

Category Theory for Quantum Natural Language Processing



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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.

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.¹ 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 oracles² and promises³ 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.

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 HHL⁴ 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].

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

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

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

⁴Named after its discoverers Harrow, Hassidim and Lloyd.

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**-complete¹ 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 [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

¹A **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.

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_θ , 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 θ 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_θ , 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: “Mi pyeryedayem mislyi posryedstvom ryechi”. The machine printed a translation almost simultaneously: “We transmit thoughts by means of speech.” The operator did not know Russian.

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*¹ 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.² 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].

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

²Compositionality 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.

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 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 GOFAI 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” behaviour¹ 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 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

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

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) algorithm¹ 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 symbolistic (spécieuse générale)* in which all truths of reason would be reduced to a kind of calculus.

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

¹We 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”¹. 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 , “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

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

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 *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.¹ 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

¹We 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].

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 correspondence 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 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 rule¹. 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 categorical 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*², 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 like \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]

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

²String 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].

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 $\mathsf{t|ket}$ compiler [Siv+20]. String diagrams are the main data structure of our QNLP algorithms: we translate the diagrams of sentences into diagrams of quantum circuits. 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.

- We¹ 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 it, 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.

¹The “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.”

- 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.

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**.

- [Fel+20] Giovanni de Felice, Elena Di Lavore, Mario Román, and Alexis Toumi. “Functorial Language Games for Question Answering”. In: *Proceedings of the 3rd Annual International Applied Category Theory Conference 2020, ACT 2020, Cambridge, USA, 6-10th July 2020*. Ed. by David I. Spivak and Jamie Vicary. Vol. 333. EPTCS. 2020, pp. 311–321. DOI: **10.4204/EPTCS.333.21**.
- [STS20] Dan Shiebler, Alexis Toumi, and Mehrnoosh Sadrzadeh. “Incremental Monoidal Grammars”. In: *CoRR* abs/2001.02296 (2020). arXiv: **2001.02296**.
- [Kar+21] Dimitri Kartsaklis, Ian Fan, Richie Yeung, Anna Pearson, Robin Lorenz, Alexis Toumi, Giovanni de Felice, Konstantinos Meichanetzidis, Stephen Clark, and Bob Coecke. “Lambeq: An Efficient High-Level Python Library for Quantum NLP”. In: *CoRR* abs/2110.04236 (2021). arXiv: **2110.04236**.
- [TK21] Alexis Toumi and Alex Koziell-Pipe. “Functorial Language Models”. In: *CoRR* abs/2103.14411 (2021). arXiv: **2103.14411**.
- [Coe+21] Bob Coecke, Giovanni de Felice, Konstantinos Meichanetzidis, and Alexis Toumi. “How to Make Qubits Speak”. In: *CoRR* abs/2107.06776 (2021). arXiv: **2107.06776**.
- [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**.

1

DisCoPy: monoidal categories in Python

Python has become the programming language of choice for most applications in both natural language processing (e.g. Stanford NLP [Man+14], NLTK [LB02] and SpaCy [HM17]) and quantum computing (with development kits like Qiskit [Cro18] and PennyLane [Ber+20] and interfaces to compilers like pytket [Siv+20]). Thus, it was the obvious choice of language for an implementation of QNLP. However, unlike functional programming languages like Haskell, Python has little support for category theory. Indeed, before the release of DisCoPy, the only existing Python framework for category theory was a module of SymPy [Meu+17] that can draw commutative diagrams in finite categories. Hence, the first step in implementing QNLP was to develop our own framework for applied category theory in Python: DisCoPy. The main feature was the drawing of string diagrams (e.g. the grammatical structure of sentences) and the application of functors (e.g. to quantum circuits, either executed on quantum hardware or classically simulated).

String diagrams have become the lingua franca of applied category theory. However, the definitions one can find in the literature usually fall into one of two extremes: either definitions by general abstract nonsense or definitions by example and appeal to intuition. On one side of the spectrum, the standard technical reference has become the *Geometry of tensor calculus* [JS91] where Joyal and Street define string diagrams as equivalence classes of labeled topological graphs embedded in the plane and then characterise them as the arrows of free monoidal

categories. On the other, *Picturing quantum processes* [CK17] contains over a thousand string diagrams but their formal definition as well as any mention of category theory are relegated to mere appendices.

This chapter contains a description of the DisCoPy package alongside an elementary list-based definition of string diagrams. The first section introduces categories and functors for the Python programmer, i.e. with no mathematical prerequisites apart from sets and monoids. The second section introduces monoidal categories for the Python programmer, defining string diagrams from first principles. The third section gives the category theoretic foundations for our definition, which we call the premonoidal approach. The fourth section defines the drawing and reading algorithms for string diagrams, which arise as the two sides of the equivalence between the premonoidal and the topological definitions. The fifth section introduces monoidal categories with extra structure (rigid, biclosed, symmetric, cartesian, hypergraph) and the inheritance mechanism which implements this hierarchy of structure. The last section discusses the relationship between our list-based premonoidal approach and the existing graph-based definitions of diagrams in symmetric monoidal categories.

1.1 Categories in Python

What are categories and how can they be useful to the Python programmer? This section will answer this question by taking the standard mathematical definitions and breaking them into *data*, which can be translated into Python code, and *axioms*, which cannot be formally verified in Python, but can be translated into test cases. The data for a category is given by a tuple $C = (C_0, C_1, \text{dom}, \text{cod}, \text{id}, \text{then})$ where:

- C_0 and C_1 are classes of *objects* and *arrows* respectively,
- $\text{dom}, \text{cod} : C_1 \rightarrow C_0$ are functions called *domain* and *codomain*,
- $\text{id} : C_0 \rightarrow C_1$ is a function called *identity*,
- $\text{then} : C_1 \times C_1 \rightarrow C_1$ is a partial function called *composition*, denoted by (\circ) .

Given two objects $x, y \in C_0$, the set¹ $C(x, y) = \{f \in C_1 \mid \text{dom}(f), \text{cod}(f) = x, y\}$ is called a *homset* and we write $f : x \rightarrow y$ whenever $f \in C(x, y)$. We denote the composition $\text{then}(f, g)$ by $f \circ g$, translated to `f >> g` in Python. The axioms for the category C are the following:

¹We will assume that this forms a set rather than a proper class, i.e. we will only work with *locally small* categories.

- $\text{id}(x) : x \rightarrow x$ for all objects $x \in C_0$,
- for all arrows $f, g \in C_1$, the composition $f \circ g$ is defined iff $\text{cod}(f) = \text{dom}(g)$, moreover we have $f \circ g : \text{dom}(f) \rightarrow \text{cod}(g)$,
- $\text{id}(\text{dom}(f)) \circ f = f = f \circ \text{id}(\text{cod}(f))$ for all arrows $f \in C_1$,
- $f \circ (g \circ h) = (f \circ g) \circ h$ whenever either side is defined for $f, g, h \in C_1$.

Note that we play with the overloaded meaning of the word *class*: we use it to mean both a mathematical collection that need not be a set, and a Python class with its methods and attributes. Reading it in the latter sense, `dom` and `cod` are *attributes* of the arrow class, `then` is a *method*, `id` is a *static method*. Thus, implementing a category in Python means nothing more than subclassing the abstract classes `Object` and `Arrow` of listing 1.1.1, and then checking that the axioms hold via some (necessarily non-exhaustive) software tests.

Listing 1.1.1. Abstract classes for categories, functors and transformations.

