

Category Theory for Quantum Natural Language Processing



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Abstract

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

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Introduction

What are quantum computers good for?

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

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]. Word meanings are first encoded in a machine-readable format, then the machine

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]. Frege [Fre84] did state what is 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.

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 GOF AI

with deep learning.

DisCo models have their roots in neuropsychology rather than AI. Indeed, they first appeared as models of the brain rather than architectures of learning machines. In their seminal work [MP43], McCulloch and Pitts give the first formal definition of neural networks and show how their “all-or-nothing” 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 the meaning of sentences as quantum processes comes with a price: they can be

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

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 symbolic (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 and *topological quantum field theories* (TQFTs). Intuitively, there is an analogy

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].

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 explanation [Ryl37] for how Aristotle arrived at such a list is that it comes from

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.

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 Ph.D. thesis [Law63] on *functorial semantics* set up a framework for model the-

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].

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

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

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

a century beforehand, Lambek [Lam58; Lam59; Lam61] had started to unravel the analogy between the derivations in categorial grammars and proof trees in mathematical logic. He then extended this analogy in *Categorial and categorial grammar* [Lam88] where he showed that these grammatical derivations are in fact arrows in *closed monoidal categories* and proposed to cast Montague semantics as a topos-valued functor. Later, he argued not “that categories should play a role in linguistics, but rather that they already do” [Lam99a]. Indeed, Hotz [Hot66] had already proved that Chomsky’s generative grammars were *free monoidal categories*, although his original German article was never translated to English and remains confidential. The idea of using functors as semantics had appeared implicitly in Knuth [Knu68] in the context-free case and was made explicit by Benson [Ben70] for unrestricted grammars. From this categorial 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*¹, 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 categorial structures (symmetric, compact closed, etc.) correspond to a hierarchy of graphical gadgets (swaps, wire bending, etc.). In *Picturing Quantum Processes* [CK17], Coecke and Kissinger introduce quantum theory with over a thousand diagrams. And the list of applications keeps growing: electronics [BF15] and chemistry [BP17], control theory [BE14] and concurrency [BSZ14], databases [BSS18] and knowledge representation [Pat17], Bayesian inference [CS12; CJ19] and causality [KU19], cognition [Bol+17] and game theory [Gha+18], functional programming [Ril18] and machine learning [FST17].

¹String 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].

If they are a great tool for writing scientific papers, string diagrams can also be a powerful data structure for developing software applications: `quantomatic` [KZ15] and its successor `PyZX` [Kv19] perform automatic rewriting of diagrams in the ZX calculus, `globular` [BKV18] and its successor `homotopy.io` [RV19] are proof assistants for higher category theory, `cartographer` [SWZ19] and `catlab` [PSV21] implement diagrams in symmetric monoidal categories, which are also implicit in the circuit data structure of the `t|ket>` compiler [Siv+20]. String diagrams are the main data structure of our QNLP algorithms: we 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.

- [Bor+19] Emanuela Boros, Alexis Toumi, Erwan Rouchet, Bastien Abadie, Dominique Stutzmann, and Christopher Kermorvant. “Automatic Page Classification in a Large Collection of Manuscripts Based on the International Image Interoperability Framework”. In: *International Conference on Document Analysis and Recognition*. 2019. DOI: **10.1109/ICDAR.2019.00126**.

- [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](https://doi.org/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](https://doi.org/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](https://arxiv.org/abs/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](https://arxiv.org/abs/2110.04236).
- [TK21] Alexis Toumi and Alex Koziell-Pipe. “Functorial Language Models”. In: *CoRR* abs/2103.14411 (2021). arXiv: [2103.14411](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/2110.10641).

1

DisCoPy: Python for the applied category theorist

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

1.1.1 Abstract categories

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` or `g << f` in Python. The axioms for the category C are the following:

- $\text{id}(x) : x \rightarrow x$ 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.

```
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:
    dom = cod = Object, Arrow

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

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

```

@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)]: ...

```

Note that annotations with dependent types are not supported by any Python implementation yet. We include them to make the thesis clearer although they do not appear in the DisCoPy code.

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 $\alpha(x) \circ G(f) = F(f) \circ \alpha(y)$ 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. *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 1.1.3. *When the class of objects and arrow are finite sets, we can draw the category as a directed multigraph with objects as nodes 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 . One commutative diagram can state a large number of equations, which can be read by diagram chasing.*

Example 1.1.4. A monoid is the same as a category with one object, i.e. every arrow (element) can be composed with (multiplied by) every other. A preorder, i.e. a set with a reflexive transitive relation, is the same as a category with at most one arrow $x \leq y$ between any two objects x and y . Functors between monoids are the same as homomorphisms, functors between preorders are monotone functions.

Example 1.1.5. Just about any class of mathematical structures will be the objects of a category with the transformations between them as arrows: the category **Set** of sets and functions, the category **Mon** of monoids and homomorphisms, the category **Preord** of preorders and monotone functions, the category **Cat** of small categories and functors, etc. There are embedding (i.e. injective on objects and arrows) functors from **Mon** and **Preord** to **Cat**, i.e. preorders and monoids form a subcategory of **Cat**. There is a functor from **Cat** to **Preord** called the preorder collapse which sends a category C to the preorder given by $x \leq y$ iff there is an arrow $f \in C(x, y)$, i.e. we forget the difference between parallel arrows. There is a faithful (i.e. injective on homsets) functor $U : \mathbf{Mon} \rightarrow \mathbf{Set}$ called the forgetful functor which sends monoids to their underlying set and homomorphisms to functions.

1.1.2 Concrete categories

Example 1.1.6. 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 $\mathbf{Pyth} \rightarrow \mathbf{Pyth}$ 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 $\eta : \mathbf{Id} \rightarrow \mathbf{List}$ 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 1.1.7. Implementation of the category **Pyth** with `type` as objects and `Function` as arrows.

```
@dataclass
class Function:
    inside: Callable
```

```

dom: type
cod: type

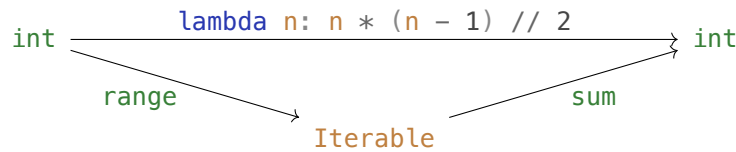
@staticmethod
def id(x: type) -> Function:
    return Function(lambda *xs: xs, x, x)

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

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

```

Example 1.1.8. 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 $f \circ g = h$.



It is read as the equation $\text{sum}(\text{range}(n)) = n * (n - 1) // 2$.

Example 1.1.9. 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 $\mathbf{FinSet} \rightarrow \mathbf{Mat}_{\mathbb{B}}$ which sends finite sets to their cardinality and functions to their graph.

Listing 1.1.10. Implementation of the Boolean rig \mathbb{B} .

```

class B:
    def __init__(self, inside: bool): self.inside = bool(inside)

```

```

__add__ = __radd__ = lambda self, other: B(self.inside or other)
__mul__ = __rmul__ = lambda self, other: B(self.inside and other)
__bool__ = lambda self: self.inside
__eq__ = lambda self, other: bool(self) == bool(other)
__repr__ = __str__ = lambda self: repr(int(self.inside))

```

`B` is like the built-in `bool` but with addition and multiplication defined as disjunction and conjunction.

Listing 1.1.11. Implementation of `MatS` with `int` as objects and `Matrix[dtype]` as arrows.

```

class Matrix:
    @classmethod
    def __class_getitem__(cls, dtype):
        class C(cls): pass
        C.dtype, C.__name__ = dtype, "Matrix[{}]" .format(dtype.__name__)
        return C

    def __init__(self, inside: list[list[dtype]], dom: int, cod: int):
        self.dom, self.cod, self.inside = dom, cod, [
            list(map(self.dtype, row)) for row in inside]

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

    def then(self, other: Matrix) -> Matrix:
        inside = [
            sum([self[i][j] * other[j][k] for j in range(other.dom)])
            for k in range(other.cod)] for i in range(self.dom)]
        return type(self)(inside, self.dom, other.cod)

    __eq__ = lambda self, other: isinstance(other, Matrix) and (
        self.inside, self.dom, self.cod) == (other.inside, other.dom, other.cod)
    __repr__ = lambda self: "Matrix[{}]({},{}, {})" .format(
        self.dtype.__name__, self.inside, self.dom, self.cod)
    __getitem__ = lambda self, key: self.inside[key]

```

Subscriptable types such as `list[list[int]]` and the `__class_getitem__` method are a new feature of Python ≥ 3.10 . By default, we fix `Matrix = Matrix[B]`, we can get real or complex matrices with `Matrix[float]` or `Matrix[complex]`. Note that this implementation is not meant to be efficient, rather it helps in making the thesis self-contained.

Example 1.1.12. The category **Circ** has natural numbers as objects and n -qubit quantum circuits as arrows $n \rightarrow n$. There is a functor $\text{eval} : \mathbf{Circ} \rightarrow \mathbf{Mat}_{\mathbb{C}}$ which sends n qubits to 2^n dimensions and evaluates each circuit to its unitary matrix.

1.1.3 Free categories

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 1.1.6: 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 correspondence 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

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 $C(-, U(y)), D(F(-), y) : C \rightarrow \mathbf{Set}$.

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:

- 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 nodes 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 1.1.13.

Listing 1.1.13. Implementation of the free category $F(\Sigma)$ with $\Sigma_0 = \mathbf{Ob}$ and $\Sigma_1 = \mathbf{Box}$.

```
@dataclass
class Ob:
    name: str
    __str__ = lambda self: self.name

@dataclass
class Arrow:
```

```

dom: Ob
cod: Ob
boxes: list[Arrow]

@classmethod
def upgrade(cls, old: Arrow) -> Arrow:
    if isinstance(old, cls): return old
    return cls(old.dom, old.cod, old.boxes)

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

def then(self, *others: Arrow) -> Arrow:
    for f, g in zip((self, ) + others, others): assert f.cod == g.dom
    dom, cod = self.dom, others[-1].cod if others else self.cod
    boxes = self.boxes + sum([other.boxes for other in others], [])
    return self.upgrade(Arrow(dom, cod, boxes))

__rshift__, __lshift__ = then, lambda self, other: other.then(self)
__len__ = lambda self: len(self.boxes)
__str__ = lambda self: '>> '.join(map(str, self.boxes))\
    if self.boxes else '{}.id({})'.format(type(self).__name__, self.dom)

@dataclass
class Box(Arrow):
    upgrade = Arrow.upgrade

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

    def __eq__(self, other):
        if isinstance(other, Box):
            return (self.name, self.dom, self.cod)\
                == (other.name, other.dom, other.cod)
        return isinstance(other, Arrow) and other.boxes == [self]

__str__ = lambda self: self.name
__hash__ = lambda self: hash(repr(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. We define the method `__str__` so that

`eval(str(f)) == f` for all `f: Arrow`, provided that the names of each object and box is in scope. 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.boxes == [f]`. 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 equal to the arrow with just itself as boxes. The main subtlety in the implementation is the class method `upgrade` which takes an `old: Arrow` as input and returns a new member of a given `cls`, subclass of `Arrow`. This allows the composition of arrows in a subclass to remain within the subclass, without having to rewrite the method `then`. This means we need to make `Arrow.id` a `classmethod` as well so that it can call `upgrade` and return an arrow of the appropriate subclass. We also need to fix `Box.upgrade = Arrow.upgrade`: when we compose a box then an arrow, we want to return a new arrow object, not a box.

Example 1.1.14. *We can define `Circuit` as a subclass of `Arrow` and `Gate` as a subclass of `Circuit` and `Box` defined by a name and a number of qubits.*

```
class Circuit(Arrow): pass

class Gate(Box, Circuit):
    upgrade = Circuit.upgrade

    def __init__(self, name: str, n_qubits: int):
        dom, cod = Ob(str(n_qubits)), Ob(str(n_qubits))
        Box.__init__(self, name, dom, cod)

Id = Circuit.id(Ob('1'))
X, Y, Z, H = [Gate(name, n_qubits=1) for name in "XYZH"]

assert (X >> Y) >> Z == X >> (Y >> Z) and X >> Id == X == Id >> X
assert isinstance(Id, Circuit) and isinstance(X >> Y, Circuit)
```

The `Functor` class listed in 1.1.15 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 `dom` and `cod` allow to define functors with arbitrary categories as domain and codomain, a `Category` is nothing more than a pair of types for its objects and arrows. For now we only use `cod` to define the image of identity arrows, otherwise the (co)domain of the functor is defined implicitly as the (co)domain of the `ob` and `ar` mappings.

We have chosen to implement functors in terms of Python `dict` rather than functions mainly because the syntax looked better for small examples. However, nothing prevents us from making the most of Python's *duck typing*: if it quacks like a `dict` and if it has a `__getitem__` method, we can use it to define functors like a `dict`. Thus, we can define functors with domains that are not finitely generated, such as the identity functor or more concretely the evaluation functor for quantum gates parameterised by a continuous angle. An equivalent solution is to subclass `Functor` and override its `__call__` method directly. The only downside is that we cannot print, save or check equality for such functors, we can only apply them to objects and arrows.

