From Randomness to Quantum Computing

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From Randomness to Quantum Computing

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From Randomness to Quantum Computing

Random numbers are used extensively in various applications in science, economy and security, ranging from cryptography to numerical simulations.

'Good' randomness is the critical resource for all these applications, but high quality randomness is neither easy to produce nor to certify. Randomness appears and is necessary almost everywhere

Random numbers had been around for more than 4,000 years, but never have they been in such demand as in our time. The oldest known dice were discovered in a 24th century B.C. tomb in the Middle East.

In 1890 statistician Francis Galton wrote that

As an instrument for selecting at random, I have found nothing superior to dice.

However, the modern world demanded a lot more randomness than dice could offer.

John von Neumann developed a *pseudo-random generator* (PRNG) around 1946: start with an initial random seed value, square it, and slice out the middle digits. A sequence obtained by repeatedly using this method exhibits *some* statistical properties of randomness.

RAND Corporation machine generated numbers using a random pulse generator: its book *A Million Random Digits with 100,000 Normal Deviates* was published in 1955.

In 1951, Ferranti Mark 1 was the first computer with a built-in random number instruction—designed by A. Turing—that could generate 20 random bits at a time using electrical noise.

All modern computers have algorithms that generate *pseudo-random numbers*.

I am convinced that the vast majority of my readers, and in fact the vast majority of scientists and even nonscientists, are convinced that they know what 'random' is. A toss of a coin is random; so is a mutation, and so is the emission of an alpha particle.... Simple, isn't it? said Kac in [34].

Well, no! Kac knew very well that randomness could be called many things, but not simple, and in fact his essay shows that randomness is complicated, and it can be described in more than one way.

Books on probability theory do not even attempt to define it. *It's like the concept of a point in geometry books.*

What's wrong with these random numbers?

The pitfalls of low quality randomness have been discovered in the Internet era. An example is the discovery in 2012 of a weakness in the encryption system used worldwide for online shopping, banking and email; the flaw was traced to the numbers a PRNG has produced [37].

Do "better" random numbers exist? Yes.

Can other methods produce "better" random numbers? Yes.

Does true or perfect random number exist? No.

Randomness is best understood through various "symptoms". Here are three of the largely accepted ones:

- (i) Unpredictability: The impossibility of any agent, acting via uniform, effective means, to predict correctly and reproducibly the outcome of an experiment using finite information extracted from the environment.
- (ii) *Incompressibility:* The impossibility to compress a random sequence.
- (iii) *Typicality:* Random sequences pass every statistical test of randomness.

The French mathematician Émile Borel, a pioneer of probability theory, argued that there is no way to formalise in an acceptable way the concept of randomness. His argument is based only one symptom of randomness, typicality, and is known as the *randomness paradox*.

A random bit-string should be "typical": it should not stand out from the crowd of other bit-strings.

Here is Borel's argument. Assume that there is a precise way to distinguish between "random bit-strings" and bit-strings which are "non-random". It does not matter how this criterion was found or operates.

Assume we have a precise **criterion** which can be applied to any bit-string and once a bit-string is given, we can say whether the bit-string is *random* or *non-random*.

Can the **criterion** be consistent? The answer is **negative**.

Indeed, choose the first bit-string which **criterion** asserts it is random. This particular bit-string is

the first bit-string satisfying the property of being random,

a property making it atypical, so non-random!

There are many random number generators:

- 1. pseudo-random generators, software produced
 - ▶ PCG, Random123, xoroshilro 128+
- 2. hardware generators, devices that generate random numbers from physical processes
 - ▶ macroscopic, e.g. coin, dice, roulette wheels, lottery machines,
 - microscopic, e.g. thermal noise, photoelectric effect, quantum effects.

In particular, there are many quantum random generators, from lab experiments to openly accessible on the internet and commercial (Quantis).

Because no current quantum random generator (QRNG) is provably better than the other generators, in particular, pseudo-random generators.

Is this so? Many advantages promised by QRNGs rely on the belief that the outcomes of quantum measurements are

intrinsically/irreducibly unpredictable.

This belief underlies:

- the use of QRNGs to produce "quantum random" sequences that are "truly unpredictable",
- the generation of cryptographic keys unpredictable to any adversary.
- Is this belief reasonable?

Notation

- Bit strings: ε (empty string), 0, 1, 00, 01, 10, 11,
- $B = \{0, 1\}$ and B^* is the set of all binary strings.
- Strings can be concatenated: from x and y get xy.
- The length of the string x is denoted by |x|

•
$$|\varepsilon| = 0, |0| = |1| = 1, |00| = |01| = |10| = |11| = 2, \dots$$

•
$$|xy| = |x| + |y|$$
.

- Let bin(n) be the binary representation of the number n + 1 without the leading 1. For example: 1 → ε, 2 → ... This is a bijection between positive integers and binary strings.
- The quasi-lexicographical order: x < y iff bin⁻¹(x) < bin⁻¹(y).

Notation

- A partial function φ from B* to B* ∪ {∞} is partially computable if there is a Turing machine working with the alphabet B that computes it. By dom(φ) we denote the domain of φ.
- ► A partially computable function from B* to B* is called computable.
- A subset S ⊆ B* is called computable if its characteristic function is computable.
- A subset S ⊆ B* is called computably enumerable (c.e.) if there is a computable function f from B* to B* such that F(B*) = S, i.e. f enumerates S.

More notation

- B^{∞} is the set of all binary infinite sequences $\mathbf{x} = x_1 x_2 \cdots x_n \cdots$.
- x(n) = x₁x₂ · · · x_n ∈ B^{*} is the prefix of length n > 0 of the sequence x.

▶ For
$$w \in B^*$$
 and $W \subset B^*$, put
 $wB^{\infty} = \{\mathbf{x} \in B^{\infty} \mid w = \mathbf{x}(|w|)\}$ and $WB^{\infty} = \bigcup_{w \in W} wB^{\infty}$.

- The family $(wB^{\infty}, w \in B^*)$ generates a σ -algebra on B^{∞} .
- The Lebesgue measure is now defined by $\mu(wB^{\infty}) = 2^{-|w|}$.
- A property P of sequences x ∈ B[∞] is true almost everywhere in the sense of µ in case the set of sequences not having the property P is a null set, i.e. µ({x | P(x) is false}) = 0.

Borel's Law of Large Numbers—the proportion of heads in a "large" number of a fair coin flips "should be" roughly 1/2—can be expressed by a property true almost everywhere in the sense of μ :

$$\mu\left(\left\{\mathbf{x}\in B^{\infty}\mid \lim_{n\to\infty}\frac{x_1+x_2+\ldots+x_n}{n}\neq\frac{1}{2}\right\}\right)=0.$$

A sequence satisfying a property false almost everywhere with respect to μ is very "particular", "not typical".

Many results in probability theory are true almost everywhere, so it is tempting to say that

a sequence **x** is "random" if it satisfies every property true almost everywhere with respect to μ .

For every sequence **x** we can define the property P_x as follows: **y** satisfies P_x if for every $n \ge 1$ there exists a natural $m \ge n$ such that $x_m \ne y_m$.

► VDWfinite

Every $P_{\mathbf{x}}$ is an asymptotic property which is true almost everywhere with respect to μ and \mathbf{x} does not have property $P_{\mathbf{x}}$. Accordingly, no sequence can verify all properties true almost everywhere with respect to μ .

The above definition is vacuous, hence *there is no true/perfect lawless sequence*.

A "universal" non-trivial property shared by all sequences was discovered by van der Waerden (see for example [30]; for the finite version see **VDWfinite**):

In every binary sequence at least one of the two symbols must occur in arithmetical progressions of every length.

There is no constructive proof for van der Waerden result: no algorithm can decide which alternative is true: 0 occurs in arithmetical progressions of every length or 1 occurs in arithmetical progressions of every length.

There is a way to overcome the above difficulty in defining randomness:

Consider only *a sequence of asymptotic properties true almost everywhere.*

But, then which sequence of properties should be chosen?

Clearly, the "larger" the chosen sequence of properties is, the "more random" will be the sequences satisfying that sequence of properties.

The notion of randomness has to have at least the properties of unpredictability, incompressibility and typicality.

Martin-Löf [39] proposal was to consider only the constructive properties constructively true almost everywhere with respect to μ .

Martin-Löf [39] defined random sequences by means of statistical tests.

A Martin-Löf test is a c.e. set $A \subset \mathbf{N} \times B^*$ such that $A_i = \{w \in B^* \mid (i, w) \in A\}$ and $\mu(A_i B^\infty) \leq 2^{-i}$, for all natural *i*. The set $\bigcap_{i\geq 0}(A_i B^\infty)$ is the (constructive null) set of all sequences which do not pass the randomness test *A*. This definition captures "typicality".

A a sequence x is Martin-Löf random if for every Martin-Löf test A,

$$\mathbf{x} \notin \bigcap_{i \ge 0} (A_i B^\infty).$$

Theorem [Martin-Löf Theorem] Constructively, with probability μ one, every sequence is Martin-Löf-random.

From Randomness to Quantum Computing

A set S of strings is prefix-free if no string in S is a proper prefix of a string in S.

- The sets $\{x \in B^* \mid |x| = n\}$, $\{1^n 0 \mid n \ge 1\}$ are prefix-free.
- The set {x₁x₁x₂x₂...x_nx_n01 | x₁x₂...x_n ∈ L} is prefix-free for every L ⊆ B*.
- The set {x₁0x₂0...x_n1 | x₁x₂...x_n ∈ L} is prefix-free for every L ⊆ B*.
- B^{*} is not prefix-free.

