QUANTUM COMPUTING FOR DATA ANALYTICS
In Brief:

- After 40 years of research, the industrialization of quantum computing has begun to transform Data Analytics & AI with benefits expected in 2–3 years.

- Computations on data in quantum systems promise new analytics opportunities and exponential speed gains for today’s most challenging business problems.

- Despite challenges in scaling quantum systems and integrating them into business data workflows, the industry progresses fast towards enterprise readiness.

- Businesses engaging in quantum incubation & readiness programs today can strategically position themselves for future disruptions.

Introduction

We live in a world of accelerating growth of the global digital economy, where digitalization of information creates big data assets and digital technologies become more powerful, accessible, and cheaper. This is reflected in entirely new business operating models and ways we interact, work, shop, and receive services. This observable acceleration and technological evolution is the result of complementary advances, from the internet, cloud and edge computing, mobile electronics to open-source collaborations. Overall, the backbone and key enabler of this progression is the semiconductor industry. Based on several physics and engineering breakthroughs and the invention of the transistor in the first half of the 20th century, the industry has rapidly evolved from special- to general-purpose computing technologies and consistently followed the performance predictions of Moore’s Law, doubling the number of transistors in integrated computing circuits about every two years.

This involved shrinking transistors to currently about 2 nanometers in size, which represents only a few atoms next to each other. However, at this level, transistors reach quantum physical limits, noise challenges, and the fabrication process becomes uneconomical. As a result, the industry reacted with new 3D hybrid stacking designs, the advancement of application-specific integrated circuits for neuromorphic computing targeting Artificial Intelligence (AI) applications, and the opening of an entire new era of information processing: Quantum Computing (QC).

The way we represent and process information, from the Abacus for arithmetic calculations in ancient times to transistors in the latest iPhone, has not changed much on a fundamental level: computations are deterministic in nature, and their logic follows our macroscopic understanding of the world. But the paradigm of information representation and processing in QC follows the quantum mechanical laws at atomic scales, which is fundamentally different from the world we are used to. While the smallest unit of information in a classical computer is a bit, a binary digit deterministically represented as either “0” or “1”, the nearest equivalent unit in a quantum computer is the qubit, a two-state quantum system probabilistically represented as a coherent superposition of both “0” and “1”.

There are many physical representations of qubits that can be manipulated for controlled computation, such as using state encodings in an atom, the spin of an electron, the polarization of a photon, or more complex systems. The rules of the game for processing quantum information are anything but intuitive. For example, reading one page at a time of a 100-page digital book written in bits tells us 1% more about the book’s information content, unlike if the book were written in entangled qubits, where information is encoded in the correlations among the pages, thus requiring a collective observation of all 100 pages at once to retrieve the book’s information content. But there are exponentially more bits needed to describe the quantum state of qubits: for example, a system with only 100 qubits would require more bits than on all hard drives in the world. With 300 qubits, it would require more bits than the number of atoms in the visible universe (see Figure 1). In turn, far greater amounts of classical information can be represented in quantum resources, which opens up new dimensions for future Big Data analytics.
Quantum Computing for Data Analytics

Introduction

This exponential scaling behavior in QC gives rise to great economical interest in using this technology to solve complex high-dimensional optimization problems much faster or to tackle those that are even impossible with today’s semiconductor technology. Tremendous progress has been made since Richard Feynman sparked the idea of QC over 40 years ago, but particularly various breakthroughs over the last 4 years have made this new computing era a near-term reality for relevant business applications. One of those has been the demonstration of quantum supremacy with Google’s 53-qubit device named Sycamore in 2019, performing a calculation in 3 minutes that would have taken the most powerful supercomputer on earth at least a few days. While this calculation admittedly had no practical use except demonstrating that classical systems cannot simulate quantum systems efficiently, it marked the opening of the Noisy Intermediate-Scale Quantum (NISQ) era. The name highlights one of today’s main engineering challenges: protecting qubits from decoherence and induced noise from the surrounding macroscopic environment controlling them. This leads to computing error rates currently of the order of $10^{-3}$ and demands intelligent error correction techniques to scale QC with hundred thousands of qubits and thus to realize its full potential for massive high-impact applications in the future Fault-Tolerant Quantum Computing (FTQC) era.

