Computer-inspired quantum experiments

Mario Krenn, Manuel Erhard and Anton Zeilinger

Abstract | The design of new devices and experiments has historically relied on the intuition of human experts. Now, design inspirations from computers are increasingly augmenting the capability of scientists. We briefly overview different fields of physics that rely on computer-inspired designs using a variety of computational approaches based on topological optimization, evolutionary strategies, deep learning, reinforcement learning or automated reasoning. Then we focus specifically on quantum physics. When designing new quantum experiments, there are two challenges: quantum phenomena are unintuitive, and the number of possible configurations of quantum experiments explodes exponentially. These challenges can be overcome by using computer-designed quantum experiments. We focus on the most mature and practical approaches to find new complex quantum experiments, which have subsequently been realized in the lab. These methods rely on a highly efficient topological search, which can inspire new scientific ideas. We review several extensions and alternatives based on various optimization and machine learning techniques. Finally, we discuss what can be learned from the different approaches and outline several future directions.

Computers have long been an indispensable tool for scientists, enabling more complex calculations or simulations. Traditionally, a computer was no more than a powerful calculator, running hard-coded algorithms. However, computers are increasingly being used in the more creative design processes in various fields of physics, augmenting the conventional intuition-based design strategies. In this Perspective article, we discuss how advanced computational methods help to design new experiments and uncover new approaches. After providing a brief overview of computer-inspired designs in physics, we focus on quantum experiments, in particular, on quantum optics experiments. We discuss how to design specific experimental configurations that can generate, transform or measure particular non-classical quantum states, such as non-classically correlated or entangled states. We will also show how exploration — design without a particular goal — can lead to new ideas.

There is an entire spectrum of approaches, from pure goal-driven tasks for the discovery of specific experimental implementations of the generation and transformation of quantum states, to computational exploration methods that help uncover and inspire new scientific ideas. In this Perspective article, we are agnostic towards the computational methodology, meaning that we do not restrict ourselves to machine learning techniques. Instead, we follow the pragmatic approach of covering all automated, computational methods that help to design and to discover new quantum experiments.

Owing to our focus on computer-inspired designs of quantum experiments, we do not cover the many interesting computational and machine learning methods in related fields such as experimental quantum Hamiltonian learning (where parameterized quantum circuits are modified to uncover coefficients of the Hamiltonian)[1,2], neural-network-enhanced quantum tomography and measurements[3–5], or control and calibration of settings in quantum experiments[6–9]. We direct the reader to reviews that cover the topics of machine learning in more detail, for physics[10] and quantum physics[11,12].

Computer-inspired designs

In this section, we overview some examples of computer-inspired designs in different areas of physics, also summarized in TABLE 1. One of the most impressive and influential examples of computer-inspired designs can be found in plasma physics in the design of nuclear fusion reactors in form of stellarators. Although stellarators had been studied since the 1950s, it was only possible to design their magnetic coils with sufficiently high quality in the late 1980s, when computers became powerful enough[13]. The most extensive experimental implementation is the billion-dollar reactor Wendelstein 7X in Greifswald, Germany, with 50 computer-designed, superconducting magnetic coils that were optimized for confinement, stability, transport and equilibrium properties as well as experimental constraints[14,15]. Wendelstein 7X produced the first stable hydrogen plasma in 2015 (REF.[16]).

In accelerator physics, computer-inspired and computer-optimized designs have a long tradition[17], from which we mention a few examples. Genetic algorithms augmented with machine learning techniques have been used to optimize the magnetic confinement configurations of National Synchrotron Light Source II (NSLS-II) storage ring at the Brookhaven National Laboratory in the United States. The goal was to maximize the dynamic aperture, a complex multiobjective function that involves, among others, the beam lifetime and energy acceptance. Several high-quality solutions have been experimentally tested[18]. Quality improvements of the beam injection at the heavy-ion synchrotron SIS18 at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany have also been achieved using genetic algorithms. The algorithm found a better set of parameters than previous simulation studies[19]. High-power radio-frequency sources, which are essential for particle accelerators, have been optimized using evolutionary algorithms. There, the evolutionary algorithm's objective is to maximize the efficiency of a klystron, by exploring the continuous space of geometric design parameters of a multicell cavity[20].

Topological optimization[21–24] has shaped the field of mechanical engineering

Table 1 | **Examples of computer-inspired designs in selected fields of physics**

Discipline	Objectives	Degrees of freedom	Approaches	Status
Plasma physics	Magnetic confinement for thermonuclear reactor[13]	Geometry of magnetic coils	High-quality plasma simulations	Wendelstein 7X[16]
Accelerator physics	Stable high-power, high-density beams[17]	Continuous magnet settings and cavity geometries	Evolutionary, gradient based	Efficient designs[19,20], PoC experiments[18]
Mechanical engineering	2D and 3D material designs[25,26]	Quasi-continuous pixel/voxel	Topological optimization[21–24]	Widely used in industry and academia
Nanophotonics	Nonlinear optics, metamaterial, topological photonics	Quasi-continuous pixel/voxel	Topological optimization[28,29]	Efficient designs, PoC experiments
Quantum circuits	Circuits for binary, gate-based, universal quantum computers	Circuit topology and parameterized gates	Deterministic[39,40], variational[43–45], machine learning[47,48], automated reasoning[54–56]	Efficient designs, PoC experiments[43]
Superconducting hardware	Fundamental multiqubit gates[57]	Circuit topology and parametrized gates	Topology search, gradient based	Efficient designs
Chemistry	Functional materials, drug candidates[58,59]	Discrete molecular graphs	Virtual screening[61–63], evolutionary[64–67], gradient based[68]	Widely used in industry and academia
Quantum experiments	Complex entangled states, quantum transformations in quantum optics	Discrete experimental topology and continuous components	Highly efficient topological search[83], evolutionary[117,119,120], reinforcement[121,124], gradient based[125,133]	PoC experiments[85–90,113,114], conceptual insights[91,93,115]

PoC, proof-of-principle experiments.

since the late 1980s[25,26]. Remarkable new aerodynamic structures have been designed using computer-aided approaches that could lead to a substantial reduction in the fuel consumption of aeroplanes[27]. The idea of topological optimization has subsequently found application in the field of nanophotonics[28,29], and has since been augmenting optimization schemes based on human intuition. Its applications range from nonlinear optics to topological photonics and nanoscale optics. Concrete examples involve highly efficient free-space-to-waveguide couplers[30], compact micrometre-scale wavelength demultiplexers for several different colours[31], highly efficient, diamond-based coupling devices[32], discovery of topological bands[33] or on-chip particle accelerators[34].

The automated design and verification of logical circuits is well established[35,36]. The quantum version is the automated synthesis of quantum circuits. In principle, the question of designing a quantum circuit for a given quantum algorithm can be solved with the Solovay–Kitaev algorithm for a universal qubit gate set[37]. Unfortunately, the algorithm leads to impractically large quantum circuits. Thus, great efforts are invested in simplifying and optimizing quantum circuits with deterministic or heuristic methods[38–40]. Furthermore, there is a need to optimize theoretical quantum circuits for hardware with architecture-specific constraints, a process known as compilation[41,42]. A very different approach is the variational optimization of quantum circuits, using hybrid quantum-classical algorithms. Two prominent examples are the variational quantum eigensolver[43,44] and the quantum approximate optimization algorithm[45]. There, a parameterized quantum circuit is optimized using an objective function. For example, to produce a desired quantum state as accurately as possible, one can use the fidelity as the objective function. However, there are challenges such as exponentially vanishing gradients[46], which shows that finding sufficiently good parameter settings requires more unconventional learning algorithms. Furthermore, how to find good initial quantum circuit topologies (which is more coarse-grained than in the nanophotonics case) is an open question[47,48]. A particular instance of quantum circuit design concerns quantum control and quantum feedback algorithms. There, the task is to find optimal quantum circuit design strategies that are adaptive and work in changing environments. Neural-network-based reinforcement learning has been demonstrated to be a viable tool to solve these tasks[49], with potential impact on quantum error correction in quantum computers. Several other machine learning techniques approach the challenges in quantum control and quantum error correction, such as REFS[50–52].

A fundamentally different approach is the application of automated reasoning, a field in artificial intelligence that has seen tremendous progress in recent years[53]. The idea is to translate the problem of quantum circuit synthesis to Boolean satisfiability (SAT) systems. Solutions to the resulting propositional formula can subsequently be found using highly efficient SAT solvers[54–56].

An extension of the family of computer-inspired designs is superconducting quantum hardware[57]. This study reports the blueprint for the first efficient, noise-insensitive coupler for four-qubit interactions, an essential element for quantum simulations. The task to design such an element is both discrete (defining the topology of the circuit from a space of roughly 10^3 possibilities, more in BOX 1) and continuous (setting the parameters of the individual elements in a circuit). It was solved by first identifying initial random guesses, subsequently optimized through gradient descent and swarm optimization.

In chemistry and material science, the computer-inspired design of molecules is widely used for discovering new drugs, functional materials or chemical reactions[58,59]. A particular challenge is the enormous search space that is estimated to be on the order of 10^{60}, even for small biomolecules[60], and without continuous parameters that could be optimized through gradient-based methods. As a result, unbiased and systematic search methods (high-throughput virtual screening)[61–63] or genetic algorithms and particle swarms[64–67] are a common tool. These discrete search problems can be solved by transforming them into continuous optimization problems[68] — which opens up the application of deep learning methods in molecular design. The advances in deep learning have also been exploited in the design of materials with new topological band structures[33].

Computer-inspired designs based on evolutionary strategies for complex, multiobjective problems are used in many other fields of science and engineering[69]. An extensive collection with more than 10,000 relevant references can be found in REF.[70].

Computer-inspired experiments

In this section, we focus on computer-inspired quantum optics experiments. We distinguish between quantum optics experiments and quantum circuits as they differ in several ways. Quantum circuits consist of a well-defined number of qubits, for which arbitrary unitary transformations are well known. In contrast, in quantum optics experiments, photons can occupy high-dimensional Hilbert spaces in several degrees of freedom, for which experimentally feasible, arbitrary transformations are not known. Photon–photon interactions are not yet possible due to the lack of strong nonlinear materials. Furthermore, high-quality deterministic single-photon sources are still an active field of research. Lasers, which have complex photon number states, are an essential tool in quantum optics that have no analogue in quantum circuits. Quantum optics can be used for quantum metrology, imaging and communication, which lead to entirely different objectives for algorithmic designs of experiments. Conceptually, quantum circuits are logical instructions for computation devices, whereas quantum experiments are closely related to physical hardware.

We will cover general high-dimensional multiparticle quantum optical systems[71,72]. Although the experimental technology has shown impressive improvements in recent years in generating[73–75], manipulating[76–80] and measuring[81,82] complex entangled quantum systems, in many cases, the lack of feasible experimental design proposals hinders further progress.

We will focus on practical alternatives to the human design of quantum experiments. For that, we define classes of practicality of algorithms for computer-designed quantum experiments (FIG. 1), which indicate the level of maturity and demonstrated applicability in the scientific domain:

- Class 0: the algorithm has re-discovered solutions to previously solved questions.
- Class I: the algorithm has uncovered solutions to previously unsolved questions.
- Class IIa: the algorithm has uncovered solutions to previously unsolved questions, which have been experimentally demonstrated.
- Class IIb: the algorithm has inspired the discovery of scientific insights or concepts.
- Class III: combination of class IIa and class IIb. The algorithm has uncovered solutions to previously unsolved questions, which have been experimentally demonstrated, and has inspired the discovery of scientific insights or concepts.
- This classification is sufficient for the moment for our purpose. In the future, however, hopefully much more surprising and far-reaching insights can be obtained from algorithms; therefore, we expect class IIb to become more fine-grained.