A prefix-free (or self-delimiting) TM is a TM whose domain is prefix-free.

- The identity ψ(x) = x, x ∈ B* is not computable by a prefix-free TM; no total function is computable by a prefix-free TM.
- The restriction of the identity ψ(x) = x to the set {1ⁿ0 | n ≥ 1} is computable by a prefix-free TM.
- The function θ(1^{|x|}0x) = x, for all x ∈ B* is computable by a prefix-free TM.
- The set of prefix-free TMs is computably enumerable.

UPFTheorem

We can effectively construct a prefix-free TM U such that for every prefix-free TM C there effectively exists a constant $c = c_{U,C}$ such that for each input string x there exists an input z with $|z| \le |x| + c$ such that U(z) = C(x).

▶ Proof

Let M be a prefix-free Turing machine. The program-size complexity $H_M(x)$ is the size in bits of the smallest program for M to compute x:

$$H_M(x) = \inf\{|p| \mid p \in B^*, M(p) = x\}.$$

When M = U is universal, then H_U is simply denoted by H.

The program-size of the sequence \mathbf{x} is given by the sequence

 $(H(\mathbf{x}(n))_{n>0})$

Examples

Iow complexity strings:

$$H(0^n) \approx \log n + c, H(1^n) \approx \log n + c$$

► intermediate complexity strings (borderline algorithmically random strings): if x* = min{p | U(p) = x}, then

$$H(x) = |x^*|, H(x^*) \ge |x^*| - c$$

high complexity strings (algorithmically random strings):

 $\max\{H(x) \mid |x| = n\} = n + H(\operatorname{bin}(n)) + c \approx n + 2\log n + c$

▶ Proof

From Randomness to Quantum Computing

The binary representation of the number 0.40626 is

 $0.011010000\cdots$

What is the complexity of the sequence

 $\mathbf{x} = 011010000 \cdots ?$

There exists c > 0 such that for each n,

 $H(\mathbf{x}(n)) \leq 2\log n + c.$

Consider the number π written in binary and let

$$0.\pi_1\pi_2\cdots\pi_n\cdots$$

be the infinite binary sequence of the fractional part of π . There is a constant c' > 0 such that for each n,

$$H(\mathbf{\Pi}(n)) \leq 2\log n + c',$$

where

$$\mathbf{\Pi}=\pi_1\pi_2\cdots\pi_n\cdots$$

What is the difference between 0.40626 and π ?

The *halting problem* requires to construct an algorithm which decides whether an arbitrary Turing machine eventually stops or not.

Theorem [Undecidability of the halting problem] The halting problem is undecidable.

Proof. Assume by absurdity the existence of a **halting program** deciding the halting problem.

Construct the Turing machine given by the program Trouble(N):

- 1. read a natural N;
- 2. generate all programs up to N bits in size;
- use the halting program to check for each generated program whether it halts;
- simulate the running of the above generated programs, and
- 5. compute the biggest value output by these programs, say o, and output 2o + 1.

The program Trouble(N) halts for every natural N.

How long is Trouble(N)? It is about $\log_2 N$ bits.

Reason: to know N we need $\log_2 N$ bits (in binary); the rest is a constant, so Trouble(N) is $\log N + O(1)$ bits.

There is a big difference between the size—in bits—of Trouble(N) and the size of the output produced by Trouble(N).

Indeed, for large enough N, Trouble(N) belongs to the set of programs having less than N bits (because $\log N + O(1) < N$).

Accordingly, Trouble(N) generates itself at some stage of the computation.

We have got a contradiction since, on one hand, Trouble(N) outputs a natural number no larger than o, but, on the other hand, it outputs 2o + 1!

As the halting problem is undecidable, we can approach the problem probabilistically. Chaitin's Omega is the "halting probability" of a prefix-free universal TM U, that is:

$$\Omega_U = \sum_{p \in \operatorname{dom}(U)} 2^{-|p|}$$

The Kraft inequality states that for a prefix-free set S,

$$\sum_{p\in S} 2^{-|p|} \le 1,$$

which implies that $\Omega_U \leq 1$; in fact, $\Omega_U \in (0, 1)$.

Theorem [Omega solves the halting problem] With the first n bits of Omega we solve the halting problem for every program of length less than or equal to n.

▶ Proof

Corollary [Incomputability of Omega]

The sequence $\omega_1 \omega_2 \cdots \omega_n \cdots$ is not computable.

Some of these bits have actually been determined. For a natural choice of the Turing machine U, the first 40 bits of $\Omega = \Omega_U$ are

000100000010000101001110111000011111010.

If we knew the first 5,000 bits, we would know if the Riemann hypothesis is correct. For the Four colour theorem we need even less bits.
OmegaMedia

$\label{eq:corollary} \begin{array}{l} \mbox{[Transcendence of Omega]} \\ \mbox{The number } \Omega \mbox{ is transcendental and } \Omega \in (0,1). \end{array}$
Theorem [Bi-immunity of Omega] The sequence $\omega_1\omega_2\cdots\omega_n\cdots$ is bi-immune, that is, no algorithm can compute exactly more than finitely many bits of ω_i . See more in [15, 20].

Theorem [Omega has almost maximum complexity] If

$$\Omega_U=0.\omega_1\omega_2\cdots\omega_n\cdots$$

then there exits a constant c > 0 such that for all $n \ge 1$,

$$H(\omega_1\omega_2\cdots\omega_n)\geq n-c.$$

Reals whose binary expansions are sequences with maximum complexity are called algorithmically random, shortly random. • Proof

Theorem [Omega is c.e.]

The number Omega is c.e., that is, the limit of an increasing computable sequence of rationals in (0, 1).

▶ Proof

So, Omega is a c.e. algorithmically random real. In fact, the converse is also true:

Theorem [Omega = c.e. and random]

The set of Omega numbers coincides with the set of c.e. random numbers.

See more in [15, 26].

Theorem

A sequence **x** is Martin-Löf random iff there exits a constant c > 0 such that for all $n \ge 1$,

 $H(\mathbf{x}(n)) \geq n-c.$

See more in [15, 26].

Corollary Every pseudo-random sequence is not Martin-Löf random. Is Martin-Löf randomness a good model of randomness?

Martin-Löf randomness

- is provably better than pseudo-randomness,
- satisfies the typicality requirement,
- satisfies the incompressibility requirement,
- it is believed to satisfy the requirement of unpredictability, but no convincing model was yet developed to test it,
- no known device for producing it has been yet designed and certified.

See more in [15, 26].

According to Oxford Dictionary, spurious means

Not being what it purports to be; false or fake. False, although seeming to be genuine. Based on false ideas or ways of thinking.

The above (dictionary) definition is semantic, hence it depends on an assumed theory: one correlation can be spurious according to one theory, but meaningful with respect to another one.

Can we give a definition of "spurious" which is independent of *any* theory (using formal deductions, mathematical calculations, computer algorithms, etc.)?

We define a spurious correlation in a very restrictive way: a correlation is spurious if it appears in a "randomly" generated database,

so it satisfies the above broad informal description.

In fact, a spurious correlation in the above sense is "meaningless" according to any reasonable definition because, by construction, its values are chosen at "random", as all data in the database.

As a consequence, such a correlation cannot provide reliable information on future developments of any type of behaviour.

Of course, there are other reasons making a correlation spurious, even within a "non-random" database.

Van der Waerden theorem

[Equidistant correlations everywhere] For any positive integers k there is a positive integer γ such that every bit string of length more than γ contains an arithmetic progression with k occurrences of the same digit or colour, i.e. a monochromatic arithmetic progression of length k.

How "large" is the set of spurious correlations, in the above sense? Fix a real number α in the open interval (0,1). A string x of length *n* can be compressed by αn bits if co

$$H(x) \leq n - \alpha n.$$

The number of strings x of length n which are compressible by αn bits is smaller than

$$2^{(1-\alpha)n} - 1$$

hence the probability that a string x of length n has $H(x) < n - \alpha n$ is smaller than

$$2^{-\alpha n} \to 0 \ (n \to \infty).$$

See more in [21].

From Randomness to Quantum Computing

From bits to qubits

From Randomness to Quantum Computing

Bits and qubits

Classical computers use bits which are physically represented by two-state classical systems (two positions of an electrical switch, two distinct voltage or current levels allowed by a circuit).

Quantum computers operate with qubits (quantum bits) which are described as quantum states (i.e. abstract, in Hilbert space) that are physically implemented by quantum systems (e.g. an atom) which are in one of two definite states.

For example, the state of a spin- $\frac{1}{2}$ particle, when measured, is always found to be in one of two possible states, represented – using Dirac bra-ket notation – as

$$|+rac{1}{2}
angle$$
 (spin-up) or $|-rac{1}{2}
angle$ (spin-down).

Formally, a qubit is denoted as

$$|0
angle$$
 or $|1
angle.$

Unlike the intermediate states of a classical bit (e.g. any voltages between the "standard" representations of 0 and 1) which can be distinguished from 0 and 1, but do not exist from an informational point of view, quantum intermediate states cannot be reliably distinguished, even in principle, from the basis states, but do have an informational "existence".

A superposition state $|\varphi\rangle$ (pronounced "ket phi") is a qubit state vector represented by a linear combination of basis states conventionally denoted by $0\rangle$ and $|1\rangle$, that is

$$|\varphi\rangle = \alpha |\mathbf{0}\rangle + \beta |\mathbf{1}\rangle,$$

where α, β are complex numbers with $\alpha^2 + \beta^2 = 1$.