Note that annotations with dependent types are not supported by any Python implementation yet. Since Python could not statically check that compositions are well-typed, DisCoPy has no type hints and raises an `AxiomError` at runtime instead.

```
class Object: ...

class Arrow:
    dom: Object, cod: Object

    @staticmethod
    def id(x: Object) -> Arrow[x, x]: ...

    def then(self, other: Arrow[self.cod, y]) -> Arrow[self.dom, y]: ...

class Functor:
    @overload
    def __call__(self, x: Object) -> Object: ...

    @overload
    def __call__(self, f: Arrow[x, y]) -> Arrow[self(x), self(y)]: ...

class Transformation:
    dom: Functor, cod: Functor

    def __call__(self, x: Object) -> Arrow[self.dom(x), self.cod(x)]: ...
```

The data for a *functor* $F : C \rightarrow D$ between two categories C and D is given by a pair of overloaded functions $F : C_0 \rightarrow D_0$ and $F : C_1 \rightarrow D_1$ such that:

- $F(\text{dom}(f)) = \text{dom}(F(f))$ and $F(\text{cod}(f)) = \text{cod}(F(f))$ for all $f \in C_1$,
- $F(\text{id}(x)) = \text{id}(F(x))$ and $F(f \circ g) = F(f) \circ F(g)$ for all $x \in C_0$ and $f, g \in C_1$.

Thus, implementing a functor in Python amounts to subclassing the `Functor` class of listing 1.1.1 (and then implementing software tests to check that the axioms hold).

The data for a *transformation* $\alpha : F \rightarrow G$ between two parallel functors $F, G : C \rightarrow D$ is given by a function from objects $x \in C_0$ to components $\alpha(x) : F(x) \rightarrow G(x)$ in D . A *natural transformation* is one where $\alpha(x) \circ F(f) = G(f) \circ \alpha(y)$ for all arrows $f : x \rightarrow y$ in C . The `Transformation` class is given in listing 1.1.1, checking that a transformation is natural cannot be done formally in Python. In the same way that there is a set Y^X of functions $X \rightarrow Y$ for any two sets X and Y , for any two categories C and D there is a category D^C with functors $C \rightarrow D$ as objects and natural transformations as arrows.

Example 1.1.2. We can define the category **Pyth** with objects the class of all Python types and arrows the class of all Python functions. Domain and codomain of may be extracted from type annotations. Identity may given by `lambda *xs: xs` and the composition by `lambda f, g: lambda *xs: f(*g(*xs))`. (The star takes care of functions with multiple arguments.) However, equality of functions in Python is undecidable so there will be no way to check the axioms hold in general.

Endofunctors **Pyth** \rightarrow **Pyth** can be thought of as some kind of data containers. For example, we can define a **List** functor which sends a type `t` to `List[t]` and a function `f` to `lambda *xs: map(f, xs)`.

There is a natural transformation $\eta : \text{Id} \rightarrow \text{List}$ from the obvious identity functor, implemented by the built-in function `id`. Its components send objects `x : t` of any type `t` to the singleton list `[x] : List[t]`.

Listing 1.1.3. Implementation of the category **Pyth** with `type` as objects and `Function` as arrows.

```
@dataclass
class Function:
    dom: type
    cod: type
    inside: Callable

    @staticmethod
```

```

def id(x: type) -> Function:
    return Function(x, x, lambda *xs: xs)

def then(self, other: Function) -> Function:
    return Function(self.dom, other.cod, lambda *xs: other(*self(*xs)))

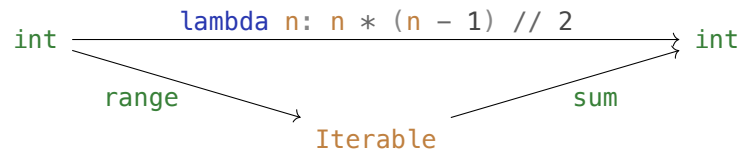
def __call__(self, *xs): return self.inside(*xs)

f = Function(int, Iterable, range)
g = Function(Iterable, int, sum)
h = Function(int, int, lambda n: n * (n - 1) // 2)
assert f.then(g)(42) == h(42) == 861

```

Example 1.1.4. When the class of objects and arrows are in fact sets, C is called a small category. For example, the category **FinSet** has the set of all finite sets as objects and the set of all functions between them as arrows. This time equality of functions between finite sets is decidable, so we can write unit tests that check that the axioms hold on specific examples.

Example 1.1.5. When the class of objects and arrow are finite sets, we can draw the category as a directed multigraphs with objects as vertices and arrows as edges, together with the list of equations between paths. A functor $F : C \rightarrow D$ from such a finite category C is called a commutative diagram in D . For example, the following commutative diagram denotes a functor $3 \rightarrow \mathbf{Pyth}$ from the finite category 3 with three objects $\{0, 1, 2\}$ and three non-identity arrow $f : 0 \rightarrow 1, g : 1 \rightarrow 2$ and $h : 0 \rightarrow 2$, with the only non-trivial composition $f \circ g = h$.



Thus, this commutative diagram is the equation $\text{sum}(\text{range}(n)) = n * (n - 1) // 2$. When the finite category is bigger than a triangle, one commutative diagram can state a large number of equations, which can be read by diagram chasing.

Example 1.1.6. The category $\mathbf{Mat}_{\mathbb{S}}$ has natural numbers as objects and $n \times m$ matrices with values in \mathbb{S} as arrows $n \rightarrow m$. The identity and composition are given by the identity matrix and matrix multiplication respectively. In order for matrix multiplication to be well-defined and for $\mathbf{Mat}_{\mathbb{S}}$ to be a category, the scalars \mathbb{S} should have at least the structure of a rig (a *riNg* without *Negatives*): a pair

of monoids $(\mathbb{S}, +, 0)$ and $(\mathbb{S}, \times, 1)$ with the first one commutative and the second a homomorphism for the first, i.e. $a \times 0 = 0 = 0 \times a$ and $(a + b) \times (c + d) = ac + ad + bc + bd$. The category $\mathbf{Mat}_{\mathbb{C}}$ is equivalent to the category of finite dimensional vector spaces and linear maps. When the scalars are Booleans with disjunction and conjunction as addition and multiplication, the category $\mathbf{Mat}_{\mathbb{B}}$ is equivalent to the category of finite sets and relations. There is a faithful functor (i.e. injective on arrows with the same domain and codomain) $\mathbf{FinSet} \rightarrow \mathbf{Mat}_{\mathbb{B}}$ which sends finite sets to their cardinality and functions to their graph.

Listing 1.1.7. Implementation of $\mathbf{Mat}_{\mathbb{B}}$ with `int` as objects and `Matrix` as arrows.

```
@dataclass
class Matrix:
    dom: int
    cod: int
    inside: list[list[bool]]

    @staticmethod
    def id(x: int) -> Matrix:
        return Matrix(x, x, [
            [i == j for i in range(x)] for j in range(x)])

    def then(self, other: Matrix) -> Matrix:
        return Matrix(self.dom, other.cod, [[
            any(self[i][j] and other[j][k] for j in range(other.dom))
            for k in range(other.cod)] for i in range(self.dom)])

    __getitem__ = lambda self, key: self.inside[key]

f = Matrix(1, 2, [[0, 1]])
g = Matrix(2, 2, [[0, 1], [1, 0]])
h = Matrix(2, 1, [[1], [0]])
assert f.then(g) == h
```

Example 1.1.8. The category **Circ** has natural numbers as objects and n -qubit quantum circuits as arrows $n \rightarrow n$. There is a functor `eval` : **Circ** \rightarrow $\mathbf{Mat}_{\mathbb{C}}$ which sends n qubits to 2^n dimensions and evaluates each circuit to its unitary matrix.