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But even in today’s NISQ era, the QC potential is expected to begin unfolding and supercharging applications in advanced data analytics: from solutions to efficiently learn complex information patterns in vast amounts of data to the supply of a new breed of talents to cope with tomorrow’s high demand for quantum information scientists, innovators, and leaders. Regardless of how long it will take us to enter the FTQC era, it is of paramount importance for every company to prepare for a quantum-accelerated world, to upskill and foster ideation of what QC could do in their industry, to strategically position themselves with quantum use cases, and to maximize the insights and business value they can gain with hybrid quantum data analytics solutions, starting today.

<table>
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<tr>
<td>100</td>
<td>“more bits than on global data stores”</td>
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<tr>
<td>300</td>
<td>“more bits than the number of atoms in visible universe”</td>
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Quantum Computing for Data Analytics

From classical to quantum computable data

Classical computers, the backbone of all digital technologies we are using today, are well established in processing structured data in form of transactions on relational databases and online analytical processing on columnar tables. Unstructured or semi-structured data exists in abundance but requires special storage (arrays or blob stores) often requiring preparation and abstraction for reasonable analytical processing on classical computers. Also, intermediate data types like dictionaries saved in key-value stores, 2D values saved in wide columns, time series databases, immutable ledgers for audit trails or entity relationships saved in graph databases lead to high transformation effort for reasonable business-relevant processing on classical computers or are losing information due to the necessary simplifications. Thus, not all of today’s data types can be analyzed efficiently on classical computers.

QC enables new analytical approaches but requires a completely new information representation on qubit registers. Before we examine quantum data analytics, we need to define required data conversions to process data with a quantum computer. All digital data must be transformed technically from the “classical environment” into a computable representation using qubits instead of binary sets. This is the main conversion path, but it is important to note that given a particular use case more conversion pathways may be considered, such as from quantum back to a classical environment or from quantum to another quantum computing environment.

Over the last 2 years, quantum computing has substantially advanced and now allows the evaluation of proof-of-concepts, but is not yet capable of processing large amounts of data as relevant in most common analytics scenarios today. Loading a complex data state into a quantum computer is costly in time due to the slow quantum processor clock rates. An increased clock rate for a high number of clock cycles would lead to noisy data and reduce the number of applicable business problems heavily. Another restriction is that nowadays quantum states can be maintained only for very short time periods, which limits the processing times and range of analytical workflows.

In addition to the limited access to real on-premise or cloud-native quantum computers, a major challenge is integrating data input and output flows into business workflows and possibly combining them with a data science lifecycle. This yields the need to educate software engineers in relevant quantum encoding and deployment patterns to provide efficient low-latency interfaces between classical bitwise computing data flows and dedicated quantum data pathways in the qubit format for selected data analytics use cases as well as back into business workflows. For example, within a quantum state preparation routine for a particular use case, the bitwise data of interest is loaded and transformed into quantum registers (memory). However, each encoding is a trade-off between the number of required qubits and the runtime for the loading process.

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Although it is common today to leverage high data volumes to solve business problems, Google’s “quantum supremacy” has already demonstrated that in quantum computing even with small amounts of data, solutions can be found for problems within a complexity domain that is very hard or even impossible to achieve using classical computers. This is a first step to a new generation of data preparation and is in line with the general trend for leveraging small data as propagated by Gartner. In other words, progress is not always driven by “just” increasing the amount of data, but by the effectiveness of different analytical approaches applied to the data for valuable insight generation.
Towards Quantum Data Analytics

Over the next few years, quantum computing is expected to discover new patterns and solutions and to provide results faster or in a more energy- and cost-efficient manner in selected analytics use cases, but only if a combination of technology-affine business analysts and applied researchers are able to efficiently use and extend business specific and technology aware methods to “quantize” the business problem and create a user accessible workflow. This quantization consists of two main challenges to address in terms of business requirements on one side and research & development feasibility on the other side.