Next, we detail the different approaches. The technologies involved are further described in BOX 1. First, we start with an algorithm for efficient topological search, which lies in class III. We then describe a method that has led to new experimental designs that have been implemented in laboratories, which lies in class IIa. One recent addition that aims specifically at conceptual insights (thus class IIb) is analysed afterwards. Finally, we overview several other promising techniques that

Box 1 | **Computer-inspired design tools**

Finding an experimental setup consists of identifying a setup topology and finding suitable component parameters. The topology of the quantum experiment is the form taken by the network of interconnections of the quantum optical components; some components can have continuous parameters (such as splitting ratios of beam splitters).

A topological search algorithm is specialized in identifying the setup topology, when the parameters for the optical components are chosen from a finite, discrete list (for example, rotation angles of wave plates that could be multiples of $\pi/8$). The search can be augmented with specific learning algorithms.

A parametric optimization starts from a setup topology that is known or conjectured to be very expressive. That means the setup has the potential to produce many different states by tuning the continuous parameters of its optical components (such as the angle of the wave plates, splitting ratios of the beam splitters or laser power). To find a suitable experimental configuration, the objective function, that is, the fidelity, can be expressed in terms of the setup parameters. This allows for the application of gradient descent, which is an iterative optimization algorithm for finding a local optimum of a differentiable function. Highly efficient optimization algorithms furthermore exploit Hessians, the second derivatives of the objective function.

Topological optimization aims to find a suitable experimental setup by starting from a very general representation of the setup and subsequently to reduce the topology of the configuration. To achieve this, abstract representations of the setups (for instance, graph-theoretical representations) can be applied.

Genetic algorithms are optimization techniques inspired by natural evolution, involving mutations and selection rules. A population of individuals (each encodes the information of one quantum experiment) are initialized. Subsequently, the best individuals are selected according to a fitness function (such as the fidelity for producing a quantum state). Their offspring are then mutated and form the next generation. This process continues iteratively; over time, the fitness of the population, and thereby the fidelity of the quantum experiment, grows.

Swarm optimization is inspired by the natural swarm intelligence, for example, in flocks of birds. The idea is that a population of individuals navigates iteratively in a search space and wants to identify the global maximum (for instance, of the fidelity). The direction of each individual is influenced by its local best solution, but also by the global best solution of the entire swarm.

Deep learning stands for algorithms that apply artificial neural networks with large numbers of layers. Often, the neural networks are trained in a supervised way. There, the user provides training examples, and the neural network is adapted such that the quality of the result improves over the span of the training. An optimal scenario will allow for the algorithm to correctly determine the class labels or predict properties for new instances.

In a reinforcement learning scenario, an agent observes and takes actions in an environment to maximize some reward function. If an agent's representation of the environment or its strategy is encoded in a large neural network, the technique is called deep reinforcement learning. The idea became widely known by the impressive results on playing computer games[163–167] and defeating world-champion Go and chess players[168]. These results motivate the application of reinforcement learning techniques to scientific environments, and in particular to the design of new quantum experiments.

Automated reasoning is a logic-based artificial intelligence technology. Informally, a computational problem is written as a logical expression of binary variables, which evaluates as true for a correct answer. Highly efficient satisfiability (SAT) solvers and various other techniques are used to find solutions to the equations efficiently. This technology has identified several proofs or counter-examples in mathematics.

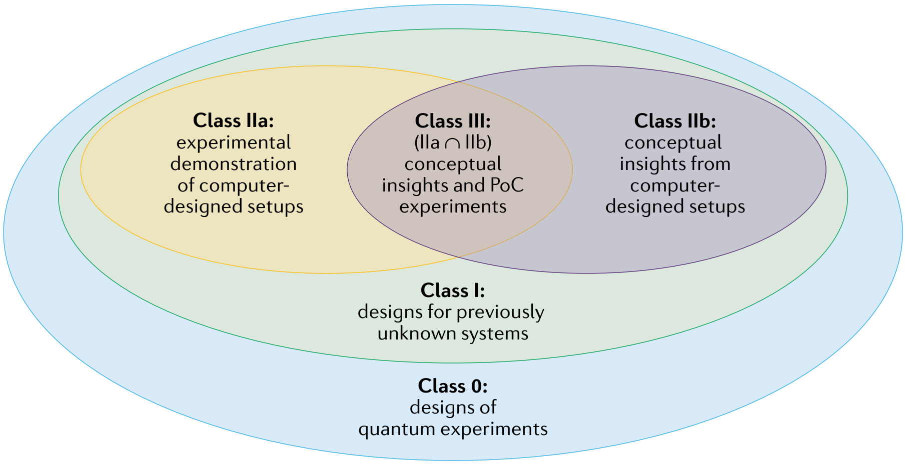

Fig. 1 | **Algorithms for designing quantum experiments.** Algorithms in classes II and III have been shown to be applicable in more practical ways of contributing to scientific research. PoC, proof-of-principle experiments.

aim to design new quantum experiments in class I. We stress that although there is a class III algorithm, approaches in other classes can be interesting for other reasons. In particular, some techniques are more generally applicable than others, whereas others are optimized for specific systems or scientific questions. Some algorithms have the potential for scientific interpretations of internal representations, while others can provide exciting features if a large amount of training data is provided. Improvements of the experimental feasibility of the computer designs are certainly expected in the future. For these reasons, we consider all presented methodologies and algorithms to be a worthwhile contribution to the difficult questions raised in experimental quantum optics. Finally, we will connect computer-inspired quantum experiments with inverse-design techniques in other fields of physics, and thereby indicate several interdisciplinary ideas that might be interesting future research questions.

Class III

We will describe a computational strategy that can be used for automated design of new quantum optics experiments, which have been realized in laboratories and have inspired new conceptual ideas. This strategy was used to find a specific experimental implementation of a quantum state or transformation, and has been used in an explorative way to uncover outliers that might be scientifically interesting. The underlying idea was first reported in REF.[83], and has since been substantially extended and improved. It led to solutions of several previously unsolved questions[83,84], many computer-designed experiments have been experimentally implemented[85–90] and it has been used to discover new scientific ideas and concepts[91–93].

The program, known as MELVIN, can be considered as a highly efficient and optimized search routine for the inherently discrete topology of quantum optical setups (the calculation of quantum states is based on symbolic transformations). The algorithm's working principle is illustrated in FIG. 2. The program has been proved successful because of several specific features. Its toolbox is chosen in such a way that all resulting solutions are experimentally feasible — that has led to several computer-inspired lab implementations. Furthermore, whereas continuous gradient-based optimization techniques are efficient in identifying (local) optima, discrete topological searches have the great advantage that their results are often interpretable for human scientists. The optical components in the setups have simple parameters (rational splitting ratios, phases are nth root of unity with small n), which makes it easy to comprehend the development of the state within the optical setup. This is in contrast to arbitrary real-valued experimental parameters, which lead to quantum states with a larger number of terms with real coefficients. Although this may be obvious, it is important for the human understanding of the underlying principles. Another notable feature is that the algorithm doesn't need to be trained, nor does it need training data. This allows the direct application to new open questions.

Although a topological search is conventionally inefficient, two core ideas substantially accelerate the identification of solutions:

1. Generalized objective functions (relaxed conditions on the objective) to increase the probability of finding potential solutions
2. Identification of necessary criteria that allow calculations to be aborted before evaluating time-expensive properties

The underlying principles are showcased by two examples that also illustrate how MELVIN can inspire not only new experimental configurations but also new conceptual ideas.

Creating a 3D Greenberger–Horne–Zeilinger state. To provide a concrete example, we discuss the application on the 3D three-partite Greenberger–Horne–Zeilinger (GHZ) state, which was the first application in REF.[83], and has been experimentally demonstrated (with some intermediate steps[85]) more than three years later[89]. The complexity of a computer-designed experiment is illustrated in FIG. 3. The initial discovery of the 3D GHZ setup in REF.[83] required roughly five central processing unit (CPU)-core hours with a Intel Core i5-2540 2.5GHz.

The 3D GHZ state can be written as

$$|\psi\rangle = \frac{1}{\sqrt{3}}(|0,0,0\rangle + |1,1,1\rangle + |2,2,2\rangle), \quad (1)$$

where $|0\rangle$, $|1\rangle$ and $|2\rangle$ are three orthogonal states, independent of their degree of freedom. To create an experimental setup for this state, some important points need to be considered.

- Assembling a quantum experiment. The algorithm starts by placing two spontaneous parametric down-conversion crystals on a virtual optical table. Setups with two crystals are very well investigated experimentally[71], so this configuration is a natural starting point. The rest of the setup is assembled from elements in the toolbox. The toolbox contains optical devices that are accessible in a quantum optics lab (FIG. 3), such as beam splitters, phase shifters, wave plates, holograms and Dove prisms. In addition to elementary transformations, adding composite devices to the toolbox can substantially speed up the search process. These devices are especially useful transformations in quantum optics, such as effective single-photon filters via quantum teleportation[94], local high-dimensional gate transformations[88] and special stable polarization transformations[95]. In the 3D GHZ state-generation example, the introduction of an interferometer-based parity sorter for spatial modes of photons (introduced in REF.[96]) can decrease the search time by a factor of roughly 25 (REF.[83]). After a certain number of elements are placed on the virtual optical table, the resulting state is calculated. For the 3D GHZ state, one of the four photons is used as a trigger to herald the generation of a three-photon state in the other three detectors. The resulting quantum state is then compared with the search target.

- Generalized objective functions. Let us illustrate how to define very general objective functions, which can greatly accelerate the search process. The main challenge is that the search space can be enormous. For example, if six photonic modes are used, and the toolbox consists of two two-input-two-output elements (each having $6\times5=30$ possible locations) and ten single-input elements (such as holograms with different mode numbers or prisms with different discrete angles; each of which can be in a certain path), this results in a choice of 120 different elements. For a standard optical experiment with 15 different elements, there are roughly $120^{15}\approx10^{31}$ different configurations. The idea is to generalize the objective function as much as possible, such that the number of correctly identified quantum experiments is as large as possible and thereby the possibility of identifying a useful solution is maximal.

The state in equation 1 is very specific, and a search for only this state is very narrow. To increase the chances of satisfying this objective state, it is necessary to formulate the target state in the most general way. In this case in particular, every local unitary transformation results in a 3D GHZ state

$$|\psi\rangle=\frac{1}{\sqrt{3}}(|a,b,c\rangle+\mathrm{e}^{i\phi_1}|\bar{a},\bar{b},\bar{c}\rangle+\mathrm{e}^{i\phi_2}|\bar{\bar{a}},\bar{\bar{b}},\bar{\bar{c}}\rangle),\qquad(2)$$

with $a\perp\bar{a}\perp\bar{\bar{a}}$ (same for b and c), and arbitrary phases ϕ_1 and ϕ_2. Even very conservative assumptions (5D mode space and eight equidistant phases) result in more than two million times more potential targets than the natural objective in equation 1. In addition, although changing the magnitude of the coefficients of the three terms changes the structure of entanglement, equal coefficients could easily be recovered just by experimentally feasible, local mode-dependent filters, which leads to the following objective state

$$|\psi\rangle=N(\gamma_1\,|a,b,c\rangle+\gamma_2\,|\bar{a},\bar{b},\bar{c}\rangle+\gamma_3\,|\bar{\bar{a}},\bar{\bar{b}},\bar{\bar{c}}\rangle),\qquad(3)$$

with coefficients $\gamma_i\in\mathbb{C}$, and N being a normalization constant. Under similarly conservative assumptions, this leads to more than 5×10^7 times as many targets as the objective state in equation 1. Importantly, if any of these targets are found, it is immediately known how to generate experimentally a 3D entangled GHZ state with fidelity $F=1$. As before, mode numbers can be adjusted by local mode transformations, and the amplitudes can be adjusted by appropriate filtering.