Example 1.1.9. Just about any class of mathematical structures as objects and their homomorphisms as arrows will form a category. For example, the category **Set** of sets and functions, the category **Mon** of monoids and homomorphisms, the category **Cat** of small categories and functors, etc. The faithful functor $U : \mathbf{Mon} \rightarrow$

Set which sends monoids to their underlying set and homomorphisms to functions is called a forgetful functor.

The main principles behind the implementation of DisCoPy follow from the concept of a *free object*. Let's start from a simple example. Given a set X , we can construct a monoid X^* with underlying set $\coprod_{n \in \mathbb{N}} X^n$ the set of all finite lists with elements in X . The associative multiplication is given by list concatenation $X^m \times X^n \rightarrow X^{m+n}$ and the unit is given by the empty list denoted $1 \in X^0$. Given a function $f : X \rightarrow Y$, we can construct a homomorphism $f^* : X^* \rightarrow Y^*$ defined by element-wise application of f (this is what the built-in `map` does in Python). We can easily check that $(f \circ g)^* = f^* \circ g^*$ and $(\text{id}_X)^* = \text{id}_{X^*}$. Thus, we have defined a functor $F : \mathbf{Set} \rightarrow \mathbf{Mon}$.

Why is this functor so special? Because it is the *left adjoint* to the forgetful functor $U : \mathbf{Mon} \rightarrow \mathbf{Set}$. An *adjunction* $F \dashv U$ between two functors $F : C \rightarrow D$ and $U : D \rightarrow C$ is a pair of natural transformations $\eta : \text{id}_C \rightarrow F \circ U$ and $\epsilon : U \circ F \rightarrow \text{id}_D$ called the *unit* and *counit* respectively. In the case of lists, we already mentioned the unit in example 1.1.2: it is the function that sends every object to a singleton list. For a monoid M , the counit $\epsilon(M) : F(U(M)) \rightarrow M$ is the monoid homomorphism that takes lists of elements in M and multiplies them. We can easily check that these two transformations are indeed natural, thus we get that *lists are free monoids*. This may be taken as a mathematical explanation for why lists are so ubiquitous in programming. Another equivalent definition of adjunction is in terms of an isomorphism $C(x, U(y)) \simeq D(F(x), y)$ which is natural¹ in $x \in C_0$ and $y \in D_0$. In the adjunction for lists, functions $X \rightarrow U(M)$ from a set X to the underlying set of a monoid M are in a natural one-to-one correspondance with monoid homomorphisms $X^* \rightarrow M$. To define a homomorphism from a free monoid, it is sufficient to define the image of each generating element.

Now we want to play the same game with categories instead of monoids. We can define a forgetful functor $U : \mathbf{Cat} \rightarrow \mathbf{Set}$ which sends a small category C to its set of objects C_0 , and its left adjoint $F : \mathbf{Set} \rightarrow \mathbf{Cat}$ which sends a set to the *discrete category* with its elements as objects and only identity arrows. However, this is a rather boring construction because forgetting the arrows of a categories is too much: the forgetful functor U is not faithful. Instead, we need to replace the category of sets with the category of *signatures*. The data for a signature is given by a tuple $\Sigma = (\Sigma_0, \Sigma_1, \text{dom}, \text{cod})$ where:

¹The isomorphism $C(x, U(y)) \simeq D(F(x), y)$ is natural in x if it is a natural transformation between the two functors $C(-, U(y)), D(F(-), y) : C \rightarrow \mathbf{Set}$.

- Σ_0 is a set of *generating objects*,
- Σ_1 is a set of *generating arrows*, which we will also call *boxes*,
- $\text{dom}, \text{cod} : \Sigma_1 \rightarrow \Sigma_0$ are the domain and codomain.

A morphism of signatures $f : \Sigma \rightarrow \Gamma$ is a pair of overloaded functions $f : \Sigma_0 \rightarrow \Gamma_0$ and $f : \Sigma_1 \rightarrow \Gamma_1$ such that $f \circ \text{dom} = \text{dom} \circ f$ and $f \circ \text{cod} = \text{cod} \circ f$. Thus, signatures and their morphisms form a category **Sig** and there is a faithful functor $U : \mathbf{Cat} \rightarrow \mathbf{Sig}$ which sends a category to its underlying signature: it forgets the identity and composition. Signatures may be thought of as directed multigraphs *with an attitude* [nLa]. Given a signature Σ , we can define a category $F(\Sigma)$ with vertices as objects and *paths as arrows*. More precisely, an arrow $f : x \rightarrow y$ is given by a length $n \in \mathbb{N}$ and a list $f_1, \dots, f_n \in \Sigma_1$ with $\text{dom}(f_1) = x$, $\text{cod}(f_n) = y$ and $\text{cod}(f_i) = \text{dom}(f_{i+1})$ for all $i < n$. Given a morphism of signatures $f : \Sigma \rightarrow \Gamma$, we get a functor $F(f) : F(\Sigma) \rightarrow F(\Gamma)$ relabeling boxes in Σ by boxes in Γ . Thus, we have defined a functor $F : \mathbf{Sig} \rightarrow \mathbf{Cat}$, it remains to show that it indeed forms an adjunction $F \dashv U$. This is very similar to the monoid case: the unit sends a box in a signature to the path of just itself, the counit sends a path of arrows in a category to their composition. Equivalently, we have a natural isomorphism $\mathbf{Cat}(F(\Sigma), C) \simeq \mathbf{Sig}(\Sigma, U(C))$: to define a functor $F(\Sigma) \rightarrow C$ from a free category is the same as to define a morphism of signatures $\Sigma \rightarrow U(C)$.

If lists are such fundamental data structures because they are free monoids, we argue that the arrows of free categories should be just as fundamental: they capture the basic notion of *data pipelines*. Free categories are implemented in the most basic module of DisCoPy, `discopy.cat`, which is sketched in listing 1.1.10.

Listing 1.1.10. Outline of the classes `Ob`, `Arrow` and `Box`.

```
@dataclass
class Ob:
    name: str

@dataclass
class Arrow:
    dom: Ob
    cod: Ob
    boxes: list[Arrow]

    @staticmethod
    def upgrade(old: Arrow) -> Arrow:
        return old
```



```

@staticmethod
def id(x: Ob) -> Arrow:
    return self.upgrade(Arrow(x, x, []))

def then(self, *others: Arrow) -> Arrow:
    if not others: return self
    for left, right in zip((self, ) + others, others):
        assert left.cod == right.dom
    return self.upgrade(Arrow(
        self.dom, others[-1].cod, self.bboxes + sum(
            [other.bboxes for other in others], [])))

__rshift__ = then

class Box(Arrow):
    def __init__(self, name: str, dom: Ob, cod: Ob):
        self.name = name
        super().__init__(dom, cod, [self])

    def __eq__(self, other):
        if not isinstance(other, Arrow): return False
        if isinstance(other, Box):
            return (self.name, self.dom, self.cod)\
                == (other.name, other.dom, other.cod)
        return other.bboxes == [self]

```

The classes `Ob` and `Arrow` for objects and arrows are implemented in a straightforward way, using the built-in `dataclass` decorator to avoid the bureaucracy of defining initialisation, equality, etc. The method `Arrow.then` accepts any number of arrows `others`, which will prove useful when defining functors. The `Box` class requires more attention: a box `f = Box('f', x, y)` is an arrow with the list of just itself as boxes, i.e. `f.bboxes == [f]`. In order for the axiom `f >> Id(y) == f == Id(x) >> f` to hold, we need to make sure that `f == Arrow(x, y, [f])`, i.e. a box is set to be equal to the arrow with just itself as boxes. The main subtlety in the implementation is the method `Arrow.upgrade` which for now is just the identity. When the user defines a subclass of `Arrow`, overriding the `upgrade` method allows the composition of objects in the subclass to remain within the subclass, without having to rewrite the methods for identity and composition.