The technology push

The challenge on the development side lies with offering algorithms and problem model suites – cousins of machine learning tools like TensorFlow, optimization tools like CPLEX, GUROBI, OR-tools or physics & chemistry simulation tools like COMSOL Multiphysics or Gaussian. These new tools (e.g., IBM’s qiskit optimization / nature or Google’s OpenFermion, TensorFlow Quantum and more) address the currently intractable parts of mature data analytics workflows. Leading examples are tasks of predicting new material properties just from the knowledge of their atomic composition, the Altzheimer disease relevant prototypic simulation of patogenous proteins and their interaction with potential drugs, and quantum Monte-Carlo methods addressing an outstanding challenge of complex electronic states of materials called “fermionic sign problem” within the in-silico workflow of calculating chemical reactions in the production or discovery of materials on real quantum hardware. Other leading technical implementations address finding patterns in data to identify clusters of similarly behaving entities or to identify outliers. These technical approaches are relevant for example in credit card transactions for fraud detection or customer preferences for movie recommendations. The endeavor to provide and apply these new computing engines is currently mainly driven by large technology corporates with extensive cash reserves in partnership with business domain and quantum application experts. Unraveling the complex map of quantum computing feasibility is currently pursued in two modes:

Figure 2: A typical technology stack of quantum applications in industry
The first mode is that of computer science, theoretical physics and mathematics, which sheds light across many of the most general and fundamental problems at the roots of seemingly infeasible business challenges across R&D (new products screening and design), logistics & production (network planning and routing, production line configuration), and sales (prediction of customer needs and recommendations). This approach developed the hand-full of first generation quantum algorithms for abstract mathematical routines (e.g., Shor’s Prime Factorization, Grover Search Algorithm, HHL Matrix Inversion Algorithm, Quantum Fourier Transform, Quantum Amplitude Estimation and more), which build on theoretical assumptions of idealized quantum computers and conceptually prove to resolve classically intractable problems at ideal precision and performance. These algorithms, although impractical until the advent of large-scale fault tolerant quantum computers, act as beacons for abstract problem fields with quantum potential and – more importantly – by excluding barren fields as object for bad R&D investments. The sweet spot lies in problem fields with complexities (a measure for “hardness of the problem”) too hard and rugged for classical computers, but not too hard for quantum computers.

The second mode and the one closer to enterprise application is that of applied researchers, engineers, and data scientists developing and empirically driving inventions for improved or new products and services. Their empirical approach is less generalistic and can therefore pay attention to more detailed structures and features in the specific and business relevant dataset at hand. Ideal solution precision irrelevant for most business requirements is traded off for practicality in the form of reduced runtime and computational resource requirements. This is achieved by heuristics which rapidly generate approximate but sufficient solutions. This approach enabled the breakthroughs in machine learning like speech detection and also enabled the second generation of quantum algorithms called variational algorithms and quantum neural networks, which enabled the drug simulations and fraud detection mentioned before. Very similar to the research concept of problem fields, whose underlying mathematical structures induce complexity and thereby enable decision support on potential quantum advantage, the deeper domain knowledge about similarities in datasets and their underlying patterns or structures are levers for technical feasibility on real quantum hardware and essentially for an guided way to quantum advantage. The sweet spot lies where the structure and patterns within the data describing the problem translate well to the structures provided by the quantum computing hardware. Examples are decision problems with many influencing factors, where small changes to the factors lead to sudden change of the considered targets. This can be the case in portfolios with assets that have complex interdependencies. In this context, complex means that the factors under consideration in the dataset are not independent enough to be treated as single factors (e.g., unrelated assets) while also not being perfectly dependent (e.g., S&P 500 and global equity), such that they all behave as one entity.