The objective can be further generalized when considering that local mode-dependent filters are experimentally simple operations. Therefore, it is conceivable to reformulate the objective into

$$\begin{aligned}|\psi\rangle=N\Big(&\gamma_1|a,b,c\rangle+\gamma_2|\bar{a},\bar{b},\bar{c}\rangle\\&+\gamma_3|\bar{\bar{a}},\bar{\bar{b}},\bar{\bar{c}}\rangle\\&+\textstyle\sum_{\ell_1,\ell_2}\gamma_{1,\ell_1,\ell_2}|\tilde{a},\ell_1,\ell_2\rangle\\&+\gamma_{2,\ell_1,\ell_2}|\ell_1,\tilde{b},\ell_2\rangle\\&+\gamma_{3,\ell_1,\ell_2}|\ell_1,\ell_2,\tilde{c}\rangle\Big),\end{aligned}\qquad(4)$$

with $\tilde{x}$ indicating a mode that is orthogonal to x, $\bar{x}$ and $\bar{\bar{x}}$, and ℓ_1 and ℓ_2 stand for two arbitray modes. This leads to a much larger number of target states recognized as successful experimental implementations of the objective state in equation 4, and for any of these solutions, it is immediately clear how to generate the state with fidelity $F=1$. With the generalization of objective function, the size of the search space (all possible experiments) stays the same, whereas the target space (all possible solutions) is enormously enlarged. This translates into a substantial speedup in the search procedure, and indicates the great importance of the definition of a general objective function. It is an interesting open question how large the speedup is. Precise estimates would require knowledge of the accessible experimental space.

Alternatively, instead of using a specific target state as an objective function, one could try to find a specific, general property of interest — which is a more general concept. In the current example, one can ask whether the entanglement shown in equation 1 is the only acceptable structure, or could other types of high-dimensional states also lead to useful solutions? The answer to this question mainly depends on the experimental goal and what the experiment should demonstrate, and shifts the focus from the generation of a specific state to the generation of a state with specific properties. For instance, one could ask whether the states

$$\begin{aligned}|\psi_1\rangle&=\frac{1}{\sqrt{3}}(|0,0,0\rangle+|1,1,1\rangle+|2,2,1\rangle),\\|\psi_2\rangle&=\frac{1}{2}(|0,0,0\rangle+|1,0,1\rangle+|2,1,0\rangle\\&\quad+|3,1,1\rangle),\end{aligned}\qquad(5)$$

should also be considered as interesting solutions. If the goal is to experimentally demonstrate genuine high-dimensional multipartite entanglement (rather than the more specific GHZ states), the answer will be yes. In that case, one can search for much more general classes of states. In this example, a Schmidt–Rank vector (SRV)[97,98] perfectly fits the task. The SRV generalizes the concept of high-dimensional entanglement to multiple particles, and denotes a vector of the dimensionalities of entanglement of every biparition. Loosely speaking, it shows the dimensionality of entanglement between one particle and the rest of the quantum state. For three

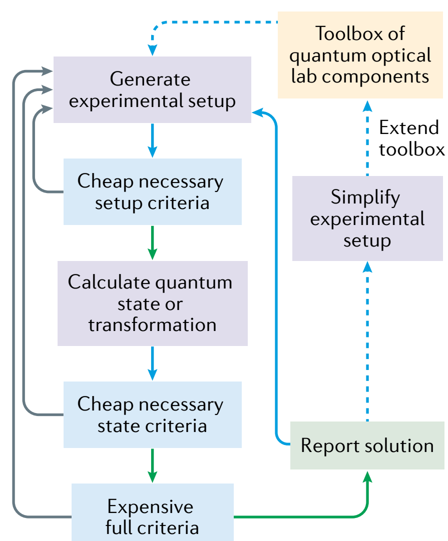

Fig. 2 | **Concept of the class III algorithm for computer-inspired experiments, MELVIN.** Experiments are assembled from a toolbox that contains all optical elements available in the laboratory. These elements are successively, randomly chosen using from a uniform distribution to avoid any bias. Then, time-inexpensive criteria are applied before calculating the full quantum state. The quantum state or transformation are calculated, then, again, time-inexpensive criteria are applied before calculating the full (usually expensive) objective function. If the experiment fulfils all criteria, it is reported to the user — otherwise, a new setup is generated. Optionally, the setup is simplified and appended to the toolbox, such that it can be used in subsequent trials to generate more complex solutions quicker. Thereby, the algorithm learns to use more successful building blocks over time. If the low-cost criteria and the expensive objective function are defined broadly, the search routine is highly efficient.

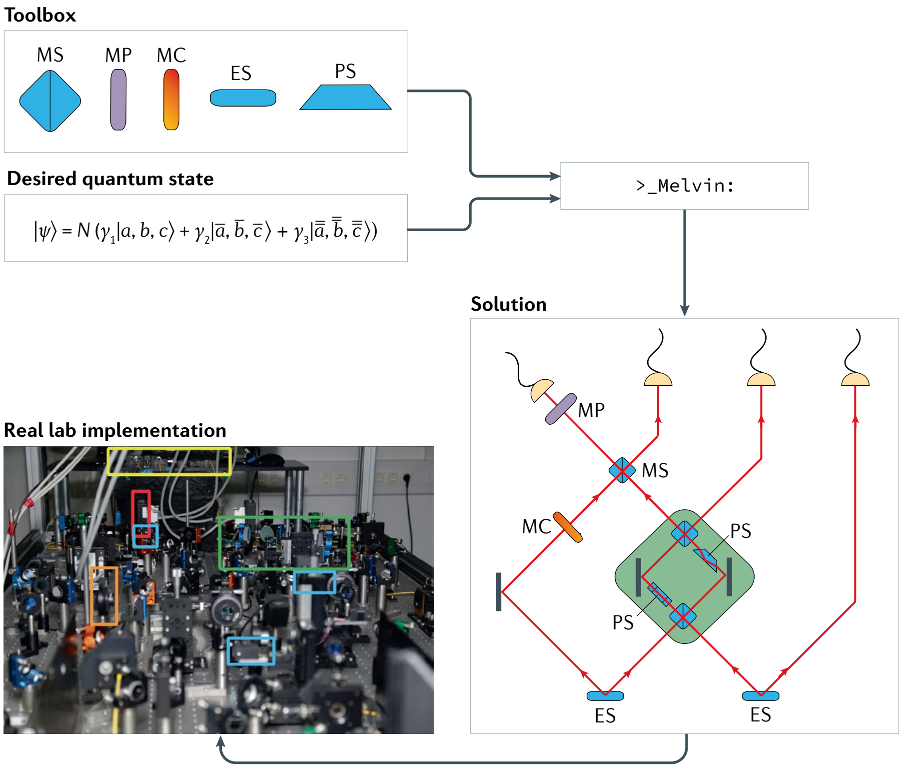

Fig. 3 | **The complexity of computer-inspired quantum experiments.** The MELVIN algorithm discovered the experimental setup for a 3D GHZ state (desired quantum state) using only the toolbox and a generalized quantum state as inputs. The toolbox contains, mode splitters (MS), mode projectors (MP), mode changers (MC), phase shifters (PS) and entanglement sources (ES). Human scientists can then implement the solution in the laboratory[89]. The symbols of the desired quantum state are defined in the main text.

particles (as in the GHZ state), the SRV of the state in equation 1 is (3,3,3) as every party is three-dimensionally entangled with the remaining state. States in equation 5 are (3,3,2)- and (4,2,2)-dimensionally entangled. The SRV gives a new way to classify high-dimensional entangled states. It can be used as the objective (instead of a direct state), which considerably increases the number of possible useful solutions.

- Speedup: identifying low-cost, necessary criteria. Calculating the final quantum state resulting from the experimental setup and evaluating the objective functions can be very time consuming. For this reason, it is desirable to find efficient methods that tell us whether the full calculation is needed.

In the GHZ example, one necessary condition for the creation of a genuine multiparty entangled state is that the quantum information from the two initial entangled pairs mixes during the evaluation of the setup. This criterion (which is generally applicable to many quantum photonic experimental states) can be applied even before the quantum state has been calculated, by investigating the structure of the generated experimental setup. If the experiment does not fulfil the criterion, it can be discarded without the calculation.After calculating the quantum state, and before evaluating the full objective function of state in equation 3 or equation 4, or the SRV (which involves the time-consuming calculation of the density matrix ranks), it is possible to analyse whether the calculated state has at least three different modes in each in each of the three photons. This criteria significantly reduces the number of states that undergo the full criteria evaluation.

Generating high-dimensional quantum gates. Let us look at another example of a generalized objective function, which has been successfully applied in the identification of high-dimensional multiphoton quantum gates[93]. The aim is to write the objective function in the most general, non-trivial way, which allows for the largest number of potential useful solutions. The simplest case is a controlled operation (CNOT) with two control modes and three target modes:

$$\begin{aligned}
\mathrm{CNOT}|0,0\rangle &= |0,0\rangle,\\
\mathrm{CNOT}|0,1\rangle &= |0,1\rangle,\\
\mathrm{CNOT}|0,2\rangle &= |0,2\rangle,\\
\mathrm{CNOT}|1,0\rangle &= |1,1\rangle,\\
\mathrm{CNOT}|1,1\rangle &= |1,2\rangle,\\
\mathrm{CNOT}|1,2\rangle &= |1,0\rangle.
\end{aligned} \tag{6}$$

The essence of this transformation needs to be extracted into an objective function. All mode numbers can be general, but there are much more degrees of freedom, which can significantly improve the chances of success. After many attempts using different objective functions, the following has lead to the first successful solution

$$\begin{aligned}
\mathrm{CNOT}|c_1, t_{1,2,3}\rangle &= |x_{1,2,3}, \bar{t}_{1,2,3}\rangle,\\
\mathrm{CNOT}|c_2, t_{1,2,3}\rangle &= |y_{1,2,3}, \bar{\bar{t}}_{1,2,3}\rangle,
\end{aligned} \tag{7}$$

where $c_{1/2}$ stands for the two different control modes and $t_{1/2/3}$ are the three target modes. x and y denote the two output control modes. Conventionally, the control photon is unchanged, but allowing the freedom of change increases the success probability. Furthermore, $\bar{t}$ and $\bar{\bar{t}}$ are target output modes, which satisfy the following criteria $\bar{t}_1 \perp \bar{t}_2 \perp \bar{t}_3$, $\bar{\bar{t}}_1 \perp \bar{\bar{t}}_2 \perp \bar{\bar{t}}_3$ and $\bar{t}_1 \perp \bar{\bar{t}}_1$, $\bar{t}_2 \perp \bar{\bar{t}}_2$ and $\bar{t}_3 \perp \bar{\bar{t}}_3$. For every proposed setup, a systematic list of 15 different modes (mode number $\ell = \pm 7$) for both the input control and target photon are used to calculate the output of the setup. If any subset of input modes leads to results that fulfil the criteria in equation 7, a control gate has likely been discovered.

An important key insight is the following: the above criteria are only necessary, not sufficient — that is, there can be solutions that are not controlled gate operations. Defining stricter criteria is not a good idea because near-miss solutions can be adjusted by human scientists into a full solution. This significantly increases the chances of finding inspirational ideas for human scientists.

Identifying solutions for complex transformations is much more computationally expensive: identifying the first high-dimensional control gate transformation has required roughly 150,000 CPU-core hours[93].

Discovery of computer-inspired concepts. Finding solutions to a predefined objective function can have a significant influence on future research. For example, the solution to the 3D GHZ state allowed the experimental investigation of statements about the local and realistic properties of the Universe[99–101]. Being able to learn new concepts or ideas from solutions found by computer algorithms would be scientifically even more interesting.

This is possible (see REF.[91]). In this case, the key insight was to use the algorithm with an objective function that allows for a large number of different classes of solutions. The objective was finding states with different SRV, as described in the previous section. The initial state, in this case, includes two spontaneous parametric down-conversion processes that each produce three-dimensionally entangled photon pairs. Informally, at a operator level, the four-photon term is the product of two pair-emission processes (each of them are three-dimensionally entangled). As a consequence, a naive limit would suggest that the maximal achievable entanglement dimensionality should be limited by $d = 3 \times 3 = 9$. After running MELVIN for roughly 50,000 CPU-core hours (with the settings explained in the previous section), it produced quantum-entangled states with 21 different SRV structures (FIG. 4). All states satisfied the natural limit of $d \leq 9$, except for one solution (highlighted in FIG. 4) that was a clear outlier, achieving 10D entanglement. The outlier shows that the native limit is wrong, and it indicates a very rare and exceptional solution, which is worth investigating further, as it might contain new techniques that have not yet been considered yet by human scientists — as was the case in this specific example.