Example 1.1.11. We can define `Circuit` as a subclass of `Arrow` with only the `upgrade` method overridden, and `Gate` as a subclass of `Circuit` and `Box` defined by a

name and a number of qubits. Now we can compose gates together and the result will be an instance of `Circuit` not merely of `Arrow`.

```
class Circuit(Arrow):
    def upgrade(old):
        return Circuit(old.dom, old.cod, old.bboxes)

class Gate(Circuit, Box):
    def __init__(self, name: str, n_qubits: int):
        Box.__init__(self, name, Ob(str(n_qubits)), Ob(str(n_qubits)))
        Circuit.__init__(self, self.dom, self.cod, self.bboxes)

H, Z, X = Gate("H", 1), Gate("Z", 1), Gate("X", 1)
assert isinstance(H >> Z >> X, Circuit)
```

The `Functor` class listed in 1.1.12 has two mappings `ob` and `ar` as attributes, from objects to objects and from boxes to arrows respectively. The domain of the functor is implicitly defined as the free category generated by the domain of the `ob` and `ar` mappings. The optional arguments `ob_factory` and `ar_factory` serve to define functors with arbitrary categories as codomain. At this point, their only use is for `ar_factory` to define identity arrows, otherwise the codomain of the functor is defined implicitly by the codomain of the `ob` and `ar` mappings.

Listing 1.1.12. Outline of the `Functor` class.

```
@dataclass
class Functor:
    ob: dict[Ob, Ob]
    ar: dict[Box, Arrow]
    ob_factory, ar_factory = Ob, Arrow

    def __call__(self, other):
        if isinstance(other, Ob):
            return self.ob[other]
        if isinstance(other, Box):
            return self.ar[other]
        if isinstance(other, Arrow):
            return self.ar_factory.id(self(other.dom)).then(
                *self(box) for box in other.bboxes)
        raise TypeError
```

Example 1.1.13. A typical *DisCoPy* script starts by defining objects and boxes:

```
x, y, z = map(Ob, "xyz")
f, g, h = Box('f', x, y), Box('g', y, z), Box('h', z, x)
```

We can define a simple relabeling functor from the free category to itself:

```
F = Functor(
    ob={x: y, y: z, z: x},
    ar={f: g, g: h, h: f})
assert F(f >> g >> h) == F(f) >> F(g) >> F(h) == g >> h >> f
```

We can interpret our arrows as Python functions:

```
G = Functor(
    ob={x: int, y: Iterable, z: int},
    ar={f: range, g: sum, h: lambda n: n * (n - 1) // 2},
    ob_factory=type, ar_factory=Function)
assert G(f >> g)(42) == G(h)(42) == 861
```

We can interpret our arrows as matrices:

```
H = Functor(
    ob={x: 1, y: 2, z: 2},
    ar={f: [[0, 1]], g: [[0, 1], [1, 0]], h: [[1], [0]]},
    ob_factory=int, ar_factory=Matrix)
assert H(f >> g) == H(h)
```

Provided we implement the methods `Functor.id` and `Functor.then`, we can even build functors into **Cat**, i.e. interpret arrows as functors:

```
I = Functor(
    ob={x: Arrow, y: Arrow, z: Tensor},
    ar={f: F, g: H}, ar_factory=Functor)
assert I(f >> g)(h) == H(F(h)) == H(f)
```

After free objects, another concept behind DisCoPy is that of a *quotient object*. Again, let's start with the example of a monoid M . Suppose we're given a binary relation $R \subseteq M \times M$, then we can construct a quotient monoid M/R with underlying set the equivalence classes of the smallest congruence generated by R . That is, the smallest relation $(\sim_R) \subseteq M \times M$ such that:

- $x \sim_R y$ for all $(x, y) \in R$,
- $x \sim_R x$ and if $x \sim_R y$ and $y \sim_R z$ then $x \sim_R z$,
- if $x \sim_R x'$ and $y \sim_R y'$ then $x \times y \sim_R x' \times y'$.

The first point says that $R \subseteq (\sim_R)$. The second says that (\sim_R) is an equivalence relation. The third says that (\sim_R) is closed under products, it is equivalent to the substitution axiom: if $x \sim_R y$ then $axb \sim_R ayb$ for all $a, b \in M$. Explicitly, the congruence (\sim_R) can be constructed in two steps: first, we define the rewriting

relation $(\rightarrow_R) \subseteq M \times M$ where $axb \rightarrow_R ayb$ for all $(x, y) \in R$ and $a, b \in M$. Second, we define (\sim_R) as the *symmetric, reflexive, transitive closure* of the rewriting relation, i.e. two elements $x, y \in M$ are equal in M/R iff they are in the same connected component of the undirected graph induced by $(\rightarrow_R) \subseteq M \times M$. Now there is a homomorphism $q : M \rightarrow M/R$ which sends monoid elements to their equivalence class with the following property: for any homomorphism $f : M \rightarrow N$ with $x \sim_R y$ implies $f(x) = f(y)$, there is a unique $f' : M/R \rightarrow N$ with $f = q \circ f'$. Intuitively, a homomorphism from a quotient M/R is nothing more than a homomorphism from M which respects the axioms R . Up to isomorphism, we can construct any monoid M as the quotient X^*/R of a free monoid X^* : take $X = U(M)$ and $R = \{(xy, z) \in X^* \times X^* \mid x \times y = z \in M\}$.

The pair $(X, R \subseteq X^* \times X^*)$ of a set of generating elements X and a binary relation R on its free monoid is called a *presentation* of the monoid $M \simeq X^*/R$. Arguably, the most fundamental computational problem is the *word problem for monoids*: given a presentation (X, R) and a pair of lists $x, y \in X^*$, decide whether $x = y$ in X^*/R . As mentioned in the introduction, it was shown to be equivalent to Turing's halting problem, and thus undecidable, by Post [Pos47] and Markov [Mar47]. The proof is straightforward: we can encode the tape alphabet and the states of a Turing machine in the set X and its transition table into the relation R , then whether the machine halts reduces to deciding $x = y$ for x and y the initial and accepting configurations respectively: a proof of equality corresponds precisely to a run of the Turing machine.

The case of quotient categories is similar, only we need to take care of objects now. Given a category C and a family of binary relations $\{R_{x,y} \subseteq C(x, y) \times C(x, y)\}_{x,y \in C_0}$, we can construct a quotient category C/R with equivalence classes as arrows. There is a functor $Q : C \rightarrow C/R$ sending each arrow to its equivalence class, and for any functor $F : C \rightarrow D$ with $(f, g) \in R_{x,y}$ implies $F(f) = F(g)$, there is a unique $F' : C/R \rightarrow D$ with $F = Q \circ F'$. Intuitively, a functor from a quotient category C/R is nothing more than a functor from C which respects the axioms R . Again, any small category C is isomorphic to the quotient $F(\Sigma)/R$ of a free category $F(\Sigma)$: take $\Sigma = U(C)$ and $R = \{(f \circ g, h) \in F(\Sigma) \times F(\Sigma) \mid f \circ g = h \in C\}$. The pair $(\Sigma, R \subseteq \coprod_{x,y \in \Sigma_0} \Sigma(x, y) \times \Sigma(x, y))$ is called a *presentation* of the category $C \simeq F(\Sigma)/R$. Since monoids are just categories with one object, the word problem for categories will be just as undecidable as for monoids.