Listing 1.1.15. Implementation of `Cat` with `Category` as objects and `Functor` as arrows.

```
Category = namedtuple("Category", ["ob", "ar"])

class DictOrCallable:
    def __class_getitem__(_, source, target):
        return dict[source, target] | Callable[[source], target]

@dataclass
class Dict:
    inside: Callable
    __getitem__ = lambda self, key: self.inside(key)

@dataclass
class Functor:
    ob: DictOrCallable[Ob, Ob]
    ar: DictOrCallable[Box, Ar]
    dom: Category
    cod: Category

    def __init__(self, ob, ar, dom=Category(Ob, Arrow), cod=Category(Ob, Arrow)):
        ob, ar = (d if hasattr(d, "__getitem__") else Dict(d) for d in (ob, ar))
        self.ob, self.ar, self.dom, self.cod = ob, ar, dom, cod

    def __call__(self, other: Ob | Arrow) -> Ob | Arrow:
        if isinstance(other, Ob): return self.ob[other]
        if isinstance(other, Box):
            result = self.ar[other]
            if isinstance(result, self.cod.ar): return result
            # This allows some nice syntactic sugar.
            return self.cod.ar(result, self(other.dom), self(other.cod))
```

```

    if isinstance(other, Arrow):
        return self.cod.ar.id(self(other.dom)).then(
            *self(box) for box in other.bboxes)
    raise TypeError

@classmethod
def id(cls, x: Category) -> Functor:
    return cls(lambda obj: obj, lambda box: box, dom=x, cod=x)

def then(self: Functor, other: Functor) -> Functor:
    assert self.cod == other.dom
    ob, ar = (
        {x: g[f[x]] for x in f} if hasattr(f, "__iter__") else (lambda x: g[f[x]])
        for f, g in [(self.ob, other.ob), (self.ar, other.ar)])
    return type(self)(ob, ar, self.dom, other.cod)

```

Example 1.1.16. *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},
    cod=Category(type, 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]]},
    cod=Category(int, Matrix))
assert H(f >> g) == H(h).transpose()

```

*We can even define functors into **Cat**, i.e. interpret arrows as functors:*

```

I = Functor(
    ob={x: Category(Ob, Arrow), y: Category(Ob, Arrow), z: Category(int, Matrix)},
    ar={f: F, g: H},
    cod=Category(Category, Functor))
assert I(f >> g)(h) == H(F(h)) == H(f)

```

1.1.4 Quotient categories

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 1.1.17. 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:

- $H \circ X = Z \circ H$ and $Z \circ X = (-1) \circ X \circ Z$,
- $f \circ f = \text{id}(1)$ and $f \circ (-1) = (-1) \circ f$ 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 $\text{cost} : F(\Sigma) \rightarrow \mathbb{R}^+$, 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.

1.1.5 Daggers, sums and bubbles

We conclude this section by discussing three extra pieces of implementation beyond the basics of category theory: daggers, 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. $(\dagger) \circ (\dagger) = \text{id}_C$. A \dagger -functor is a functor between \dagger -categories that commutes with the dagger, thus we get a category $\dagger - \mathbf{Cat}$. For example, the conjugate transpose defines a dagger on the category \mathbf{Mat}_S , the adjoint defines a dagger on the category \mathbf{Circ} and the evaluation $\mathbf{Circ} \rightarrow \mathbf{Mat}_S$ is a \dagger -functor. The free \dagger -category is constructed as follows. Define the functor $\dagger : \mathbf{Sig} \rightarrow \mathbf{Sig}$ which sends a signature Σ to $\dagger(\Sigma)$ with $\dagger(\Sigma)_0 = \Sigma_0$ and $\dagger(\Sigma)_1 = \{-1, 1\} \times \Sigma_1$ with $\text{dom}(b, f) = \text{cod}(f)$ if $b = -1$ else $\text{dom}(f)$ and symmetrically for **cod**. Then the free dagger category is the quotient category $F(\dagger(\Sigma))/R$ for the congruence generated by $(1, f) \circ (-1, f) \rightarrow_R \text{id}(\text{dom}(f))$ and $(-1, f) \circ (1, f) \rightarrow_R \text{id}(f.\text{cod})$.

DisCoPy implements free \dagger -categories by adding an attribute `is_dagger: bool` to boxes and a method `Arrow.dagger`, shortened to the postfix operator `[::-1]`, which reverses the order of boxes and negates `is_dagger` elementwise. The normal form is computable in linear time but it has not been implemented yet. In order to implement the syntactic sugar `f[::-1] == f.dagger()`, we need to override the `__getitem__` method. In general, DisCoPy defines indexing `f[i]` and slicing `f[start:stop:step]` so that `f[key].boxes == f.boxes[key]` for any `key: int` and any `key: slice` with `key.step` in `(-1, 1, None)`. Although the case of negative indices (i.e. counting backwards from the end of the list) is implemented in DisCoPy, its interaction with list reversal is too complex to be listed here.

Listing 1.1.18. Implementation of free \dagger -categories and \dagger -functors.

```
class Arrow(cat.Arrow):
    def dagger(self):
        return self.upgrade(Arrow(
            self.cod, self.dom, [box.dagger() for box in self.boxes[::-1]]))

    def __getitem__(self, key: int | slice) -> Arrow:
        if isinstance(key, int): return self.upgrade(self.boxes[key])
        if key.step not in (-1, 1, None): raise IndexError
        if key.step == -1:
            for i in (key.start, key.stop):
                if i is not None and i < 0: ...
            stop, start = (
```

```

        None if i is None else i + 1 for i in (key.stop, key.start))
    return self[start:stop].dagger()
    dom, cod = self[key.start].dom, self[key.stop].cod
    return self.upgrade(Arrow(dom, cod, self.boxes[key]))

class Box(cat.Box, Arrow):
    upgrade = Arrow.upgrade

    def __init__(self, name: str, dom: Ob, cod: Ob, is_dagger=False):
        self.is_dagger = is_dagger; cat.Box.__init__(self, name, dom, cod)

    def dagger(self):
        return Box(self.name, self.cod, self.dom, not self.is_dagger)

class Functor(cat.Functor):
    dom = cod = Category(Ob, Arrow)

    def __call__(self, other):
        if isinstance(other, Box) and other.is_dagger:
            return self(other.dagger()).dagger()
        return super().__call__(other)

```

Listing 1.1.19. Implementation of $\mathbf{Mat}_{\mathbb{S}}$ as a \dagger -category.

```

def transpose(self: Matrix) -> Matrix:
    inside = [[self[j][i] for j in range(self.dom)] for i in range(self.cod)]
    return type(self)(inside, self.cod, self.dom)

def map(self: Matrix, func: Callable[[Number], Number]) -> Matrix:
    inside = [list(map(func, row)) for row in self.inside]
    return type(self)(inside, self.dom, self.cod)

Matrix.transpose, Matrix.map = transpose, map
Matrix.conjugate = lambda self: self.map(lambda x: x.conjugate())
Matrix.dagger = lambda self: self.conjugate().transpose()

```

Example 1.1.20. We can implement a simulator for 1-qubit circuits as a \dagger -functor.

```

Circuit.eval = Functor(
    ob={Ob('1'): 2},
    ar={X: [[0, 1], [1, 0]],
        Y: [[0, -1j], [1j, 0]],
        Z: [[1, 0], [0, -1]],
        H: [[x / sqrt(2) for x in row] for row in [[1, 1], [1, -1]]],
    cod=Category(int, Matrix[complex]))

```

We can check that every circuit is unitary, i.e. its dagger is also its inverse.

```
for c in [Id, X, Y, Z, H, X >> Y >> Z >> H]:
    assert (c >> c[::-1]).eval() == Id.eval() == (c[::-1] >> c).eval()
```

We can check the equations given in the presentation of example 1.1.17.

```
assert (Z >> H).eval() == (H >> X).eval()
assert (Z >> X).eval() == (X >> Z).eval().map(lambda x: -x)
for gate in [H, Z, X]: assert (gate >> gate).eval() == Id.eval()
```

A category C has *sums*, or equivalently C is *commutative-monoid-enriched*, when it comes equipped with a commutative monoid $(+, 0)$ on each homset $C(x, y)$ such that $f \circ 0 = 0 \circ f$ 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 commutative-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. A commutative-monoid-enriched category with one object is precisely a rig. Given a signature Σ , we construct the free category with sums $F^+(\Sigma)$ by taking the free commutative monoid over each homset of $F(\Sigma)$, i.e. arrows $f : x \rightarrow y$ in $F^+(\Sigma)$ are *bags* (also called *multisets*) of arrows $f_i : x \rightarrow y$ in $F(\Sigma)$.

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. Checking equality of bags is the same as checking equality of lists sorted by any arbitrary ordering. DisCoPy functors are commutative-monoid-enriched, i.e. a formal sum of arrows can be interpreted as a concrete sum of matrices.

Listing 1.1.21. Implementation of free sum-enriched categories and functors.

```
class Arrow(cat.Arrow):
    def __add__(self, other):
        self, other = map(Sum.upgrade, (self, other))
        return Sum(self.terms + other.terms, self.dom, self.cod)

    def __eq__(self, other):
        return other.terms == [self] \
            if isinstance(other, Sum) else super().__eq__(other)

    def then(self, other: Arrow) -> Arrow:
        return Sum.upgrade(self).then(other) \
            if isinstance(other, Sum) else super().then(other)
```

```

@staticmethod
def zero(dom: Ob, cod: Ob) -> Arrow: return Sum([], dom, cod)

__lt__ = lambda self, other: hash(self) < hash(other) # An arbitrary order.

class Sum(cat.Box, Arrow):
    def __init__(self, terms: list[Arrow], dom: Ob, cod: Ob):
        assert all(f.dom == dom and f.cod == cod for f in terms)
        self.terms, name = terms, "Sum({}, {}, [{}])".format(
            dom, cod, ", ".join(map(str, terms)))
        cat.Box.__init__(self, name, dom, cod)

    def __eq__(self, other):
        if isinstance(other, Sum):
            return (self.dom, self.cod, sorted(self.terms))\
                == (other.dom, other.cod, sorted(other.terms))
        return self.terms == [other]

    def upgrade(old: cat.Arrow) -> Sum:
        return old if isinstance(old, Sum) else Sum([old], old.dom, old.cod)

    def then(self, other):
        terms = [f.then(g) for f in self.terms for g in Sum.upgrade(other).terms]
        return Sum(terms, self.dom, other.cod)

class Functor(cat.Functor):
    dom = cod = Category(Ob, Arrow)

    def __call__(self, other):
        if isinstance(other, Sum):
            unit = self.cod.ar.zero(self(other.dom), self(other.cod))
            return sum([self(f) for f in other.terms], unit)
        return super().__call__(other)

```

Listing 1.1.22. Implementation of \mathbf{Mat}_S as a category with sums.

```

def __add__(self: Matrix, other: Matrix) -> Matrix:
    inside = [[x + y for x, y in zip(u, v)]
               for u, v in zip(self.inside, other.inside)]
    return type(self)(inside, self.dom, self.cod)

@classmethod
def zero(cls, dom: int, cod: int) -> Matrix:
    return Matrix[cls.dtype]([[0 for _ in range(cod)] for _ in range(dom)], dom, cod)

```

A *bubble* on a (subcategory of a) category C is a pair of unary operators $\beta_{\text{dom}}, \beta_{\text{cod}} : C_0 \rightarrow C_0$ on objects and a unary operator between homsets $\beta : C(x, y) \rightarrow C(\beta_{\text{dom}}(x), \beta_{\text{cod}}(y))$ for (some) pairs of objects $x, y \in C_0$. Given a signature Σ and a pair $\beta_{\text{dom}}, \beta_{\text{cod}} : C_0 \rightarrow C_0$, we construct the free category with bubbles $F(\Sigma^\beta)$ by induction on the maximum level n of bubble nesting: take the signature $\Sigma^\beta = \bigcup_{n \in \mathbb{N}} \Sigma_n^\beta$ for $\Sigma_0^\beta = \Sigma$ and $\Sigma_{n+1}^\beta = \Sigma + \{\beta(f) \mid f \in F(\Sigma_n^\beta)\}$. That is, box in Σ^β is a box in Σ_n^β for some $n \in \mathbb{N}$. A box in Σ_n^β is either a box in Σ or an arrow $f : x \rightarrow y$ in $F(\Sigma_{n-1}^\beta)$ that we have put inside a bubble $\beta(f) : \beta_{\text{dom}}(x) \rightarrow \beta_{\text{cod}}(y)$.

Example 1.1.23. Any endofunctor $\beta : C \rightarrow C$ also defines a bubble, thus we can define a bubble-preserving functor $F(U(C)^\beta) \rightarrow C$ which interprets bubbles as functor application. Any functor between two categories C and D defines a bubble on their disjoint union $C + D$ (i.e. with objects $C_0 + D_0$ and arrows $C_1 + D_1$). These functor bubbles have also been called functorial boxes [Mel06].

Example 1.1.24. An exponential rig is a one-object category \mathbb{S} with sums and a bubble $\exp : \mathbb{S} \rightarrow \mathbb{S}$ which is a homomorphism from sum to product, i.e. $\exp(a+b) = \exp(a)\exp(b)$ and $\exp(0) = 1$. Any rig \mathbb{S} is an exponential rig by taking $\exp(a) = 1$ for all $a \in \mathbb{S}$. Non-trivial examples include the complex numbers as well as the Boolean rig with negation. Thus, exponential rigs provide enough syntax to define the matrices of most quantum gates, as well as any propositional logic formula.

Example 1.1.25. Matrix exponential is a bubble on the subcategory of square matrices, with the property that $\exp(f+g) = \exp(f) \circ \exp(g)$ whenever $f \circ g = g \circ f$. Also, any function $\mathbb{S} \rightarrow \mathbb{S}$ yields a bubble on $\mathbf{Mat}_{\mathbb{S}}$ given by element-wise application. For example, we can define a bubble on the category $\mathbf{Mat}_{\mathbb{B}}$ of Boolean matrices which sends each matrix f to its entrywise negation \bar{f} .

DisCoPy implements free bubbles with `Bubble`, a subclass of `Box` which we attach to the arrow class with `Arrow.bubble = Bubble`. `Bubble` has attributes `inside: Arrow`, `dom: Ob` and `cod: Ob` as well as `name: str`. DisCoPy functors interpret bubbles with `name = "method"` as the application of `method` in the codomain category. The resulting syntax with bubbles is strictly more expressive than that of free categories alone. For example, element-wise negation cannot be expressed as a composition: there is no matrix $N : x \rightarrow x$ in $\mathbf{Mat}_{\mathbb{B}}$ such that $N \circ f = \bar{f}$ for all $f : x \rightarrow y$. This is also the case for the element-wise application of any non-linear function such as the rectified linear units (ReLU) used in machine learning. 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.

Listing 1.1.26. Implementation of free categories with bubbles and their functors.