Investigations of the experimental setup to create this outlier solution have shown that it contained an implicit usage of a method pioneered in 1991, known as the Zou–Wang–Mandel technique[102]. The technique was not part of the toolbox, it was not allowed explicitly by the rules of the algorithm and it was not known to the authors of REF.[91] before the discovery by the algorithm. Instead, the solution contained a non-local interferometer, which was allowed, but not enforced in any way by the human operators. The nonlinear interferometer enabled the implicit usage of the Zou–Wang–Mandel technique.

When it was understood that and how the Zou–Wang–Mandel technique can be used in the context of high-dimensional, multipartite entanglement generation, the human scientists were able to generalize it to many different cases, and has since been known as entanglement by path identity[91]. Soon after, it was understood that this type of entanglement generation is closely related to and can efficiently be described by graph theory[92,103–105].

The example above shows how computer algorithms can not only find solutions to explicitly defined problems but can also — accidentally[106] — lead to the discovery of new ideas and concepts that maybe would have never been found by human scientists.

Class IIa

Quantum experiments using the path degree of freedom as a carrier of information have seen enormous progress over the past few years[72,107–109]. Efficient algorithms for decomposing high-dimensional, single-photon transformations into experimental setups are well known for unitary[110,111] or non-unitary[112] cases. However, in the presence of more than one photon, or quantum information carried by more than one degree of freedom, finding suitable experimental configurations is very challenging, even if one has access to well-controlled setups.

To experimentally investigate processes that depend on non-unitarity, such as dynamics involving parity–time symmetry[113] and deterministic quantum cloning exploiting non-unitarity[114], scientists have relied on computer algorithms to design the experimental setups (FIG. 5a). The algorithm iteratively increases the experimental setup (in the form of FIG. 5b) block by block. Each block consists of eight independent, continuous parameters (settings of half-wave plates and quarter-wave plates), two input and output paths as well as two loss paths.

The algorithm starts with one block and optimizes the free parameters towards its objective function. If the difference between the optimized state and the target state is too large, the algorithm extends the setup by another block and continues to optimize the new parameters. This process continues until the algorithm has found a setting with n blocks of $8n$ parameters that can reach the target function.

The topology of a setup with three blocks is shown in FIG. 5b, as it was used in REF.[114] to perform deterministic, non-unitary quantum

2,2,2	3,2,2	4,2,2	~~5,2,2~~	~~6,2,2~~	~~7,2,2~~	~~8,2,2~~	~~9,2,2~~	~~10,2,2~~
	3,3,2	4,3,2	5,3,2	6,3,2	~~7,3,2~~	~~8,3,2~~	~~9,3,2~~	~~10,3,2~~
	3,3,3	4,3,3	5,3,3	6,3,3	7,3,3	8,3,3	9,3,3	~~10,3,3~~
		4,4,2	5,4,2	6,4,2	7,4,2	8,4,2	9,4,2	10,4,2
		4,4,3	5,4,3	5,4,3	7,4,3	8,4,3	9,4,3	10,4,3
		4,4,4	5,4,4	6,4,4	7,4,4	8,4,4	9,4,4	10,4,4
			5,5,2	6,5,2	7,5,2	8,5,2	9,5,2	10,5,2
			5,5,3	6,5,3	7,5,3	8,5,3	9,5,3	10,5,3
			5,5,4	6,5,4	7,5,4	8,5,4	9,5,4	10,5,4
			5,5,5	6,5,5	7,5,5	8,5,5	9,5,5	10,5,5
				6,6,2	7,6,2	8,6,2	9,6,2	10,6,2
				6,6,3	7,6,3	8,6,3	9,6,3	10,6,3
				6,6,4	7,6,4	8,6,4	9,6,4	10,6,4
				6,6,5	7,6,5	8,6,5	9,6,5	10,6,5
				6,6,6	7,6,6	8,6,6	9,6,6	10,6,6
					7,7,2	8,7,2	9,7,2	10,7,2
					7,7,3	8,7,3	9,7,3	10,7,3

Fig. 4 | **Concrete example of how a computer-discovered outlier can inspire new ideas, concepts or technology in experimental quantum optics.** A table of Schmidt–Rank vectors (SRVs) for three-photon entangled quantum states, as investigated using MELVIN for a span of roughly 50,000 hours. The green cells represent cases where solutions have been found. For white cells, no solutions have been found, and black cells show algebraically impossible SRVs[97]. The red rectangle indicates an outlier solution that has a significantly larger entanglement dimensionality than any other solutions discovered. This surprising solution has subsequently been investigated by human scientists. It indeed contains a special case of a new experimental concept, which has subsequently been interpreted, understood and generalized[91]. This example demonstrates that computer algorithms can inspire new scientific ideas and concepts, which has a widely unexplored potential that goes far beyond experimental quantum information science.

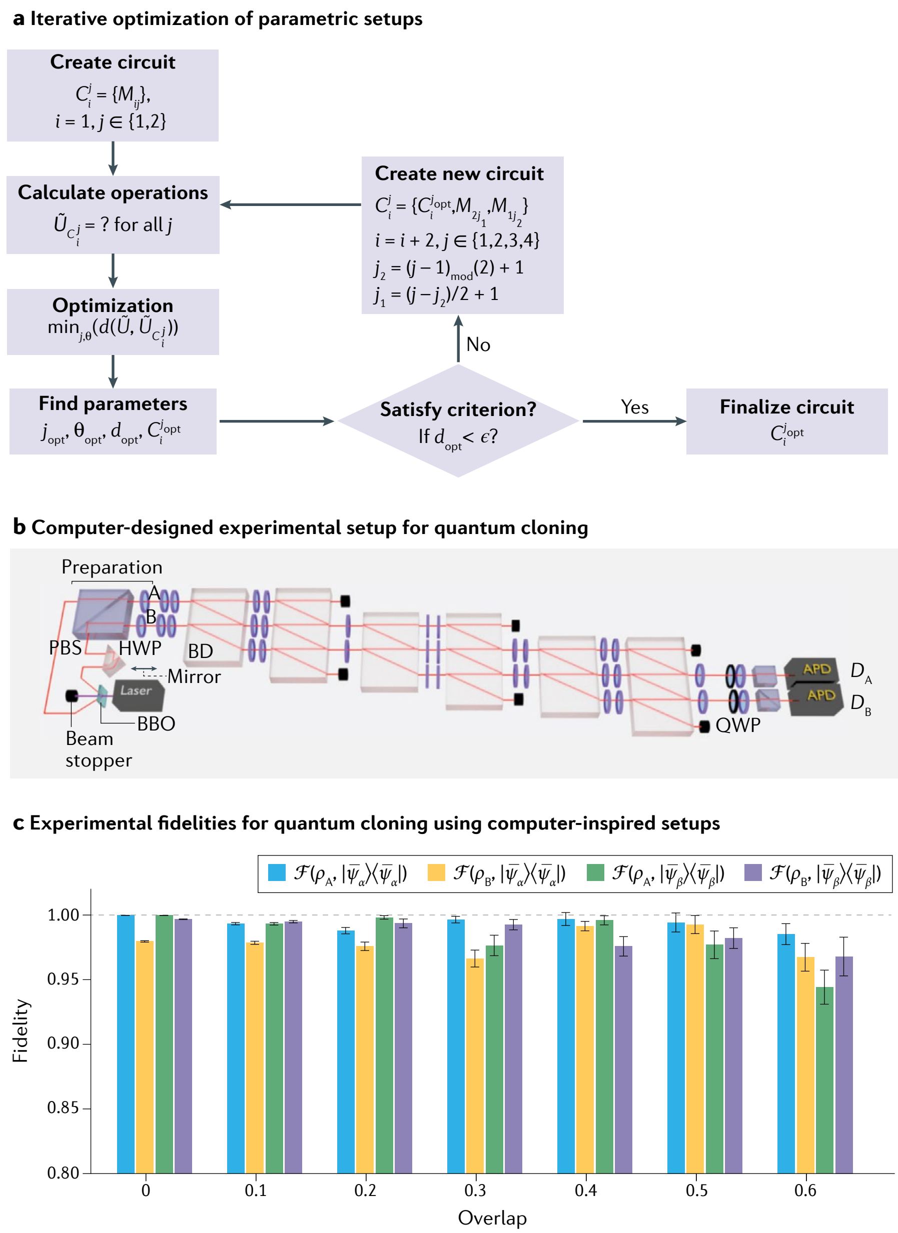

Fig. 5 | **Example of a class IIa algorithm. a** | The concept of the algorithm is to start building an entire setup from continuously parametrized building blocks. The program starts with one building block M and optimizes its free parameters (for example, angle settings of half-wave and quarter-wave plates, which are described by the vector $\boldsymbol{\theta}$). C defines the whole circuit, with indices i and j (mod stands for a modulo operation, opt stands for the optimized indices). If the target operation U can not be reached within a certain quality ε (measured by a distance function $d(.,.)$), the algorithm adds another basic building block with continuous parameters and continues to optimize the angle setting until it reaches the specified target quality. **b** | A setup for performing deterministic, non-unitary quantum cloning, with three sets of building blocks. BD stands for beam displacer, which are polarization-dependent objects. The purple elements between the BDs are wave plates, and the black boxes are loss elements. Discovering this setup took 30 min on an Intel Core i5 notebook with 1.6 GHz and 8 GB random access memory using Wolfram Mathematica. **c** | High-quality experimental results for the fidelity F of quantum-cloned states ρ and ψ. Error bars are estimated by error analysis in Monte Carlo, assuming Poissonian counting statistics. APD, avalanche photodiode; BBO, barium borate optical crystal; D_A and D_B, detectors; HWP, half-wave plate; PBS, polarizing beam splitter; QWP, quarter-wave plate. Adapted with permission from REF.[114], APS.

cloning. This complex experimental configuration was implemented experimentally, resulting in a very-high-quality average fidelity of beyond 98% (FIG. 5c).

The algorithm is in the class IIa because it has demonstrated its ability to design setups for previously unsolved questions, and its solutions have been practical such that they where experimentally implemented in the laboratory. Finally, it will be interesting to understand how new scientific insights and ideas can be extracted from this approach (which would correspond to class III).

Class IIb

A new design algorithm — named THESEUS — aims specifically at conceptual insights and scientific understanding[115]. The main idea is to use a physics-inspired, graph-theoretical representation[92], which was initially discovered using MELVIN. Each quantum optics setup (including probabilistic and deterministic sources, linear optics elements with or without post-selection) corresponds to a weighted, edge-coloured graph. Likewise, every graph can be translated into one of several different experimental schemes, such as bulk optics, integrated photonics or entanglement by path identity.

The initial state is a complete graph, with weighted multicoloured edges between each vertex. An objective function can be defined as a nonlinear function in terms of weights ω of the graph, which is then solved using a gradient-based optimization algorithm that furthermore exploits the second-order derivatives (Hessians) of the objective function. During the optimization, a set of weights are uncovered that maximize the fidelity of the target state. If the fidelity is beyond a certain threshold, one edge is removed from the original graph, and the objective function is optimized again. These steps continue iteratively until no more edges of the graph can be removed. In these cases, the graphs are usually small enough that they can be conceptually interpreted and generalized by human scientists. Furthermore, the graphs can be directly translated into different quantum optics experimental schemes.