A qubit is a unit vector in the space C^2 , so for each qubit $|x\rangle$, there are two (complex) numbers $a, b \in C$ such that

$$|x\rangle = a|0\rangle + b|1\rangle = \left(egin{array}{c} a \\ b \end{array}
ight),$$
 (1)

where

$$|0
angle = \left(egin{array}{c} 1 \ 0 \end{array}
ight), \; |1
angle = \left(egin{array}{c} 0 \ 1 \end{array}
ight),$$

and $|a|^2 + |b|^2 = 1$.

We can perform a measurement that projects the qubit onto the basis $\{|0\rangle, |1\rangle\}$. Then we will obtain the outcome $|1\rangle$ with probability $|b|^2$, and the outcome $|0\rangle$ with probability $|a|^2$.

With the exception of limit cases a = 0 and b = 0, the measurement irrevocably disturbs the state:

If the value of the qubit is initially unknown, then there is no way to determine a and b with any conceivable measurement.

However, after performing the measurement, the qubit is in a known state (either $|0\rangle$ or $|1\rangle$); this state is typically different from the previous state.

The above facts point out an important difference between qubits and classical bits. There is no problem in measuring a classical bit without disturbing it, so we can decode all of the information that it encodes. If we have a classical bit with a fixed, but unknown value (0 or 1), then we can only say that there is a probability that the bit has the value 0, and a probability that the bit has the value 1, and these two probabilities add up to 1. When we measure the bit, we acquire additional information; after measurement, we will know completely the value of the bit. The ability of quantum systems to exist in a "blend" of all their allowed states simultaneously is known as the Principle of Superposition.

Even though a qubit can be put in a superposition (1), it contains no more information than a classical bit, in spite of its having infinitely many states. The reason is that information can be extracted only by measurement. But, as we have argued, for any measurement of a qubit with respect to a given orthonormal basis, there are only two possible results, corresponding to the two vectors of the basis. It is not possible to capture more information measuring in two different bases because the measurement changes the state. Even worse, quantum states cannot be cloned, hence it's impossible to measure a qubit in two different ways (even, indirectly, by using a copy trick, that is copying and measuring the copy).

Quantum randomness

From Randomness to Quantum Computing

With the understanding acquired on randomness we will look at the best candidate of randomness, quantum randomness.

- How can we produce quantum randomness?
- What is the physical "reason" of quantum randomness?
- What is the quality of quantum randomness?
- Is quantum randomness better than pseudo-randomness?

Quantum randomness is not true randomness



Nature, doi:10.1038/news.2010.181, 14 April 2010.

From Randomness to Quantum Computing

Quantum randomness is not true randomness



QUANTIS

TRUE RANDOM NUMBER GENERATOR EXPLOITING QUANTUM PHYSICS

QUANTIS is a physical random number generator exploiting an elementary quantum optics process. Photons light particles - are sent one by one onto a semi-transparent mirror and detected. The exclusive events (reflection - transmission) are associated to "0" - "1" bit values. The operation of Quantis is continuously monitored to ensure immediate detection of a failure and disabling of the random bit stream. The product exists in four versions:

- USB device random stream of 4Mbits/sec
- PCI Express (PCIe) board random stream of 4Mbits/sec
- PCI board random stream of 4Mbits/sec and 16Mbits/sec
- OEM component random stream of 4Mbits/sec

Select the product of interest for more information.

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PRODUCTS

True Random Number Generators (TRNG)

- Quantis-USB
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 Quantis-PCI
- Quantis-OEM

Indeterminism and quantum randomness

Quantum randomness is

- postulated and
- generally reduced to the indeterminism of quantum measurements: because the outcome is indeterministic there is no way to predict it, hence it is random.

However, indeterminism does not imply randomness and randomness does not imply indeterminism:

- pseudo-randomness,
- coin-tossing (chaoticity),
- Omega number,
- Schrödinger equation.

Value indefiniteness is a central notion to this discussion. Informally, for a given quantum system in a particular state, we say that an observable is value definite if the measurement of that observable is predetermined to take a (potentially hidden) value.

In defining it we are guided by Einstein, Podolsky and Rosen famous analysis in [27] which can be encapsulated in the following

EPR principle: If, without in any way disturbing a system, we can predict with certainty the value of a physical quantity, then there exists a definite value prior to observation corresponding to this physical quantity.

See more in [7, 8, 9].

EPR principle justifies also

Eigenstate principle: If a quantum system is prepared in a state $|\psi\rangle$, then the projection observable $P_{\psi} = |\psi\rangle\langle\psi|$ is value definite.

- Admissibility: Definite values must not contradict the statistical quantum predictions for compatible observables on a single quantum.
- Noncontextuality of definite values: The outcome obtained by measuring a value definite observable (a preexisting physical property) is *noncontextual*, i.e. it does not depend on other compatible observables which may be measured alongside the value definite observable.
- Eigenstate principle: If a quantum system is prepared in the state $|\psi\rangle$, then the projection observable $P_{\psi} = |\psi\rangle \langle \psi|$ is value definite.

Assume the above three hypotheses.

Theorem

Assume a quantum system prepared in the state $|\psi\rangle$ in dimension $n \geq 3$ Hilbert space \mathfrak{C}^n , and let $|\phi\rangle$ be any state neither orthogonal nor parallel to $|\psi\rangle$, i.e. $0 < |\langle\psi|\phi\rangle| < 1$. Then the projection observable $P_{\psi} = |\phi\rangle \langle\phi|$ is value indefinite.

Theorem

The set of value indefinite observables has constructive measure 1, that is, almost all observables are value indefinite.

Value indefiniteness and unpredictability

EPR principle: If, without in any way disturbing a system, we can predict with certainty the value of a physical quantity, then there exists a definite value prior to observation corresponding to this physical quantity.

Conversely, if no unique element of physical reality corresponding to a particular physical quantity exists, this is reflected by the physical quantity being value indefinite.

If a physical property is value indefinite we cannot predict with certainty the outcome of any experiment measuring this property.

If we assert of an observable event that it is unpredictable we do not mean, of course, that it is logically or physically impossible for anybody to give a correct description of the event in question before it has occurred; for it is clearly not impossible that somebody may hit upon such a description accidentally. What is asserted is that certain rational methods of prediction break down in certain cases—the methods of prediction which are practised in physical science. We present a non-probabilistic model of prediction based on the ability of a computable operating agent to correctly predict using finite information extracted from the system of the specified experiment, [10].

Predictions should remain correct in any arbitrarily long (but finite) set of repetitions of the experiment.

Consider a physical experiment *E* producing a single bit. We consider an experiment *E* producing a single bit $x \in \{0, 1\}$.

An example of such an experiment is the measurement of a photon's polarisation after it has passed through a 50-50 beam splitter.

With a particular trial of E we associate the parameter λ (the state of the universe) which fully describes the trial. While λ is not in its entirety an obtainable quantity, we can view it as a resource that one can extract finite information from in order to predict the outcome of the experiment E.

An extractor is a (deterministic) function $\lambda \mapsto \langle \lambda \rangle$ mapping reals to rationals.

For example, $\langle \lambda \rangle$ may be an encoding of the result of the previous trial of *E*, or the time of day the experiment is performed.

A predictor for E is an algorithm (computable function) P_E which halts on every input and outputs **0** or **1** or prediction withheld.

 P_E can utilise as input the information $\langle \lambda \rangle$, but, as required by EPR, must be passive, i.e. must not disturb or interact with E in any way.

A predictor P_E provides a correct prediction using the extractor $\langle \rangle$ for a trial of E with parameter λ if, when taking as input $\langle \lambda \rangle$, it outputs **0** or **1** and this output is equal to the result of the experiment.

The predictor P_E is $k, \langle \rangle$ -correct if there exists an $n \ge k$ such that when E is repeated n times with associated parameters $\lambda_1, \ldots, \lambda_n$ producing the outputs x_1, x_2, \ldots, x_n , P_E outputs the sequence $P_E(\langle \lambda_1 \rangle), P_E(\langle \lambda_2 \rangle), \ldots, P_E(\langle \lambda_n \rangle)$ with the following two properties:

(i) no prediction in the sequence is incorrect, and (ii) in the sequence there are k correct predictions.

The outcome x of a single trial of the experiment E performed with parameter λ is predictable (with certainty) if there exist an extractor $\langle \rangle$ and a predictor P_E which is

1.
$$k, \langle \rangle$$
-correct for all k , and
2. $P_E(\langle \lambda \rangle) = x$.

Theorem 3

If *E* is an experiment measuring a quantum value indefinite observable, then every predictor P_E using any extractor $\langle \rangle$ is not $k, \langle \rangle$ -correct, for all k.

Theorem 4

In an infinite repetition of *E* as considered above, no single bit x_i of the generating infinite sequence $x_1x_2...$ can be predicted.

epr principle: If a repetition of measurements of an observable generates a computable sequence, then this implies these observables were value definite.

Theorem [7]

Assume the epr and Eigenstate principles. An infinite repetition of the experiment E measuring a quantum value indefinite observable generates an incomputable (even bi-immune) infinite sequence $x_1x_2...$

Generalised beam QRNG producing maximum unpredictable, incomputable sequences



Figure: Generalised beam QRNG
Realisation of the generalised beam QRNG with qutrits



Figure: Realisation of a QRNG with superconducting circuits on a chip (gray). A qutrit (yellow) is coupled to a read out (red) and control circuitries. Near quantum limited Josephson parametric amplifier (JPA) can be used to discriminate all possible outcomes of the protocol with certainty including false runs. Fast programmable gate array (FPGA) can be used to provide the correction pulses to reinitialise the qutrit in its ground state right after the end of the protocol run. [36]

The quantum gate model

From Randomness to Quantum Computing

Quantum computing was first introduced by Yuri I. Manin in 1980 and Richard Feynman in 1982 and intensively researched afterwards.