```
class Bubble(Box):
    def __init__(self, inside: Arrow, dom=None, cod=None, name="bubble"):
        self.inside, dom, cod = inside, dom or inside.dom, cod or inside.cod
        name = "Bubble({}, {}, {}, {})".format(inside, dom, cod, name)
        super().__init__(name, dom, cod)

Arrow.bubble = Bubble

class Functor(cat.Functor):
    def __call__(self, other):
        if isinstance(other, Bubble):
            return getattr(self.cod.ar, other.name)(
                self(other.inside), self(other.dom), self(other.cod))
        return super().__call__(other)
```

Example 1.1.27. We can encode the architecture of a neural network as an arrow with sums and bubbles, encoding vector addition and non-linear activation function respectively. The evaluation of the neural network on some input vector for some parameters is given by the application of a sum-and-bubble-preserving functor into $\mathbf{Mat}_{\mathbb{R}}$. The hyper-parameters (i.e. the number of neurons at each layer) are given by the image of the functor on objects.

```
Matrix.ReLU = lambda self, _, _ : self.map(lambda x: max(x, 0))

vector, bias = Box('vector', x, y), Box('bias', x, x)
ones, weights = Box('ones', x, y), Box('weights', y, z)
network = ((vector + (bias >> ones)) >> weights).bubble(name="ReLU")

F = Functor(
    ob={x: 1, y: 4, z: 2},
    ar={vector: [[1.2, -2.3, 3.4, -4.5]],
        bias: [[-3.14]], ones: [[1, 1, 1, 1]],
        weights: [[5.6, -6.7, 7.8, -8.9],
                  [9.0, -0.1, 2.3, -3.4]]},
    cod=Category(int, Matrix[float]))

assert F(network) == F(vector).map(lambda x: x + F(bias)[0][0])\
    .then(F(weights)).map(lambda x: max(0, x))
```

Example 1.1.28. *We can implement propositional logic with boxes as propositions, composition as conjunction, sum as disjunction and bubble as negation. The evaluation of a formula in a model corresponds to the application of a sum-and-bubble-preserving functor into $\mathbf{Mat}_{\mathbb{B}}(1,1)$.*

```
Matrix.dtype, Matrix._not = B, lambda self, _, _ : self.map(lambda x: not x)

class Formula(Arrow):
    _not = lambda self: self.bubble(name="_not")

class Proposition(Box, Formula):
    def __init__(self, name): Box.__init__(self, name, Ob('1'), Ob('1'))

def model(data: dict[Proposition, bool]):
    return Functor(Ob={Ob('1'): 1},
                  ar={p: [[data[p]] for p in data},
                  dom=Category(Ob, Formula),
                  cod=Category(int, Matrix[B]))

p, q = map(Proposition, "pq")
p_implies_q = (q._not() >> p)._not()
not_p_or_q = p._not() + q

for a, b in itertools.product([0, 1], [0, 1]):
    F = Formula.model({p: a, q: b})
    assert F(p_implies_q) == not (not F(q) and F(p)) \
           == F(not_p_or_q) == not F(p) or F(q)
```

Remark 1.1.29. *The constructions for dagger, sums and bubbles all commute with each other. Moreover, there is cube of faithful functors which embed free categories in free \dagger -categories with sums and bubbles. Thus, they are all implemented by default in the same class `Arrow`.*

1.2 Diagrams in Python

1.2.1 Abstract monoidal categories

In the previous section, we introduced the idea of arrows in free categories as abstract 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* $(f \circ g) \otimes (f' \circ g') = (f \otimes g) \circ (f' \otimes g')$ holds for all arrows $f, f', g, g' \in C_1$.

We will use the following terminology: an object x is called a *system*, an arrow $f : 1 \rightarrow x$ from the unit is called a *state* of the system 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*.

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

Example 1.2.2. *A monoidal category with one object is a commutative monoid. Indeed in any monoidal category, the interchange law implies that scalars form a commutative monoid, by the following Eckmann-Hilton argument:*

$$\begin{aligned} a \circ b &= 1 \otimes a \circ b \otimes 1 = (1 \circ b) \otimes (a \circ 1) = b \otimes a \\ &= (b \circ 1) \otimes (1 \circ a) = b \otimes 1 \circ 1 \otimes a = b \circ a \end{aligned}$$

Example 1.2.3. *A monoidal category with at most one arrow between any two objects is called a preordered monoid. The functoriality axiom implies that the preorder is in fact a pre-congruence, i.e. $a \leq b$ and $c \leq d$ implies $a \times c \leq b \times d$.*

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.

Given the presentation of a monoid (X, R) with $R \subseteq X^* \times X^*$, we can construct a preordered monoid with $(\leq_R) = \bigcup_{n \in \mathbb{N}} R^n \subseteq X^* \times X^*$ the (non-symmetric) reflexive transitive closure of R . Thus, the inequality problem (i.e. given two lists $x, y \in X^*$ and a presentation (X, R) , decide whether $x \leq_R y$) is a generalisation of the word problem for monoids.

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 the only effect is discarding, i.e. the constant function into the singleton. **FinSet** is also monoidal with the empty set 0 as unit and disjoint union as tensor.

Example 1.2.5. For any category C , there is a monoidal category C^C where the objects are endofunctors with composition as tensor and the arrows are natural transformations $\alpha : F \rightarrow F', \beta : G \rightarrow G'$ with vertical composition $(\alpha \otimes \beta)(x) : G(F(x)) \rightarrow G'(F'(x))$ as tensor.

1.2.2 Concrete monoidal categories

Example 1.2.6. 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 that every monoidal category is monoidally equivalent¹ to a strict one.

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 @ Id >> Id @ g != Id @ g >> f @ Id`. As we will discuss in section 1.5, **Pyth** is in fact a premonoidal category. The states, i.e. the functions

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.

$f : () \rightarrow t$, 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.

Listing 1.2.7. Implementation of **Pyth** as a (non-strict pre)monoidal category.

```
def tensor(self: Function, other: Function) -> Function:
    dom, cod = tuple[self.dom, other.dom], tuple[self.cod, other.cod]
    return Function(dom, cod, lambda x, y: (self(x), self(y)))
```

Example 1.2.8. 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 `tuple[True, t1]` and `tuple[False, t2]`¹, i.e. a term $(b, x): t1 + t2$ is a pair of a Boolean $b: \text{bool}$ 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 1.2.9. The category \mathbf{Mat}_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 S is commutative, \mathbf{Mat}_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.

Listing 1.2.10. Implementation of \mathbf{Mat}_S as a monoidal category with Kronecker product as tensor.

```
def tensor(self: Matrix, other: Matrix) -> Matrix:
    dom, cod = self.dom * other.dom, self.cod * other.cod
    inside = [[self[i_dom][i_cod] * other[j_dom][j_cod]
               for i_cod in range(self.cod) for j_cod in range(other.cod)]
              for i_dom in range(self.dom) for j_dom in range(other.dom)]
    return type(self)(inside, dom, cod)
```

Example 1.2.11. 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.

¹What we really mean is `tuple[Literal[True], t1] | tuple[Literal[False], t2]`.

1.2.3 Free monoidal categories

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 $\mathbf{dom}, \mathbf{cod} : \Sigma_1 \rightarrow \Sigma_0^*$ 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 $f_{\circ} \mathbf{dom} = \mathbf{dom}_{\circ} f^*$ and $f_{\circ} \mathbf{cod} = \mathbf{cod}_{\circ} f^*$. 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 1.2.12. *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 1.2.13. *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 $\mathbf{dom}, \mathbf{cod} : C_1 \rightarrow C_0^*$,
- a function $\mathbf{id} : C_0^* \rightarrow C_1$ and a (partial) operation $\mathbf{then} : C_1 \times C_1 \rightarrow C_1$,
- 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 1.2.14. 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 .

In the cases of monoidal categories where the objects are the natural numbers with addition as tensor, such as **FinSet** with disjoint union, **Mat_S** with direct sum or **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 also called *coloured PROs*, this is the same thing as a foo-monoidal category. For example, we can take all the Python types as colours and define **Pyth** as a foo-monoidal category with `list[type]` as objects.

Listing 1.2.15. Implementation of the foo-monoidal category **Pyth** with `list[type]` as objects and **Function** as arrows.

```

untuple = lambda *xs: xs[0] if len(xs) == 1 else xs

class Function(cat.Function):
    dom: list[type]
    cod: list[type]

    def tensor(self, other: Tensor) -> Tensor:
        def inside(*xs):
            left, right = xs[:len(self.dom)], xs[len(self.dom):]
            return untuple(*(tuple(self(left)) + tuple(other(right))))
        return Function(inside, self.dom + other.dom, self.cod + other.cod)

```

In the case of **Mat_S** with Kronecker product as tensor, we can define an equivalent category **Tensor_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.

Listing 1.2.16. Implementation of the foo-monoidal category **Tensor_S** \simeq **Mat_S** with `list[int]` as objects and **Tensor[dtype]** as arrows.

```

from functools import reduce as foldl
product = lambda x: foldl(lambda a, b: a * b, x, 1)

class Tensor(Matrix):
    dom: list[int]
    cod: list[int]

    def downgrade(self) -> Matrix:
        return Matrix[self.dtype](self.inside, product(self.dom), product(self.cod))

    @classmethod
    def id(cls, x: list[int]) -> Tensor:
        return cls(Matrix.id(product(x)).inside, x, x)

    def then(self, other: Tensor) -> Tensor:
        inside = self.downgrade().then(other.downgrade()).inside
        return type(self)(inside, self.dom, other.cod)

    def tensor(self, other: Tensor) -> Tensor:
        inside = self.downgrade().tensor(other.downgrade()).inside
        return type(self)(inside, self.dom + other.dom, self.cod + other.cod)

```

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 1.2.17. *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 $\text{dom}(x, f, y) = x\text{dom}(f)y$ and $\text{cod}(x, f, y) = x\text{cod}(f)y$. 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 1.2.18. *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 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 nodes 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 $(1, f, 1) \circ (1, g, 1) \leftarrow_R (x, g, 1) \circ (1, f, y)$. For the composition of two scalars $a : 1 \rightarrow 1$ and $b : 1 \rightarrow 1$, we can apply interchangers indefinitely $a \circ b \rightarrow_R b \circ a \rightarrow_R a \circ b$: this is the Eckmann-Hilton argument. Delpeuch and Vicary [DV18] give a quadratic solution to the word problem for free monoidal categories, i.e. deciding when two diagrams are equal.

Theorem 1.2.19 ([DV18]). *The equality of diagrams is decidable in linear time in the connected case, and quadratic in the general case. The right interchanger is confluent and for connected diagrams, i.e. when the Eckmann-Hilton argument does not apply, it reaches a normal form in a cubic number of steps.*

Proof. The linear-time algorithm for the connected case works by reduction to isomorphism of planar maps. In the general case, computing the tree of connected components of the diagram takes quadratic time. The cubic worst-case for normal forms is given in example 1.3.7. \square

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. Then, 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 equated by the interchanger.

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 . In the next section, we will show that this construction is in fact equivalent to the topological definition of diagrams as labeled graphs embedded in the plane.

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

```
@dataclass
class Ty(Ob):
    objects: list[Ob | str]

    def __init__(self, objects=[]):
        self.objects = [x if isinstance(x, Ob) else Ob(x) for x in objects]
        super().__init__("{}".format(' @ '.join([x.name for x in self.objects])))

    @classmethod
    def upgrade(cls, old: Ob) -> Ty:
        if isinstance(old, cls): return old
        return cls(old.objects) if isinstance(old, Ty) else cls(old)

    def tensor(self, *others: Ty) -> Ty:
        if all(isinstance(other, Ty) for other in others):
            return self.upgrade(Ty(
                self.objects + sum([other.objects for other in others], [])
            ))
        return NotImplemented # This will allow whiskering on the left.

    __matmul__ = tensor
    __getitem__ = lambda self, key: self.upgrade(Ty([self.objects[key]]))
    __pow__ = lambda self, n: self.upgrade(Ty(n * self.objects))
    __len__ = lambda self: len(self.objects)
```

The implementation of the class `Ty` for types (i.e. lists of objects) is straightforward, it is sketched in listing 1.2.20. The only subtlety is in the 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 redefine the `tensor` method.

Example 1.2.21. *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): self.n = n
    objects = property(lambda self: n * [Ob('1')])
    upgrade = staticmethod(lambda old: Qubits(len(old)))
    __str__ = lambda self: "qubit ** {}".format(len(self))

qubit = Qubits(1)
assert qubits ** 0 == Qubits(0) and qubits ** 42 == Qubits(42)
assert isinstance(qubit ** 0, Qubits) and isinstance(qubit ** 42, Qubits)
```

The implementation of `Layer` as a subclass of `cat.Box` is sketched in listing 1.2.22. 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 1.2.22. 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 = "{} @ {} @ {}".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 of layers. The `interchange` method takes an integer `i < len(self.layers)` and returns the diagram with boxes `i` and `i + 1` interchanged, or raises an `AssertionError` if they are connected. It also takes an optional argument `left: bool` which allows to choose between left and right in case we're interchanging an effect then a state. The optional `down: bool` allows to interchange `i - 1` and `i` instead. Although for now it is redundant, we will override it in a meaningful way in section 1.4.3.

