

# Category Theory for Quantum Natural Language Processing



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A thesis submitted for the degree of  
*Doctor of Philosophy*

December 20, 2021



# Abstract

This thesis introduces a framework for quantum natural language processing (QNLP) based on a simple yet powerful analogy between computational linguistics and quantum mechanics: grammar as entanglement. The grammar of a sentence connects the meaning of words in the same way that entanglement connects the states of quantum systems, they are both structures of information flow. We turn this language-to-qubit analogy into an algorithm that maps the grammatical structure of sentences onto the architecture of parameterised quantum circuits. We then use a hybrid classical-quantum algorithm to train the model on some data-driven task so that evaluating the circuits computes the meaning of sentences. The implementation of these QNLP models led to the development of DisCoPy, a Python library for computing with string diagrams based on a premonoidal approach to computational category theory (Chapter 1). We formalise our QNLP models as monoidal functors from grammar to quantum circuits and we introduce the idea of functorial learning, i.e. learning structure-preserving functors from diagram-like data (Chapter 2). In order to learn optimal functor parameters via gradient descent, we introduce the notion of diagrammatic differentiation, a graphical calculus for computing the gradient of quantum circuits and string diagrams in general (Chapter 3).



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# Introduction

## What are quantum computers good for?

Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

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*Simulating Physics with Computers,*  
Feynman (1981)

Quantum computers harness the principles of quantum theory such as superposition and entanglement to solve information-processing tasks. In the last 42 years, quantum computing has gone from theoretical speculations to the implementation of machines that can solve problems beyond what is possible with classical means. This section will sketch a brief and biased history of the field and of its future challenges.

In 1980, Benioff [Ben80] takes the abstract definition of a computer and makes it physical: he designs a quantum mechanical system whose time evolution encodes the computation steps of a given Turing machine. In retrospect, this may be taken as the first proof that quantum mechanics can simulate classical computers. The same year, Manin [Man80] looks at the opposite direction: he argues that it would take exponential time for a classical computer to simulate a generic quantum system. Feynman [Fey82; Fey85] comes to the same conclusion and suggests a way to simulate quantum mechanics much more efficiently: building a quantum computer!

So what are quantum computers good for? Feynman's intuition gives us a first, trivial answer: at least quantum computers could simulate quantum mechanics efficiently. Deutsch [Deu85] makes the question formal by defining quantum Turing machines and the circuit model. Deutsch and Jozsa [DJ92] design the first quantum algorithm and prove that it solves *some* problem exponentially faster than any classical *deterministic* algorithm.<sup>1</sup> Simon [Sim94] improves on their result by designing a problem that a quantum computer can solve exponentially faster than any classical algorithm. Deutsch-Jozsa and Simon relied on oracles<sup>2</sup> and promises<sup>3</sup> and their problems have little practical use. However, they inspired Shor's algorithm [Sho94] for prime factorisation and discrete logarithm. These two problems are believed to require exponential time for a classical computer and their hardness is at the basis of the public-key cryptography schemes currently used on the internet.

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<sup>1</sup>A classical *randomised* algorithm solves the problem in constant time with high probability.

<sup>2</sup>An oracle is a black box that allows a Turing machine to solve a certain problem in one step.

<sup>3</sup>The input is promised to satisfy a certain property, which may be hard to check.

In 1997, Grover provides another application for quantum computers: “searching for a needle in a haystack” [Gro97]. Formally, given a function  $f : X \rightarrow \{0, 1\}$  and the promise that there is a unique  $x \in X$  with  $f(x) = 1$ , Grover’s algorithm finds  $x$  in  $O(\sqrt{|X|})$  steps, quadratically faster than the optimal  $O(|X|)$  classical algorithm. Grover’s algorithm may be used to brute-force symmetric cryptographic keys twice bigger than what is possible classically [BBD09]. It can also be used to obtain quadratic speedups for the exhaustive search involved in the solution of NP-hard problems such as constraint satisfaction [Amb04]. Independently, Bennett et al. [Ben+97] prove that Grover’s algorithm is in fact optimal, adding evidence to the conjecture that quantum computers cannot solve these NP-hard problems in polynomial time. Chuang et al. [CGK98] give the first experimental demonstration of a quantum algorithm, running Grover’s algorithm on two qubits.

Shor’s and Grover’s discovery of the first real-world applications sparked a considerable interest in quantum computing. The core of these two algorithms has then been abstracted away in terms of two subroutines: phase estimation [Kit95] and amplitude amplification [Bra+02], respectively. Making use of both these subroutines, the HHL<sup>1</sup> algorithm [HHL09] tackles one of the most ubiquitous problems in scientific computing: solving systems of linear equations. Given a matrix  $A \in \mathbb{R}^{n \times n}$  and a vector  $b \in \mathbb{R}^n$ , we want to find a vector  $x$  such that  $Ax = b$ . Under some assumptions on the sparsity and the condition number of  $A$ , HHL finds (an approximation of)  $x$  in time logarithmic in  $n$  when a classical algorithm would take quadratic time simply to read the entries of  $A$ . This initiated a new wave of enthusiasm for quantum computing with the promise of exponential speedups for machine learning tasks such as regression [WBL12], clustering [LMR13], classification [RML14], dimensionality reduction [LMR14] and recommendation [KP16]. The narrative is appealing: machine learning is about finding patterns in large amounts of data represented as high-dimensional vectors and tensors, which is precisely what quantum computers are good at. The argument can be formalised in terms of complexity theory: HHL is BQP-complete<sup>2</sup> hence if there is an exponential advantage for quantum algorithms at all there must be one for HHL.