THESEUS significantly outperforms other algorithms in terms of discovery speed. In particular, for the discovery of the first 50 SRV states THESEUS requires 15 minutes whereas MELVIN used hundreds of hours. Similarly, whereas MELVIN requires 150,000 CPU-core hours to discover the first high-dimensional CNOT gate, THESEUS found it within one second. THESEUS was able to uncover several experimental setups for previously unknown, or infeasible, tasks. Among them, are the first high-dimensional GHZ states with more than four photons, heralded high-dimensional Bell states and GHZ states, and significantly more efficient high-dimensional quantum gates. In each of the cases, the human scientists were able to conceptually understand the solution, which was demonstrated in an experiment by using the computer design and generalizing it without performing any further computations. Further comparisons with other computational approaches, scopes and limitations of THESEUS are yet to be investigated.

Class I

The algorithms described in the previous sections have led to experimental designs that were subsequently successfully implemented in laboratories (class IIa) or have led to new scientific insights (class IIb or class III). The approaches discussed in this section have not yet demonstrated the same level of maturity, which is a challenge for future research. Nonetheless, class I algorithms use new optimization and machine learning approaches that could in the future lead to exciting practical developments.

Evolutionary strategies. To design quantum optics experimental setups for efficient quantum metrology[116], a genetic algorithm approach has been demonstrated[117]. Evolutionary strategies have gained a lot of attention in machine learning because they are scalable alternatives to reinforcement algorithms[118].

The algorithm Tachikoma[117] (named after the artificial intelligence robots in the famous anime *Ghost in the Shell*) has access to a toolbox of experimentally available elements. However, in contrast to REF.[83], the toolbox is filled with continuous-variable quantum optical technologies. The experimental elements include a squeezing operator, displacement operators, beam splitters with variable transmission rates, a phase operator, photon-number-sensitive measurements and quadrature measurements. The continuous parameters are further restricted to resemble experimentally feasible operations, such that the final results are practically achievable states.

The algorithm starts with a population of randomly assembled initial experiments, chosen from the toolbox. Those initial solutions then undergo evolutionary optimization, by mutating the experimental setups and selecting the best candidates as offspring for the next generation. The selection criteria are based on a fitness function that involves the phase-measuring capability for a given number of average photon numbers. Tachikoma uncovered several promising candidate setups that more than double the phase measurement precision compared with the best-known, practical state.

In the three years since the original publication, the approach has been significantly improved. In one extension[119], the authors showed how the usage of deep neural networks can lead to a speedup in finding a useful output state. The idea is to train a neural network to classify the photon number distribution of a given state into one out of six categories (which involves cat states, squeezed cat states, cubic phases and others). The network helps to guide the search in the right direction, and only later, the computational expensive fitness functions are evaluated within the genetic algorithm. Thereby, several useful quantum states have been discovered.

The approach used for Tachikoma has also been significantly advanced in AdaQuantum[120] (named after Ada Lovelace, the world's first computer programmer). By improving both the numerical simulation and refining the search algorithm, the authors of AdaQuantum were able to improve the speed by another factor of five over their own best result. Furthermore, a higher noise and photon-loss tolerance was demonstrated, which is essential in real experiments (FIG. 6a). If these designs are indeed experimentally feasible and yield the predicted phase measurement precision, they could become an important reference in experimental quantum metrology.

The computations for AdaQuantum were executed for 96 hours on 16 cores of the University of Nottingham's High-Performance Computing facility. Further improvements of the algorithm could enable the optimization in the much larger space of three optical modes. This would not only improve the resulting measurement precision but also allow the algorithm to explore even more unorthodox solutions, which physicists could then try to understand. Finding the underlying conceptual reasons for the designs produced by AdaQuantum could uncover new insights for human scientists, thus it is an exciting future research direction.

Reinforcement learning. In REF.[121], the authors used a reinforcement learning algorithm (called Projective Simulations[122,123]) in the environment of quantum experiments and quantum states. The agent acts in the same environment[83] as MELVIN. Its task is to build an optical experiment using a toolbox of optical elements. The reward of the environment depends on the entanglement property of the resulting quantum state. Over time, the agent learns to choose optical elements in such a way that it finds more interesting quantum states. With this approach, the algorithm re-discovered solutions that have been previously discovered by MELVIN. Furthermore, it autonomously finds ways to simplify the experiments, which previously has only been achieved in a hard-coded way. The algorithm's internal representation shows that it learned to build specific optical devices that have been used by humans for many years, such as a special type of interferometer[96].

After confirming that the reinforcement learning approach works for re-discovery tasks, a similar algorithm was targeted to identify new quantum communication protocols[124]. The projective simulation reinforcement learning algorithm[121,122] has subsequently been applied to challenging tasks where solutions are not well studied and understood by human scientists[124]. There, the algorithm discovered a quantum repeater that in theory shows better performance in realistic, asymmetrical situations than the best-known previous solution (FIG. 6b); hence, the algorithm lies in the class I. It would be exciting if the proposed experimental setup was implemented in experiments, and the predicted performance was confirmed. Furthermore, it would be fascinating to understand which new conceptual insights scientists can extract from the solutions of the agent. Those are important open questions for the future.

Supervised classification. In machine learning, it is commonly believed that one of the keys to success is the use of appropriate representations and the availability of sufficient amounts of data (either provided by a supervisor or generated on the fly in the form of self-supervision). If such a dataset can be provided, supervised learning methods can be used to model quantum optical experiments and thereby potentially substantially reduce the number of required search steps compared with an entirely unguided search. In REF.[125], a deep recurrent neural network in the form of a long short-term memory network[126] was able to model and predict complex entanglement properties of a state that is the output of a quantum experiment (FIG. 6c). The network receives as an input an optical element sequence and is trained to predict the corresponding SRV, discussed before. The training data consist of hundreds of thousands of examples, extended from the table in FIG. 4. The long short-term memory network shows much better than random prediction qualities, which is a necessary and promising first step towards a deep generative model for quantum experiments based on deep reinforcement learning. This approach suggests that the production of large, interesting training datasets for

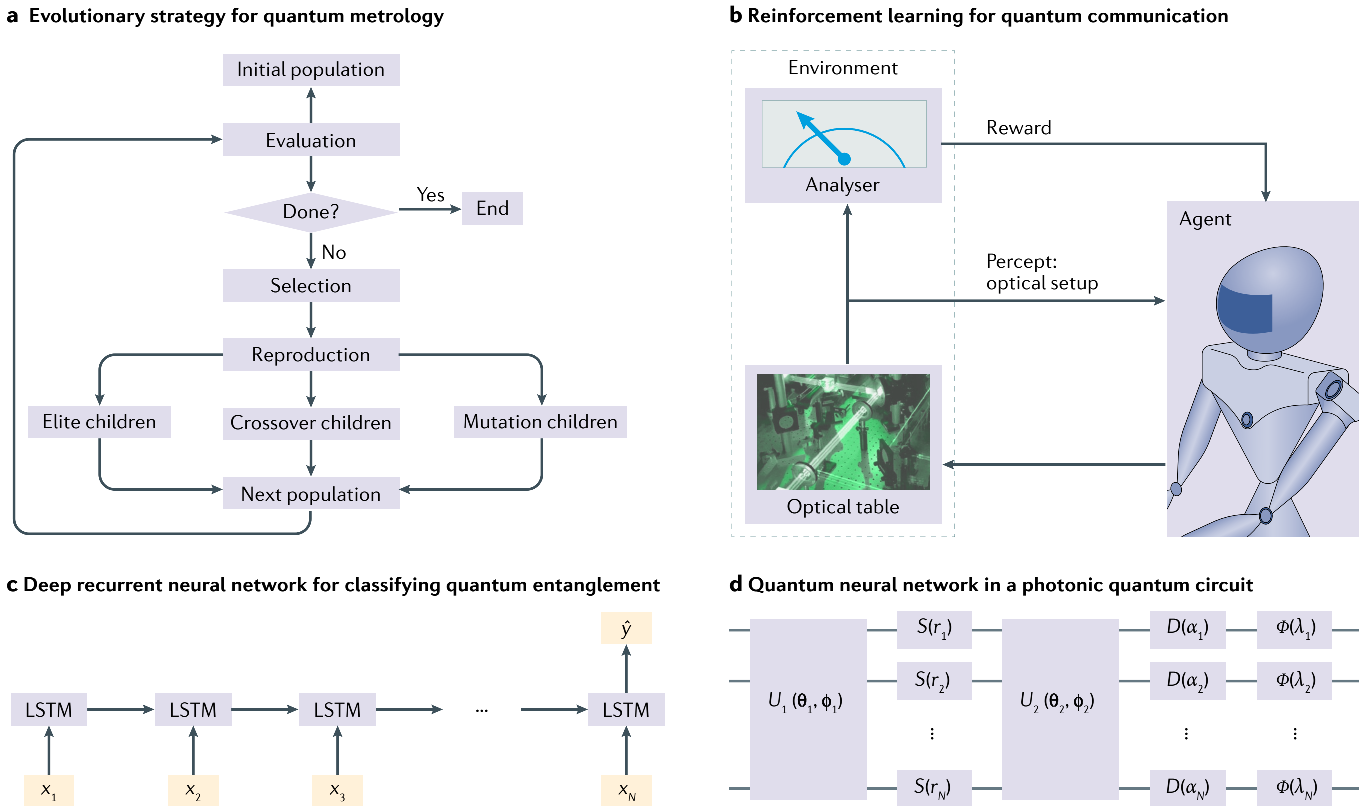

Fig. 6 | **Examples of class I algorithms for computer-inspired quantum experiments using various optimization and machine learning techniques. a** | A genetic algorithm for designing new methods in quantum metrology. An initial, random population undergoes an evolutionary process. The individual setups, which form the population, are selected according to their fitness. The best ones are mutated and form the next generation. **b** | The concept of a reinforcement learning algorithm for designing quantum communication schemes. An agent performs actions in an environment (changing quantum communication scheme), which changes the state of the environment. The agent receives a reward according to the quality of the action. **c** | The concept of a reinforcement learning algorithm for designing quantum optics experiments. An agent performs actions in an environment (changing the setup), which changes the state of the environment. The agent receives a reward according to the quality of the action. Here, x_i stand for optical elements and y is the predicted SRV class. **d** | A photonic quantum circuit can be parametrized continuously, thus gradient-based optimization techniques are possible. The individual elements of the circuits are unitary transformations U_i, squeezing S, displacement D and non-Gaussian gates Φ, with continuous parameters, $r, \alpha, \boldsymbol{\theta}, \boldsymbol{\phi}, \lambda$. LSTM, long short-term memory. Panel **a** reprinted with permission from REF.[120], IOP Publishing; Panel **b** adapted with permission from REF.[121], PNAS. Panel **d** reprinted with permission from REF.[133], IOP Publishing.

quantum optics experiments could become a benchmark to compare inverse-design algorithms and fuel machine learning approaches for the design of quantum optics experiments.

Gradient-based optimization in quantum photonic circuits. Integrated on-chip photonics allow for access to arbitrary unitary operations[110] that are continuously parameterized and can span a large discrete[107,108,127–129] or continuous[130–132] Hilbert space.

Gradient-based optimization of quantum states and quantum transformations is ideally suited for such systems. In REF.[133], the aim is to find optimal quantum circuit settings to produce useful quantum systems for continuous-variable (CV) quantum architectures. A variational quantum circuit (called CV quantum neural networks) is used, its gates and connectivities (that is its topology) being fixed, but all the gates containing free parameters[134] (FIG. 6d). The authors find implementations for important states such as NOON states, which are essential in quantum metrology[116] and Gottesman–Kitaev–Preskill states, which can be used for error correction in CV quantum computing[135]. In addition, the task of the algorithm (which is based on the Strawberry Fields software platform[136]) is to find implementations for cubic phase gates, which is a crucial basis element for CV quantum computation[137], and the quantum Fourier transform. All the predicted results have theoretical fidelity larger than 99%. It would be exciting to see whether those promising solutions that are in theory of significantly higher quality than previously known ones are experimentally feasible to be implemented and whether extracting scientific understanding from those high-quality solutions is possible.