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 1.2.23. 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)

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

    def tensor(self, other: Diagram | Ty) -> Diagram:
        if isinstance(other, Ty): other = self.id(other)
        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))

    def interchange(self, i: int, left=False, down=True) -> Diagram: ...
    def normal_form(self, left=False) -> Diagram: ...
    def draw(self, **params): ...

    __matmul__, __rmatmul__ = tensor, lambda self, other:\
        other @ self if isinstance(other, Diagram) else self.id(other) @ self
```

Again, we have a class method `upgrade` which takes an old `cat.Arrow` and turns it into a new object of type `cls`, a given subclass of `Diagram`. This means we do not need to repeat the code for identity or composition which is already

implemented by `cat.Arrow`. In turn, when the user defines a subclass of `Diagram`, they do not need to repeat the code for identity, composition or tensor. The implementation of `monoidal.Box` as a subclass of `cat.Box` and `Diagram` is relatively straightforward, we only need to make sure that a box is equal to the diagram of just itself. We need to be careful with the order of inheritance however, diagram equality is defined in terms of box equality, so if we had `Box.__eq__ = Diagram.__eq__` then checking equality would enter an infinite loop. We also want the `upgrade` method of `Box` to be that of `Diagram`.

Listing 1.2.24. Outline of the class `monoidal.Box`.

```
class Box(cat.Box, Diagram):
    upgrade = Diagram.upgrade

    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 isinstance(other, Box): return cat.Box.__eq__(self, other)
        return isinstance(other, Diagram) and other.layers == [Layer.upgrade(self)]
```

Example 1.2.25. We can define `Circuit` as a subclass of `Diagram`. `Gate` and `Ket` are subclasses of `Circuit` and `Box`. Now we can compose and tensor gates together and the result will be an instance of `Circuit`.

```
class Circuit(Diagram): pass

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

class Ket(Circuit, Box):
    def __init__(self, *bits: bool):
        self.bits, dom, cod = bits, Qubits(0), Qubits(len(bits))
        name = "Ket({})".format(', '.join(map(str, bits)))
        Box.__init__(self, name, dom, cod)

Gate.upgrade = Ket.upgrade = Circuit.upgrade

H, CX = Gate("H", n_qubits=1), Gate("CX", n_qubits=2)
Id, sqrt2 = Circuit.id(qubit), Gate("sqrt(2)", n_qubits=0)
assert isinstance(sqrt2 @ Ket(0, 0) >> H @ Id >> CX, Circuit)
```

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 1.2.26. Implementation of monoidal functors.

```
class Functor(cat.Functor):
    dom = cod = Category(Ty, Diagram)

    def __call__(self, other):
        if isinstance(other, Ty):
            return self.cod.ob(sum([self(x) for x in other.objects], []))
        if isinstance(other, Ob):
            result = self.ob[other] if other in self.ob else self.ob[Ty(other)]
            if isinstance(result, self.cod.ob): return result
            return self.cod.ob([result]) # Allows some nice syntactic sugar.
        if isinstance(other, Layer):
            left, box, right = other
            return id_left @ self(box) @ id_right
        return super().__call__(other)
```

Note that the domain the dictionary `ob` can be either an `Ob` or a `Ty` of length 1.

Example 1.2.27. We can simulate quantum circuits by applying a functor from `Circuit` to `Tensor`.

```
class Eval(Functor):
    def __init__(self):
        ob = {Ob('1'): 2}
        ar = {H: [[x / sqrt(2) for x in row] for row in [[1, 1], [1, -1]]],
              CX: [[i == j for j in [0, 1, 2, 3]] for i in [0, 1, 3, 2]],
              sqrt2: [[sqrt(2)]]}
        super().__init__(ob, ar, cod=Category(tuple[int], Tensor[complex]))

    def __call__(self, other):
        if isinstance(other, Ket):
            if not other.bits: return Tensor.id([])
            head, *tail = other.bits
            return Tensor[complex]([[head, not head]], [], [2]) @ self(Ket(*tail))
        return super().__call__(other)
```

```
Circuit.eval = Eval()
circuit = sqrt2 @ Ket(0, 0) >> H @ Id >> CX
superposition = Ket(0, 0) + Ket(1, 1)
assert circuit.eval() == superposition.eval()
```

Remark 1.2.28. *DisCoPy uses a more compact encoding of diagrams than their list of layers. Indeed, a diagram is uniquely specified by a domain, a list of boxes and a list of offsets, i.e. the length of the type to the left of each box.*

```

Encoding = namedtuple("Encoding", ["dom", "boxes_and_offsets"])

def encode(diagram: Diagram) -> Encoding:
    return Encoding(diagram.dom, [(box, len(left)) for left, box, _ in diagram.layers])

def decode(encoding: Encoding) -> Diagram:
    diagram = Diagram.id(encoding.dom)
    for box, offset in encoding.boxes_and_offsets:
        left, right = result.cod[:offset], result.cod[offset + len(box.dom):]
        diagram >= Diagram.id(left) @ box @ Diagram.id(right)
    return diagram

x, y, z = map(Ty, "xyz")
f, g, h = Box('f', x, y), Box('g', y, z), Box('h', y @ z, x)
encoding = Encoding(dom=x @ y, boxes_and_offsets=[(f, 0), (g, 1), (h, 0)])
assert decode(encoding) == f @ g >> h and encode(f @ g >> h) == encoding

```

1.2.4 Quotient monoidal categories

Once we have defined freeness, we need to define quotients. The quotient C/R of a monoidal category C by a binary relation $R \subseteq \coprod_{x,y \in C_0^*} C(x, y) \times C(x, y)$ is the quotient category for the rewriting relation \rightarrow_R where:

$$u \circ b \otimes f \otimes c \circ v \rightarrow_R u \circ b \otimes g \otimes c \circ v$$

for all $(f, g) \in R$, $u : a \rightarrow b \otimes \text{dom}(f) \otimes c$ and $v : b \otimes \text{cod}(f) \otimes c \rightarrow d$. Intuitively, if we can equate f and g then we can equate them in any context, i.e. with any objects b and c tensored on the left and right and any arrows u and v composed above and below. A proof that two diagrams are equal in the quotient can itself be thought of as a diagram in three dimensions, i.e. the movie of a diagram being rewritten into another. These higher-dimensional diagrams will be mentioned in section 1.6. Again, every monoidal category C is isomorphic to the quotient of a free monoidal category $C = F(\Sigma)/R$: take $\Sigma = U(C)$ and the relation $R \subseteq F(U(C)) \times F(U(C))$ given by every binary composition and tensor.

Why should computer scientists care about diagrams? One reason is that they are free data structures in the same sense that lists are free: they are a two-dimensional generalisation of lists. Another reason is that they allow an elegant

definition of a Turing-complete problem: given a finite monoidal signature Σ and a pair of lists $x, y \in \Sigma_0^*$, decide whether there is a diagram $f : x \rightarrow y$ in $F(\Sigma)$. Indeed, the word problem for monoids (which is equivalent to the halting problem for Turing machines) reduces to the existence problem for diagrams: given the presentation of a monoid X^*/R , take objects $\Sigma_0 = X$ and boxes $\Sigma_1 = R$ with $\text{dom}, \text{cod} : \Sigma_1 \hookrightarrow X^* \times X^* \rightarrow X^*$ the left and right hand-side of each related pair. For any pair $x, y \in X^*$, we have that $x \leq_R y$ if and only if there is a diagram $f : x \rightarrow y$ in $F(\Sigma)$: the preordered monoid generated by the relation R is the preorder collapse of the free monoidal category $F(\Sigma)$. While monoid presentations define *decision problems* (i.e. with a Boolean output), free monoidal categories naturally define *function problems*: given a pair of types, output a diagram.

If we compose the two reductions together, we get a free monoidal category where diagrams are the possible runs of a given Turing machine. Moreover, a monoidal functor from the category of one machine to another corresponds to a reduction between the problems they solve, the domain machine being simulated by the codomain. Thus, we could very well take finite monoidal signatures as our definition of machine and diagrams as our definition of computation: algorithmic complexity is given by the size of signatures, time and space complexity are given by the length and width¹ of diagrams. Now if two-dimensional diagrams encode computations on one-dimensional lists, we can think of three-dimensional diagrams either as computations on two-dimensional data, or as higher-order computations. For example, the optimisation steps of a (classical or quantum) compiler can be thought of as a three-dimensional diagram, with (classical or quantum) circuits as domain and codomain.

1.2.5 Daggers, sums and bubbles

As in the previous section, we introduce three extra pieces of implementation: daggers, sums and bubbles. A \dagger -monoidal category is a monoidal category with a dagger (i.e. an identity-on-objects involutive contravariant endofunctor) that is also a monoidal functor, a \dagger -monoidal functor is both a \dagger -functor and a monoidal functor. They are implemented by adding a `dagger` method to the `Layer` class.

Listing 1.2.29. Implementation of free \dagger -monoidal categories.

```
def dagger(self: Layer) -> Layer:
    return Layer(self.left, self.box.dagger(), self.right)
```

¹The width of a diagram is the maximum width of its layers, which is not preserved by interchangers. In the diagrams generated by Turing machines, we cannot apply interchangers anyway: every box is connected to the next by the head of the machine.

A monoidal category is commutative-monoid-enriched when it has sums that distribute over the tensor, i.e. $(f + f') \otimes (g + g') = f \otimes g + f \otimes g' + f' \otimes g + f' \otimes g'$ and $f \otimes 0 = 0 = 0 \otimes f$. They are implemented by a method `Sum.tensor`.

Listing 1.2.30. Implementation of free monoidal categories with sums.

```
def tensor(self: Sum, other: Sum) -> Sum:
    dom, cod = self.dom @ other.dom, self.cod @ other.cod
    return Sum([f @ g for f in self.terms for g in other.terms], dom, cod)
```

Bubbles for monoidal categories are the same as bubbles for categories, their implementation requires no extra work. As we mentioned in the previous section, bubbles do give us a strictly more expressive syntax however: they can encode operations on arrows that cannot be expressed in terms of composition or tensor.

Example 1.2.31. *As in example 1.1.23, any monoidal endofunctor $\beta : C \rightarrow C$ also defines a bubble on the monoidal category C , we can define a bubble-preserving functor $F(U(C)^\beta) \rightarrow C$ which interprets bubbled diagrams as functor application. However, the disjoint union $C + D$ of two monoidal categories does not yield a well-defined monoidal category: we cannot tensor arrows of C with those of D . Thus, the case of monoidal functors $C \rightarrow D$ requires diagrams with different colours (for the inside and the outside of the bubble) which we will mention in section 1.4.*

Example 1.2.32. *We can implement the Born rule as a bubble on `Circ` interpreted as element-wise squared amplitude. We can also implement any classical post-processing as a bubble.*

```
Bra = lambda *bits: Ket(*bits)[::-1]
Born_rule = lambda x: abs(x) ** 2
Circuit.measure = lambda self: self.bubble(name="squared_amplitude")
Tensor.squared_amplitude = lambda self: self.map(Born_rule)

assert (Ket(0) >> H >> Bra(0)).measure().eval()[0][0] == .5

biased_ReLU = lambda x: max(0, 2 * x - 1)
Circuit.post_process = lambda self: self.bubble(name="non_linearity")
Tensor.non_linearity = lambda self: self.map(biased_ReLU)

circuit = Ket(0, 0) >> H @ Id >> CX >> Bra(0, 0)
post_processed_circuit = circuit.measure().post_process()
assert post_processed_circuit.eval()[0][0] \
    == biased_ReLU(Born_rule(circuit.eval()[0][0]))
```

Example 1.2.33. We can implement the formulae of first-order logic using Peirce's existential graphs. They are the first historical examples of string diagrams as well as the first definition of first-order logic [BT98; BT00; MZ16; HS20]. Bubbles, which Peirce calls cuts, encode negation. The evaluation of a formula in a finite model corresponds to the application of a bubble-preserving functor into $\mathbf{Mat}_{\mathbb{B}}$.

```
class Formula(Diagram):
    cut = lambda self: self.bubble(name="_not")

class Predicate(Box, Formula):
    def __init__(self, name): Box.__init__(self, name, Ty(), Ty('x'))

def model(size, data: dict[Predicate, list[bool]]):
    Functor(ob={Ty('x'): size},
           ar={p: [data[p]] for p in data},
           dom=Category(Ty, Formula),
           cod=Category(list[int], Tensor[B]))

men, mortal = map(Predicate, ("men", "mortal"))
all_men_are_mortal = (men.cut() >> mortal.dagger()).cut()

for a, b, c, d in itertools.product(*4 * [[0, 1]]):
    F = model(size=2, {men: [a, b], mortal: [c, d]})
    assert F(all_men_are_mortal) == all(
        not F(men)[i][0] or F(mortal)[i][0] for i in range(2))
```

We get to the end of this section and the reader may have noticed that we have not drawn a single diagram yet: drawing will be the topic of the next section. This absence of drawing intends to demonstrate that diagrams are not only a great tool for visual reasoning, they can also be thought of as a *data structure for abstract pipelines*. Monoidal functors then allow to evaluate these abstract pipelines in terms of concrete computation, be it Python functions, tensor operations or quantum circuits. This abstract programming style, defining programs in terms of composition rather than arguments-and-return-value, is called *point-free* or *tacit programming*. Because of the difficulty of writing any kind of complex program in that way, it has also been called the *pointless style*. DisCoPy provides a `@diagramize` decorator which allows the user to define diagrams using the standard syntax for Python functions instead of the point-free syntax. Given `dom: Ty`, `cod: Ty` and `boxes: list[Box]` as parameters, it adds to each box a `__call__` method which takes the objects of its domain as input and returns the objects of its codomain.

Example 1.2.34. We can define quantum circuits as Python functions on qubits.