What does it mean to implement a quotient category in Python? Since presentations of categories are as expressive as Turing machines, we might as well avoid

solving the halting problem and just use a Python function to define equality of arrows. Implementing a quotient category is nothing more than implementing a free category and an equality function that respects the axioms of a congruence. One straightforward way is to define equality of arrows f, g in a free category $F(\Sigma)$ to be the equality of their interpretation $\llbracket f \rrbracket = \llbracket g \rrbracket$ under a functor $\llbracket - \rrbracket : F(\Sigma) \rightarrow D$ into a concrete category D where equality is decidable. Another method is to define a *normal form* method which takes an arrow and returns the representative of its equivalence class, then identity of arrow is identity of their normal forms.

Example 1.1.14. Take the signature Σ with one object $\Sigma_0 = \{1\}$ and four arrows $\Sigma_1 = \{Z, X, H, -1\}$ for the Z , X and Hadamard gate and the global (-1) phase. Let's define the relation R induced by:

- $HX = ZH$ and $ZX = (-1)XZ$,
- $ff = 1$ and $f(-1) = (-1)f$ for all $f \in \Sigma_1$.

The quotient $F(\Sigma)/R$ is a subcategory of the category **Circ** of quantum circuits, it is isomorphic to the quotient induced by the interpretation $\llbracket - \rrbracket : F(\Sigma) \rightarrow \mathbf{Mat}_{\mathbb{C}}$. Suppose we're given a functor $\mathbf{cost} : F(\Sigma) \rightarrow \mathbb{R}^+$, we can define the normal form of a circuit f to be the representative of its equivalence class with the lowest cost. Thus, deciding equality of circuits reduces to solving circuit optimisation perfectly.

We conclude this section by discussing three extra pieces of implementation beyond the basics of category theory: dagger, sums and bubbles. A *dagger* for a category C can be thought of as a kind of time-reversal for arrows. More precisely, a dagger is a contravariant endofunctor $\dagger : C \rightarrow C^{op}$, i.e. from the category to its opposite with **dom** and **cod** swapped, which is the identity on objects and an involution, i.e. $(\dagger) \circ (\dagger) = \text{id}_C$. DisCoPy implements free \dagger -categories by adding an attribute `_dagger: bool` to boxes and a method `Arrow.dagger`, shortened to the postfix `[::-1]`, which reverses the order of boxes and negates `_dagger` elementwise. A \dagger -functor is a functor between \dagger -categories which commutes with the dagger, they are implemented by adding a case to the code for functor application to define `F(box) = F(box[::-1])[::-1]` whenever `box._dagger` is true. For example, the conjugate transpose defines a dagger on the category $\mathbf{Mat}_{\mathbb{S}}$, the adjoint defines a dagger on the category **Circ** and the evaluation $\mathbf{Circ} \rightarrow \mathbf{Mat}_{\mathbb{S}}$ is a \dagger -functor.

A category C has *sums*, or equivalently C is *monoid-enriched*, when it comes equipped with a commutative monoid $(+, 0)$ on each homset $C(x, y)$ such that $f \circ 0 = 0 = 0 \circ f$ and $(f + f') \circ (g + g') = f \circ g + f \circ g' + f' \circ g + f' \circ g'$ for all arrows f, g, f', g' .

A functor $F : C \rightarrow D$ between categories with sums is monoid-enriched when $F(0) = 0$ and $F(f + g) = F(f) + F(g)$. For example, the category $\mathbf{Mat}_{\mathbb{S}}$ has sums given by elementwise addition of matrices. In DisCoPy, free categories with sums are implemented by `Sum`, a subclass of `Box` with an attribute `terms: list[Arrow]`. The method `then` is straightforward: the composition of a sum is the sum of the compositions of its terms. Defining equality requires some extra care however: we want an arrow to be equal to the sum of just itself, we also want two sums to be equal when their list of terms are permutations of each other. DisCoPy functors are monoid-enriched, i.e. formal sum of arrows can be interpreted as a concrete sum of matrices.

By a *bubble* we mean an operator which takes an arrow in a category C and puts it into a box. More formally, a bubble is a pair of functions $b_{\text{dom}}, b_{\text{cod}} : C_0 \rightarrow C_0$ between objects and a unary operator between homsets $b : C(x, y) \rightarrow C(b_{\text{dom}}(x), b_{\text{cod}}(y))$ for each pair of objects $x, y \in C_0$. DisCoPy implements the free category with bubbles via a `Bubble` class initialised by `dom, cod: Ob` and an attribute `inside: Arrow`. DisCoPy functors automatically respect bubbles, i.e. we have that $F(b(f)) = b(F(f))$ for all arrows f . Thus, we can interpret arrows with bubbles as arbitrary operations on the codomain of our interpretation functors. For example, we can define a negation bubble on the category $\mathbf{Mat}_{\mathbb{B}}$ of Boolean matrices: it is the identity on objects and sends each matrix f to its entrywise negation \bar{f} . The resulting syntax with bubbles is strictly more expressive than that of free categories alone: negation cannot be expressed as a composition, there is no matrix n in $\mathbf{Mat}_{\mathbb{B}}$ such that $f \circ n = \bar{f}$ for all matrices f . As we will discuss in Chapter 3, differentiation of parameterised matrices cannot be expressed as a composition either, but it is a unary operator between homsets, i.e. a bubble.

1.2 String diagrams in Python

In the previous section, we introduced the idea of arrows in free categories as formal data pipelines and functor application as their evaluation in concrete categories such as `Pyth`, `Mat` or `Circ` where the computation happens. For now, our pipelines are rather basic because they are linear: we cannot express functions of multiple arguments, nor tensors of order higher than 2, nor circuits with multiple qubits in any explicit way. In this section, we move from the one-dimensional syntax of arrows in free categories to the two-dimensional syntax of *string diagrams*,

the arrows of free *monoidal categories*. The data for a (strict¹) monoidal category C is that of a category together with: an object $1 \in C_0$ called the *unit* and a pair of overloaded binary operations called the *tensor* on objects $\otimes : C_0 \times C_0 \rightarrow C_0$ and on arrows $\otimes : C_1 \times C_1 \rightarrow C_1$, translated to `@` in Python. The axioms for monoidal categories are the following:

- $(C_0, \otimes, 1)$ and $(C_1, \otimes, \text{id}(1))$ are monoids,
- the tensor defines a functor $\otimes : C \times C \rightarrow C$, i.e. the following *interchange law* $(f \circ g') \otimes (g \circ f') = (f \otimes g) \circ (f' \otimes g')$ holds for all arrows $f, f', g, g' \in C_1$.

We will use the following terminology: an arrow $f : 1 \rightarrow x$ from the unit is called a *state* of the object x , an arrow $f : x \rightarrow 1$ into the unit is called an *effect* of x and an arrow $a : 1 \rightarrow 1$ from the unit to itself is called a *scalar*. The interchange law implies that the scalars form a commutative monoid, by the following Eckmann-Hilton argument:

$$a \circ b = 1 \otimes a \circ b \otimes 1 = (1 \circ b) \otimes (a \otimes 1) = b \otimes a \quad (1.1)$$

$$= (b \circ 1) \otimes (1 \circ a) = b \otimes 1 \circ 1 \otimes a = b \circ a \quad (1.2)$$

A functor $F : C \rightarrow D$ between monoidal categories C and D is (strict²) monoidal whenever it is also a monoid homomorphism on objects and arrows. Thus, monoidal categories themselves form a category **MonCat** with monoidal functors as arrows. A transformation $\alpha : F \rightarrow G$ between two monoidal functors $F, G : C \rightarrow D$ is monoidal itself when $\alpha(x \otimes y) = \alpha(x) \otimes \alpha(y)$ for all objects $x, y \in C$.