Numerical experimental design for heralded photonic entanglement. Heralded sources of three-photon GHZ states are the basis of several proposals for the resource states of photonic, measurement-based quantum computation[138,139].

Recently, REF.[140] reported the most efficient circuit known so far that can generate three-photon GHZ states. The discovered setup requires reliable deterministic single-photon sources, for which impressive progress has been reported recently[141]. The generation of heralded states requires ancilla particles. The idea in REF.[140] is to start with a ten-path setup, and an input state in the form of $|1,1,1,1,1,1,0,0,0,0\rangle$, which represents photon number states, meaning that the first six paths contain photons, where three of the photons are used as ancilla photons. Using the approach of factorizing unitary matrices in REF.[111], it is possible to numerically optimize the corresponding unitary transformation that transforms the initial state into the desired GHZ state. The transformation of the input state to the heralded GHZ state is not unique. This additional freedom has been exploited to reduce the complexity of the experimental setup, by minimizing the number of non-trivial optical components such as beam splitters. The result is a small setup for generating a three-particle GHZ state. The idea for reducing the optical components leads to an efficient generation probability for a heralded three-qubit GHZ of $P = 1/54$.

A generalization of the experimental setup (for instance, to a larger number of photons or higher dimensions) has not yet been shown. However, the relatively small number of optical components (only 12 beam splitters and a number of phase shifters) might allow for intuitive interpretations and potentially the extraction of abstract underlying concepts, which can be applied elsewhere. Furthermore, the systematic optimization step that reduces the number of elements might find applications in many other quantum design tasks and has excellent potential for extracting scientific insights from the experimental setups. In that case, the algorithm would become a member of the class IIb.

Outlook

The defining characteristic of computer-designed quantum experiments in class IIb or class III is the possibility of extracting inspirations for conceptual and scientific understanding. We argue that this was made possible because of the topological search and topological optimization. Whereas most other approaches involve, at least partly, the optimization of continuous parameters, computer-inspired quantum experiments of these classes are designed mainly through course-grained topological optimization. As a consequence, solutions contain clearly identifiable patterns, and the resulting quantum states are sparse. These properties facilitate interpretability[84,91,93]. It would be interesting to apply a similar approach in other fields, especially in the computer-inspired designs of quantum circuits and superconducting hardware[57]. Although a purely topological search is probably much slower in identifying optimal solutions, it might lead to more interpretable solutions. An interesting related challenge is to understand how to improve interpretability in solutions of continuous optimization strategies.

The target states researched for quantum optical experiments could potentially directly be investigated through nanophotonics[28]. For example, one could envision a nano-photonic structure that directly emits high-dimensional multiphotonic entangled states. Alternatively, a highly efficient and stable generalization of computer-designed holographic transformations[142–144] or scattering[145–147] to multiphotonic states could potentially significantly reduce experimental complexities in bulk optics.

The field of computer-inspired molecular design in chemistry has similar questions to those discussed in this Perspective article. The discrete objects (atoms) form an enormous search space of 10^{40}–10^{60} possibilities, even for relatively small molecules. It has been shown how this discrete optimization problem can be formulated in a continuous manner[68]. Continuous optimization allows for the exploitation of gradient descent, and thus the application of modern deep learning methods, an active field both in academia and industry[58,59]. Like molecules, quantum experiments can be interpreted as graphs[148]; thus, the design of new quantum setups can benefit from the developments in computer-inspired molecular design.

Topological search and the verification of electric circuits have long been using automated reasoning technologies, which have seen remarkable progress over the past decade[53,149,150]. Similar techniques have also been explored for gate-based qubit quantum circuits[54–56]. Reformulating the search for the topologies of quantum optical experiments as a propositional formula (where all variables have logical values, that is, they are either true or false) would be a fascinating field of research.

Furthermore, it would be useful to find ways to make the algorithm's results and internal representation of the problem easier to interpret physically and intuitively. This would help humans understand and learn new concepts and design rules from the discovered solutions. One way could be through interpretable neural networks[151,152] in the physical context[153–156]. These can be applied to deep generative models for complex scientific structures such as functional molecules or quantum experiments[148].

An important question is how can unexpected solutions be identified more systematically? These solutions have the potential to stimulate new creative insights that humans have not thought of yet[106,157], and are particularly desirable in the scientific context.

Interestingly, the algorithms outlined in this Perspective article can not only be applied to the design of quantum experiments but also have been used to find solutions for questions in theoretical quantum information[158]. Many problems in the foundations of entanglement theory are of discrete nature[159–162] and can be great targets to apply the methods described here. Solutions to questions in theoretical quantum information (rather than experimental design) might be directly interpretable and lead to conceptual insights.

The size of a quantum system increases exponentially with the number of involved particles, which leads to enormous storage and computation requirements. Classical computers will be limited to evaluating the entire state of a quantum system beyond certain system sizes. However, quantum systems below ten photons can be stored and evaluated on standard notebooks. We argue that for many design questions, the solutions can be generalizable from the solutions for small systems. However, it remains an important question to consider how to design large quantum experiments.

Even partial answers to these questions could lead to new, exciting computer-inspired ideas. We believe that such algorithms will become tools to augment human scientist's creativity.

Code availability

Example codes both for Wolfram Mathematica and for Python (using SymPy) can be found at https://github.com/XuemeiGu/MelvinPython/.

Mario Krenn[1,2,3,4]✉, *Manuel Erhard*[1,2]✉ *and Anton Zeilinger*[1,2]✉

[1]*Vienna Center for Quantum Science and Technology (VCQ), Faculty of Physics, University of Vienna, Vienna, Austria.*

[2]*Institute for Quantum Optics and Quantum Information (IQOQI) Vienna, Austrian Academy of Sciences, Vienna, Austria.*

[3]*Department of Chemistry and Computer Science, University of Toronto, Toronto, Ontario, Canada.*

[4]*Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada.*

✉*e-mail: mario.krenn@univie.ac.at; manuel.erhard@univie.ac.at; anton.zeilinger@univie.ac.at*

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1. Wang, J. et al. Experimental quantum Hamiltonian learning. *Nat. Phys.* **13**, 551–555 (2017).
2. Gentile, A. A. et al. Learning models of quantum systems from experiments. Preprint at https://arxiv.org/abs/2002.06169 (2020).
3. Torlai, G. et al. Neural-network quantum state tomography. *Nat. Phys.* **14**, 447–450 (2018).
4. Palmieri, A. M. et al. Experimental neural network enhanced quantum tomography. *npj Quantum Inf.* **6**, 20 (2020).
5. Gebhart, V. & Bohmann, M. Neural-network approach for identifying nonclassicality from click-counting data. *Phys. Rev. Res.* **2**, 023150 (2020).
6. Weidner, C. & Anderson, D. Z. Experimental demonstration of shaken-lattice interferometry. *Phys. Rev. Lett.* **120**, 263201 (2018).