However, the exponential speedup of HHL comes with some caveats, thoroughly analysed by Aaronson [Aar15]. Two of these challenges are common to many quantum algorithms: 1) the efficient encoding of classical data into quantum states and 2) the efficient extraction of classical data via quantum measurements. Indeed, what HHL really takes as input is not a vector  $b$  but a quantum state  $|b\rangle = \sum_{i=1}^n b_i |i\rangle$  called its amplitude encoding. Either the input vector  $b$  has enough structure that we can describe it with a simple, explicit formula. This is the case for example in the calculation of electromagnetic scattering cross-sections [CJS13]. Or we assume that our classical data has been loaded onto a quantum random-access memory (qRAM) that can prepare the state in logarithmic time [GLM08]. Not only is qRAM a daunting challenge from an engineering point of view, in some cases it also requires too much error correction for the state preparation to be efficient

<sup>1</sup>Named after its discoverers Harrow, Hassidim and Lloyd.

<sup>2</sup>A BQP-complete problem is one that is polynomial-time equivalent to the circuit model, the hardest problem that a quantum computer can solve with bounded error in polynomial time.



[Aru+15]. Symmetrically, the output of HHL is not the solution vector  $x$  itself but a quantum state  $|x\rangle$  from which we can measure some observable  $\langle x|M|x\rangle$ . If preparing the state  $|b\rangle$  requires a number of gates exponential in the number of qubits, or if we need exponentially many measurements of  $|x\rangle$  to compute our classical output, then the quantum speedup disappears.

Shor, Grover and HHL all assume *fault-tolerant* quantum computers [Sho96]. Indeed, any machine we can build will be subject to noise when performing quantum operations, errors are inevitable: we need an error correcting code that can correct these errors faster than they appear. This is the content of the *quantum threshold theorem* [AB08] which proves the possibility of fault-tolerant quantum computing given physical error rates below a certain threshold. One noteworthy example of such a quantum error correction scheme is Kitaev’s toric code [Kit03] and the general idea of topological quantum computation [Fre+03] which offers the long-term hope for a quantum computer that is fault-tolerant “by its physical nature”. However this hope relies on the existence of quasi-particles called Majorana zero-modes, which as of 2021 has yet to be experimentally demonstrated [Bal21].

The road to large-scale fault-tolerant quantum computing will most likely be a long one. So in the meantime, what can we do with the noisy intermediate-scale quantum machines we have available today, in the so-called NISQ era [Pre18]? Most answers involve a hybrid classical-quantum approach where a classical algorithm is used to optimise the preparation of quantum states [McC+16]. Prominent examples include the quantum approximate optimisation algorithm (QAOA [FGG14]) for combinatorial problems such as maximum cut and the variational quantum eigensolver (VQE [Per+14]) for approximating the ground state of chemical systems. These variational algorithms depend on the choice of a parameterised quantum circuit called the *ansatz*, based on the structure of the problem and the resources available. Some families of ansätze such as instantaneous quantum polynomial-time (IQP) circuits are believed to be hard to simulate classically even at constant depth [SB09], opening the door to potentially near-term NISQ speedups.

Although the hybrid approach first appeared in the context of machine learning [Ban+08], the idea of using parameterised quantum circuits as machine learning models went mostly unnoticed for a decade [BLS19]. It was rediscovered under the name of quantum neural networks [FN18] then implemented on two-qubits [Hav+19], generating a new wave of attention for quantum machine learning. The idea is straightforward: 1) encode the input vector  $x \in \mathbb{R}^n$  as a quantum state  $|\phi_x\rangle$  via the ansatz of our choice, 2) initialise a random vector of parameters  $\theta \in \mathbb{R}^d$  and encode it as a measurement  $M_\theta$ , again via some choice of ansatz 3) take the probability  $y = \langle \phi(x)|M_\theta|\phi(x)\rangle$  as the prediction of the model. A classical algorithm then uses this quantum prediction as a subroutine to find the optimal parameters  $\theta$  in some data-driven task such as classification.

One of the many challenges on the way to solving real-world problems with parameterised quantum circuits is the existence of *barren plateaus* [McC+18]: with random circuits as ansatz, the probability of non-zero gradients is exponentially small in the number of qubits and our classical optimisation gets lost in a flat landscape. One can help but notice the striking similarity with the vanishing gradient problem

for classical neural networks, formulated twenty years earlier [Hoc98]. Barren plateaus do not appear in circuits with enough structure such as quantum convolutional networks [Pes+21], they can also be mitigated by structured initialisation strategies [Gra+19]. Another direction is to avoid gradients altogether and use *kernel methods* [SK19]: instead of learning a measurement  $M_\theta$ , we use our NISQ device to estimate the distance  $|\langle \phi_{x'} | \phi_x \rangle|^2$  between pairs of input vectors  $x, x' \in \mathbb{R}^n$  embedded in the high-dimensional Hilbert space of our ansatz. We then use a classical support vector machine to find the optimal hyperplane that separates our data, with theoretical guarantees to learn quantum models at least as good as the variational approach [Sch21].