Quantum algorithms are probabilistic and give the correct answer with high probability; the probability of failure can be decreased by repeating the algorithm.

Quantum computing

- In 1985 Deutsch constructed the first model of quantum computer by quantisation of the universal Turing machine.
- In 1994 Shor designed a quantum algorithm for factoring integers in polynomial (quantum) time in the size of the input; the problem whether there is a classical polynomial algorithm for factoring is still open.
- ► Two years later Grover discovered a quantum algorithm for searching an unsorted *N*-entry database in O(√*N*) time and O(log *N*) space: this algorithm is optimal within the quantum computing model for black box oracles.

The most popular model of quantum computing is probably the *circuit (gate) model* in which quantum algorithms are built from a small set of quantum gates.

Adiabatic quantum computing, proposed in 2000, relies on the adiabatic theorem to do calculations.

A quantum computer is a computation system that makes direct use of quantum-mechanical phenomena, such as superposition and entanglement, to perform operations on data.

Classical computers encode data into binary digits (bits) using classical physical systems – e.g. the position of gear teeth in Babbage's differential engine, a memory element or wire carrying a binary signal, in contemporary machines – which are always in one of two definite states (0 or 1).

Typically, the system is described by one or more continuous parameters, for example, voltage. Such a parameter is used to separate the space into two well-defined regions chosen to represent 0 and 1. Manufacturing imperfections, local perturbations may affect, so signals are periodically restored toward these regions to prevent them from drifting away.

References: [22, 31, 42].

The quantum evolution of a qubit is described by a "unitary operator", that is an operator induced by a unitary matrix.¹

Any unitary operator $U : \mathbf{C}^2 \to \mathbf{C}^2$ can be viewed as a single qubit gate. Considering the basis $\{|0\rangle, |1\rangle\}$, the transformation is fully specified by its effect on the basis vectors. In order to obtain the associated matrix of an operator U, we put the coordinates of $U|0\rangle$ in the first column and the coordinates of $U|1\rangle$ in the second one.

¹A quadratic matrix A of order n over **C** is *unitary* if $AA^{\dagger} = I$ (the identity $n \times n$ matrix); A^{\dagger} is the transposed conjugate matrix of A.

From Randomness to Quantum Computing

So, the general form of a transformation that acts on a single qubit is a 2×2 matrix

$$\mathsf{A} = \left(egin{array}{c} \mathsf{a} & \mathsf{b} \\ \mathsf{c} & \mathsf{d} \end{array}
ight),$$

which transforms the qubit state $\alpha |0\rangle + \beta |1\rangle$ into the state $(\alpha a + \beta b)|0\rangle + (c\alpha + d\beta)|1\rangle$:

1

$$\left(\begin{array}{cc} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{array}\right) \left(\begin{array}{c} \alpha \\ \beta \end{array}\right) = \left(\begin{array}{c} \alpha \mathbf{a} + \beta \mathbf{b} \\ \mathbf{c} \alpha + \mathbf{d} \beta \end{array}\right).$$

We may think of logic gates as transformations. For example, the NOT transformation which interchanges the vectors $|0\rangle$ and $|1\rangle$, is the matrix

NOT
$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
.

It flips that state of its input,

NOT
$$|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle,$$

and

$$\mathsf{NOT} \ |1\rangle = \left(\begin{array}{c} 0 & 1 \\ 1 & 0 \end{array} \right) \left(\begin{array}{c} 0 \\ 1 \end{array} \right) = \left(\begin{array}{c} 1 \\ 0 \end{array} \right) = |0\rangle.$$

Quantum gate model

The square-root of NOT (introduced by Deutsch) is the transformation

$$\begin{array}{rcl} \sqrt{\mathsf{NOT}} & |0\rangle & \rightarrow & \frac{1}{2}(1+i)|0\rangle + \frac{1}{2}(1-i)|1\rangle, \\ \\ & & \\ & |1\rangle & \rightarrow & \frac{1}{2}(1-i)|0\rangle + \frac{1}{2}(1+i)|1\rangle, \end{array}$$

$$\sqrt{\text{NOT}} = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}.$$
$$\sqrt{\text{NOT}} \cdot \sqrt{\text{NOT}} = \text{NOT} , \qquad (2)$$

and

$$\sqrt{\text{NOT}} \cdot \sqrt{\text{NOT}}^{\dagger}$$
$$= \frac{1}{4} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix} \begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix} = I.$$

The square-root of NOT is a typical "quantum" gate in the sense that it is impossible to have a single-input/single-output classical binary logic gate that satisfies (2). Indeed, any classical binary

$\sqrt{\text{NOT}}_{\text{classical}}$

gate is going to output a 0 or a 1 for each possible input 0/1. Assume that we have such a classical square-root of NOT gate acting as a pair of transformations

$$\sqrt{\text{NOT}}_{\text{classical}}(0) = 1, \sqrt{\text{NOT}}_{\text{classical}}(1) = 0.$$

Then, two consecutive applications of it will not flip the input!

Finally we consider the Hadamard transformation H is defined by

$$egin{array}{rcl} |0
angle &
ightarrow &rac{1}{\sqrt{2}}(|0
angle+|1
angle)\ H&:\ &|1
angle &
ightarrow &rac{1}{\sqrt{2}}(|0
angle-|1
angle)\ ,\ H&=rac{1}{\sqrt{2}}\left(egin{array}{rcl} 1&1\ 1&-1\end{array}
ight). \end{array}$$

This transformation has a number of important applications. When applied to $|0\rangle$, *H* creates a superposition state

$$rac{1}{\sqrt{2}}(\ket{0}+\ket{1}).$$

The simplest way to illustrate the power of quantum computing is to solve the so-called Deutsch's problem. Consider a Boolean function $f : \{0,1\} \rightarrow \{0,1\}$ and suppose that we have a black box to compute it. We would like to know whether f is constant (that is, f(0) = f(1)) or balanced $(f(0) \neq f(1))$. To make this test classically, we need two computations of f, f(0) and f(1) and one comparison. Is it possible to do it better? The answer is affirmative, and here is a quantum solution.

Suppose that we have a quantum black box to compute f. Consider the transformation U_f which applies to two qubits, $|x\rangle$ and $|y\rangle$ and produces $|x\rangle|y \oplus f(x)\rangle$.² This transformation flips the second qubit if f acting on the first qubit is 1, and does nothing if f acting on the first qubit is 0.

 $^{^{2}}$ By \oplus we denote, as usual, the sum modulo 2.

The black box is "quantum", so we can chose the input state to be a superposition of $|0\rangle$ and $|1\rangle$. Assume first that the second qubit is initially prepared in the state $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Then,

$$U_f\left(|x\rangle \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right)$$

= $|x\rangle \frac{1}{\sqrt{2}}(|0 \oplus f(x)\rangle - |1 \oplus f(x)\rangle)$
= $(-1)^{f(x)}|x\rangle \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$

Next take the first qubit to be $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle).$ The black box produces

$$\begin{split} &U_f\left(\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\right)\\ &=\frac{1}{\sqrt{2}}((-1)^{f(0)}|0\rangle+(-1)^{f(1)}|1\rangle)\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\\ &=\frac{1}{2}(-1)^{f(0)}(|0\rangle+(-1)^{f(0)\oplus f(1)}|1\rangle)(|0\rangle-|1\rangle). \end{split}$$

Next perform a measurement that projects the first qubit onto the basis

$$rac{1}{\sqrt{2}}(\ket{0}+\ket{1}), rac{1}{\sqrt{2}}(\ket{0}-\ket{1}).$$

Neglecting the sign and normalisation, we obtain

- $(|0\rangle |1\rangle)$ if the function f is balanced and
- $(|0\rangle + |1\rangle)$ in the opposite case.

The quantum algorithm solving Deutsch's problem is:

1. Start with a closed physical system prepared in the quantum state $|01\rangle\,.$

- 2. Evolve the system according to H.
- 3. Evolve the system according to U_f .
- 4. Evolve the system according to H.

5. Measure the system. If the result is the second possible output, the f is constant; if the result is the fourth possible output, then f is balanced.

To prove the correctness of the quantum algorithm, we shall show that the first and third possible outputs can be obtained with probability zero, while one (and only one) of the second and the fourth outcomes will be obtained with probability one, and the result solves correctly Deutsch's problem.

To this aim we follow step-by-step the quantum evolution described by the above algorithm.

In Step 1 we start with a closed physical system prepared in the quantum state $\left|01\right\rangle$:

$$V = \left(egin{array}{c} 0 \\ 1 \\ 0 \\ 0 \end{array}
ight)$$

After Step 2 the system has evolved in the state (which is independent of f):

$$HV = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \times \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}$$

.