7. Cimini, V. et al. Calibration of quantum sensors by neural networks. *Phys. Rev. Lett.* **123**, 230502 (2019).
8. Youssry, A., Chapman, R. J., Peruzzo, A., Ferrie, C. & Tomamichel, M. Modeling and control of a reconfigurable photonic circuit using deep learning. *Quantum Sci. Technol.* **5**, 025001 (2020).
9. You, C. et al. Identification of light sources using machine learning. *Appl. Phys. Rev.* **7**, 021404 (2020).
10. Carleo, G. et al. Machine learning and the physical sciences. *Rev. Mod. Phys.* **91**, 045002 (2019).
11. Dunjko, V. & Briegel, H. J. Machine learning & artificial intelligence in the quantum domain: a review of recent progress. *Rep. Prog. Phys.* **81**, 074001 (2018).
12. Lamata, L. Quantum machine learning and quantum biomimetics: a perspective. *Mach. Learn. Sci. Technol.* **1**, 033002 (2020).
13. Fasoli, A. et al. Computational challenges in magnetic-confinement fusion physics. *Nat. Phys.* **12**, 411 (2016).
14. Helander, P. Theory of plasma confinement in non-axisymmetric magnetic fields. *Rep. Prog. Phys.* **77**, 087001 (2014).
15. Pedersen, T. S. et al. Confirmation of the topology of the Wendelstein 7-X magnetic field to better than 1: 100,000. *Nat. Commun.* **7**, 13493 (2016).
16. Wolf, R. et al. Major results from the first plasma campaign of the Wendelstein 7-X stellarator. *Nucl. Fusion* **57**, 102020 (2017).
17. Hofler, A. et al. Innovative applications of genetic algorithms to problems in accelerator physics. *Phys. Rev. Spec. Top. Accel. Beams* **16**, 010101 (2013).
18. Li, Y., Cheng, W., Yu, L. H. & Rainer, R. Genetic algorithm enhanced by machine learning in dynamic aperture optimization. *Phys. Rev. Accel. Beams* **21**, 054601 (2018).
19. Appel, S. et al. Optimization of heavy-ion synchrotrons using nature-inspired algorithms and machine learning. In *13th International Computational Accelerator Physics Conference (ICAP'18)* 15–21 (JACOW, 2019).
20. Pierrick, H., Juliette, P., Claude, M. & Franck, P. Klystron efficiency optimization based on a genetic algorithm. In *2019 International Vacuum Electronics Conference (IVEC)* 1–2 (IEEE, 2019).
21. Bentley, P. *Evolutionary Design by Computers* (Morgan Kaufmann, 1999).
22. Bendsøe, M. P. *Topology Optimization* (Springer, 2009).
23. van Dijk, N. P., Maute, K., Langelaar, M. & Van Keulen, F. Level-set methods for structural topology optimization: a review. *Struct. Multidiscipl. Optim.* **48**, 437–472 (2013).
24. Sigmund, O. On the usefulness of non-gradient approaches in topology optimization. *Struct. Multidiscipl. Optim.* **43**, 589–596 (2011).
25. Bendsøe, M. P. & Kikuchi, N. Generating optimal topologies in structural design using a homogenization method. *Comput. Methods Appl. Mech. Eng.* **71**, 197–224 (1988).
26. Xie, Y. M. & Steven, G. P. A simple evolutionary procedure for structural optimization. *Comput. Struct.* **49**, 885–896 (1993).
27. Aage, N., Andreassen, E., Lazarov, B. S. & Sigmund, O. Giga-voxel computational morphogenesis for structural design. *Nature* **550**, 84–86 (2017).
28. Molesky, S. et al. Inverse design in nanophotonics. *Nat. Photon.* **12**, 659–670 (2018).
29. Yao, K., Unni, R. & Zheng, Y. Intelligent nanophotonics: merging photonics and artificial intelligence at the nanoscale. *Nanophotonics* **8**, 339–366 (2019).
30. Shen, B., Wang, P., Polson, R. & Menon, R. Integrated metamaterials for efficient and compact free-space-to-waveguide coupling. *Opt. Express* **22**, 27175–27182 (2014).
31. Su, L., Piggott, A. Y., Sapra, N. V., Petykiewicz, J. & Vuckovic, J. Inverse design and demonstration of a compact on-chip narrowband three-channel wavelength demultiplexer. *ACS Photon.* **5**, 301–305 (2017).
32. Dory, C. et al. Inverse-designed diamond photonics. *Nat. Commun.* **10**, 3309 (2019).
33. Peano, V., Sapper, F. & Marquardt, F. Rapid exploration of topological band structures using deep learning. Preprint at https://arxiv.org/abs/1912.03296 (2019).
34. Sapra, N. V. et al. On-chip integrated laser-driven particle accelerator. *Science* **367**, 79–83 (2020).
35. Sheeran, M., Singh, S. & Stålmarck, G. Checking safety properties using induction and a SAT-solver. In *International Conference on Formal Methods in Computer-aided Design* (eds Hunt Jr, W. A. & Johnson, S. D.) 127–144 (Springer, 2000).
36. Saeedi, M. & Markov, I. L. Synthesis and optimization of reversible circuits–a survey. *ACM Comput. Surv.* **45**, 21 (2013).
37. Dawson, C. M. & Nielsen, M. A. The Solovay–Kitaev algorithm. https://arxiv.org/abs/quant-ph/0505030 (2005).
38. Maslov, D., Dueck, G. W., Miller, D. M. & Negrevergne, C. Quantum circuit simplification and level compaction. *IEEE Trans. Comput. Des. Integr. Circuits Syst.* **27**, 436–444 (2008).
39. Bocharov, A., Roetteler, M. & Svore, K. M. Efficient synthesis of probabilistic quantum circuits with fallback. *Phys. Rev. A* **91**, 052317 (2015).
40. Nam, Y., Ross, N. J., Su, Y., Childs, A. M. & Maslov, D. Automated optimization of large quantum circuits with continuous parameters. npj *Quantum Inf.* **4**, 23 (2018).
41. Martinez, E. A., Monz, T., Nigg, D., Schindler, P. & Blatt, R. Compiling quantum algorithms for architectures with multi-qubit gates. *New J. Phys.* **18**, 063029 (2016).
42. Maslov, D. Basic circuit compilation techniques for an ion-trap quantum machine. *New J. Phys.* **19**, 023035 (2017).
43. Peruzzo, A. et al. A variational eigenvalue solver on a photonic quantum processor. *Nat. Commun.* **5**, 4213 (2014).
44. McClean, J. R., Romero, J., Babbush, R. & Aspuru-Guzik, A. The theory of variational hybrid quantum-classical algorithms. *New J. Phys.* **18**, 023023 (2016).
45. Farhi, E., Goldstone, J. & Gutmann, S. A quantum approximate optimization algorithm. Preprint at https://arxiv.org/abs/1411.4028 (2014).
46. McClean, J. R., Boixo, S., Smelyanskiy, V. N., Babbush, R. & Neven, H. Barren plateaus in quantum neural network training landscapes. *Nat. Commun.* **9**, 4812 (2018).
47. Sim, S., Johnson, P. D. & Aspuru-Guzik, A. Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms. *Adv. Quantum Technol.* **2**, 1900070 (2019).
48. Rattew, A. G., Hu, S., Pistoia, M., Chen, R. & Wood, S. A domain-agnostic, noise-resistant evolutionary variational quantum eigensolver for hardware-efficient optimization in the Hilbert space. Preprint at https://arxiv.org/abs/1910.09694 (2019).
49. Fösel, T., Tighineanu, P., Weiss, T. & Marquardt, F. Reinforcement learning with neural networks for quantum feedback. *Phys. Rev. X* **8**, 031084 (2018).
50. Friis, N., Melnikov, A. A., Kirchmair, G. & Briegel, H. J. Coherent controlization using superconducting qubits. *Sci. Rep.* **5**, 18036 (2015).
51. Bukov, M. et al. Reinforcement learning in different phases of quantum control. *Phys. Rev. X* **8**, 031086 (2018).
52. Fösel, T., Krastanov, S., Marquardt, F. & Jiang, L. Efficient cavity control with SNAP gates. Preprint at https://arxiv.org/abs/2004.14256 (2020).
53. Brakensiek, J., Heule, M., Mackey, J. & Narváez, D. The resolution of Keller's conjecture. In *International Joint Conference on Automated Reasoning* (eds Peltier, N. & Sofronie-Stokkermans, V.) 48–65 (Springer, 2020).
54. Wille, R., Przigoda, N. & Drechsler, R. A compact and efficient SAT encoding for quantum circuits. In *2013 Africon* 1–6 (IEEE, 2013).
55. Meuli, G., Soeken, M. & De Micheli, G. SAT-based CNOT, T quantum circuit synthesis. In *International Conference on Reversible Computation* (eds Kari, J. & Ulidowski, I.) 175–188 (Springer, 2018).
56. Wille, R., Burgholzer, L. & Zulehner, A. Mapping quantum circuits to IBM QX architectures using the minimal number of SWAP and H operations. In *Proc. 56th Annual Design Automation Conference 2019* 142 (ACM, 2019).
57. Menke, T. et al. Automated discovery of superconducting circuits and its application to 4-local coupler design. Preprint at https://arxiv.org/abs/1912.03322 (2019).
58. Sanchez-Lengeling, B. & Aspuru-Guzik, A. Inverse molecular design using machine learning: generative models for matter engineering. *Science* **361**, 360–365 (2018).
59. Gromski, P. S., Henson, A. B., Granda, J. M. & Cronin, L. How to explore chemical space using algorithms and automation. *Nat. Rev. Chem.* **3**, 119–128 (2019).
60. Virshup, A. M., Contreras-García, J., Wipf, P., Yang, W. & Beratan, D. N. Stochastic voyages into uncharted chemical space produce a representative library of all possible drug-like compounds. *J. Am. Chem. Soc.* **135**, 7296–7303 (2013).
61. Robbins, D. W. & Hartwig, J. F. A simple, multidimensional approach to high-throughput discovery of catalytic reactions. *Science* **333**, 1423–1427 (2011).
62. Gómez-Bombarelli, R. et al. Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. *Nat. Mater.* **15**, 1120–1127 (2016).
63. Lyu, J. et al. Ultra-large library docking for discovering new chemotypes. *Nature* **566**, 224–229 (2019).
64. O'Boyle, N. M., Campbell, C. M. & Hutchison, G. R. Computational design and selection of optimal organic photovoltaic materials. *J. Phys. Chem. C* **115**, 16200–16210 (2011).
65. Chen, X., Du, W., Qi, R., Qian, F. & Tianfield, H. Hybrid gradient particle swarm optimization for dynamic optimization problems of chemical processes. *Asia Pac. J. Chem. Eng.* **8**, 708–720 (2013).
66. Jensen, J. H. A graph-based genetic algorithm and generative model/Monte Carlo tree search for the exploration of chemical space. *Chem. Sci.* **10**, 3567–3572 (2019).
67. Nigam, A., Friederich, P., Krenn, M. & Aspuru-Guzik, A. Augmenting genetic algorithms with deep neural networks for exploring the chemical space. Preprint at https://arxiv.org/abs/1909.11655 (2020).
68. Gómez-Bombarelli, R. et al. Automatic chemical design using a data-driven continuous representation of molecules. *ACS Cent. Sci.* **4**, 268–276 (2018).
69. Coello, C. A. C. et al. *Evolutionary Algorithms for Solving Multi-objective Problems* Vol. 5 (Springer, 2007).
70. Coello, C. A. C. List of references on evolutionary multiobjective optimization. *Delta* http://delta.cs.cinvestav.mx/~ccoello/EMOO/emoopage.html (2017).
71. Pan, J.-W. et al. Multiphoton entanglement and interferometry. *Rev. Mod. Phys.* **84**, 777–838 (2012).
72. Flamini, F., Spagnolo, N. & Sciarrino, F. Photonic quantum information processing: a review. *Rep. Prog. Phys.* **82**, 016001 (2018).
73. Graffitti, F., Kundys, D., Reid, D. T., Brańczyk, A. M. & Fedrizzi, A. Pure down-conversion photons through sub-coherence-length domain engineering. *Quantum Sci. Technol.* **2**, 035001 (2017).
74. Lenzini, F. et al. Active demultiplexing of single photons from a solid-state source. *Laser Photon. Rev.* **11**, 1600297 (2017).
75. Wang, X.-L. et al. 18-qubit entanglement with six photons' three degrees of freedom. *Phys. Rev. Lett.* **120**, 260502 (2018).
76. Luo, Y.-H. et al. Quantum teleportation in high dimensions. *Phys. Rev. Lett.* **123**, 070505 (2019).
77. Bornman, N. et al. Ghost imaging using entanglement-swapped photons. *npj Quantum Inf.* **5**, 63 (2019).
78. Wang, H. et al. Boson sampling with 20 input photons and a 60-mode interferometer in a 10^{14}-dimensional Hilbert space. *Phys. Rev. Lett.* **123**, 250503 (2019).
79. Hu, X.-M. et al. Experimental multi-level quantum teleportation. Preprint at https://arxiv.org/abs/1904.12249 (2019).
80. Llewellyn, D. et al. Chip-to-chip quantum teleportation and multi-photon entanglement in silicon. *Nat. Phys.* **16**, 148–153 (2020).
81. Bavaresco, J. et al. Measurements in two bases are sufficient for certifying high-dimensional entanglement. *Nat. Phys.* **14**, 1032–1037 (2018).
82. Ahn, D. et al. Adaptive compressive tomography with no a priori information. *Phys. Rev. Lett.* **122**, 100404 (2019).
83. Krenn, M., Malik, M., Fickler, R., Lapkiewicz, R. & Zeilinger, A. Automated search for new quantum experiments. *Phys. Rev. Lett.* **116**, 090405 (2016).
84. Gao, X., Krenn, M., Kysela, J. & Zeilinger, A. Arbitrary *d*-dimensional Pauli X gates of a flying qudit. *Phys. Rev. A* **99**, 023825 (2019).
85. Malik, M. et al. Multi-photon entanglement in high dimensions. *Nat. Photon.* **10**, 248–252 (2016).
86. Schlederer, F., Krenn, M., Fickler, R., Malik, M. & Zeilinger, A. Cyclic transformation of orbital angular momentum modes. *New J. Phys.* **18**, 043019 (2016).
87. Wang, F. et al. Generation of the complete four-dimensional bell basis. *Optica* **4**, 1462–1467 (2017).
88. Babazadeh, A. et al. High-dimensional single-photon quantum gates: concepts and experiments. *Phys. Rev. Lett.* **119**, 180510 (2017).
89. Erhard, M., Malik, M., Krenn, M. & Zeilinger, A. Experimental Greenberger–Horne–Zeilinger entanglement beyond qubits. *Nat. Photon.* **12**, 759–764 (2018).
90. Kysela, J., Erhard, M., Hochrainer, A., Krenn, M. & Zeilinger, A. Experimental high-dimensional entanglement by path identity. *Proc. Natl Acad. Sci. USA* (in the press).
91. Krenn, M., Hochrainer, A., Lahiri, M. & Zeilinger, A. Entanglement by path identity. *Phys. Rev. Lett.* **118**, 080401 (2017).