Random quantum circuits may be unsuitable for machine learning, but they play a crucial role in the quest for *quantum advantage*, the experimental demonstration of a quantum computer solving a task that cannot be solved by classical means in any reasonable time. We are back to Feynman’s original intuition: sampling from a random quantum circuit is the perfect candidate for such a task. The end of 2019 saw the first claim of such an advantage with a 53-qubit computer [Aru+19]. The claim was almost immediately contested by a classical simulation of 54 qubits in two and a half days [Ped+19] then in five minutes [Yon+21]. Zhong et al. [Zho+20] made a new claim with a 76-photon linear optical quantum computer followed by another with a 66-qubit computer [Wu+21; Zhu+21]. They estimate that a classical simulation of the sampling task they completed in a couple of hours would take at least ten thousand years.

Now that quantum computers are being demonstrated to compute something beyond classical, the question remains: can they compute something *useful*?

## Why should we make NLP quantum?

A girl operator typed out on a keyboard the following Russian text in English characters: “Mipyeryedayem mislyi posryedstvom ryechi”. The machine printed a translation almost simultaneously: “We transmit thoughts by means of speech.” The operator did not know Russian.

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*New York Times* (8th January 1954)

The previous section hinted at the fact that quantum computing cannot simply solve any problem faster. There needs to be some structure that a quantum computer can exploit: its own structure in the case of physics simulation or the group-theoretic structure of cryptographic protocols in Shor’s algorithm. So why should we expect quantum computers to be any good at natural language processing (NLP)? This section will argue that natural language shares a common structure with quantum theory, in the form of two linguistic principles: *compositionality* and *distributionality*.

The history of artificial intelligence (AI) starts in 1950 with a philosophical question from Turing [Tur50]: “Can machines think?” reformulated in terms of a game, now known as the Turing test, in which a machine tries to convince a

human interrogator that it is human too. In order to put human and machine on an equal footing, Turing suggests to let them communicate only via written language: his thought experiment actually defined an NLP task. Only four years later, NLP goes from philosophical speculation to experimental demonstration: the IBM 701 computer successfully translated sentences from Russian to English such as “They produce alcohol out of potatoes.” [Hut04]. With only six grammatical rules and a 250-word vocabulary taken from organic chemistry and other general topics, this first experiment generated a great deal of public attention and the overly-optimistic prediction that machine translation would be an accomplished task in “five, perhaps three” years.

Two years later, Chomsky [Cho56; Cho57] proposes a hierarchy of models for natural language syntax which hints at why NLP would not be solved so fast. In the most expressive model, which he argues is the most appropriate for studying natural language, the parsing problem is in fact Turing-complete. Let alone machine translation, merely deciding whether a given sequence of words is grammatical can go beyond the power of any physical computer. Chomsky’s parsing problem is a linguistic reinterpretation of an older problem from Thue [Thu14], now known as the *word problem for monoids*<sup>1</sup> and proved undecidable by Post [Pos47] and Markov [Mar47] independently. This reveals a three-way connection between theoretical linguistics, computer science and abstract algebra which will pervade much of this thesis. But if we are interested in solving practical NLP problems, why should we care about such abstract constructions as formal grammars?

Most NLP tasks of interest involve natural language *semantics*: we want machines to compute the *meaning* of sentences. Given the grammatical structure of a sentence, we can compute its meaning as a function of the meanings of its words. This is known as the *principle of compositionality*, usually attributed to Frege.<sup>2</sup> It was already implicit in Boole’s *laws of thought* [Boo54] and then made explicit by Carnap [Car47]. Montague [Mon70a; Mon70b; Mon73] applied this principle in linguistics for the first time, arguing that there is “no important theoretical difference between natural languages and the artificial languages of logicians”. From a theoretical principle, one may argue that compositionality became the basis of the symbolic approach to NLP, also known as *good old-fashioned AI* (GOFAI) [Hau89]. Word meanings are first encoded in a machine-readable format, then the machine can compose them to answer complex questions. This approach culminated in 2011 with IBM Watson defeating a human champion at *Jeopardy!* [LF11].

The same year, Apple deploy their virtual assistant in the pocket of millions of users, soon followed by internet giants Amazon and Google. While Siri, Alexa and their competitors have made NLP mainstream, none of them make any explicit use of formal grammars. Instead of the complex grammatical analysis and knowledge representation of expert systems like Watson, the AI of these next-generation NLP machines is powered by deep neural networks and machine learning

<sup>1</sup>Historically, Thue, Markov and Post were working with *semigroups*, i.e. unitless monoids.

<sup>2</sup>Compositionality does not appear in any of Frege’s published work [Pel01]. What Frege [Fre84] did state is now known as the *context principle*: “it is enough if the sentence as whole has meaning; thereby also its parts obtain their meanings”. This can be taken as a kind of dual to compositionality: the meanings of the words are functions of the meaning of the sentence.

of big data. Although their architecture got increasingly complex, these neural networks implement a simple statistical concept: *language models*, i.e. probability distributions over sequences of words. Instead of the compositionality of symbolic AI, these statistical methods rely on another linguistic principle, *distributionality*: words with similar distributions have similar meanings. Intuitively,