Example 1.2.1. The category **Pyth** is monoidal with unit `()` and `tuple[t1, t2]` as the tensor of types `t1` and `t2`. Given two functions `f` and `g`, we can define their tensor `f @ g = lambda x, y: f(x), g(y)`.

There are two caveats however. First, **Pyth** is not strict monoidal: `(x, (y, z))` is not strictly equal to `((x, y), z)` but only naturally isomorphic, similarly for `(((), x) != x != (x, ()))`. These natural isomorphisms are subject to coherence conditions which make sure that all the ways to rebracket `((x, y), z), w` into `(x, (y, (z, w)))` are the same. In practice, this bureaucracy of parenthesis does not pose any problem: MacLane's coherence theorem [Mac71, p. VII] makes sure

¹We will assume that our monoidal categories are strict, i.e. the axioms for monoids are equalities rather than natural isomorphisms subject to coherence conditions.

²We will assume that our monoidal functors are strict, i.e. $F(x \otimes y) = F(x) \otimes F(y)$ and $F(1) = 1$ are equalities rather than natural transformations.

that every monoidal category is monoidally equivalent¹ to a strict one. In the case of **Pyth**, there is an equivalent monoidal structure with flattened tuples instead: $(t1 @ t2) @ t3 = t1 @ (t2 @ t3) = \text{tuple}[t1, t2, t3]$.

Second, the interchange law only holds for the subcategory of **Pyth** with pure functions as arrows. Indeed, if the functions **f** and **g** are impure (e.g. they call **random** or **print**) then their tensor **f @ g** will depend on the order in which they are evaluated, i.e. $f @ \text{Id} \gg \text{Id} @ g \neq \text{Id} @ g \gg f @ \text{Id}$. As we will discuss in the next section, **Pyth** is in fact a premonoidal category. The states, i.e. the functions $f : () \rightarrow t$, can be identified with their value $f() : t$. There is only one pure effect, i.e. a unique pure function $f : t \rightarrow ()$ called discarding, and thus a unique pure scalar. If we take all impure functions into account, the scalars form a non-commutative monoid of side-effects.

Example 1.2.2. With some effort, we can also make **Pyth** monoidal with the tagged union as tensor on objects and **typing.NoReturn** as unit. Given two types **t1**, **t2**, their tagged union $t1 + t2$ is the union of the types $\text{tuple}[\text{True}, t1]$ and $\text{tuple}[\text{False}, t2]$ ², i.e. a term $(b, x) : t1 + t2$ is a pair of a Boolean **b**: **bool** and a term $x : t1$ if **b** else $x : t2$. Given two functions **f**, **g** we can define their tensor $f + g = \text{lambda } b, x : (b, f(x) \text{ if } b \text{ else } g(x))$.

Example 1.2.3. Every monoid *M* can also be seen as a discrete monoidal category, i.e. with only identity arrows.

Example 1.2.4. The category **FinSet** is monoidal with the singleton 1 as unit and Cartesian product as tensor. Again, this is not a strict monoidal category but it is equivalent to one: take the category with natural numbers $m, n \in \mathbb{N}$ as objects and functions $[m] \rightarrow [n]$ as arrows for $[n] = \{0, 1, \dots, n-1\}$. The states can be identified with elements and discarding is the only effect. **FinSet** is also monoidal with the empty set 0 as unit and disjoint union as tensor.

Example 1.2.5. The category $\mathbf{Mat}_{\mathbb{S}}$ is monoidal with addition of natural numbers as tensor on objects and the direct sum $f \oplus g = \begin{pmatrix} f & 0 \\ 0 & g \end{pmatrix}$ as tensor on arrows. When the rig \mathbb{S} is commutative, $\mathbf{Mat}_{\mathbb{S}}$ is also monoidal with multiplication of natural numbers as tensor on objects and the Kronecker product as tensor on arrows. The inclusion functor $\mathbf{FinSet} \rightarrow \mathbf{Mat}_{\mathbb{B}}$ is monoidal in two ways: it sends disjoint unions to direct sums and Cartesian products to Kronecker products.

¹An equivalence of categories is an adjunction where the unit and counit are in fact natural isomorphisms. It is a monoidal equivalence when they are also monoidal transformations.

²What we really mean is $\text{tuple}[\text{Literal}[\text{True}], t1] \mid \text{tuple}[\text{Literal}[\text{False}], t2]$.

Example 1.2.6. *The category **Circ** is monoidal with addition of natural numbers as tensor on objects and parallel composition of circuits as tensor on arrows. The evaluation functor $\text{eval} : \mathbf{Circ} \rightarrow \mathbf{Mat}_{\mathbb{C}}$ is monoidal: it sends the parallel composition of circuits to the Kronecker product of their unitary matrices.*

Now, what does it mean to implement a monoidal category in Python? Again, nothing more than defining a pair of classes for objects and arrows with a **tensor** method that satisfies the axioms. Less trivially, we want to implement the arrows of *free monoidal categories* which can then be interpreted in arbitrary monoidal categories via the application of monoidal functors: this is the content of the **discopy.monoidal** module. As in the case of free categories, free monoidal categories will be the image of a functor $F : \mathbf{MonSig} \rightarrow \mathbf{MonCat}$, the left adjoint to the forgetful functor $U : \mathbf{MonCat} \rightarrow \mathbf{MonSig}$ from monoidal categories to *monoidal signatures*. A monoidal signature Σ is a monoidal category without identity, composition or tensor: a pair of sets Σ_0, Σ_1 and a pair of functions $\text{dom}, \text{cod} : \Sigma_1 \rightarrow \Sigma_0^*$ from boxes to lists of objects. A morphism of monoidal signatures $f : \Sigma \rightarrow \Gamma$ is a pair of functions $f : \Sigma_0 \rightarrow \Gamma_0$ and $f : \Sigma_1 \rightarrow \Gamma_1$ with $f \circ \text{dom} = \text{dom} \circ f^*$ and $f \circ \text{cod} = \text{cod} \circ f^*$. Thus, we have defined the category **MonSig** of monoidal signatures and their morphisms. In order to define the forgetful functor $U : \mathbf{MonCat} \rightarrow \mathbf{MonSig}$, we will need the following technical lemma.

Definition 1.2.7. *A monoidal category C is foo (free on objects) when its monoid of objects $(C_0, \otimes, 1)$ is a free monoid $C_0 = X^*$ generated by some set of objects X .*

Lemma 1.2.8. *Every monoidal category is monoidally equivalent to a foo one.*

Proof. Given a monoidal category C , we construct C' with objects C_0^* the free monoid over the objects of C and $C'(x, y) = C(\epsilon_{C_0^*}(x), \epsilon_{C_0^*}(y))$ for $\epsilon_{C_0} : C_0^* \rightarrow C_0$ the counit of the list adjunction. That is, an arrow $f : x \rightarrow y$ between two lists $x, y \in C_0^*$ in C' is an arrow $f : \epsilon_{C_0}(x) \rightarrow \epsilon_{C_0}(y)$ between their multiplication in C . From left to right, the monoidal equivalence $C \simeq C'$ sends every object $x \in C_0$ to its singleton list $x \in C_0^*$ and every arrow to itself, from right to left it sends every list to its multiplication and every arrow to itself. \square

This means we can take the data for a monoidal category C to be the following:

- a class C_0 of *generating objects* and a class C_1 of arrows,
- domain and codomain functions $\text{dom}, \text{cod} : C_1 \rightarrow C_0^*$,
- a function $\text{id} : C_0^* \rightarrow C_1$ and a (partial) operation $\text{then} : C_1 \times C_1 \rightarrow C_1$,

- an operation on arrows $\mathbf{tensor} : C_1 \times C_1 \rightarrow C_1$ with $\mathbf{dom}(f \otimes g) = \mathbf{dom}(f)\mathbf{dom}(g)$ and $\mathbf{cod}(f \otimes g) = \mathbf{cod}(f)\mathbf{cod}(g)$.