```

kets0 = Ket(0, 0)

@diagramize(dom=Qubits(2), cod=Qubits(2), boxes=[sqrt2, kets0, H, CX])
def circuit():
    sqrt2(); qubit0, qubit1 = kets0
    return CX(H(qubit0), qubit1)

assert circuit == sqrt2 @ kets0 >> H @ Id >> CX

```

The underlying algorithm constructs a graph with nodes for each object of the domain and the codomain of each box, as well as of the whole diagram. There is an edge from a codomain node of a box (or a domain node of the whole diagram) to the domain node of another (or a codomain node of the whole diagram) whenever they are connected. There is also a node for each box and an edge from that box node to its domain and codomain nodes. First, we initialise the graph of the identity diagram and feed the objects of its codomain as input to the decorated function. When a box is applied to a list of nodes, it adds edges going into each object of its domain and returns nodes for each object of its codomain. Finally, the return value of the decorated function is taken as the codomain of the whole diagram.

Listing 1.2.35. Translation from **Diagram** to **Graph**.

We use the graph data structure from NetworkX [HSSC08].

```

from networkx import Graph

Node = namedtuple('Node', ['kind', 'label', 'i', 'j'])

def diagram2graph(diagram: Diagram) -> Graph:
    graph = Graph()
    scan = [Node('dom', x, i, -1) for i, x in enumerate(diagram.dom)]
    graph.add_edges(zip(scan, scan))
    for j, (left, box, _) in enumerate(diagram.layers):
        box_node = Node('box', box, -1, j)
        dom_nodes = [Node('dom', x, i, j) for i in enumerate(box.dom)]
        cod_nodes = [Node('cod', x, i, j) for i in enumerate(box.cod)]
        graph.add_edges(zip(scan[len(left): len(left @ box.dom)], dom_nodes))
        graph.add_edges(zip(dom_nodes, len(box.dom) * [box_node]))
        graph.add_edges(zip(len(box.cod) * [box_node], cod_nodes))
        scan = scan[len(left):] + cod_nodes + scan[len(left @ box.dom):]
    graph.add_edges(zip(scan, [
        Node('cod', x, i, len(diagram)) for i, x in enumerate(diagram.cod)]))
    return graph

```

The `graph2diagram` algorithm which translates the resulting graph into a diagram will be covered in the next section. It will allow to automatically read *pictures of diagrams* (i.e. matrices of pixels) and translate them into `Diagram` objects. Note that in order to construct a `monoidal.Diagram` we need to assume *plane graphs* as input, i.e. graphs with an embedding in the plane. We also need to assume that every codomain node is connected to exactly one domain node. In sections 1.4 and 1.6 we will discuss the case of diagrams induced by non-planar graphs, with potentially multiple edges between domain and codomain nodes. Listing 1.2.35 shows the implementation of the inverse translation `diagram2graph` which outputs only planar graphs as we will show in the next section by constructing their embedding in the plane, i.e. their drawing.

1.3 Drawing & reading

The previous section defined diagrams as a data structure based on lists of layers, in this section we define *pictures of diagrams*. Concretely, such a picture will be encoded in a computer memory as a bitmap, i.e. a matrix of colour values. Abstractly, we will define these pictures in terms of topological subsets of the Cartesian plane. We first recall the topological definition from Joyal's and Street's unpublished manuscript *Planar diagrams and tensor algebra* [JS88] and then discuss the isomorphism between the two definitions. In one direction, the isomorphism sends a `Diagram` object to its drawing. In the other direction, it reads the picture of a diagram and translates it into a `Diagram` object, i.e. its domain, codomain and list of layers.

1.3.1 Labeled generic progressive plane graphs

A *topological graph*, also called 1-dimensional cell complex, is a tuple (G, G_0, G_1) of a Hausdorff space G and a pair of a closed subset $G_0 \subseteq G$ and a set of open subsets $G_1 \subseteq P(G)$ called *nodes* and *wires* respectively, such that:

- G_0 is discrete and $G - G_0 = \bigcup G_1$,
- each wire $e \in G_1$ is homeomorphic to an open interval and its boundary is contained in the nodes $\partial e \subseteq G_0$.

From a topological graph G , one can construct an undirected graph in the usual sense by forgetting the space G , taking G_0 as nodes and edges $(x, y) \in G_0 \times G_0$

for each $e \in G_1$ with $\partial e = \{x, y\}$. A topological graph is finite (planar) if its undirected graph is finite (planar, i.e. there is some embedding in the plane).

A *plane graph* between two real numbers $a < b$ is a finite, planar topological graph G with an embedding in $\mathbb{R} \times [a, b]$. We define the domain $\text{dom}(G) = G_0 \cap \mathbb{R} \times \{a\}$, the codomain $\text{cod}(G) = G_0 \cap \mathbb{R} \times \{b\}$ as lists of nodes ordered by horizontal coordinates and the set $\text{boxes}(G) = G_0 \cap \mathbb{R} \times (a, b)$. We require that:

- $G \cap \mathbb{R} \times \{a\} = \text{dom}(G)$ and $G \cap \mathbb{R} \times \{b\} = \text{cod}(G)$, i.e. the graph touches the horizontal boundaries only at domain and codomain nodes,
- every domain and codomain node $x \in G \cap \mathbb{R} \times \{a, b\}$ is in the boundary of exactly one wire $e \in G_1$, i.e. wires can only meet at box nodes.

A plane graph is *generic* when the projection on the vertical axis $p_1 : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is injective on $G_0 - \mathbb{R} \times \{a, b\}$, i.e. no two box nodes are at the same height. From a generic plane graph, we can get a list $\text{boxes}(G) \in G_0^*$ ordered by height. A plane graph is *progressive* (also called *recumbent* by Joyal and Street) when p_1 is injective on each wire $e \in G_1$, i.e. wires go from top to bottom and do not bend backwards.

From a progressive plane graph G , one can construct a directed graph by forgetting the space G , taking G_0 as nodes and edges $(x, y) \in G_0 \times G_0$ for each $e \in G_1$ with $\partial e = \{x, y\}$ and $p_1(x) < p_1(y)$. We can also define the domain and the codomain of each box node $\text{dom}, \text{cod} : \text{boxes}(G) \rightarrow G_1^*$ with $\text{dom}(x) = \{e \in G_1 \mid \partial e = \{x, y\}, p_1(x) < p_1(y)\}$ the wires coming in from the top and $\text{cod}(x) = \{e \in G_1 \mid \partial e = \{x, y\}, p_1(x) > p_1(y)\}$ the wires going out to the bottom, these sets are linearly ordered as follows. Take some $\epsilon > 0$ such that the horizontal line at height $p_1(x) - \epsilon$ crosses each of the wires in the domain. Then list $\text{dom}(x) \in G_1^*$ in order of horizontal coordinates of their intersection points, i.e. $e < e'$ if $p_0(y) < p_0(y')$ for the projection $p_0 : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ and $y^{(\prime)} = e^{(\prime)} \cap \{p_1(x) - \epsilon\} \times \mathbb{R}$. Symmetrically we define the list of codomain nodes $\text{cod}(x) \in G_1^*$ with a horizontal line at $p_1 + \epsilon$.

A *labeling* of progressive plane graph G by a monoidal signature Σ is a pair of functions from wires to objects $\lambda : G_1 \rightarrow \Sigma_0$ and from boxes to boxes $\lambda : \text{boxes}(G) \rightarrow \Sigma_1$ which commutes with the domain and codomain. From an lgpp (*labeled generic progressive plane*) graph, one can construct a **Diagram**.

Listing 1.3.1. Translation from labeled generic progressive plane graphs to **Diagram**.

```
def read( G,  $\lambda : G_1 \rightarrow \text{Ty}$ ,  $\lambda : \text{boxes}(G) \rightarrow \text{Box}$  ) -> Diagram:
    dom = [  $\lambda(e)$  for  $x \in \text{dom}(G)$  for  $e \in G_1$  if  $x \in \partial e$  ]
    boxes = [  $\lambda(x)$  for  $x \in \text{boxes}(G)$  ]
    offsets = [  $\text{len}( G_1 \cap \{p_0(x)\} \times \mathbb{R} )$  for  $x \in \text{boxes}(G)$  ]
    return decode(dom, zip(boxes, offsets))
```

1.3.2 From diagrams to graphs and back

In the other direction, there are many possible ways to draw a given **Diagram** as a lgpp graph, i.e. to embed its graph into the plane. Vicary and Delpuch [DV18] give a linear-time algorithm to compute such an embedding with the following disadvantage: the drawing of a tensor $f \otimes g$ does not necessarily look like the horizontal juxtaposition of the drawings for f and g . For example, if we tensor an identity with a scalar, the wire representing the identity will wiggle around the node representing the scalar. DisCoPy uses a quadratic-time drawing algorithm with the following design decision: we make every wire a straight line and as vertical as possible. We first initialise the lgpp graph of the identity with a constant spacing between each wire, then for each layer we update the embedding so that there is enough space for the output wires of the box before we add it to the graph.

Listing 1.3.2. Outline of **Diagram.draw** from **Diagram** to **PlaneGraph**.

```
Embedding = dict[Node, tuple[float, float]]
PlaneGraph = tuple[Graph, Embedding]

def draw(self: Diagram) -> PlaneGraph:
    graph = diagram2graph(self)
    def make_space(scan: list[Node], box: Box, offset: int) -> float:
        """ Update the graph to make space and return the left of the box. """
    box_nodes = [Node('box', box, -1, j) for j, box in enumerate(self.boxes)]
    dom_nodes = scan = [Node('dom', x, i, -1) for i, x in enumerate(self.dom)]
    position = {node: (i, -1) for i, node in enumerate(dom_nodes)}
    for j, (left, box, _) in enumerate(self.layers):
        box_node, left_of_box = Node('box', box, -1, j), make_space(scan, box, offset)
        position[box_node] = (left_of_box + max(len(box.dom), len(box.cod)) / 2, j)
        for kind, epsilon in (('dom', -.1), ('cod', .1)):
            for i, x in enumerate(getattr(box, kind)):
                position[Node(kind, x, i, j)] = (left_of_box + i, j + epsilon)
```

```

box_cod_nodes = [Node('cod', x, i, j) for i, x in enumerate(box.cod)]
scan = scan[:len(left)] + box_cod_nodes + scan[len(left @ box.dom):]
for i, x in enumerate(self.cod):
    position[Node('cod', x, i, len(self))] = (position[scan[i]][0], len(self))
return graph, position

```

```
Diagram.draw = draw
```

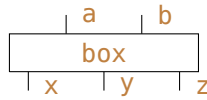
Note that when we draw the plane graph for a diagram, we do not usually draw the box nodes as points. Instead, we draw them as boxes, i.e. a box node $x \in \text{boxes}(G)$ is depicted as the rectangle with corners $(l, p_1(x) \pm \epsilon)$ and $(r, p_1(x) \pm \epsilon)$ for $l, r \in \mathbb{R}$ the left- and right-most coordinate of its domain and codomain nodes. In this way, we do not need to draw the in- and out-going wires of the box node: they are hidden by the rectangle. Exceptions include *spider boxes* where we draw the box node (the head) and its outgoing wires (the legs of the spider) as well as *swap*, *cup* and *cap boxes* where we do not draw the box node at all, only its outgoing wires which are drawn as Bézier curves to look like swaps, cups and caps respectively. These special boxes will be discussed, and drawn, in section 1.4.

Example 1.3.3. Drawing of a box, an identity, a layer, a composition and a tensor.

```

a, b, c, x, y, z, w = map(Ty, "abcxyzw")
Box('box', a @ b, x @ y @ z).draw()

```



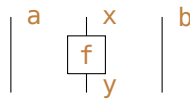
```
Diagram.id(x @ y @ z).draw()
```



```

layer = a @ Box('f', x, y) @ b
layer.draw()

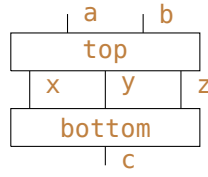
```



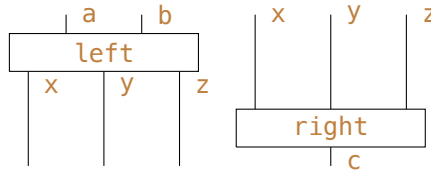
```

top, bottom = Box('top', a @ b, x @ y @ z), Box('bottom', x @ y @ z, c)
(top >> bottom).draw()

```

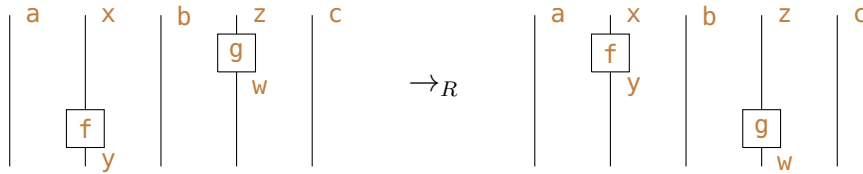


```
left, right = Box('left', a @ b, x @ y @ z), Box('right', x @ y @ z, c)
(left @ right).draw()
```



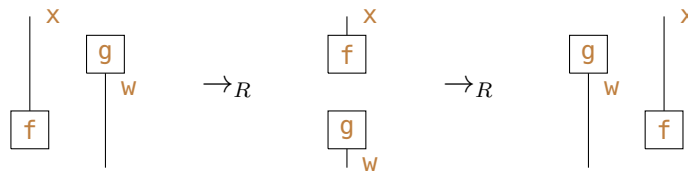
Example 1.3.4. Drawing of the interchanger in the general case.

```
f, g = Box('f', x, y), Box('g', z, w)
(a @ f @ b @ g @ c).interchange(0).draw(); (a @ f @ b @ g @ c).draw()
```



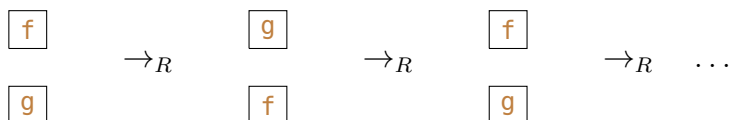
Example 1.3.5. Drawing of the interchangers for an effect then a state.