92. Krenn, M., Gu, X. & Zeilinger, A. Quantum experiments and graphs: multiparty states as coherent superpositions of perfect matchings. *Phys. Rev. Lett.* **119**, 240403 (2017).
93. Gao, X., Erhard, M., Zeilinger, A. & Krenn, M. Computer-inspired concept for high-dimensional multipartite quantum gates. *Phys. Rev. Lett.* **125**, 050501 (2020).
94. Wang, X.-L. et al. Quantum teleportation of multiple degrees of freedom of a single photon. *Nature* **518**, 516–519 (2015).
95. Anwer, H., Nawareg, M., Cabello, A. & Bourennane, M. Experimental test of maximal tripartite nonlocality using an entangled state and local measurements that are maximally incompatible. *Phys. Rev. A* **100**, 022104 (2019).
96. Leach, J., Padgett, M. J., Barnett, S. M., Franke-Arnold, S. & Courtial, J. Measuring the orbital angular momentum of a single photon. *Phys. Rev. Lett.* **88**, 257901 (2002).
97. Huber, M. & de Vicente, J. I. Structure of multidimensional entanglement in multipartite systems. *Phys. Rev. Lett.* **110**, 030501 (2013).
98. Huber, M., Perarnau-Llobet, M. & de Vicente, J. I. Entropy vector formalism and the structure of multidimensional entanglement in multipartite systems. *Phys. Rev. A* **88**, 042328 (2013).
99. Ryu, J. et al. Multisetting Greenberger–Horne–Zeilinger theorem. *Phys. Rev. A* **89**, 024103 (2014).
100. Lawrence, J. Rotational covariance and Greenberger–Horne–Zeilinger theorems for three or more particles of any dimension. *Phys. Rev. A* **89**, 012105 (2014).
101. Lawrence, J. Many-qutrit Mermin inequalities with three measurement bases. Preprint at https://arxiv.org/abs/1910.05869 (2019).
102. Zou, X., Wang, L. J. & Mandel, L. Induced coherence and indistinguishability in optical interference. *Phys. Rev. Lett.* **67**, 318–321 (1991).
103. Gu, X., Erhard, M., Zeilinger, A. & Krenn, M. Quantum experiments and graphs II: quantum interference, computation, and state generation. *Proc. Natl Acad. Sci. USA* **116**, 4147–4155 (2019).
104. Gu, X., Chen, L., Zeilinger, A. & Krenn, M. Quantum experiments and graphs. III. High-dimensional and multiparticle entanglement. *Phys. Rev. A* **99**, 032338 (2019).
105. Krenn, M., Gu, X. & Soltész, D. Questions on the structure of perfect matchings inspired by quantum physics. In *Proc. 2nd Croatian Combinatorial Days* (eds Došlić, T. & Martinjak, I) 57–70 (Faculty of Civil Engineering, University of Zagreb, 2019).
106. Lehman, J. et al. The surprising creativity of digital evolution: a collection of anecdotes from the evolutionary computation and artificial life research communities. *Artif. Life* **26**, 274–306 (2020).
107. Wang, J., Sciarrino, F., Laing, A. & Thompson, M. G. Integrated photonic quantum technologies. *Nat. Photon.* **14**, 273–284 (2020).
108. Feng, L.-T., Guo, G.-C. & Ren, X.-F. Progress on integrated quantum photonic sources with silicon. *Adv. Quantum Technol.* **3**, 1900058 (2020).
109. Slussarenko, S. & Pryde, G. J. Photonic quantum information processing: a concise review. *Appl. Phys. Rev.* **6**, 041303 (2019).
110. Reck, M., Zeilinger, A., Bernstein, H. J. & Bertani, P. Experimental realization of any discrete unitary operator. *Phys. Rev. Lett.* **73**, 58–61 (1994).
111. Clements, W. R., Humphreys, P. C., Metcalf, B. J., Kolthammer, W. S. & Walmsley, I. A. Optimal design for universal multiport interferometers. *Optica* **3**, 1460–1465 (2016).
112. Tischler, N., Rockstuhl, C. & Słowik, K. Quantum optical realization of arbitrary linear transformations allowing for loss and gain. *Phys. Rev. X* **8**, 021017 (2018).
113. Xiao, L. et al. Observation of critical phenomena in parity-time-symmetric quantum dynamics. *Phys. Rev. Lett.* **123**, 230401 (2019).
114. Zhan, X. et al. Experimental quantum cloning in a pseudo-unitary system. *Phys. Rev. A* **101**, R010302 (2020).
115. Krenn, M., Kottmann, J., Tischler, N. & Aspuru-Guzik, A. Conceptual understanding through efficient inverse-design of quantum optical experiments. Preprint at https://arxiv.org/abs/2005.06443 (2020).
116. Giovannetti, V., Lloyd, S. & Maccone, L. Advances in quantum metrology. *Nat. Photon.* **5**, 222–229 (2011).
117. Knott, P. A search algorithm for quantum state engineering and metrology. *New J. Phys.* **18**, 073033 (2016).
118. Salimans, T., Ho, J., Chen, X., Sidor, S. & Sutskever, I. Evolution strategies as a scalable alternative to reinforcement learning. Preprint at https://arxiv.org/abs/1703.03864 (2017).
119. O'Driscoll, L., Nichols, R. & Knott, P. A hybrid machine learning algorithm for designing quantum experiments. *Quantum Mach. Intell.* **1**, 5–15 (2019).
120. Nichols, R., Mineh, L., Rubio, J., Matthews, J. C. & Knott, P. A. Designing quantum experiments with a genetic algorithm. *Quantum Sci. Technol.* **4**, 045012 (2019).
121. Melnikov, A. A. et al. Active learning machine learns to create new quantum experiments. *Proc. Natl Acad. Sci. USA* **115**, 1221–1226 (2018).
122. Briegel, H. J. & De las Cuevas, G. Projective simulation for artificial intelligence. *Sci. Rep.* **2**, 400 (2012).
123. Briegel, H. J. On creative machines and the physical origins of freedom. *Sci. Rep.* **2**, 522 (2012).
124. Wallnöfer, J., Melnikov, A. A., Dür, W. & Briegel, H. J. Machine learning for long-distance quantum communication. *PRX Quantum* **1**, 010301 (2020).
125. Adler, T. et al. Quantum optical experiments modeled by long short-term memory. Preprint at https://arxiv.org/abs/1910.13804 (2019).
126. Hochreiter, S. & Schmidhuber, J. Long short-term memory. *Neural Comput.* **9**, 1735–1780 (1997).
127. Qiang, X. et al. Large-scale silicon quantum photonics implementing arbitrary two-qubit processing. *Nat. Photon.* **12**, 534–539 (2018).
128. Wang, J. et al. Multidimensional quantum entanglement with large-scale integrated optics. *Science* **360**, 285–291 (2018).
129. Lu, L. et al. Three-dimensional entanglement on a silicon chip. *npj Quantum Inf.* **6**, 30 (2020).
130. Weedbrook, C. et al. Gaussian quantum information. *Rev. Mod. Phys.* **84**, 621–669 (2012).
131. Lenzini, F. et al. Integrated photonic platform for quantum information with continuous variables. *Sci. Adv.* **4**, eaat9331 (2018).
132. Zhang, G. et al. An integrated silicon photonic chip platform for continuous-variable quantum key distribution. *Nat. Photon.* **13**, 839–842 (2019).
133. Arrazola, J. M., et al. Machine learning method for state preparation and gate synthesis on photonic quantum computers. *Quantum Sci. Technol.* **4**, 024004 (2019).
134. Killoran, N. et al. Continuous-variable quantum neural networks. *Phys. Rev. Res.* **1**, 033063 (2019).
135. Menicucci, N. C. Fault-tolerant measurement-based quantum computing with continuous-variable cluster states. *Phys. Rev. Lett.* **112**, 120504 (2014).
136. Killoran, N. et al. Strawberry fields: a software platform for photonic quantum computing. *Quantum* **3**, 129 (2019).
137. Sabapathy, K. K., Qi, H., Izaac, J. & Weedbrook, C. Production of photonic universal quantum gates enhanced by machine learning. *Phys. Rev. A* **100**, 012326 (2019).
138. Gimeno-Segovia, M., Shadbolt, P., Browne, D. E. & Rudolph, T. From three-photon Greenberger–Horne–Zeilinger states to ballistic universal quantum computation. *Phys. Rev. Lett.* **115**, 020502 (2015).
139. Zaidi, H. A., Dawson, C., van Loock, P. & Rudolph, T. Near-deterministic creation of universal cluster states with probabilistic Bell measurements and three-qubit resource states. *Phys. Rev. A* **91**, 042301 (2015).
140. Gubarev, F. et al. Improved heralded schemes to generate entangled states from single photons. Preprint at https://arxiv.org/abs/2004.02691 (2020).
141. Wang, H. et al. On-demand semiconductor source of entangled photons which simultaneously has high fidelity, efficiency, and indistinguishability. *Phys. Rev. Lett.* **122**, 113602 (2019).
142. Morizur, J.-F. et al. Programmable unitary spatial mode manipulation. *J. Opt. Soc. A* **27**, 2524–2531 (2010).
143. Fontaine, N. K. et al. Laguerre–Gaussian mode sorter. *Nat. Commun.* **10**, 1865 (2019).
144. Brandt, F., Hiekkamäki, M., Bouchard, F., Huber, M. & Fickler, R. High-dimensional quantum gates using full-field spatial modes of photons. *Optica* **7**, 98–107 (2020).
145. Rotter, S. & Gigan, S. Light fields in complex media: mesoscopic scattering meets wave control. *Rev. Mod. Phys.* **89**, 015005 (2017).
146. Fickler, R., Ginoya, M. & Boyd, R. W. Custom-tailored spatial mode sorting by controlled random scattering. *Phys. Rev. B* **95**, 161108 (2017).
147. Leedumrongwatthanakun, S. et al. Programmable linear quantum networks with a multimode fibre. *Nat. Photon.* **14**, 139–142 (2020).
148. Krenn, M., Häse, F., Nigam, A., Friederich, P. & Aspuru-Guzik, A. SELFIES: a robust representation of semantically constrained graphs with an example application in chemistry. *MLST* (in the press).
149. Heule, M. J., Kullmann, O. & Marek, V. W. Solving and verifying the boolean pythagorean triples problem via cube-and-conquer. In *International Conference on Theory and Applications of Satisfiability Testing* (eds Creignou, N. & Le Berre, D.) 228–245 (Springer, 2016).
150. Heule, M. J. & Kullmann, O. The science of brute force. *Commun. ACM* **60**, 70–79 (2017).
151. Higgins, I. et al. beta-VAE: learning basic visual concepts with a constrained variational framework. In *ICLR 2017* (2017).
152. Chen, T. Q., Li, X., Grosse, R. B. & Duvenaud, D. K. Isolating sources of disentanglement in variational autoencoders. *Adv. Neural Inf. Process. Syst.* **21**, 2610–2620 (2018).
153. Lusch, B., Kutz, J. N. & Brunton, S. L. Deep learning for universal linear embeddings of nonlinear dynamics. *Nat. Commun.* **9**, 4950 (2018).
154. Roscher, R., Bohn, B., Duarte, M. F. & Garcke, J. Explainable machine learning for scientific insights and discoveries. *IEEE Access* **8**, 42200–42216 (2020).
155. Iten, R., Metger, T., Wilming, H., Del Rio, L. & Renner, R. Discovering physical concepts with neural networks. *Phys. Rev. Lett.* **124**, 010508 (2020).
156. Nautrup, H. P. et al. Operationally meaningful representations of physical systems in neural networks. Preprint at https://arxiv.org/abs/2001.00593 (2020).
157. Lehman, J. et al. The surprising creativity of digital evolution: a collection of anecdotes from the evolutionary computation and artificial life research communities. *Artif. Life* **26**, 274–306 (2020).
158. Pavičić, M., Waegell, M., Megill, N. D. & Aravind, P. Automated generation of Kochen–Specker sets. *Sci. Rep.* **9**, 6765 (2019).
159. Goyeneche, D., Alsina, D., Latorre, J. I., Riera, A. & Życzkowski, K. Absolutely maximally entangled states, combinatorial designs, and multiunitary matrices. *Phys. Rev. A* **92**, 032316 (2015).
160. Bengtsson, I. & Życzkowski, K. *Geometry of Quantum States: An Introduction to Quantum Entanglement* (Cambridge Univ. Press, 2017).
161. Horodecki, P., Rudnicki, L. & Zyczkowski, K. Five open problems in quantum information. Preprint at https://arxiv.org/abs/2002.03233 (2020).
162. Bharti, K., Haug, T., Vedral, V. & Kwek, L.-C. Machine learning meets quantum foundations: a brief survey. Preprint at https://arxiv.org/abs/2003.11224 (2020).
163. Mnih, V. et al. Human-level control through deep reinforcement learning. *Nature* **518**, 529–533 (2015).
164. Vinyals, O. et al. Grandmaster level in StarCraft II using multi-agent reinforcement learning. *Nature* **575**, 350–354 (2019).
165. Jaderberg, M. et al. Human-level performance in 3D multiplayer games with population-based reinforcement learning. *Science* **364**, 859–865 (2019).
166. Pathak, D., Agrawal, P., Efros, A. A. & Darrell, T. Curiosity-driven exploration by self-supervised prediction. In *Proc. IEEE Conference on Computer Vision and Pattern Recognition Workshops* 16–17 (IEEE, 2017).
167. Burda, Y. et al. Large-scale study of curiosity-driven learning. Preprint at https://arxiv.org/abs/1808.04355 (2019).
168. Silver, D. et al. A general reinforcement learning algorithm that masters chess, shogi, and Go through self-play. *Science* **362**, 1140–1144 (2018).

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