This principle may be traced back to Wittgenstein’s *Philosophical Investigations*: “the meaning of a word is its use in the language” [Wit53], usually shortened into the slogan *meaning is use*. It was then formulated in the context of computational linguistics by Harris [Har54], Weaver [Wea55] and Firth [Fir57], who coined the famous quotation: “You shall know a word by the company it keeps!” Before deep neural networks took over, the standard way to formalise distributionality had been *vector space models* [SWY75]. We have a set of  $N$  words appearing in a set of  $M$  documents and we simply count how many times each word appears in each document to get a  $M \times N$  matrix. We normalise it with a weighting scheme like tf-idf (term frequency by inverse document frequency), factorise it (via e.g. singular value decomposition or non-negative matrix factorisation) and we’re done! The columns of the matrix encode the meanings of words, taking their inner product yields a measure of word similarity which can then be used in tasks such as classification or clustering. This method has the advantage of simplicity and it works surprisingly well in a wide range of applications from spam detection to movie recommendation [TP10]. Its main limitation is that a sentence is represented not as a sequence but as a *bag of words*, the word vectors will be the same whether the corpus contained “dog bites man” or “man bites dog”. A standard way to fix this is to compute vectors not for words in isolation but for  $n$ -grams, windows of  $n$  consecutive words for some fixed size  $n$ . However the fix has its own limits: if  $n$  is too small we cannot detect any long-range correlations, if it is too big then the matrix is so sparse that we cannot detect anything at all.

In contrast, the recurrent neural networks (RNNs) of Rumelhart, Hinton and Williams [RHW86] are inherently sequential and their internal state can encode arbitrarily long-range correlations. At each step, the network processes the next word in a sequence and updates its internal state. This internal memory can then be used to predict the rest of the sequence, or fed as input to another network e.g. for translation into another language. Once the obstacles to training were overcome (such as the vanishing gradients mentioned above), RNN architectures such as long short-term memory (LSTM) [HS97] set records in a variety of NLP tasks such as language modeling [SMH11], speech recognition [GMH13] and machine translation [SVL14]. The purely sequential approach of RNNs turned out to be limited: when the network is done reading, the information from the first word has to propagate through the entire text before it can be translated. Bidirectional RNNs [SP97] fix this issue by reading both left-to-right and right-to-left. Nonetheless, it is somewhat unsatisfactory from a cognitive perspective (humans manage to understand text without reading backward, why should a machine do that?) and also harder to use in online settings where words need to be processed one at a time.

Attention mechanisms provide a much more elegant solution: instead of assuming that the “company” of a word is its immediate left and right neighbourhood,

we let the neural network itself learn which words are relevant to which. First introduced as a way to boost the performance of RNNs on translation tasks [BCB16], attention has then become the basis of the *transformer model* [Vas+17]: a stack of attention mechanisms which process sequences without recurrence altogether. Starting with BERT [Dev+19], transformers have replaced RNNs as the state-of-the-art NLP model, culminating with the GPT-3 language generator authoring its own article in *The Guardian* [GPT20]: “A robot wrote this entire article. Are you scared yet, human?”

Indeed *why* should we be scared? Because we are ignorant of *how* the robot wrote the article and we cannot explain what in its billions of parameters made it write the way it did. Transformers and neural networks in general are *black boxes*: we can probe the way they map inputs to outputs, but if we look at the terabytes of weights in between, we find no interpretation of the mapping. Moreover without explainability there can be no fairness: if we cannot explain how its decisions are made, we can hardly prevent the network from reproducing the discriminations present both in the datasets and in the assumptions of the data scientist. We argue that explainable AI requires to make the distributional black boxes transparent by endowing them with a compositional structure: we need *compositional distributional* (DisCo) models that reconcile symbolic GOF AI with deep learning.

DisCo models have their roots in neuropsychology rather than AI. Indeed, they first appeared as models of the brain rather than architectures of learning machines. In their seminal work [MP43], McCulloch and Pitts give the first formal definition of neural networks and show how their “all-or-nothing” behaviour<sup>1</sup> allow them to encode a fragment of propositional logic. Hebb [Heb49] then introduced the first biological mechanism to explain learning and structured perception: “neurons that fire together, wire together”. These computational models of the brain became the basis of *connectionism* [Smo87; Smo88] and the *neurosymbolic* [Hil97] approach to AI: high-level symbolic reasoning emerges from low-level neural networks. An influential example is Smolensky’s *tensor product representation* [Smo90], where discrete structures such as lists and trees are embedded into the tensor product of two vector spaces, one for variables and one for values. Concretely, a list  $x_1, \dots, x_n$  of  $n$  vectors of dimension  $d$  is represented as a tensor  $\sum_{i \leq n} |i\rangle \otimes x_i \in \mathbb{R}^n \otimes \mathbb{R}^d$ . Smolensky [Smo90] is also the first to make the analogy between the distributional representations of compositional structures in AI and the group representations of quantum physics. He argues that symbolic structures embed in neural networks in the same way that the symmetries of particles embed in their state space: via *representation theory*, a precursor of *category theory* which we discuss in the next section.

Clark and Pulman [CP07b] propose to apply this tensor product representation to NLP, but they note its main weakness: lists of different lengths do not live in the same space, which makes it impossible to compare sentences with different grammatical structures. The categorical compositional distributional (DisCoCat) models of Clark, Coecke and Sadrzadeh [CCS08; CCS10] overcome this issue by taking the analogy with quantum one step further. Word meanings and grammatical structure are to linguistics what quantum states and entanglement

<sup>1</sup>A neuron’s response is either maximal or zero, regardless of the stimulus strength.

structure are to physics. DisCoCat word meanings live in vector spaces and they compose with tensor products: the states of quantum theory do too. Grammar tells you how words are connected and how information flows in a sentence and in the same way, entanglement connects quantum states and tells you how information flows in a complex quantum system. This analogy allows to borrow well-established mathematical tools from quantum theory, and it was implemented on classical hardware with some empirical success on small-scale tasks such as sentence comparison [Gre+10] and word sense disambiguation [GS11; KSP13]. However representing the meaning of sentences as quantum processes comes with a price: they can be exponentially hard to simulate classically.