After Step 3 the quantum system is in the state (which *depends* upon f):

$$U_{f}HV = \begin{pmatrix} 1-f(0) & f(0) & 0 & 0 \\ f(0) & 1-f(0) & 0 & 0 \\ 0 & 0 & 1-f(1) & f(1) \\ 0 & 0 & f(1) & 1-f(1) \end{pmatrix} \times \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}$$
$$= \begin{pmatrix} \frac{1}{2} - f(0) \\ -\frac{1}{2} + f(0) \\ \frac{1}{2} - f(1) \\ -\frac{1}{2} + f(1) \end{pmatrix}.$$

After Step 4, the quantum state of the system has become:

$$HU_{f}HV = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \times \begin{pmatrix} \frac{1}{2} - f(0) \\ -\frac{1}{2} + f(0) \\ \frac{1}{2} - f(1) \\ -\frac{1}{2} + f(1) \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ 1 - f(0) - f(1) \\ 0 \\ f(1) - f(0) \end{pmatrix}.$$

Finally, in Step 5 we *measure* the current state of the system, that is, the state HU_fHV , and we get:

- 1. output 1 with probability $p_1 = 0$,
- 2. output 2 with probability $p_2 = (1 f_Q(|0\rangle) f_Q(|1\rangle))^2$,
- 3. output 3 with probability $p_3 = 0$,
- 4. output 4 with probability $p_4 = (f_Q(|1\rangle) f_Q(|0\rangle))^2$.

To conclude:

- ▶ if $f_Q(|0\rangle) = f_Q(|1\rangle)$, then $f(0) + f(1) = 0 \pmod{2}$, f(1) - f(0) = 0; consequently, $p_2 = 1, p_4 = 0$.
- ▶ if $f_Q(|0\rangle) \neq f_Q(|1\rangle)$, then f(0) + f(1) = 1, f(1) f(0) = -1or f(1) - f(0) = 1; consequently, $p_2 = 0$, $p_4 = 1$.
- the outputs 1 and 3 have each probability zero.

So, Deutsch's problem was solved with only one computation of f. The explanation consists in the ability of a quantum computer to be in a blend of states: we can compute f(0) and f(1), but also, and more importantly, we can extract some information about f which tells us whether f(0) is equal or not to f(1).

Can we match classically this complexity?

The claim made more than 30 years ago in [24] and still maintained in 2018 is **negative**. This claim **false** appears in many books on quantum computing with the notable exception of [42]. See more in [17, 5, 6, 33].

Deutsch's problem was solved with only one use of U_f . The solution is probabilistic, and the result is obtained with probability one. Its success relies on the following three facts:

- the "embedding" of f into f_Q (see also the discussion in Mermin [41], end of section C, p. 11),
- ► the ability of the quantum computer to be in a superposition of states: we can check whether f_Q(|0⟩) is equal or not to f_Q(|1⟩) not by computing f_Q on |0⟩) and |1⟩, but on a superposition of |0⟩) and |1⟩, and
- the possibility to extract the required information with just one measurement.

We *de-quantise Deutsch's algorithm*, see [17, 33], in the following way. We consider **Q** the set of rationals, and the space $\mathbf{Q}[i] = \{a + bi \mid a, b \in \mathbf{Q}\}, (i = \sqrt{-1})$. We embed the original function f in $\mathbf{Q}[i]$ and we define the classical analogue C_f of the quantum evolution U_f acting from $\mathbf{Q}[i]$ to itself as follows:

$$C_f(a+bi) = (-1)^{0 \oplus f(0)} a + (-1)^{1 \oplus f(1)} bi.$$
(3)

The four different possible bit-functions f induce the following four functions C_f from $\mathbf{Q}[i]$ to $\mathbf{Q}[i]$ (\bar{x} is the conjugate of x):

$$C_{00}(x) = \bar{x}, \text{ if } f(0) = 0, f(1) = 0,$$

$$C_{01}(x) = x, \text{ if } f(0) = 0, f(1) = 1,$$

$$C_{10}(x) = -x, \text{ if } f(0) = 1, f(1) = 0,$$

$$C_{11}(x) = -\bar{x}, \text{ if } f(0) = 1, f(1) = 1.$$

Deutsch's problem becomes the following:

A function f is chosen from the set $\{C_{00}, C_{01}, C_{10}, C_{11}\}$ and the problem is to determine, with a single query, which type of function it is, balanced or constant. The following *deterministic* classical algorithm solves the problem:

Given f, calculate $(i-1) \times f(1+i)$. If the result is real, t is balanced; otherwise, the function is constant.

Indeed, the algorithm is correct because if we calculate $(i-1) \times f(1+i)$ we get:

$$(i-1) \times C_{00}(1+i) = (i-1)(1-i) = 2i,$$

 $(i-1) \times C_{01}(1+i) = (i-1)(1+i) = -2,$
 $(i-1) \times C_{10}(1+i) = (i-1)(-1-i) = 2,$
 $(i-1) \times C_{11}(1+i) = (i-1)(i-1) = -2i.$

If the answer is real, then the function is balanced, and if the answer is imaginary, then the function is constant.

From Randomness to Quantum Computing

Two-dimensionality can be obtained in various other simpler ways. For example, we can choose as space the set $Z[\sqrt{2}] = \{a + b\sqrt{2} \mid a, b \in Z\}$, where $\overline{a + b\sqrt{2}} = a - b\sqrt{2}$. Using a similar embedding function as (3),

$$C_f(a+b\sqrt{2}) = (-1)^{0\oplus f(0)}a + (-1)^{1\oplus f(1)}b\sqrt{2}$$

now acting on $\mathbf{Z}[\sqrt{2}]\text{, we get the solution:}^3$

Given f, calculate $(\sqrt{2}-1) \times f(1+\sqrt{2})$. If the result is rational, then the function is balanced; otherwise, the function is constant.

³In fact we don't need the whole set $Z[\sqrt{2}]$, but its finite subset $\{a + b\sqrt{2} \mid a, b \in \mathbb{Z}, |a|, |b| \leq 3\}$.

From Randomness to Quantum Computing

Can the quantum gate model simulate any Turing machine? No.

The reason is that all function computable by the quantum gate model are **total**. The halting problem for the quantum gate model is trivial. See more in [12].

Quantum annealing

From Randomness to Quantum Computing

Adiabatic quantum computing (AQC) is an alternative to the quantum gate model. Results by [28, 11] "suggest" that the two models of quantum computing are polynomially equivalent.

More general references about AQC and D-Wave machine: [40, 18, 3].

One distinction between the two models is their discrete versus analog natures: the quantum gate mode is discrete while AQC is continuum.

Adiabatic in AQC refers to a process in which there is no transfer of energy between the system and its environment. This a thermal (not quantum) property; its name is used here metaphorically.

AQC uses the propensity of physical systems – classical or quantum – to minimise their free energy. *Quantum annealing* is free energy minimisation in a quantum system.

Adiabatic quantum computing (cont.)

An AQC algorithm that computes an exact or approximate solution of an optimisation problem encoded in the ground state – its lowest-energy state – of a Hamiltonian (the operator corresponding to the total energy of the system).



Figure: AQC example

The algorithm starts at an initial state H_I that is easily obtained, then evolves adiabatically by changing to the Hamiltonian H_F . The qubit states are read at the end of the transition.

From Randomness to Quantum Computing

An example of evolution is $H = (1 - t)H_I + tH_F$ as the time t increases monotonically from 0 to 1. During the entire computation, the system must stay in a valid ground state.

If the system can reach its ground state we get an exact solution; if it can only reach a local minimum, then we get an approximate solution.

The slower the evolution process the better the approximate (possibly exact) solution is obtained.
AQC is based on the 1928 Born-Fock adiabatic theorem which accounts for the adiabatic evolution of quantum states when the change in the time-dependent Hamiltonian is sufficiently slow:

A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.

- Quantum Annealing (QA) is a heuristic approach originally designed for solving hard combinatorial optimisation problems.
- QA is not as powerful as AQC in (i.e. it can not simulate any quantum gate).
- It is debatable whether QA can provide any actual speedup over classical algorithms.
- QA is relatively easy to engineer.

The D-Wave computers are produced by the Canadian company D-Wave Systems.

D-Wave One (2011) operates on a 128 qubit chipset.

D-Wave Two (2013) works with 512 qubits.

D-Wave 2X (2015) is a 1024 qubit quantum computer.

D-Wave 2000Q (2017) operates with 2048 qubits.

D-Wave Systems describes their machines as using quantum annealing to improve convergence of the system's energy towards the ground state energy of an QUBO problem.

Moore-like growth in hardware (number of qubits)







The Quadratic Unconstrained Binary Optimisation (QUBO) is an **NP**-hard mathematical problem consisting in the minimisation of a quadratic objective function

$$z = \mathbf{x}^T Q \mathbf{x},$$

where **x** is a *n*-vector of binary variables and *Q* is a symmetric $n \times n$ matrix:

$$x^* = \min_{\mathbf{x}} \sum_{i \ge j} x_i Q_{(i,j)} x_j$$
, where $x_i \in \{0, 1\}$.

D-Wave solves only one problem: QUBO. Really?

The computer architecture consists of qubits arranged with a host configuration as a subgraph of a Chimera graph which consists of an $M \times N$ two-dimensional lattice of blocks, with each block consisting of 2*L* vertices (a complete bipartite graph $K_{L,L}$), in total 2*MNL* variables.

The D-Wave One has M = N = L = 4 for a maximum of 128 qubits.

D-Wave qubits are loops of superconducting wire, the coupling between qubits is magnetic wiring and the machine itself is supercooled.

To index a qubit we use four numbers (i, j, u, k), where

- ▶ (*i*, *j*) indexes the (row, column) of the block,
- $u \in \{0,1\}$ is the left/right bipartite half of $K_{L,L}$ and
- 0 < k < L is the offset within the bipartite half.

Qubits indexed by (i, j, u, k) and (i', j', u', k') are neighbours if and only if

1.
$$i = i'$$
 and $j = j'$ and $[(u, u') = (0, 1) \text{ or } (u, u') = (1, 0)]$ or
2. $i = i' \pm 1$ and $j = j'$ and $u = u'$ and $u = 0$ and $k = k'$ or
3. $i = i'$ and $j = j' \pm 1$ and $u = u'$ and $u = 1$ and $k = k'$.