The axioms for the objects to be a monoid now come for free, we only need to require that tensor on arrows is a monoid with the interchange law. With this definition of (free-on-objects) monoidal category, we can define the forgetful functor $U : \mathbf{MonCat} \rightarrow \mathbf{MonSig}$: it forgets the identity, composition and tensor on arrows, but not the tensor on objects which is free.

Example 1.2.9. Take a monoid M seen as a discrete monoidal category, we get an equivalent monoidal category M' with objects the free monoid M^* and an isomorphism $x_1 \dots x_n \rightarrow y_1 \dots y_m$ whenever $x_1 \times \dots \times x_n = y_1 \times \dots \times y_m$ in M .

Example 1.2.10. In the cases of monoidal categories where the objects are the natural numbers with addition as tensor, such as \mathbf{FinSet} with disjoint union, $\mathbf{Mat}_{\mathbb{S}}$ with direct sum or \mathbf{Circ} , the monoid of objects is already free: $(\mathbb{N}, +, 0)$ is the free monoid generated by the singleton set. These monoidal categories are also called PROs (for PROduct categories). When the objects are generated by a more-than-one-element set they are called coloured PROs, but a coloured PRO is precisely a foo monoidal category.

Example 1.2.11. In the case of $\mathbf{Mat}_{\mathbb{S}}$ with Kronecker product as tensor, we can define an equivalent category $\mathbf{Tensor}_{\mathbb{S}}$ where the objects are lists of natural numbers and the arrows $f : x_1 \dots x_n \rightarrow y_1 \dots y_m$ are $(x_1 \times \dots \times x_n) \times (y_1 \times \dots \times y_m)$ matrices, i.e. tensors of order $m+n$. Note that we could define yet another equivalent category where the objects are lists of prime numbers instead.

Now how do we go on constructing the left adjoint $F : \mathbf{MonSig} \rightarrow \mathbf{MonCat}$? In the same way that lists in the free monoid X^* can be defined as equivalence classes of expressions built from generators in X , product and unit, we can construct the arrows of the free monoidal category $F(\Sigma)$ as equivalence classes of expressions built from boxes in Σ_1 , identity, composition and tensor. In order to find good representatives for these equivalence classes, we will need the following technical lemma.

Definition 1.2.12. Given a monoidal signature Σ , we define a signature of layers $L(\Sigma)$ with Σ_0^* as objects and triples $(x, f, y) \in \Sigma_0^* \times \Sigma_1 \times \Sigma_0^*$ as boxes with $\mathbf{dom}(x, f, y) = x\mathbf{dom}(f)y$ and $\mathbf{cod}(x, f, y) = x\mathbf{cod}(f)y$. Given a morphism of monoidal signatures $f : \Sigma \rightarrow \Gamma$, we get a morphism between their signatures of layers $L(f) : L(\Sigma) \rightarrow L(\Gamma)$. Thus, we have defined a functor $L : \mathbf{MonSig} \rightarrow \mathbf{Sig}$.

Lemma 1.2.13. *Fix a monoidal signature Σ . Every well-typed expression built from boxes in Σ_1 , identity of objects in Σ_0^* , composition and tensor is equal to:*

$$\text{id}(x) \text{ for } x \in \Sigma_0^* \quad \text{or} \quad \text{id}(x_1) \otimes f_1 \otimes \text{id}(y_1) \circ \dots \circ \text{id}(x_n) \otimes f_n \otimes \text{id}(y_n)$$

for some list of layers $(x_1, f_1, y_1), \dots, (x_n, f_n, y_n) \in L(\Sigma)$.

Proof. By induction on the structure of well-typed expressions. The only non-trivial case is for the tensor $f \otimes g$ of two expressions $f : x \rightarrow y$ and $g : z \rightarrow w$, where we need to apply the interchange law to push the tensor through the composition $f \otimes g = (f \circ \text{id}(y)) \otimes (\text{id}(z) \circ g) = f \otimes \text{id}(z) \circ \text{id}(y) \otimes g$. \square

We now have all the ingredients to define the free monoidal category $F(\Sigma)$: it is a quotient $F(L(\Sigma))/R$ of the free category generated by the signature of layers $L(\Sigma)$. Its objects, which we call *types*, are lists in the free monoid Σ_0^* . Its arrows, which we call *diagrams*, are paths with lists in Σ_0^* as vertices and layers $(x, f : s \rightarrow t, y) \in L(\Sigma)$ as edges $xsy \rightarrow xty$. The equality of diagrams is the smallest congruence generated by the *right interchanger*:

$$(axb, g, c) \circ (a, f, bwc) \rightarrow_R (a, f, bzc) \circ (ayb, g, c)$$

for all types $a, b, c \in \Sigma_0^*$ and boxes $f : x \rightarrow y$ and $g : z \rightarrow w$. That is, we can interchange two consecutive layers whenever the output of the first box is not connected to the input of the second, i.e. there is an identity arrow $\text{id}(b)$ separating them. Note that for an effect $f : x \rightarrow 1$ followed by a state $g : 1 \rightarrow y$, we have two options: we can apply the right interchanger $(1, f, 1) \circ (1, g, 1) \rightarrow_R (1, g, x) \circ (y, f, 1)$ or its opposite $(1, f, 1) \circ (1, g, 1) \leftarrow_R (x, g, 1) \circ (1, f, y)$. Delpeuch and Vicary [DV18] give a quadratic solution to the word problem for monoidal categories, i.e. deciding when two diagrams are equal.

Theorem 1.2.14 ([DV18]). *The equality of diagrams is decidable in linear time in the connected case, and quadratic in the general case. For connected diagrams, i.e. when the Eckmann-Hilton argument does not apply, the right interchanger is confluent and it reaches a normal form in a cubic number of steps.*

Now that we have defined the equality of diagrams, there remains to define the tensor operation. First, we define the *whiskering* $f \otimes z$ of a diagram f by an object $z \in \Sigma_0^*$ on the right: we tensor z to the right-hand side of each layer (x_i, f_i, y_i) , i.e. $f \otimes z = (x_1, f_1, y_1 z) \circ \dots \circ (x_n, f_n, y_n z)$ and symmetrically for the whiskering $z \otimes f$

on the left. Now we can define the tensor $f \otimes g$ of two diagrams $f : x \rightarrow y$ and $g : z \rightarrow w$ in terms of whiskering $f \otimes g = f \otimes z \circ y \otimes g$. Note that we could have chosen to define $f \otimes g = x \otimes g \circ f \otimes w$, the two definitions are related by the interchanger.

We can check that we have indeed defined a monoidal category $F(\Sigma)$. Given a morphism of monoidal signatures $f : \Sigma \rightarrow \Gamma$, we get a monoidal functor $F(f) : F(\Sigma) \rightarrow F(\Gamma)$ by relabeling: we have defined a functor $F : \mathbf{MonSig} \rightarrow \mathbf{MonCat}$. We now have to show that it is indeed the left adjoint of $U : \mathbf{MonCat} \rightarrow \mathbf{MonSig}$. This is very similar to the monoid case. The unit $\eta_\Sigma : \Sigma \rightarrow U(F(\Sigma))$ sends objects to themselves and boxes $f : x \rightarrow y \in \Sigma$ to diagrams $(1, f, 1) \in L(\Sigma)$, i.e. the layer with empty lists on both sides of f . The counit $\epsilon_C : F(U(C)) \rightarrow C$ is the functor which sends diagrams with boxes in C to their evaluation, i.e. the formal composition and tensor of diagrams in $F(U(C))$ is sent to the concrete composition and tensor of arrows in C .