If DisCoCat models are intractable for classical computers, why not use a quantum computer instead? Zeng and Coecke [ZC16] answered this question with the first quantum natural language processing (QNLP) algorithm<sup>1</sup> and the proof of a quadratic speedup on a sentence classification task. Wieber et al. [Wie+19] later defined a QNLP algorithm based on a generalisation of the tensor product representation and proved it is BQP-complete: if any quantum algorithm has an exponential advantage, then in principle there must be one for QNLP. However promising they may be, both algorithms assume fault-tolerance and they are at least as far away from solving real-world problems as Grover and HHL.

This is where the work presented in this thesis comes in: we show it is possible to implement DisCoCat models on the machines available today. The author and collaborators [Mei+20b; Coe+20] introduced the first NISQ-friendly framework for QNLP by translating DisCoCat models into variational quantum algorithms. We then implemented this framework and demonstrated the first QNLP experiment on a toy question-answering task [Mei+20a] and more recent experiments showed empirical success on a larger-scale classification task [Lor+21]. Our framework was later applied to machine translation [Abb+21; VN21], word-sense disambiguation [Hof21] and even to generative music [Mir+21]. Future experiments will have to demonstrate that QNLP is more than a mere analogy and that it can achieve *quantum advantage on a useful task*. But before we can discuss our implementation in detail, we have to make the DisCoCat analogy formal.

## How can category theory help?

I should still hope to create a kind of *universal symbolic* (*spécieuse générale*) in which all truths of reason would be reduced to a kind of calculus.

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*Letter to Nicolas Remond, Leibniz (1714)*

“Every sufficiently good analogy is yearning to become a functor” [Bae06] and we will see that the analogy behind DisCoCat models is indeed a functor. Coecke et al. [CGS13] make a meta-analogy between their models of natural language

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<sup>1</sup>We do not consider previous algorithms that are inspired by quantum theory but run on classical computers such as the frameworks of Chen [Che02] and Blacoe et al. [BKL13].

and *topological quantum field theories* (TQFTs). Intuitively, there is an analogy between regions of spacetime and quantum processes: both can be composed either in sequence or in parallel. TQFTs formalise this analogy: they assign a quantum system to each region of space and a quantum process to each region of spacetime, in a way that respects sequential and parallel composition. In the same structure-preserving way, DisCoCat models assign a vector space to each grammatical type and a linear map to each grammatical derivation. Both TQFTs and DisCoCat can be given a one-sentence definition in terms of category theory: they are examples of *functors into the category of vector spaces*.

How can the same piece of general abstract nonsense (category theory’s nickname) apply to both quantum gravity and natural language processing? And how can this nonsense be of any help in the implementation of QNLP algorithms? This section will answer with a brief and biased history of category theory and its applications to quantum physics and computational linguistics, from an abstract framework for meta-mathematics to a concrete toolbox for NLP on quantum hardware. First, a short philosophical digression on the etymology of the words “functor” and “category” shall bring some light to their divergent meanings in mathematics and linguistics.

The word “functor” first appears in Carnap’s *Logical syntax of language* [Car37] to describe what would be called a *function symbol* in a modern textbook on first-order logic. He introduces them as a way to reduce the laws of empirical sciences like physics to the pure syntax of his formal logic, taking the example of a *temperature functor*  $T$  such that  $T(3) = 5$  means “the temperature at position 3 is 5”<sup>1</sup>. In the linguistics community, this meaning has then drifted to become synonymous with *function words* such as “such”, “as”, “with”, etc. These words do not refer to anything in the world but serve as the grammatical glue between the *lexical words* that describe things and actions. They represent less than one thousandth of our vocabulary but nearly half of the words we speak [CP07a].

Categories (from the ancient Greek *κατηγορία*, “that which can be said”) have a much older philosophical tradition. In his *Categories* [Ari66], Aristotle first makes the distinction between the simple forms of speech (the things that are “said without any combination” such as “man” or “arguing”) and the composite ones such as “a man argued”. He then classifies the simple, atomic things into ten categories: “each signifies either substance or quantity or qualification or a relative or where or when or being-in-a-position or having or doing or being-affected”. A common explanation [Ryl37] for how Aristotle arrived at such a list is that it comes from the possible *types of questions*: the answer to “What is it?” has to be a substance, the answer to “How much?” a quantity, etc. Although he was using language as a tool, his system of categories aims at classifying things in the world, not forms of speech: it was meant as an *ontology*, not a grammar. In his *Critique of Pure Reason* [Kan81], Kant revisits Aristotle’s system to classify not the world, but the mind: he defines categories of understanding rather than categories of being. The idea that every object (whether in the world or in the mind) is an object of a certain type has then become foundational in mathematical logic and Russell’s

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<sup>1</sup>MacLane [Mac38] would later remark that Carnap’s formal language cannot express the coordinate system for positions, nor the scale in which temperature is measured.