Figure: D-Wave architecture: a subgraph of a Chimera graph with L = N = 4.

In the Figure above shows for L = N = 4 (and M > 2) the structure of an initial part of a Chimera graph where the two half partitions of the bipartite graphs $K_{L,L}$ (blocks) are drawn horizontally and vertically, respectively.

The linear index (qubit id of the vertices) from the four tuple (i, j, u, k) is the value 2NLi + 2Lj + Lu + k.

- 1. State the problem. (Example: maximum-independent-set problem.)
- 2. Reformulate the problem as a QUBO. (Example: reformulate the integer programming optimisation problem as an equivalent QUBO.)
- 3. Decompose a large problem. (Example: use branch-and-bound methods to divide a large problem into smaller subproblems.)
- 4. Minor embedding problem. (Example: minor embed the QUBO graph into a Chimera graph.)
- 5. Submitting the problem to the D-Wave machine.

Recall that an independent set in a graph is a set S of vertices such that for every two vertices in S, there is no edge connecting them.

Maximum Weighted Independent Set (MWIS) Problem:

- *Input:* A graph G = (V, E) with positive vertex weights $w : V \to \mathbb{R}^+$.
- Task: Find an independent set $V' \subseteq V$ such that $\sum_{v \in V'} w(v)$ is as large as possible.

Fact

For every graph G = (V, E) with positive vertex weights $w : V \to \mathbb{R}^+$, the largest weighted independent set of G is equal to $\sum_{v \in V} w(v)$ minus the smallest weighted vertex cover of G.

Proof: The set $V' \subseteq V$ is an independent set of weight $W_1 = \sum_{v \in V'} w(v)$ if and only if $V'' = V \setminus V'$ is a vertex cover of weight $W_2 = \sum_{v \notin V'} w(v)$.

Since $W_1 + W_2 = \sum_{v \in V} w(v)$ the statement was proved.

Fix an input graph G = (V, E) with positive vertex weights $w : V \to \mathbb{R}^+$. Let $W = \max\{w(v) \mid v \in V\}$. We build a QUBO matrix of dimension n = |V| such that:

$$Q_{(i,j)} = \begin{cases} -w(v_i), & \text{if } i = j, \\ > W, & \text{if } i < j \text{ and } ij \in E. \\ 0, & \text{otherwise.} \end{cases}$$
(4)

A vertex-weighted graph and its MWIS QUBO matrix.



Theorem

The QUBO formulation given in (4) solves the MWIS Problem.

Proof: Let \mathbf{x} be a Boolean vector corresponding to an optimal solution to the QUBO formulation (4).

Let $D(\mathbf{x}) = \{v_i \mid x_i = 1\}$ be the vertices selected by \mathbf{x} .

If D(x) is an independent set then −x^TQx is its weighted sum.

For two different solutions \mathbf{x}_1 and \mathbf{x}_2 , which correspond to independent sets, the smallest value of $\mathbf{x}_1^T Q \mathbf{x}_1$ and $\mathbf{x}_2^T Q \mathbf{x}_2$ is better.

Correctness of the formulation

Next assume D(x) is not an independent set and prove that the objective function corresponding to D(x) can be improved.

Indeed, there must be two vertices v_i and v_j in $D(\mathbf{x})$ such that $v_i v_j$ is an edge in the graph.

Let $\mathbf{x}_1 = \mathbf{x}$ but set $x_i = 0$, i.e. $D(\mathbf{x}_1) = D(\mathbf{x}) \setminus \{i\}$. We then have

$$\mathbf{x}_1^T Q \mathbf{x}_1 < \mathbf{x}^T Q \mathbf{x} - W + w(v_i) \leq \mathbf{x}^T Q \mathbf{x}.$$

We repeat the process of improving x until we get an independent set, hence the optimal value of the QUBO holds for some independent set. By the second paragraph of this proof, we know that a maximum weighted independent set corresponds to x^* . See more in [25].

D-Wave architecture is designed to do quantum annealing to solve QUBOs but it is not a complete graph.

In order to "solve" a QUBO problem with the D-Wave machine the logical qubits – the variables in the QUBO formulation – have to be "mapped" onto the physical qubits of the Chimera graph – the graph architecture of the machine –, a process known as "embedding".

Each logical qubit corresponds (via the embedding) to one or more connected physical qubits, called *chain*. *The number of physical qubits is severely limited*.

The *efficiency* of an embedding is measured by the number of physical qubits, the maximum chain and the density of the QUBO matrix.

Minor embeddings

A minor embedding of a graph $G_1 = (V_1, E_1)$ onto a graph $G_2 = (V_2, E_2)$ is a function $f : V_1 \to 2^{V_2}$ that satisfies the following three conditions:

- 1. The sets of vertices f(u) and f(v) are disjoint for $u \neq v$.
- 2. For all $v \in V_1$, there is a subset of edges $E' \subseteq E_2$ such that G' = (f(v), E') is connected.
- 3. If $\{u, v\} \in E_1$, then there exist $u', v' \in V_2$ such that $u' \in f(u), v' \in f(v)$ and $\{u', v'\}$ is an edge in E_2 .

For the minor embedding f defined above, G_1 is referred to as the guest graph while G_2 is called the *host graph*.

We view a QUBO matrix Q as a weighted adjacency matrix (guest graph) to be embedded onto the D-Wave's Chimera graph (host graph).

Quantum supremacy

From Randomness to Quantum Computing

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What is quantum supremacy?

The quantum computational advantage for simulating quantum systems was first stated by Feynman in 1981. What is the justification of Feynman's insight? According to the data processing inequality [23], (classical) post-processing cannot increase information. This suggests that to run an accurate classical simulation of a quantum system one must know a lot about the system before the simulation is started. Manin [38] and Feynman [29] have argued that a quantum computer might not need to have so much knowledge.

This line of reasoning seemingly inspired Deutsch [24] to state

The postulate of quantum computation: Computational devices based on quantum mechanics will be computationally superior compared to digital computers. A spectacular support for this postulate came from Shor's 1994 polynomial factoring quantum algorithm [48] in spite of the fact that the problem whether factoring is in **P** was, and still is, open.

In 2011 the syntagm "quantum supremacy" was coined and discussed by J. Preskill in his Rapporteur talk "Quantum Entanglement and Quantum Computing" [46] at the 25th *Solvay Conference on Physics* (Brussels, Belgium, 19–22 October 2011):

We therefore hope to hasten the onset of the era of quantum supremacy, when we will be able to perform tasks with controlled quantum systems going beyond what can be achieved with ordinary digital computers. Recently, quantum supremacy was described in [13] as follows:

Quantum supremacy is achieved when a formal computational task is performed with an existing quantum device which cannot be performed using any known algorithm running on an existing classical supercomputer in a reasonable amount of time. Note the imprecision in the above formulation: the comparison is made with "any known algorithm running on an existing classical supercomputer" and the classical computation takes "a reasonable amount of time". Can this imprecision be decreased or, even better, eliminated?

Quantum supremacy suggests a misleading comparison between classical and quantum computing: if a quantum computer can outdo **any** classical computer on one problem we have quantum supremacy, even if classical computers could be at least as good as quantum ones in solving many (most) other problems. Put it bluntly, *quantum supremacy, if achieved, won't make classical computing obsolete.* A quantum computational supremacy experiment has to prove both a lower bound and an upper bound.

In Google's proposed experiment [43] the upper bound is given by a quantum algorithm (running on a quantum computer with 49 qubits) sampling from the output distribution of pseudo-random quantum circuits built from a universal gate set—a mathematical fact and an engineering artefact (the construction of the quantum machine)

The lower bound is necessary for proving that no classical computer can simulate the sampling in reasonable time.

Proving lower bounds is notoriously more difficult than demonstrating upper bounds.

Criteria for quantum computational supremacy

Harrow and Montanaro [32] have proposed a reasonable list of criteria for a quantum supremacy experiment:

- 1. a well-defined computational problem,
- a quantum algorithm solving the problem which can run on a near-term hardware capable of dealing with noise and imperfections,
- 3. an amount of computational resources (time/space) allowed to any classical competitor,
- 4. a small number of well-justified complexity-theoretic assumptions,
- 5. a verification method that can efficiently distinguish between the performances of the quantum algorithm from **any** classical competitor using the allowed resources.

Is the quest for quantum computational supremacy worthwhile?

Apart publicity and marketing, is the effort of demonstrating the quantum computational supremacy justified? What are the (possible) benefits? Can the claim of quantum computational supremacy be falsified?

The main benefit could be foundational and philosophical: a better understanding of the nature of quantum mechanics through its computational capabilities. A successful quantum supremacy experiment could be a complement to Bell experiment: the later refuted local hidden models of quantum mechanics, while the former *seems* to invalidate the Extended Church-Turing, a foundational principle of classical complexity theory which ensures that the polynomial time class **P** is well defined. Is the quest for quantum computational supremacy worthwhile?

The Thesis places strong constraints, one of them being that *the model of computation is digital*. For example, analog computers are excluded because they assume infinite arithmetic precision. Furthermore, it is known that an infinite precision calculator with operations +, x, =0?, can factor integers in polynomial time (see [47, 49]).

But, are quantum computers a "reasonable" model of computation? Are quantum systems digital? At first glance quantum computers (and, more generally, quantum systems) appear to be analog devices, since a quantum gate is described by a unitary transformation, specified by complex numbers; a more in-depth analysis is still required. Is the quest for quantum computational supremacy worthwhile?