```
f, g = Box('f', x, Ty()), Box('g', Ty(), w)
(f >> g).interchange(0).draw()
(f >> g).draw()
(f >> g).interchange(0, left=True).draw()
```



Example 1.3.6. Drawing of the Eckmann-Hilton argument.

```
f, g = Box('f', Ty(), Ty()), Box('g', Ty(), Ty())
(f @ g).draw()
(f @ g).interchange(0).draw()
(f @ g).interchange(0).interchange(0).draw()
```



Example 1.3.7. *The following spiral diagram is the cubic worst-case for interchanger normal form. It is also the quadratic worst-case for drawing, at each layer of the first half we need to update the position of every preceding layer in order to make space for the output wires.*

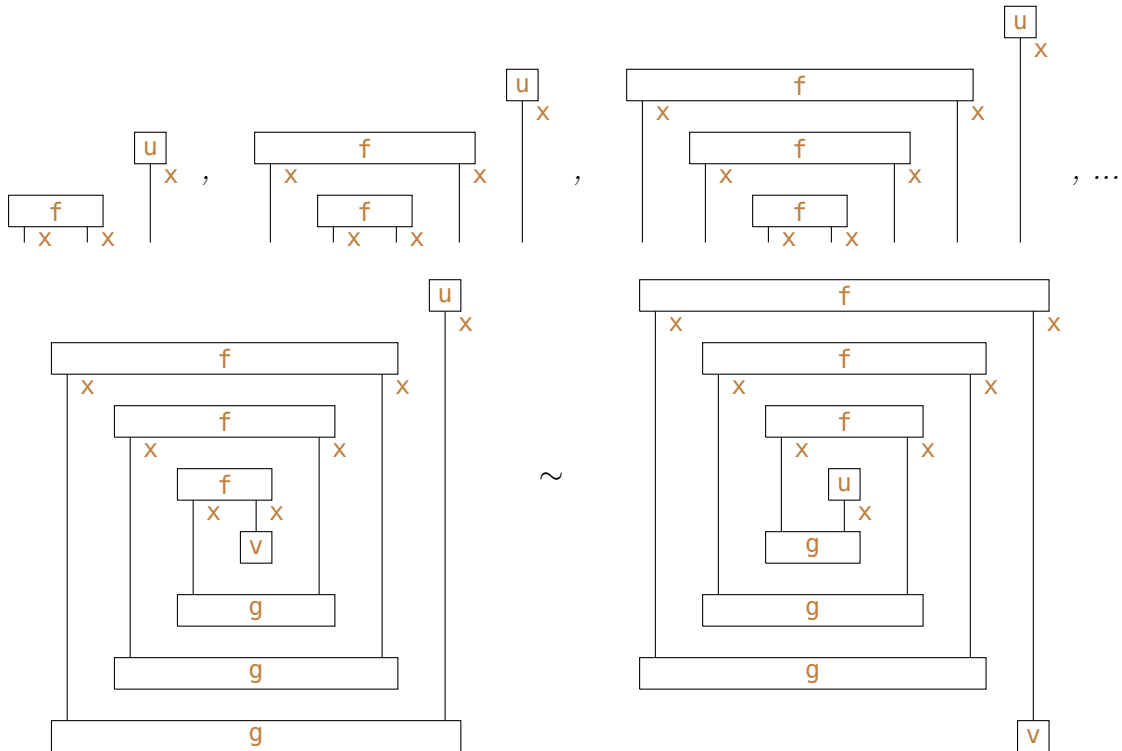
```

x = Ty('x')
f, g = Box('f', Ty(), x @ x), Box('g', x @ x, Ty())
u, v = Box('u', Ty(), x), Box('v', x, Ty())

def spiral(length: int) -> Diagram:
    diagram, n = u, length // 2 - 1
    for i in range(n): diagram >=> Id(x ** i) @ f @ Id(x ** (i + 1))
    diagram >=> Id(x ** n) @ v @ Id(x ** n)
    for i in range(n): diagram >=> Id(x ** (n - i - 1)) @ g @ Id(x ** (n - i - 1))
    return diagram

diagram = spiral(8)
for i in [1, 2, 3]: diagram[:i + 1].draw()
diagram.draw(); diagram.normal_form().draw()

```



Next, we define the inverse translation `graph2diagram`.

Listing 1.3.8. Translation from `PlaneGraph` to `Diagram`.

```

def graph2diagram(graph: Graph, position: Embedding) -> Diagram:
    dom = Ty(*[node.label for node in graph.nodes if node.kind == 'dom' and node.j == -1])
    boxes = [node.label for node in graph.nodes if node.kind == 'box']
    scan, offsets = [Node('dom', x, i, -1) for i, x in enumerate(dom)], []
    for j, box in enumerate(boxes):
        left_of_box = position[Node('dom', box.dom[0], 0, j)][0]\
            if box.dom else position[Node('box', box, -1, j)][0]
        offset = len([node for node in scan if position[node][0] < left_of_box])
        box_cod_nodes = [Node('cod', x, i, j) for i, x in enumerate(box.cod)]
        scan = scan[:offset] + box_cod_nodes + scan[offset + len(box.dom):]
        offsets.append(offset)
    return decode(dom, zip(boxes, offsets))

```

Theorem 1.3.9. `graph2diagram(self.draw()) == self` for all `self: Diagram`.

Proof. By induction on `n = len(self.layers)`. If `not len(self.layers)` we get that `dom == self.dom` and `boxes == offsets == []`. If the theorem holds for `self`, it holds for `self >> Layer(left, box, right)`. Indeed, we have:

- `dom == self.dom` and `boxes == self.boxes + [box]`
- `(x, Node('cod', self.cod[i], i, n)) in graph` for `i, x in enumerate(scan)`

Moreover, the horizontal coordinates of the nodes in `scan` are strictly increasing, thus we get the desired `offsets == self.offsets + [len(left)]`. \square

From a labeled generic progressive plane graph, we get a unique diagram *up to deformation*. A deformation $h : G \rightarrow G'$ between two labeled plane graphs G, G' is a continuous map $h : G \times [0, 1] \rightarrow \mathbb{R} \times \mathbb{R}$ such that:

- $h(G, t)$ is a plane graph for all $t \in [0, 1]$, $h(G, 0) = G$ and $h(G, 1) = G'$,
- $x \in \text{boxes}(G)$ implies $h(x, t) \in \text{boxes}(h(G, t))$ for all $t \in [0, 1]$,
- $h(G, t) \models \lambda = \lambda$ for all $t \in [0, 1]$, i.e. the labels are preserved throughout.

A deformation is progressive (generic) when $h(G, t)$ is progressive (generic) for all $t \in [0, 1]$. We write $G \sim G'$ when there exists some deformation $h : G \rightarrow G'$, this defines an equivalence relation.

Theorem 1.3.10. For all lgpp graphs G , `Diagram.draw(graph2diagram(G))` $\sim G$ up to generic progressive deformation.

Proof. By induction on the length of `boxes(G)`. If there are no boxes, G is the graph of the identity and we can deform it so that each wire is vertical with constant spacing. If there is one box, G is the graph of a layer and we can cut it in three vertical slices with the box node and its outgoing wires in the middle. We can apply the case of the identity to the left and right slices, for the middle slice we make the wires straight with a constant spacing between the domain and codomain. Because G is generic, we can cut a graph with $n > 2$ boxes in two horizontal slices between the last and the one-before-last box, then apply the case for layers and the induction hypothesis. To glue the two slices back together while keeping the wires straight, we need to make space for the wires going out of the box.

This deformation is indeed progressive, i.e. we never bend wires we only make them straight. It is also generic, i.e. we never move a box node past another. \square

Theorem 1.3.11. *There is a progressive deformation $h : G \rightarrow G'$ between two lgpp graphs iff `graph2diagram(G) == graph2diagram(G')` up to interchanger.*

Proof. By induction on the number n of *coincidences*, the times at which the deformation h fails to be generic, i.e. two or more boxes are at the same height. WLOG (i.e. up to continuous deformation of deformations) this happens at a discrete number of time steps $t_1, \dots, t_n \in [0, 1]$. Again WLOG at each time step there is at most two boxes at the same height, e.g. if there are two boxes moving below a third at the same time, we deform the deformation so that they move one after the other. The list of boxes and offsets is preserved under generic deformation, thus if $n = 0$ then `graph2diagram(G) == graph2diagram(G')` on the nose. If $n = 1$, take `i: int` the index of the box for which the coincidence happens and `left: bool` whether it is a left or right interchanger, then `graph2diagram(G).interchange(i, left) == graph2diagram(G')`. Given a deformation with $n + 1$ coincidences, we can cut it in two time slices with 1 and n coincidences respectively then apply the cases for $n = 1$ and the induction hypothesis.

For the converse, a proof of `graph2diagram(G) == graph2diagram(G')`, i.e. a sequence of n interchangers, translates into a deformation with n coincidences. DisCoPy can output these proofs as videos using `Diagram.normalize` to iterate through the rewriting steps and `Diagram.to_gif` to produce a `.gif` file. \square

1.3.3 A natural isomorphism

We have established an isomorphism between the class of lgpp graphs (up to progressive deformation) and the class of `Diagram` objects (up to interchanger).

It remains to show that this actually forms an isomorphism of monoidal categories. That is for every monoidal signature Σ , there is a monoidal category $G(\Sigma)$ with objects Σ_0^* and arrows the equivalence classes of lgpp graphs with labels in Σ . The domain and codomain of an arrow is given by the labels of the domain and codomain of the graph. The identity $\text{id}(x_1 \dots x_n)$ is the graph with wires $(i, a) \rightarrow (i, b)$ for $i \leq n$ and $a, b \in \mathbb{R}$ the horizontal boundaries. The tensor of two graphs G and G' is given by horizontal juxtaposition, i.e. take $w = \max(p_0(G)) + 1$ the right-most point of G plus a margin and set $G \otimes G' = G \cup \{(p_0(x) + w, p_1(x)) \mid x \in G'\}$. The composition $G \circ G'$ is given by vertical juxtaposition and connecting the codomain nodes of G to the domain nodes of G' . That is, $G \circ G' = s^+(G) \cup s^-(G') \cup E$ for $s^\pm(x) = (p_0(x), \frac{p_1(x) \pm (b-a)}{2})$ and wires $s^+(\text{cod}(G)_i) \rightarrow s^-(\text{dom}(G')_i) \in E$ for each $i \leq \text{len}(\text{cod}(G)) = \text{len}(\text{dom}(G'))$.

The deformations for the unitality axioms are straightforward: there is a deformation $G \circ \text{id}(\text{cod}(G)) \sim G \sim \text{id}(\text{dom}(G)) \circ G$ which contracts the wires of the identity graph, the unit of the tensor is the empty diagram so we have an equality $G \otimes \text{id}(1) = G = \text{id}(1) \otimes G$. The deformations for the associativity axioms are better described by the hand-drawn diagrams of Joyal and Street in figure 1.1.

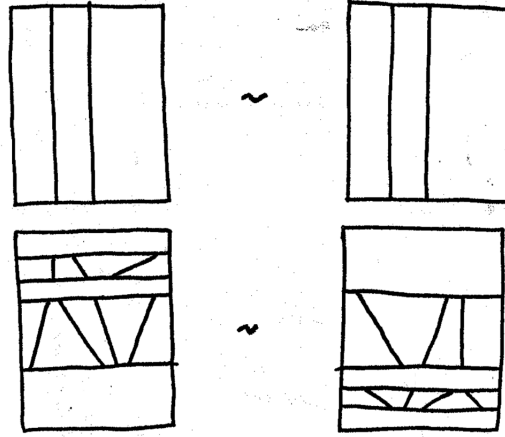


Figure 1.1: Deformations for the associativity of tensor and composition.

The interchange law holds on the nose, i.e. $(G \otimes G') \circ (H \otimes H') = (G \circ H) \otimes (G' \circ H')$, as witnessed by figure 1.2, the hand-drawn diagram which is the result of both sides.

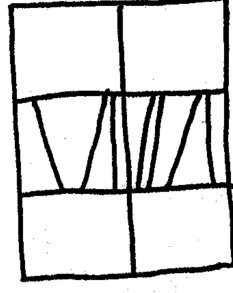


Figure 1.2: The graph of the interchange law.

Thus, we have defined a monoidal category $G(\Sigma)$. Given a morphism of monoidal signatures $f : \Sigma \rightarrow \Gamma$, there is a functor $G(f) : G(\Sigma) \rightarrow G(\Gamma)$ which sends a graph to itself relabeled with $f \circ \lambda$, its image on arrows is given in listing 1.3.12. Hence, we have defined a functor $G : \mathbf{Monsig} \rightarrow \mathbf{MonCat}$ which we claim is naturally isomorphic to the free functor $F : \mathbf{Monsig} \rightarrow \mathbf{MonCat}$ defined in the previous section.

Listing 1.3.12. Implementation of the functor $G : \mathbf{Monsig} \rightarrow \mathbf{MonCat}$.