*theory of types* [Rus03]. The same idea has also had a great influence in linguistics and especially in the *categorial grammar* tradition initiated by Ajdukiewicz [Ajd35] and Bar-Hillel [Bar53; Bar54], where categories have now become synonymous with *grammatical types* such as nouns, verbs, etc.

Independently of their use in linguistics, Eilenberg and MacLane [EM42a; EM42b; EM45] gave categories and functors their current mathematical definition. Inspired by Aristotle’s categories of things and Kant’s categories of thoughts, they defined categories as types of *mathematical structures*: sets, groups, spaces, etc. Their great insight was to focus not on the content of the objects (elements, points, etc.) but on the composition of the *arrows* between them: functions, homomorphisms, continuous maps, etc. Applying the same insight to categories themselves, what really matters are the arrows between them: *functors*, maps from one category to another that preserve the form of arrows.<sup>1</sup> A prototypical example is Poincaré’s construction of the fundamental group of a topological space [Poi95], which can be defined as a functor from the category of (pointed) topological spaces to that of groups: every continuous map between spaces induces a homomorphism between their fundamental groups, in a way that respects composition and identity. Thus, the abstraction of category theory allowed to formalise the analogies between topology and algebra, proving results about one using methods from the other. It was then used as a tool for the foundation of algebraic geometry by the school of Grothendieck [GD60], which brought the analogy between geometric shapes and algebraic equations to a new level of abstraction and led to the development of *topos theory*.

The establishment of category theory as an independent discipline and as a foundation for mathematics owes much to the work of Lawvere. His influential Ph.D. thesis [Law63] on *functorial semantics* set up a framework for model theory where logical theories are categories and their models are functors. He then undertook the axiomatisation of the category of sets [Law64] and the category of categories [Law66]. The resulting notion of elementary topos [Law70b] subsumed Grothendieck’s definition and emphasised the foundational concept of *adjunction* [Law69; Law70a]. “Adjoint functors arise everywhere” became the slogan of MacLane’s classic textbook *Categories for the working mathematician* [Mac71]. Lambek [Lam68; Lam69; Lam72] used the related notion of *cartesian closed categories* to extend the Curry-Howard correspondance between logic and computation into a trinity with category theory: proofs and programs are arrows, logical formulae and data types are objects. The discovery of this three-fold connection resulted in a wide range of applications of category theory to theoretical computer science, surveyed in Scott [Sco00].

This unification of mathematics, logic and computer science has been followed by an ongoing program of categorical foundations for physics, initiated by Lawvere’s topos-theoretic treatment of classical dynamics [Law79] and continuum physics [LS86] with Schanuel. As we mentioned at the start of this section, the work of Atiyah [Ati88], Baez and Dolan [BD95] on TQFTs showed categories and functors to be essential tools in the grand unification project of quantum

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<sup>1</sup>We can play the same game again: what matters are not so much the functors themselves but the *natural transformations* between them, which is what category theory was originally meant to define. To keep playing that game is to fall in the rabbit hole of infinity category theory [RV16].



gravity [Bae06]. This now quaternary analogy between physics, mathematics, logic and computation was popularised by Baez and Stay in their *Rosetta Stone* [BS09]. On more concrete grounds, this connection between category theory and quantum physics appeared in Selinger’s proposal of a quantum programming language [Sel04] and the development of a quantum lambda calculus [VT04; SV06; SV+09]. The same insight blossomed in the school of *categorical quantum mechanics* (CQM) led by Abramsky and Coecke [AC04; AC08], where quantum processes are arrows in *compact closed categories*. This approach culminated in the *ZX calculus* of Coecke and Duncan [CD08; CD11], a categorical axiomatisation which was proved complete for qubit quantum computing [JPV18; HNW18] with applications including error correction [Cha+18; GF19], circuit optimisation [Kv20; Dun+20; dBW20], compilation [CSD20; dD20] and extraction [Bac+20].

In quantum computing as well, adjunction is fundamental: it underlies the definition of entanglement and the proof of correctness for the *teleportation protocol*. Back in 2004 when Coecke first presented this result at the McGill category theory seminar, Lambek immediately pointed out the analogy with his *pregroup grammars* [Lam99b; Lam01] where adjunction is the only grammatical rule<sup>1</sup>. Half a century beforehand, Lambek [Lam58; Lam59; Lam61] had started to unravel the analogy between the derivations in categorial grammars and proof trees in mathematical logic. He then extended this analogy in *Categorial and categorial grammar* [Lam88] where he showed that these grammatical derivations are in fact arrows in *closed monoidal categories* and proposed to cast Montague semantics as a topos-valued functor. Later, he argued not “that categories should play a role in linguistics, but rather that they already do” [Lam99a]. Indeed, Hotz [Hot66] had already proved that Chomsky’s generative grammars were *free monoidal categories*, although his original German article was never translated to English and remains confidential. The idea of using functors as semantics had appeared implicitly in Knuth [Knu68] in the context-free case and was made explicit by Benson [Ben70] for unrestricted grammars. From this categorical formulation of linguistics, Lambek [Lam10] first suggested the analogy between linguistics and physics which is the basis of this thesis: *pregroup reductions as quantum processes*.