What does it take to refute the claim of quantum computational supremacy? This amounts to prove that any computation performed by any quantum computer can be simulated by a classical machine in polynomial time, a weaker form of the Extended Church-Turing Thesis. This statement cannot be proved for the same reasons the Church-Turing Thesis cannot be proved: obviously, they may be disproved.

The paper [44] presents efficient classical boson sampling algorithms and a theoretical analysis of the possibility of scaling boson sampling experiments; it concludes that "near-term quantum supremacy via boson sampling is unlikely". The proposed experiment is not about solving a problem: it is the computational task of sampling from the output distribution of pseudo-random quantum circuits built from a universal gate set.

This computational task is difficult because as the grid size increases, the *memory needed to store everything increases classically exponentially*. But, do we *really need* to store everything?

The required memory for a $6 \times 4 = 24$ -qubit grid is just 268 megabytes, less than the average smartphone, but for a $6 \times 7 = 42$ -qubit grid it jumps to 70 terabytes, roughly 10,000 times that of a high-end PC. Google has used Edison, a supercomputer housed by the US National Energy Research Scientific Computing Center and ranked 72 in the Top500 List [1], to simulate the behaviour of the grid of 42 qubits.

The classical simulation stopped at this stage because going to the next size up was thought to be currently impossible: a 48-qubit grid would require 2,252 petabytes of memory, almost double that of the top supercomputer in the world. The path to quantum computational supremacy was obvious: if Google could solve the problem with a 50-qubit quantum computer, it would have beaten every other computer in existence.

Simple and clear!

Google was on track to deliver before the end of 2017!

Let us note that many, if not most, discussions about quantum computational supremacy focus on the most exciting possibilities of quantum computers, namely the upper bound.

What about the lower bound? Google's main article on this topic [13] refers cautiously to the lower bound in the abstract:

We extend previous results in computational complexity to argue more formally that this sampling task must take exponential time in a classical computer.

They do not claim to have a proof for the lower bound, just a "better formal argument".

Proving the lower bound...

Memory assumption. Sampling this distribution classically requires a direct numerical simulation of the circuit, with computational cost exponential in the number of qubits.

The assumption was corroborated by the statement:

Storing the state of a 46–qubit system takes nearly a petabyte of memory and is at the limit of the most powerful computers. [43]

The **Memory assumption** is crucial for the proposed lower bound, and, indeed, this was confirmed very soon. The paper [45] proved that a supercomputer can simulate sampling from random circuits with low depth (layers of gates) of up to 56 qubits.

Better results have been quickly announced, see for example [14]. The limits of classical simulation are not only known, but hard to predict.

In spite of this, IBM has announced a prototype of a 50-qubit quantum computer, stating that it "aims to demonstrate capabilities beyond today's classical systems" with quantum systems of this size [2].

Digression: again about the importance of lower bounds

Ewin Tang (an 18-year-old undergraduate student at UT Austin) has recently proved [50] that classical computers can solve the "recommendation problem" – given incomplete data on user preferences for products, can one quickly and correctly predict which other products a user will prefer? – with performance comparable to that of a quantum computer.

Is this significant? **Yes**, because quantum computer scientists had considered this problem to be one of the best examples of a problem that quantum computers can solve exponentially faster than their classical ones.

The quantum solution in [35] was hailed as one of the first examples in *quantum machine learning and big data* that would be unlikely to be done classically...

According to [4]

The successful classical simulation does not undercut the rationale for quantum supremacy experiments. The truth, ironically, is almost the opposite: it being possible to simulate 49–qubit circuits using a classical computer is a precondition for Google's planned quantum supremacy experiment, because it's the only way we know to check such an experiment's results!

The goal is to get via quantum computing as far as you can up the mountain of exponentiality provided people still see you from the base. Why? Because it's there. "It is not the mountain we conquer but ourselves", as Edmund Hillary aptly said.
Three lessons

- Do not to underestimate the importance of mathematical modelling and proving (lower bounds, in particular).
- A trend in quantum computing is emerging: when a problem is solved efficiently in quantum computing, it draws more attention and often produces better classical alternatives than existed before. Some of the new efficient classical solutions, see for example [17, 5, 6, 33, 50], have been directly inspired by the quantum work.
- The conversation on quantum computing, quantum cryptography and their applications needs an infusion of modesty (if not humility), more technical understanding and clarity as well as less hype. Raising false expectations could be harmful for the field.

The race continues! See more in [16].

Supplementary material

From Randomness to Quantum Computing

Let $s_1 \cdots s_n$ be a binary string. A monochromatic arithmetic progression of length k is a substring

 $s_i s_{i+t} s_{i+2t} \cdots s_{i+(k-1)t}$

 $1 \le i \le i + (k-1)t \le n$ with all characters equal (0 or 1) for some t > 0.

Van der Waerden finite theorem

For every natural k there is a natural n > k such that every string of length n contains a monochromatic arithmetic progression of length k.

VDW

Let C_i be a computably enumeration of all prefix-free TMs and construct the prefix-free TM U by

$$U(1^i 0x) = C_i(x).$$

▶ USTheorem

Proof

To prove that $H(x^*) \ge |x^*| - c$ we construct the prefix-free TM

$$D(p) = U(U(p))$$

and pick the constant *c* coming from the universality theorem (applied to *U* and *D*). Take $x = y^*$, $z = x^*$. One has:

$$D(z) = U(U(z)) = U(U(x^*)) = U(x) = U(y^*) = y,$$

SO

$$H_D(y) \le |z| = |x^*| = H(x),$$

 $|x| = |y^*| = H(y) \le H_D(y) + c \le H(x) + c.$

StringComplexity

From Randomness to Quantum Computing

Given $\omega_1 \omega_2 \cdots \omega_n$ we run in parallel U(p) on various programs till we get enough programs p_1, \ldots, p_N such that

$$\sum_{i=1}^{N} 2^{-|p_i|} \geq 0.\omega_1 \omega_2 \cdots \omega_n.$$

Every program q with $|q| \le n$, different from all p_i 's above, doesn't stop as otherwise

$$\Omega < 0.\omega_1\omega_2\cdots\omega_n + 2^{-n} \leq \sum_{i=1}^N 2^{-p_i} + 2^{-|q|} \leq \Omega,$$

a contradiction.
• OmegaHaltTheorem

Define M as follows: on input x compute y = U(x) and the smallest number of programs $p_1, \ldots, p_t \in \text{dom}(U)$ (if they exist) with

$$\sum_{i=1}^t 2^{-|p_i|} \ge 0.y.$$

Let M(x) be the first (in quasi-lexicographical order) string not belonging to the set $\{U(p_1), U(p_2), \ldots, U(p_t)\}$ if both y and t exist, and $M(x) = \infty$ if $U(x) = \infty$ or t does not exist. If $M(x) < \infty$ and x' is a string with U(x) = U(x'), then M(x) = M(x').

Applying this to an arbitrary x with $M(x) < \infty$ and the program $x' = (U(x))^*$ yields

$$H_M(M(x)) \le |x'| = H_U(U(x)).$$
 (5)

Furthermore, by the universality of U there is a constant c > 0 with

$$H_U(M(x)) \le H_M(M(x)) + c, \tag{6}$$

for all x with $M(x) < \infty$.

Take $U(x) = \omega_1 \cdots \omega_n$. From the construction of M (and the fact that Omega solves the halting problem) we conclude that $H_U(M(x)) \ge n$. Using (6) and (5) we obtain

$$egin{array}{rcl} &\leq & H_U(M(x))\ &\leq & H_M(M(x))+c\ &\leq & H_U(U(x))+c\ &= & H_U(\omega_1\omega_2\cdots\omega_n)+c. \end{array}$$

The sequence of rationals $r_N = \sum_{i=1}^N 2^{-|f(i)|}$, where f is a computable enumeration of the domain of U, is computable, increasing and converges to Ω .

CEOmegaTheorem

Van der Waerden theorem

For any positive integers k there is a positive integer γ such that every bit string of length more than γ contains an arithmetic progression with k occurrences of the same digit or colour, i.e. a monochromatic arithmetic progression of length k.

SpuriousCorrelations

The CBS drama TV show Numb3rs,

http://www.cbs.com/primetime/numb3rs/,

season 5; episode 5; scene 6) includes the following dialogue:

LARRY: Ah, Charles, my ambulatory reference book. Chaitin's Omega Constant...?

CHARLIE: Omega equals .00787499699. Why, what're you working on? (sees the file, reacts) Oh. FBI file.

The math is explained at http://numb3rs.wolfram.com/505. Incomputability of Omega

Graph isomorphism

From Randomness to Quantum Computing

The **graph isomorphism problem** is the computational problem of determining whether two finite graphs are isomorphic.

Instance: Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ with $|V_1| = |V_2|$ and $|E_1| = |E_2|$. Question: Determine whether there exists a bijective edge-

invariant vertex mapping (isomorphism) $f: V_1 \rightarrow V_2.$

The mapping f is edge-invariant if for every pair of vertices $\{u, v\}$, we have $uv \in E_1$ iff $f(u)f(v) \in E_2$.

This is one of a very few problems in **NP** that is neither known to be solvable in polynomial time nor **NP**-complete.

QUBO direct formulation for the graph isomorphism problem

Following [19] we present a QUBO objective function F for the graph isomorphism problem which requires n^2 binary variables represented by a binary vector $\mathbf{x} \in \mathbb{Z}_2^{n^2}$:

$$\mathbf{x} = (x_{0,0}, x_{0,1}, \dots, x_{0,n-1}, x_{1,0}, x_{1,1}, \dots, x_{1,n-1},$$

$$\ldots, x_{n-1,0}, \ldots, x_{n-1,n-1}).$$

The equality $x_{i,i'} = 1$ encodes the property that the function f maps the vertex v_i in G_1 to the vertex $v_{i'}$ in G_2 : $f(v_i) = v_{i'}$.