```
SigMorph = tuple[dict[Ob, Ob], dict[Box, Box]]

def G(f: SigMorph) -> Callable[[Graph], Graph]:
    def G_of_f(graph: Graph) -> Graph:
        relabel = lambda node: Node('box', f[1][node.label], node.i, node.j)\
            if node.kind == 'box'\
            else Node(node.kind, f[0][node.label], node.i, node.j)
        return Graph(map(relabel, graph.edges))
    return G_of_f
```

Theorem 1.3.13. *There is a natural isomorphism $F \simeq G$.*

Proof. From theorems 1.3.10 and 1.3.11, we have an isomorphism between **Diagram** and **PlaneGraph** given by $d2g = \mathbf{Diagram.draw}$ and $g2d = \mathbf{graph2diagram}$, up to deformation and interchanger respectively. Now define the image of F on arrows $F = \lambda f: \mathbf{Functor}(ob=f[0], ar=f[1])$. Given a morphism of monoidal signatures $f: \mathbf{SigMorph}$ we have the following two naturality squares.

$$\begin{array}{ccc}
 \mathbf{Diagram} & \xrightarrow{d2g} & \mathbf{PlaneGraph} \\
 F(f) \downarrow & & \downarrow G(f) \\
 \mathbf{Diagram} & \xrightarrow{d2g} & \mathbf{PlaneGraph}
 \end{array}
 \quad \text{and} \quad
 \begin{array}{ccc}
 \mathbf{PlaneGraph} & \xrightarrow{g2d} & \mathbf{Diagram} \\
 G(f) \downarrow & & \downarrow F(f) \\
 \mathbf{PlaneGraph} & \xrightarrow{g2d} & \mathbf{Diagram}
 \end{array}$$

□

1.3.4 Daggers, sums and bubbles

As in the previous sections, we now discuss the drawing of daggers, sums and bubbles. When we draw a diagram in the free \dagger -monoidal category, we add some asymmetry to the drawing of each box so that it looks like the vertical reflection of its dagger.

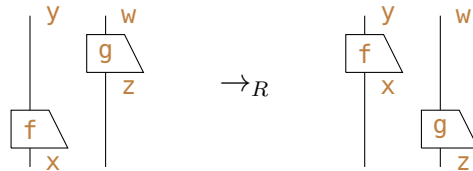
Example 1.3.14. Drawing of the axiom for unitaries.

```
f, g = Box('f', x, y), Box('g', z, w)
(f >> f[::-1]).draw(); Diagram.id(x).draw(); (f[::-1] >> f).draw(); Diagram.id(y).draw()
```



Example 1.3.15. Drawing of the axiom for \dagger -monoidal categories.

```
f, g = Box('f', x, y), Box('g', z, w)
(f @ g)[::-1].draw(); (f[::-1] @ g[::-1]).draw()
assert (f @ g)[::-1].normal_form() == f[::-1] @ g[::-1]
```

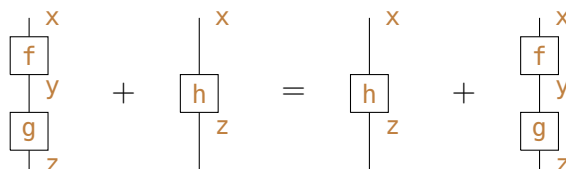


When we draw a sum, we just draw each term with an addition symbol in between. More generally, `drawing.equation` allows to draw any list of diagrams and `drawing.Equation` allows to draw equations within equations.

Example 1.3.16. Drawing of a commutativity equation.

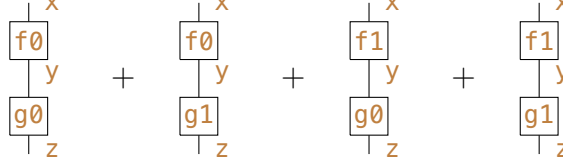
```
from discopy import drawing

f, g, h = Box('f', x, y), Box('g', y, z), Box('h', x, z)
drawing.equation(drawing.Equation(f >> g, h, symbol='$+$'),
                 drawing.Equation(h, f >> g, symbol='$+$'))
```

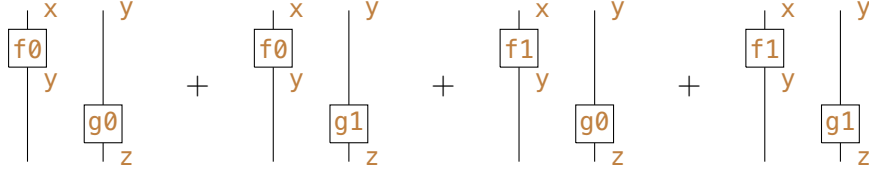


Example 1.3.17. Drawing a composition and tensor of sums.

```
f0, g0 = Box("f0", x, y), Box("g0", y, z)
f1, g1 = Box("f1", x, y), Box("g1", y, z)
((f0 + f1) >> (g0 + g1)).draw()
```



```
((f0 + f1) @ (g0 + g1)).draw()
```

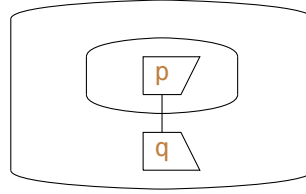
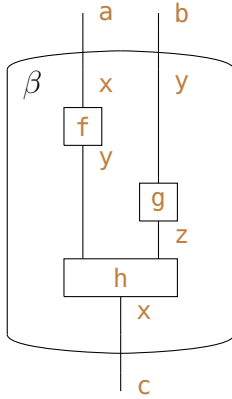


The case of drawing bubbles is more interesting. One solution would be to draw the bubble as a rectangle like any other box, then draw the content of the bubble inside the rectangle. However, this would require some clever scaling so that the boxes of the diagram inside the bubble have the same size as the boxes outside, i.e. we would need to add more complexity to our drawing algorithm. The solution implemented in DisCoPy is to apply a faithful functor `downgrade` : $F(\Sigma^\beta) \rightarrow F(\Sigma \cup \text{open}^\beta \cup \text{close}^\beta)$ from the free monoidal category with bubbles $F(\Sigma^\beta)$ to the free monoidal category generated by the following signature. Take the objects $\text{open}_0^\beta = \text{close}_0^\beta = \Sigma_0 + \{\bullet\}$ and boxes for opening $\text{open}^\beta(x) : \beta_{\text{dom}}(x) \rightarrow \bullet \otimes x \otimes \bullet$ and closing $\text{close}^\beta(x) : \bullet \otimes x \otimes \bullet \rightarrow \beta_{\text{cod}}(x)$ bubbles for each type $x \in \Sigma_0^*$. Now define $\text{downgrade}(\text{f.bubble}()) = \text{open}^\beta(\text{f.dom}) \circ (\bullet \otimes \text{f} \otimes \bullet) \circ \text{close}^\beta(\text{f.cod})$ for any diagram `f` inside a bubble. That is, we draw a bubble as its opening, its inside with identity wires on both sides then its closing. The \bullet -labeled wires are drawn with Bézier curves so that the bubble looks a bit closer to a circle than a rectangle. In the case of bubbles that are length-preserving on objects, we also want to override the drawing of its opening and closing boxes so that the wires go straight through the bubble rather than meeting at the box node.

Example 1.3.18. Drawing of a bubbled diagram and a first-order logic formula.

```
f, g, h = Box('f', x, y), Box('g', y, z), Box('h', y @ z, x)
(f @ g >> h).bubble(dom=a @ b, cod=c, name="$\\beta$").draw()
```

```
men, mortal = Predicate('p'), Predicate('q')
(men.cut() >> mortal.dagger()).cut().draw()
```



1.3.5 Automatic diagram recognition

We conclude this section with an application of theorem 1.3.13 to *automatic diagram recognition*: turning pictures of diagrams into diagrams. In listing 1.3.1, we described an abstract reading algorithm which took lgpp graphs as input and returned diagrams. We make it a concrete algorithm by taking *bitmaps* as input: grids of Boolean pixels describing a black-and-white picture. The algorithm `read` listed below takes as input a pair of bitmaps for the box nodes and the wires of the plane graph, it returns a `Diagram`. It is more general than the `graph2diagram` algorithm of listing 1.3.1 where we assumed that the embedding of the graph looked like the output of `Diagram.draw`. i.e. that edges are straight vertical lines. Indeed, our reading algorithm will accept *any bitmaps* as input and always return a valid diagram, however bended the edges are. If the bitmaps indeed represent a progressive generic plane graph G , then we get `read(G).draw() ~ G` up to progressive generic deformation. If not, the output will still be a diagram but its drawing may not look anything like the input.

Listing 1.3.19. Implementation of the abstract reading algorithm of listing 1.3.1.

```
from numpy import array, argmin
from skimage.measure import regionprops, label

def read(box_pixels: array, wire_pixels: array) -> Diagram:
    connected_components = lambda img: regionprops(label(img))
    box_nodes, wires = map(connected_components, (box_pixels, wire_pixels))
    source, target, length, width = [], [], len(box_pixels), len(box_pixels[0])
    critical_heights = [0] + [int(node.centroid[0]) for node in box_nodes] + [length]
    for wire, region in enumerate(wires):
        top, bottom = (minmax(i for i, _ in region.coords) for minmax in (min, max))
        source.append(argmin(abs(array(critical_heights) - top)))
        target.append(argmin(abs(array(critical_heights) - bottom)))
```

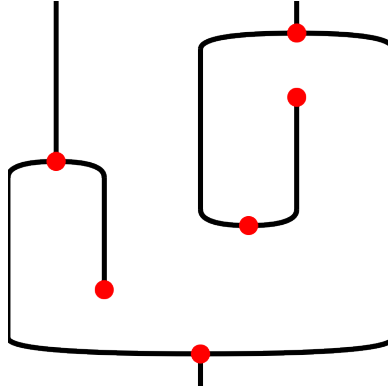
```