It is remarkable that Lambek could foresee QNLP without *string diagrams*<sup>2</sup>, probably the most powerful tool in the hands of the applied category theorist. They first appeared in another confidential article from Hotz [Hot65] as a formalisation of the diagrams commonly used in electronics. Penrose [Pen71] then used the same notation as an informal shortcut for tedious tensor calculations, and later applied it to relativity theory with Rindler [PR84]. Joyal and Street [JS88; JS91; JS95] gave the first topological definition of string diagrams and characterised them as the arrows of free monoidal categories. At first a piece of mathematical folklore that was hand-drawn on blackboards and rarely included in publications, string diagrams were published at a much bigger scale with the advent of typesetting tools

<sup>1</sup>See [Coe19] for a first-hand account of this story and a praise of Jim Lambek.

<sup>2</sup>String diagrams do not appear in any of Lambek’s published work. Instead, he either uses lines of equations, proof trees or “underlinks” for pregroup adjunctions [Lam08]. He admits “not having had the patience to absorb” the topological definition of Joyal-Street string diagrams [Lam10].

like  $\text{\LaTeX}$  and  $\text{\textit{TikZ}}$ . Selinger’s survey [Sel10], makes the hierarchy of categorical structures (symmetric, compact closed, etc.) correspond to a hierarchy of graphical gadgets (swaps, wire bending, etc.). In *Picturing Quantum Processes* [CK17], Coecke and Kissinger introduce quantum theory with over a thousand diagrams. And the list of applications keeps growing: electronics [BF15] and chemistry [BP17], control theory [BE14] and concurrency [BSZ14], databases [BSS18] and knowledge representation [Pat17], Bayesian inference [CS12; CJ19] and causality [KU19], cognition [Bol+17] and game theory [Gha+18], functional programming [Ril18] and machine learning [FST17].

If they are a great tool for writing scientific papers, string diagrams can also be a powerful data structure for developing software applications: *quantomatic* [KZ15] and its successor *PyZX* [Kv19] perform automatic rewriting of diagrams in the ZX calculus, *globular* [BKV18] and its successor *homotopy.io* [RV19] are proof assistants for higher category theory, *cartographer* [SWZ19] and *catlab* [PSV21] implement diagrams in symmetric monoidal categories, which are also implicit in the circuit data structure of the *t|ket* compiler [Siv+20]. String diagrams are the main data structure of our QNLP algorithms: we first construct diagrams for sentences, apply a functor to translate them into quantum circuits and then send them as instructions to a quantum computer. As none of the existing category theory software was flexible enough, we had to implement our own: *DisCoPy* [Fel+20], a Python library for computing with functors and diagrams in monoidal categories. *DisCoPy* then became the engine underlying *lambeq* [Kar+21], a high-level library for experimental QNLP. Although its development was driven by the implementation of *DisCoCat* models on quantum computers, *DisCoPy* was designed as a general-purpose toolkit for applied category theory. It is freely available (as in free beer and in free speech) at:

<https://github.com/oxford-quantum-group/discopy>

In conclusion, category theory can really be a *theory of anything*: from algebraic geometry and quantum gravity to natural language processing. There is a striking analogy between category theory and string diagrams as a universal graphical language and the *characteristica universalis* and *calculus ratiocinator* dreamt by Leibniz three hundred years ago, a formal language and computational framework that would be able to express all of mathematics, science and philosophy. Indeed, not only can categories be tools for the working mathematicians and scientists, they can also be of help to the philosophers. In the footsteps of Grassmann’s *Ausdehnungslehre* [Gra44] and his project of an algebraic formalisation of Hegel, Lawvere [Law89; Law91; Law92; Law96] set out to formulate Hegelian dialectics in terms of adjunctions. This led to the ongoing effort of Schreiber, Corfield and their collaborators on the nLab [SCn21] to translate *Wissenschaft Der Logik* [Heg12] in terms of category theory. Not only can it accommodate the absolute idealism of Hegel, category theory can also deal with the pragmatism of Peirce [Pei06], who developed first-order logic independently of Frege using what was later recognised as the first string diagrams [BT98; BT00; MZ16; HS20]. String diagrams have also been used to model Wittgenstein’s language games as functors from a grammar to a category of games [HL18]. In recent work [FTC20], we applied these functorial language games to question answering, going from philosophy to NLP via category theory.

## Contributions

The first chapter is an extended version of the DisCoPy paper [FTC20]. It emerged from a dialectic teacher-student collaboration with Giovanni de Felice: implementing our own category theory library was a way to teach him Python programming. Bob Coecke then added the capital letters to the name of DisCoPy.

- We<sup>1</sup> give an elementary definition of string diagrams for monoidal categories. Our construction decomposes the free monoidal category construction into three basic steps: 1) a layer monad on the category of monoidal signatures, 2) the free premonoidal category as a free category of layers and 3) the free monoidal category as a quotient by interchangers. To the best of our knowledge, this *premonoidal approach* had been relegated to mathematical folklore: it was known by those who knew, yet it never appeared in print.
- We prove the equivalence between our elementary definition and the topological definition of Joyal and Street [JS88]. One side of this equivalence underlies the drawing algorithm of DisCoPy, the other side is the basis of a prototype for an automatic diagram recognition algorithm.
- We describe our object-oriented implementation of monoidal category theory. The hierarchy of categorical structures (monoidal, closed, rigid, etc.) is encoded in a hierarchy of Python classes and an inheritance mechanism implements the free-forgetful adjunctions between them.
- We discuss the relationship between our premonoidal approach and the existing graph-based data structures for diagrams in symmetric monoidal categories.

The second chapter deals with QNLP, building on [Mei+20a; Coe+20; Mei+20b]. It was joint work with Bob Coecke, Giovanni de Felice and Konstantinos Meichanetzidis. Although we were working in the same office, Stefano Gogioso arrived at the same ideas independently with his collaborator Nicolò Chiappori.