For this mapping we need to pre-compute n^2 binary constants $e_{i,j}$, $0 \le i < n$ and $0 \le j < n$: $e_{i,j} = 1$ if $ij \in E_2$.

QUBO direct formulation for the graph isomorphism problem

The objective function $F(\mathbf{x})$ has the following form:

$$F(\mathbf{x}) = H(\mathbf{x}) + \sum_{ij \in E_1} P_{i,j}(\mathbf{x}),$$
(7)

where

$$H(\mathbf{x}) = \sum_{0 \le i < n} \left(1 - \sum_{0 \le i' < n} x_{i,i'} \right)^2 + \sum_{0 \le i' < n} \left(1 - \sum_{0 \le i < n} x_{i,i'} \right)^2,$$
(8)

and

$$P_{i,j}(\mathbf{x}) = \sum_{0 \le i' < n} \left(x_{i,i'} \sum_{0 \le j' < n} x_{j,j'} (1 - e_{i',j'}) \right).$$
(9)

From Randomness to Quantum Computing

The function F consists of two parts, $H(\mathbf{x})$ and $\sum_{ij \in E_1} P_{i,j}(\mathbf{x})$. Each part serves as a penalty for the case when the function f is not an isomorphism.

• The first part *H* ensures that *f* is a bijective function:

H = 0 iff the function f encoded by the vector **x** is a bijection.

• The second term ensures that *f* is edge-invariant:

 $\sum_{ij\in E_1} P_{i,j}(\mathbf{x}) > 0 \text{ iff there exists an edge } uv \in E_1 \text{ such that}$ $f(u)f(v) \notin E_2.$

Assume that

$$x^* = \min_{\mathbf{x}} F(\mathbf{x}).$$

Then, the mapping f can be 'decoded' from the values of the variables $x_{i,i'}$ using an additional partial function D. Let \mathcal{F} be the set of all bijections between V_1 and V_2 .

Then $D : \mathbb{Z}_2^{n^2} \to \mathcal{F}$ is a partial 'decoder' function that re-constructs the vertex mapping f from the vector \mathbf{x} , if such f exists.

QUBO direct formulation for the graph isomorphism problem

The domain of *D* contains all vectors $\mathbf{x} \in \mathbb{Z}_2^{n^2}$ that can be 'decoded' into a bijective function *f*:

$$\operatorname{dom}(D) = \left\{ \mathbf{x} \in \mathbb{Z}_2^{n^2} \; \middle| \; \sum_{0 \le i' < n} x_{i,i'} = 1, \text{ for all } 0 \le i < n \right.$$
$$\operatorname{and} \sum_{0 \le i < n} x_{i,i'} = 1, \text{ for all } 0 \le i' < n \right\},$$

and

$$D(\mathbf{x}) = egin{cases} f, & ext{if } \mathbf{x} \in ext{dom}(D), \ ext{undefined}, & ext{otherwise}, \end{cases}$$

where $f: V_1 \rightarrow V_2$ is a bijection such that $f(v_i) = v_{i'}$ iff $x_{i,i'} = 1$.

From Randomness to Quantum Computing

QUBO direct formulation for the graph isomorphism problem

The following two lemmata will be used to prove correctness of the objective function F in (7).

Lemma

For every $\mathbf{x} \in \mathbb{Z}_2^{n^2}$, $H(\mathbf{x}) = 0$ iff $D(\mathbf{x})$ is defined (in this case $D(\mathbf{x})$ is a bijection).

Lemma

Let $\mathbf{x} \in \mathbb{Z}_2^{n^2}$ and assume that $D(\mathbf{x})$ is a bijective function. Then, $\sum_{ij \in E_1} P_{i,j}(\mathbf{x}) = 0$ iff the mapping $f = D(\mathbf{x})$ is edge-invariant.

Theorem

For every $\mathbf{x} \in \mathbb{Z}_2^{n^2}$, $F(\mathbf{x}) = 0$ iff the mapping $f : V_1 \to V_2$ defined by $f = D(\mathbf{x})$ is an isomorphism.

The matrix QUBO can only contain quadratic terms, so some terms of $F(\mathbf{x})$ have to be modified in such a way that this condition is satisfied and the optimal solutions of (??) are preserved. To this aim two operations will be performed.

First, any constant term is ignored because removing it does not modify the optimal solutions of (??): the value of $F(\mathbf{x})$ is reduced by a constant amount for all $\mathbf{x} \in \mathbb{Z}_2^n$.

Second, as all variables $x_{i,i'}$ are binary, we replace $x_{i,i'}$ with $x_{i,i'}^2$ for all $x_{i,i'}$ with no effect on the value of $F(\mathbf{x})$.

QUBO direct formulation for the graph isomorphism problem: the graph P_3

Consider the path graph P_3 of order 3 and two copies represented as G_1 with edges $E_1 = \{\{0,1\},\{1,2\}\}$ and G_2 with edges $E_2 = \{\{0,1\},\{0,2\}\}$. It is easy to see there are two possible isomorphisms between G_1 and G_2 , where we require vertex 1 of G_1 to be mapped to vertex 0 of G_2 .

The QUBO formulation requires $3^2=9$ variables and the binary variable vector $\bm{x}\in\mathbb{Z}_2^9$ is:

$$\mathbf{x} = (x_{0,0}, x_{0,1}, x_{0,2}, x_{1,0}, x_{1,1}, x_{1,2}, x_{2,0}, x_{2,1}, x_{2,2}).$$

By expanding (8) we get:

$$\begin{split} \mathcal{H}(\mathbf{x}) &= (1 - (x_{0,0} + x_{0,1} + x_{0,2}))^2 + (1 - (x_{1,0} + x_{1,1} + x_{1,2}))^2 \\ &+ (1 - (x_{2,0} + x_{2,1} + x_{2,2}))^2 + (1 - (x_{0,0} + x_{1,0} + x_{2,0}))^2 \\ &+ (1 - (x_{0,1} + x_{1,1} + x_{2,1}))^2 + (1 - (x_{0,2} + x_{1,2} + x_{2,2}))^2 \end{split}$$

From Randomness to Quantum Computing

QUBO direct formulation for the graph isomorphism problem: the graph P_3

Finally we obtain the following penalty terms:

$$\begin{aligned} & P_{0,1} = x_{0,0}x_{1,0} + x_{0,1}(x_{1,1} + x_{1,2}) + x_{0,2}(x_{1,1} + x_{1,2}), \\ & P_{1,2} = x_{1,0}x_{2,0} + x_{1,1}(x_{2,1} + x_{2,2}) + x_{1,2}(x_{2,1} + x_{2,2}). \end{aligned}$$

The objective function $F(\mathbf{x})$ can only contains quadratic terms, so we need to process some of the penalty terms before we can encode them in a QUBO instance. Finally, for all elements $x_{i,i'}$ in \mathbf{x} we map the variable $x_{i,i'}$ to the index $d(x_{i,i'}) = 3i + i' + 1$ (between 1 and 9) and then the entry $Q_{(d(x_{i,i'}),d(x_{j,j'}))}$ is assigned the coefficient of the term $x_{i,i'}x_{i,j'}$ in $F(\mathbf{x})$.

As for each pair $x_{i,i'}$ and $x_{j,j'}$ there are two possible equivalent terms, $x_{i,i'}x_{j,j'}$ and $x_{j,j'}x_{i,i'}$, as a convention, we will use the term that is be mapped to the upper-triangular part of Q.

QUBO direct formulation for the graph isomorphism problem: the graph P_3

The upper-triangular matrix representation of Q is:

| variables | <i>x</i> 0,0 | $x_{0,1}$ | $x_{0,2}$ | $x_{1,0}$ | $x_{1,1}$ | $x_{1,2}$ | <i>x</i> _{2,0} | $x_{2,1}$ | <i>x</i> _{2,2} |
|-------------------------|--------------|-----------|-----------|-----------|-----------|-----------|-------------------------|-----------|-------------------------|
| X0,0 | -2 | 2 | 2 | 3 | 0 | 0 | 2 | 0 | 0 |
| <i>x</i> _{0,1} | | -2 | 2 | 0 | 3 | 1 | 0 | 2 | 0 |
| <i>x</i> _{0,2} | | | -2 | 0 | 1 | 3 | 0 | 0 | 2 |
| <i>x</i> _{1,0} | | | | -2 | 2 | 2 | 3 | 0 | 0 |
| $x_{1,1}$ | | | | | -2 | 2 | 0 | 3 | 1 |
| $x_{1,2}$ | | | | | | -2 | 0 | 1 | 3 |
| X2,0 | | | | | | | -2 | 2 | 2 |
| x _{2.1} | | | | | | | | -2 | 2 |
| X2.2 | | | | | | | | | -2 |

Table: QUBO matrix for P_3

We have removed a constant value of 6 from $F(\mathbf{x})$ when encoding it into Q, so the value of the optimal solution of $f(\mathbf{x}) = \mathbf{x}^T Q \mathbf{x}$ will be decreased by 6, obtaining the following two optimal solutions:

 $\mathbf{x}_1 = (0, 1, 0, 1, 0, 0, 0, 0, 1)$ and $\mathbf{x}_2 = (0, 0, 1, 1, 0, 0, 0, 1, 0)$.

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