Listing 1.2.15. Outline of the class `monoidal.Ty`.

```
class Ty(Ob):
    def __init__(self, *objects: Ob | str):
        self.objects = [x if isinstance(x, Ob) else Ob(x) for x in objects]
        super().__init__(name="Ty({})".format(
            ', '.join([x.name for x in self.objects])))

    @staticmethod
    def upgrade(old: Ob) -> Ty:
        return old if isinstance(old, Ty) else Ty(old)

    def tensor(self, *others: Ty) -> Ty:
        if any(not isinstance(other, Ty) for other in others):
            return NotImplemented # This allows whiskering on the left.
        return self.upgrade(Ty(*self.objects + sum(
            [other.objects for other in others], [])))

    __matmul__ = tensor
```

The implementation of the class `Ty` for types (i.e. lists of objects) is straightforward, it is sketched in listing 1.2.15. The only subtlety is in the static method `upgrade` which allows the user to subclass `Ty` in a way that the tensor of subclassed objects stays within the subclass, without having to override the `tensor` method.

Example 1.2.16. We can define a `Qubits` subclass and be sure that the tensor of qubits is still an instance of `Qubits`, not merely `Ty`.

```

class Qubits(Ty):
    def __init__(self, n: int):
        super().__init__(self, n * [Ob("qubit")])

    def upgrade(old):
        return Qubits(len(old.bboxes))

qubit = Qubits(1)
assert qubit @ qubit == Qubits(2) and isinstance(qubit @ qubit, Qubits)

```

The implementation of `Layer` as a subclass of `cat.Box` is sketched in listing 1.2.17. It has methods `__matmul__` and `__rmatmul__` for whiskering on the right and left respectively, and `upgrade` for turning boxes into layers with units on both sides.

Listing 1.2.17. Outline of the class `monoidal.Layer`.

```

class Layer(cat.Box):
    def __init__(self, left: Ty, box: cat.Box, right: Ty):
        self.left, self.box, self.right = left, box, right
        name = "Layer({}, {}, {})".format(left, box, right)
        dom, cod = left @ box.dom @ right, left @ box.cod @ right
        super().__init__(name, dom, cod)

    def __matmul__(self, other: Ty) -> Layer:
        return Layer(self.left, self.box, self.right @ other)

    def __rmatmul__(self, other: Ty) -> Layer:
        return Layer(other @ self.left, self.box, self.right)

    @staticmethod
    def upgrade(old: cat.Box) -> Layer:
        return old if isinstance(old, Layer) else Layer(Ty(), old, Ty())

```

Now we have all the ingredients to define `Diagram` as a subclass of `Arrow` with instances of `Layer` as boxes. The `tensor` method is defined in terms of left and right whiskering. The `interchange` method takes an integer `i < len(self.layers)` and returns the diagram with layers `i` and `i + 1` interchanged, or raises an `AxiomError` if their boxes are connected. It also takes an optional argument `left: bool` which allows to choose between left and right interchangers. The `normal_form` method applies `interchange` until it reaches a normal form, or raises `NotImplementedError` if the diagram is disconnected. The `draw` method renders the diagram as an image, it implements the drawing algorithm discussed in the next section.

Listing 1.2.18. Outline of the class `monoidal.Diagram`.

```

class Diagram(cat.Arrow):
    def __init__(self, dom: Ty, cod: Ty, layers: list[Layer]):
        self.layers = layers
        super().__init__(dom, cod, boxes=layers)

    def tensor(self, other: Diagram) -> Diagram:
        dom, cod = self.dom @ other.dom, self.cod @ other.cod
        layers = [layer @ other.dom for layer in self.layers]
        layers += [self.cod @ layer for layer in other.layers]
        return self.upgrade(Diagram(dom, cod, layers))

    __matmul__ = tensor

    def interchange(self, i: int, left=False) -> Diagram: ...

    def normal_form(self, left=False) -> Diagram: ...

    def draw(self, **params): ...

    @staticmethod
    def upgrade(old: cat.Arrow) -> Diagram:
        if isinstance(old, Diagram): return old
        layers = list(map(Layer.update, old.boxes))
        dom, cod = map(Ty.upgrade, (old.dom, old.cod))
        return Diagram(dom, cod, layers)

    @staticmethod
    def subclass(ar_factory):
        def upgrade(old: cat.Arrow) -> ar_factory:
            if not isinstance(old, Diagram): old = Diagram.upgrade(old)
            return ar_factory(old.dom, old.cod, old.layers)
        ar_factory.upgrade = staticmethod(upgrade)
        return ar_factory

```

Again, we have an `upgrade` method which takes an old `cat.Arrow` and turns it into a new object of type `Diagram`. This means we do not need to repeat the code for identity or composition which is already implemented by `cat.Arrow`. The `subclass` method adds an appropriate `upgrade` method to `ar_factory`, a given subclass of `Diagram`. When the user defines a subclass of `Diagram`, they only need to use the decorator `@Diagram.subclass` without having to repeat the code for identity, composition or tensor.

Example 1.2.19. We can define `Circuit` as a subclass of `Diagram` with only the `upgrade` method overridden, and `Gate` as a subclass of `Circuit` and `Box`. Now we can compose and tensor gates together and the result will be an instance of `Circuit`.

```
@Diagram.subclass
class Circuit(Diagram): ...

class Gate(Circuit, Box):
    def __init__(self, name: str, n_qubits: int):
        Box.__init__(self, name, Qubits(n_qubits), Qubits(n_qubits))
        Circuit.__init__(self, self.dom, self.cod, self.layers)

H, CX, Id = Gate("H", 1), Gate("CX", 2), Circuit.id(Qubits(1))
assert isinstance(H @ Id >> CX, Circuit)
```

The implementation of `monoidal.Box` as a subclass of `Diagram` and `cat.Box` is relatively straightforward, we only need to make sure that a box is equal to the diagram of just itself.

Listing 1.2.20. Outline of the class `monoidal.Box`.

```
class Box(Diagram, cat.Box):
    def __init__(self, name: str, dom: Ty, cod: Ty):
        cat.Box.__init__(self, name, dom, cod)
        Diagram.__init__(self, dom, cod, [Layer.upgrade(self)])

    def __eq__(self, other):
        if not isinstance(other, Diagram): return False
        if isinstance(other, Box):
            return cat.Box.__eq__(self, other)
        return other.layers == [Layer.upgrade(self)]
```

The `monoidal.Functor` class is a subclass of `cat.Functor`. It overrides the `__call__` method to define the image of types and layers, and it delegates to its superclass for the image of objects, boxes and composition.

Listing 1.2.21. Outline of the class `monoidal.Functor`.

```
class Functor(cat.Functor):
    def __call__(self, other):
        if isinstance(other, Ty):
            return self.ob_factory.tensor(
                *[self(x) for x in other.objects])
        if isinstance(other, Layer):
            left, box, right = other
            return self(left) @ self(box) @ self(right)
        return super().__call__(other)
```

1.3 The premonoidal approach

1.4 Drawing and reading

1.5 Adding extra structure

1.6 Related & future work

2

Quantum natural language processing

3

Diagrammatic differentiation

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