- We define QNLP models as functors from grammar to quantum circuits and show that any DisCoCat model can be implemented in this way.
- We develop a rewriting strategy for the resulting circuits which reduces both the required number of qubits and the amount of post-selection. The underlying algorithm, called *snake removal*, computes the normal form of diagrams in rigid monoidal categories.
- We introduce a hybrid classical-quantum algorithm to train QNLP models on a question-answering task. The underlying idea of *functorial learning*, i.e. learning structure-preserving functors from diagram-like data, provides a theoretical framework for machine learning on structured data.

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<sup>1</sup>The “we” of this section refers to the author of this thesis. Although we believe that science is collaboration and that the notion of personal contribution is obsolete, it is in fact required by university regulations: “Where some part of the thesis is not solely the work of the candidate or has been carried out in collaboration with one or more persons, the candidate shall submit a clear statement of the extent of his or her own contribution.”

The third chapter introduces *diagrammatic differentiation*, a graphical calculus for computing the gradients of parameterised diagrams which applies to the training of QNLP models but also to functorial learning in general. Most of the material has been published in joint work with Richie Yeung and Giovanni de Felice [TYF21].

- We generalise the dual number construction from rings to monoidal categories. Dual diagrams are formal sums of a string diagram (the real part) and its derivative with respect to some parameter (the epsilon part).
- We introduce graphical gadgets called bubbles, which can encode arbitrary unary operators on monoidal categories. In particular, they encode differentiation of diagrams and allow to express the standard rules of calculus (linearity, product, chain) entirely in terms of diagrams.
- We study diagrammatic differentiation for the ZX calculus. In the pure case, this allows to compute the gradients of linear maps with respect to phase parameters. In the mixed classical-quantum case, this yields a definition of the parameter-shift rules used in quantum machine learning.
- We define the gradient of QNLP models and parameterised functors in general.

## Publications

The material presented in this thesis builds on the following publications.

- [Mei+20b] Konstantinos Meichanetzidis, Stefano Gogioso, Giovanni de Felice, Nicolò Chiappori, Alexis Toumi, and Bob Coecke. “Quantum Natural Language Processing on Near-Term Quantum Computers”. In: *Proceedings 17th International Conference on Quantum Physics and Logic, QPL 2020, Paris, France, June 2 - 6, 2020*. Ed. by Benoît Valiron, Shane Mansfield, Pablo Arrighi, and Prakash Panangaden. Vol. 340. EPTCS. 2020, pp. 213–229. DOI: 10.4204/EPTCS.340.11. arXiv: 2005.04147.
- [FTC20] Giovanni de Felice, Alexis Toumi, and Bob Coecke. “DisCoPy: Monoidal Categories in Python”. In: *Proceedings of the 3rd Annual International Applied Category Theory Conference, ACT*. Vol. 333. EPTCS, 2020. DOI: 10.4204/EPTCS.333.13.
- [Coe+20] Bob Coecke, Giovanni de Felice, Konstantinos Meichanetzidis, and Alexis Toumi. “Foundations for Near-Term Quantum Natural Language Processing”. In: *CoRR* abs/2012.03755 (2020). arXiv: 2012.03755.
- [Mei+20a] Konstantinos Meichanetzidis, Alexis Toumi, Giovanni de Felice, and Bob Coecke. “Grammar-Aware Question-Answering on Quantum Computers”. In: *ArXiv e-prints* (2020). arXiv: 2012.03756.

- [TYF21] Alexis Toumi, Richie Yeung, and Giovanni de Felice. “Diagrammatic Differentiation for Quantum Machine Learning”. In: *Proceedings 18th International Conference on Quantum Physics and Logic, QPL 2021, Gdansk, Poland, and Online, 7-11 June 2021*. Ed. by Chris Heunen and Miriam Backens. Vol. 343. EPTCS. 2021, pp. 132–144. DOI: 10.4204/EPTCS.343.7.

During his DPhil, the author has also published the following articles.

- [FMT19] Giovanni de Felice, Konstantinos Meichanetzidis, and Alexis Toumi. “Functorial Question Answering”. In: *Proceedings Applied Category Theory 2019, ACT 2019, University of Oxford, UK*. Vol. 323. EPTCS. 2019. DOI: 10.4204/EPTCS.323.6.
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- [McP+21] Lachlan McPheat, Gijs Wijnholds, Mehrnoosh Sadrzadeh, Adriana Correia, and Alexis Toumi. “Anaphora and Ellipsis in Lambek Calculus with a Relevant Modality: Syntax and Semantics”. In: *CoRR* abs/2110.10641 (2021). arXiv: 2110.10641.



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- John C. Platt, Chris Quintana, Eleanor G. Rieffel, Pedram Roushan, Nicholas C. Rubin, Daniel Sank, Kevin J. Satzinger, Vadim Smelyanskiy, Kevin J. Sung, Matthew D. Trevithick, Amit Vainsencher, Benjamin Villalonga, Theodore White, Z. Jamie Yao, Ping Yeh, Adam Zalcman, Hartmut Neven, and John M. Martinis. “Quantum Supremacy Using a Programmable Superconducting Processor”. In: *Nature* 574.7779 (Oct. 2019), pp. 505–510. DOI: 10.1038/s41586-019-1666-5.
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