All the previously described research and technical approaches can be grouped into 3 technical application areas:

1. **Simulation & Sampling** – random sampling for approximating properties of complex systems (e.g., material / drug property prediction) and optimizing complex decisions (e.g., large scale telecom / utilities / rail network recovery or planning)

2. **Search & Optimization** – algorithms and heuristics which discover a route towards the desired solutions (e.g., Grover-search, Max-Cut optimization)

3. **Machine Learning & Pattern Recognition** – projecting the problem into quantum space to enable new viewpoints and discover patterns in data (e.g., credit fraud detection)
The business pull

The second challenge of addressing the business needs and translating business requirements lies with technology-oriented business analysts and quantitative experts with deep understanding of business logic. They are challenged to assess the application design and provide guidance on trade-offs offered by the technology (e.g., between runtime and precision) in order to transform the technology investment into business value. The pattern behind the approach is industry agnostic and spans the entire value chain, generating valuable insights across various types of data and enabling three types of application:

1. **Descriptive Analytics**: a more precise description of typically uncertain business situations based on additional data and analytics [Figure 3] – “descriptive Analytics”

2. **Predictive Analytics**: creating and correcting predictions on the impact of actions to shape and adapt potential outcomes of business decisions “predictive Analytics”

3. **Prescriptive Analytics**: support of decision-making by enabling the evaluation and prioritization of complex alternatives for actions – [see Figure 4] “prescriptive Analytics”

Applying the appropriate methods from the three technical application areas to the appropriate areas of business [Figure 4] enables the connection between technology and business by leveraging the problem and data structures and deciding on the right quantum software development kit, algorithm, hardware, and workflow tooling. Based on this technology architecture, we can follow the process to bridge from business requirements to quantum computing workflow results.

![Figure 3: The business and management challenge of assessing the status quo, setting goals and actions to achieve them under uncertainty / incomplete information](image)

![Figure 4: Additional data to reduce uncertainties and support actions provided by data analytics and advanced analytics – describing and predicting scenarios with machine learning and simulation and prescribing actions through optimization to correct and improve](image)
Eventually, quantum computing will become widely available, allowing everyone who uses Quantum Computing to solve challenges and rapidly utilize the power of new algorithms to overcome classical boundaries. The primary challenge will still be to identify the business problems and use cases that can be translated efficiently into quantum-computable structures leveraging quantum computable routines. This is where a clear advantage for first movers and early adopters will arise. While others first need to understand how to adapt to a new way of solving business critical objectives, companies that have been working with a QC stack for quite some time will already have that skillset and talent in place. Moreover, a huge part of realizing the desired business impact with a technology is not only to have it integrated in the enterprise-wide infrastructure, but also involve business stakeholders in the design process of the new solution. Another very important aspect is the variety of development speed in the quantum computing realm. Some use cases and fields of application might arise earlier than others (e.g., optimization vs. QML), yielding yet another advantage for early adopters.

90% of organizations will partner with consulting companies or full-stack providers to accelerate quantum computing innovation through 2023, according to Gartner².
First movers will gradually improve their quantum skills and simultaneously understand where to harness the power of quantum as soon as it is available and simultaneously understand. One possibility to embark on the journey is a quantum readiness or incubation program as illustrated in Figure 5.

In this way it might be possible to leverage quantum computers as co-processors even in cloud & big data pipelines. Thus, the imperative in discovering and piloting high potential use cases is a critical check that has to be performed periodically and frequently. Within this discovery process, several aspects have to be covered, ranging from data encoding & loading methods to utilizing new Quantum Computing tools or processors. Rigorous due diligence in assessing the data quality and structure is the basis of success and facilitates the selection of appropriate algorithms / solvers for the instance at hand. The first practical advantages will rely on hybrid methods, orchestrated efficiently on a combination of quantum computers interfaced with classical computers. This approach uses the best of both worlds, combining easy pre-processing and highly flexible cloud setup with new quantum algorithms.

The time to start your quantum journey is now!
Quantum Computing for Data Analytics

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