sampling tasks are natural candidates for testing and proving the potential of quantum computers. Therefore, our statistical analysis is expected to be useful for various near term experimental efforts for NISQ computers, including future attempts for ‘quantum supremacy’ demonstrations.

Acknowledgment The numerical work in this paper was done by the R Package and Wolfram Mathematica. We are grateful to Larry Goldstein for insightful comments and questions and to Alexander Vlasov for helpful comments on the Google data and other matters. We are also thankful to members of the Google team and especially to John Martinis and Sergio Boixo for helpful discussions.

References


10 Appendix: Some proofs

Proof of (27), Proposition 4.1: In order to compute \( \text{Var}(U_{g(w)} = \log(w)) \) we use the approximation (valid for large \( M \)) \( w_i = z_i/M \), and we assume \( z_i \sim \text{Exp}(1) \). We need the following facts:

\[
\int_0^\infty (\log(z) + \gamma)^2 (z - 1)e^{-z}dz = 0 \text{ and } \int_0^\infty (\log(z) + \gamma)^2 e^{-z}dz = \pi^2/6 \approx 1.6449 \quad (46)
\]

where \( \gamma \) is Euler’s constant. The first equation in (46) shows that in this case \( A = 1 \); see (26). The second equation, with \( w = z/M \) implies \( B = -\gamma - \log(M) \), and \( EW = \phi - \gamma - \log(M) \). Thus

\[
\text{Var}[\log(\tilde{w}_j)] = E E^w[(\log(w_i) - EW)^2 | \{w_i\}] = E\left\{ \sum_{i=1}^{M} (\log(w_i) - EW)^2(\phi w_i + (1 - \phi)/M) \right\}
\]

\[
= E\left\{ (\log(z/M) - EW)^2[\phi w + (1 - \phi)] \right\} = \int_0^\infty (\log(z) - \phi + \gamma)^2[\phi(z - 1) + 1]e^{-z}dz,
\]

and the above integrals imply

\[
\int_0^\infty (\log(z) - \phi + \gamma)^2[\phi(z - 1) + 1]e^{-z}dz
\]

\[
= \int_0^\infty [(\log(z) + \gamma)^2 + \phi^2 - 2\phi(\log(z) + \gamma)][\phi(z - 1) + 1]e^{-z}dz
\]

\[
= \int_0^\infty [(\log(z) + \gamma)^2]e^{-z}dz + \phi^2 - 2\phi^2 + 2\phi\gamma - 2\phi\gamma = \pi^2/6 - \phi^2.
\]

We obtain that \( U_{g(z)} = \log(z) = \frac{1}{N} \sum_{i=1}^{N} \log(\tilde{w}_i) + \gamma + \log(M) \) and

\[
\text{Var}(U_{f(z)} = \log(z)) \approx \frac{1}{N}(\pi^2/6 - \phi^2) \approx \frac{1}{N}(1.6449 - \phi^2).
\]

Proof of (36)

The expectation \( EW \) taken with respect to the sampling rule (34) and then over \( \{w_i\}_1^M \) can be expressed after some calculations as

\[
EW = \phi + M^2\phi_{ro}E\left[ \left( \sum_{|y| \neq 0} w_{x\oplus y} B_q(y)/D \right)^2 \right] + (1 - \phi_g) - 1
\]

\[
= M^2\phi_{ro}E\left[ \left( \sum_{|y| \neq 0} w_{x\oplus y} B_q(y)/D \right)^2 \right] - \phi_{ro}, \quad (47)
\]

35
where \( D := \sum_{|y| \neq 0} B_q(y) = 1 - (1 - q)^n \). Since this is the sum over \( N \) iid terms divided by \( N \) the expectation reduces to only one term. The \( M \) terms of (34) all have the same expectation, so we can multiply by \( M \) instead of summing. Thus, the term \( \phi \) in (47) arises from

\[
M \phi \sum_{i=1}^{M} E(v_i w_i) = M^2 \phi E[w_{x(i)}] E[\sum_{|y| \neq 0} w_{x(i) \oplus y} B_q(y)/D] = \phi,
\]

since \( E(w_{x(i)} w_{x(i) \oplus y}) = E[w_{x(i)}] E[w_{x(i) \oplus y}] = 1/M^2 \) for \( |y| \neq 0 \). The new part to compute is \( C := M^2 E\left[ \left( \sum_{|y| \neq 0} w_{x \oplus y} B_q(y) \right)^2 \right] \) for any fixed \( x \). For off-diagonal terms in the sum of squares, that is, terms of the form \( w_{(x \oplus y)w_{x \oplus y'}} \) with \( y' \neq y \), we have \( E w_{(x \oplus y)w_{x \oplus y'}} = 1/M^2 \). However, if \( M \) is not large relative to \( N \) we may have repetitions in the sample, and when \( z_{x \oplus y} = z_{x \oplus y'} \), their product has expectation of \( 2/M(M+1) \) rather than \( 1/M^2 \). This implies that for relatively small \( M \) we underestimate \( EW \) if we assume \( E w_{(x \oplus y)w_{x \oplus y'}} = 1/M^2 \). We now assume \( M \) large and therefore (with possible underestimation) the total probability of the off-diagonal elements in \( C \) is \( \sum_{y \neq y', 1 \leq |y|, |y'| \leq n} B_q(y)B_q(y')/M^2 \).

For the diagonal terms the expectations satisfy \( E w_{x \oplus y} w_{x \oplus y} = 2/M(M+1) \). We have

\[
A := \sum_{|y| \neq 0} B_q(y)^2 = \sum_{k=1}^{n} \binom{n}{k} q^{2k} (1-q)^{2n-2k} = [q^2 + (1-q)^2]^{n} - (1-q)^{2n},
\]

and therefore

\[
B := \sum_{y \neq y', 1 \leq |y|, |y'| \leq n} B_q(y)B_q(y') = [1 - (1 - q)^n]^2 - \{[q^2 + (1-q)^2]^n - (1-q)^{2n} \}.
\]

Therefore, for large \( M \)

\[
C := 2AM/(M+1) + B \approx [1 - (1 - q)^n]^2 + [q^2 + (1-q)^2]^n - (1-q)^{2n}.
\]

It follow that

\[
EW = \phi_r C/D^2 - \phi_{ro} = \phi_{ro} [C/D^2 - 1],
\]

which is (36).

The computation of \( Var(W) \) is rather cumbersome and will not be presented here. For data analysis purposes we shall compute it by simulations.