scan = [wire for wire, node in enumerate(source) if node == 0]
dom, boxes_and_offsets = Ty('x') ** len(scan), []
for depth, box_node in enumerate(box_nodes):
    input_wires = [wire for wire in scan if target[wire] == depth + 1]
    output_wires = [wire for wire, node in enumerate(source) if node == depth + 1]
    dom, cod = Ty('x') ** len(input_wires), Ty('x') ** len(output_wires)
    box = Box('box_{}_{}'.format(len(dom), len(cod)), dom, cod)
    height, left = map(int, box_node.centroid)
    left_of_box = [wire for wire in scan if wire not in input_wires
                   and dict(wires[wire].coords).get(height, width) < left]
    offset = max(len(left_of_box), 0)
    boxes_and_offsets.append((box, offset))
    scan = scan[:offset] + output_wires + scan[offset + len(input_wires):]
return decode(dom, boxes_and_offsets)

```

We use the `array` data structure of NumPy [vCV11] for bitmaps. We compute the connected components of box and wire pixels with Scikit-Image [Wal+14], using their default ordering by lexicographic order of top-left pixel. We then define a list of critical heights: the top of the picture, the height of the centroid of each box component, then the bottom of the picture. For each wire component, we define its source and target as the closest critical height to its top-most and bottom-most pixel. We define the domain of the diagram as the list of wires with the domain as source. We then scan through the picture top to bottom, keeping a list `scan` of the open wires at each height. For each box, we find its input wires in this list and define the offset as the number of wires left of the box node that are not inputs, then we update `scan` with the output wires. We get an encoding `dom`, `boxes_and_offsets` which yields a valid diagram by construction.

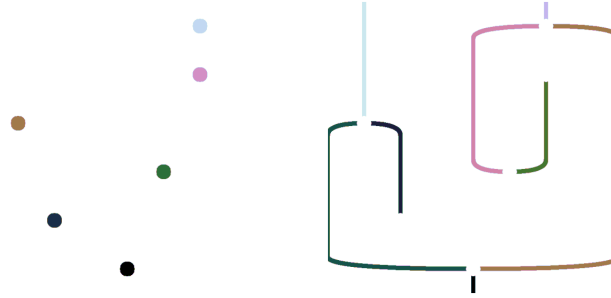
Example 1.3.20. *Suppose we take the following picture of a diagram as input, where the red pixels are boxes and the black pixels are wires:*



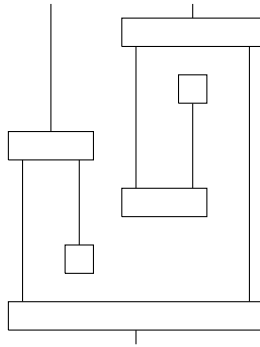
We count $\{1, \dots, 6\}$ boxes and 8 wires

$$\{0 \rightarrow 3, 0 \rightarrow 1, 1 \rightarrow 4, 1 \rightarrow 6, 2 \rightarrow 4, 3 \rightarrow 6, 3 \rightarrow 5, 6 \rightarrow 7\}$$

for 0 and 7 the domain and codomain of the whole diagram respectively.

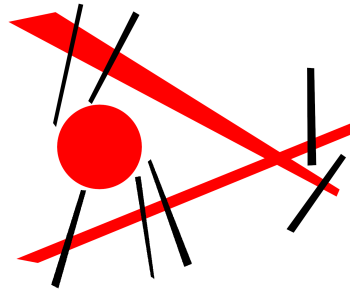


From this, we reconstruct the following diagram by scanning top to bottom:



which is indeed equal to the input picture, up to generic progressive deformation.

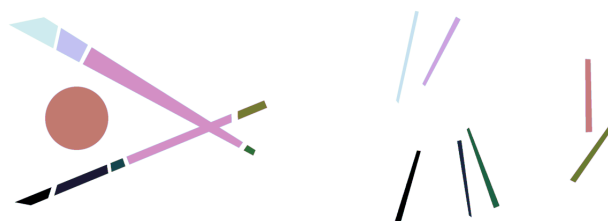
Example 1.3.21. Suppose we start from the following pastiche of Kandinsky's Punkt und linie zu fläche (point and line on the plane):



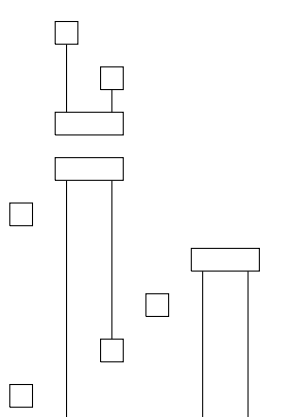
We count $\{1, \dots, 9\}$ boxes and 7 wires

$$\{0 \rightarrow 3, 1 \rightarrow 3, 2 \rightarrow 4, 4 \rightarrow 8, 4 \rightarrow 9, 6 \rightarrow 10, 6 \rightarrow 10\}$$

for 0 and 10 the domain and codomain of the whole diagram respectively.



From this, we reconstruct the following diagram by scanning top to bottom:



which looks nothing like the input because Kandinsky's abstract paintings are not generic progressive plane graphs.

What could be the applications of such a reading algorithm? Of course, real-world pictures do not come in clean red and black bitmaps. We need some more computer vision to label each pixel as belonging either to a box, a wire or the background. This can be achieved by training a convolutional neural network on a large number of example pictures, each annotated with their red and black bitmaps. Once we have trained the machine to classify whether pixels belong to a box or wire, we can also train it to output the label of each pixel, i.e. the label of the box or wire it belongs to. With enough training data, we could automatically turn pictures of Bob's blackboard into circuits that we can execute on a quantum computer. Less trivially, this could be applied to *document layout analysis*: from the picture of say, a hand-drawn calendar from the middle ages, we could train our recognition algorithm to output a diagram that encodes the structure of the calendar. In previous work [Bor+19], we trained convolutional neural networks to extract lines of text in medieval manuscripts, but we had to exclude calendars from our analysis due to the complexity of their layouts. Our diagram recognition machines would enhance the automated analysis of such hand-drawn documents with structured layouts.

Our simple algorithm is robust to any deformation of lgpp graph, but there is much room for improvement. The easiest assumption to remove is genericity, i.e. boxes need not be at distinct heights. Non-generic progressive plane graphs, i.e. with potentially horizontal wires between boxes at the same height, have been characterised as the arrows of free *double categories*. Delpeuch [Del20] shows how they can be encoded as lgpp graphs with an extra label on each wire for whether it is horizontal or vertical. We can also remove the progressivity assumption, i.e. wires can bend backwards. We have two options: either a) we write a geometric algorithm than can find the endpoints of any bended wire, or b) we train another neural network to detect each point of non-progressivity, i.e. the cups and caps where the vertical derivative of a wire changes sign. Such non-progressive plane graphs can be encoded as lgpp graphs with *cups and caps boxes*, they are the arrows of free *pivotal categories* which we discuss in section 1.4.2.

Next, we can get rid of the planarity assumption: the projection of the topological graph onto the plane need not be an embedding, i.e. wires can cross. We can improve our reading algorithm in a similar way: either a) some geometric algorithm or b) some black-box neural network that can detect the points of non-planarity, i.e. the intersection of wires. Such non-planar progressive graphs can be encoded as lgpp graphs with *swap boxes*, they are the arrows of free *symmetric monoidal categories* which we discuss in section 1.4.3. Non-planar non-progressive graphs, i.e. where wires can bend and swap, are the arrows of free *compact closed categories*, which play the starring role in categorical quantum mechanics.

Finally, we can even remove the graph assumption: wires need not be homeomorphic to an open interval. We merely require that they are one-dimensional open subsets of the plane, i.e. wires can split and merge. We do not even need to assume that their boundary is in the nodes of the graph, i.e. wires can start or end anywhere in the plane. Again, we can improve our reading algorithm by encoding such hypergraphs (i.e. where wires can have any number of sources and targets) as lgpp graphs with *spider boxes* for the splits, merges, starts and ends of each wire. Labeled hypergraphs are the arrows of free *hypergraph categories*, which we discuss in section 1.4.4. In section 1.6, we discuss the relationship between this definition of hypergraph diagrams as (equivalence classes of) planar diagrams with swap and spider boxes and the more traditional graph-based definition.

1.4 Adding extra structure

This section looks at the implementation of monoidal categories with extra structure: rigid, symmetric, hypergraph and cartesian closed categories.

1.4.1 Cartesian closed categories

1.4.2 Rigid categories & wire bending

In sections 1.1 and 1.2 we discussed the fundamental notion of *adjunction* with the example of free-forgetful functors. The definition of left and right adjoints in terms of unit and counit natural transformations makes sense in **Cat**, but it can be translated in the context of any monoidal category C . An object $x^l \in C_0$ is the left adjoint of $x \in C_0$ whenever there are two arrows $\text{cup}(x) : x^l \otimes x \rightarrow 1$ and $\text{cap}(x) : 1 \rightarrow x \otimes x^l$ (also called counit and unit) such that:

- $\text{cap}(x) \otimes x \circ x \otimes \text{cup}(x) = \text{id}(x),$

$$\begin{array}{c} x \\ \text{cup}(x) \\ x^l \end{array} = \begin{array}{c} x \\ \text{id}(x) \end{array}$$

- $x^l \otimes \text{cap}(x) \circ \text{cup}(x) \otimes x^l = \text{id}(x^l).$

$$\begin{array}{c} x^l \\ \text{cap}(x) \\ x \end{array} = \begin{array}{c} x^l \\ \text{id}(x^l) \end{array}$$

This is equivalent to the condition that the functor $x^l \otimes - : C \rightarrow C$ is the left adjoint of $x \otimes - : C \rightarrow C$. Symmetrically, $x^r \in C_0$ is the right-adjoint of $x \in C_0$ if x is its left adjoint. We say that C is *rigid* (also called *autonomous*) if every object has a left and right adjoint. From this definition we can deduce a number of properties:

- adjoints are unique up to isomorphism,
- adjoints are monoid anti-homomorphisms, i.e. $(x \otimes y)^l \simeq y^l \otimes x^l$ and $1^l \simeq 1$,
- left and right adjoints cancel, i.e. $(x^l)^r \simeq x \simeq (x^r)^l$,

We say that C is strictly rigid whenever these isomorphisms are in fact equalities, again one can show that any rigid category is monoidally equivalent to a strict one. One can also show that cups and caps compose by nesting:

- $\mathbf{cup}(x \otimes y) = y^l \otimes \mathbf{cup}(x) \otimes y \circ \mathbf{cup}(y),$

$$\begin{array}{c} \text{Diagram 1: A cup with two inputs, } x \text{ (left) and } y \text{ (right), and one output, } (x \otimes y)^l \text{ (bottom).} \\ \text{Diagram 2: A cup with two inputs, } x \otimes y \text{ (left) and } y^l \text{ (right), and one output, } x^l \text{ (bottom).} \\ \text{Diagram 3: A cup with two inputs, } x \text{ (left) and } y^l \text{ (right), and one output, } x^l \text{ (bottom).} \end{array}$$

- $\mathbf{cap}(x \otimes y) = \mathbf{cap}(x) \circ x \otimes \mathbf{cap}(y) \otimes x^l,$

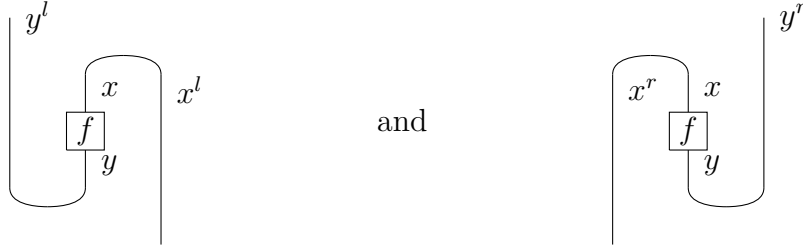
$$\begin{array}{c} \text{Diagram 1: A cap with two inputs, } (x \otimes y)^l \text{ (left) and } x^l \text{ (right), and one output, } x \otimes y \text{ (bottom).} \\ \text{Diagram 2: A cap with two inputs, } y^l \text{ (left) and } x^l \text{ (right), and one output, } x \otimes y \text{ (bottom).} \\ \text{Diagram 3: A cap with two inputs, } y^l \text{ (left) and } x \text{ (right), and one output, } y \text{ (bottom).} \end{array}$$

- and $\mathbf{cup}(1) = \mathbf{cap}(1) = \mathbf{id}(1).$

The first two equations are drawn as diagrams in a non-foo monoidal category, i.e. with wire for composite types and explicit boxes for equality. The last two equations would be drawn as the equality of empty diagrams. This can be taken as an inductive definition, once we have defined the cups and caps for generating objects, we have defined them for all types. Thus, we can take the data for a (strictly) rigid category C to be that of a free-on-objects monoidal category together with:

- a pair of unary operators $(-)^l, (-)^r : C_0 \rightarrow C_0$ on generating objects,
- and a pair of functions $\mathbf{cup}, \mathbf{cap} : C_0 \rightarrow C_1$ witnessing that x^l and x^r are the left and right adjoints of each generating object $x \in C_0$.

Diagrams in rigid categories are more flexible than monoidal categories: we can bend wires. They owe their name to the fact that they are less flexible than *pivotal categories*. For any rigid category C , there are two contravariant endofunctors, called the left and right *transpose* respectively. They send objects to their left and right adjoints, and each arrow $f : x \rightarrow y$ to



When these two functors are naturally isomorphic, C is called *pivotal*: we can rotate diagrams by 360 degrees. We say C is strictly pivotal when left and right transpose are equal. This is the case for any rigid category C with a dagger structure: the dagger of the cup (cap) for an object x is the cap (cup) of its left-adjoint x^l . When this is the case, C is called \dagger -pivotal.

Example 1.4.1. Recall from example 1.2.5 that for any category C , the category C^C of endofunctors and natural transformations is monoidal. Its subcategory with endofunctors that have both left and right adjoints is rigid. Its subcategory with endofunctors that have equal left and right adjoints is pivotal.

Example 1.4.2. $\text{Tensor}_{\mathbb{S}}$ is \dagger -pivotal with left and right adjoints given by list reversal, cups and caps by the Kronecker delta $\text{cup}(n)(i, j) = \text{cap}(n)(i, j) = 1$ if $i = j$ else 0. Note that for tensors of order greater than 2, the diagrammatic transpose defined in this way differs from the usual algebraic transpose: the former reverses list order while the latter is the identity on objects.

Example 1.4.3. Circ is \dagger -pivotal with the preparation of the Bell state as cap and the post-selected Bell measurement as cup (both are scaled by $\sqrt{2}$). The snake equations yield a proof of correctness for the (post-selected) quantum teleportation protocol.

Example 1.4.4. A rigid category which is also a preordered monoid (i.e. with at most one arrow between any two objects) is called a (quasi)¹ pregroup, their application to NLP will be discussed in section 2.1. A commutative pregroup is a (preordered) group: left and right adjoints coincide with the multiplicative inverse.

Natural examples of non-free non-commutative pregroups are hard to come by. One exception is the monoid of monotone unbounded integer functions with composition as multiplication and pointwise order. The left adjoint of $f : \mathbb{Z} \rightarrow \mathbb{Z}$ is defined such that $f^l(m)$ is the minimum $n \in \mathbb{Z}$ with $m \leq f(n)$ and symmetrically $f^r(m)$ is the maximum $n \in \mathbb{N}$ with $f(n) \leq m$.

¹In his original definition [Lam99b], Lambek also requires that pregroups are *partial orders*, i.e. preorders with antisymmetry $x \leq y$ and $y \leq x$ implies $x = y$. This implies that pregroups are strictly rigid, but also that they cannot be free on objects: $\text{cup}(x) \otimes \text{id}(x) : x \otimes x^l \otimes x \rightarrow x$ and $\text{id}(x) \otimes \text{cap}(x) : x \rightarrow x \otimes x^l \otimes x$ together would imply $x = x \otimes x^l \otimes x$.

Any monoidal functor $F : C \rightarrow D$ between two rigid categories C and D preserves left and right adjoints up to isomorphism, we say it is strict when it preserves them up to equality. Thus, we have defined a subcategory **RigidCat** \hookrightarrow **MonCat**. We define a *rigid signature* Σ as a monoidal signature where the generating objects have the form $\Sigma_0 \times \mathbb{Z}$. We identify $x \in \Sigma_0$ with $(x, 0) \in \Sigma_0 \times \mathbb{Z}$ and define the left and right adjoints $(x, z)^l = (x, z - 1)$ and $(x, z)^r = (x, z + 1)$. The objects Σ_0 are called *basic types*, their iterated adjoints $\Sigma_0 \times \mathbb{Z}$ are called *simple types*. The integer $z \in \mathbb{Z}$ is called the *adjunction number* of the simple type $(x, z) \in \Sigma_0 \times \mathbb{Z}$ by Lambek and Preller [PL07] and its *winding number* by Joyal and Street [JS88]. Again, a morphism of rigid signatures $f : \Sigma \rightarrow \Gamma$ is a pair of functions $f : \Sigma_0 \rightarrow \Gamma_0$ and $f : \Sigma_1 \rightarrow \Gamma_1$ which commute with domain and codomain.

There is a forgetful functor $U : \mathbf{RigidCat} \rightarrow \mathbf{RigidSig}$ which sends any strictly-rigid foo-monoidal category to its underlying rigid signature. We now describe its left-adjoint $F^r : \mathbf{RigidSig} \rightarrow \mathbf{RigidCat}$. Given a rigid signature Σ , we define a monoidal signature $\Sigma^r = \Sigma \cup \{\text{cup}(x)\}_{x \in \Sigma_0} \cup \{\text{cap}(x)\}_{x \in \Sigma_0}$. The free rigid category is the quotient $F^r(\Sigma) = F(\Sigma^r)/R$ of the free monoidal category by the snake equations R . That is, the objects are lists of simple types $(\Sigma_0 \times \mathbb{Z})^*$, the arrows are equivalence classes of diagrams with cup and cap boxes. This is implemented in the `rigid` module of DisCoPy as outlined below.

Listing 1.4.5. Implementation of objects and types of free rigid categories.

```
@dataclass
class Ob(cat.Ob):
    z: int

    l = property(lambda self: Ob(self.name, self.z - 1))
    r = property(lambda self: Ob(self.name, self.z + 1))

    @classmethod
    def upgrade(cls, old: cat.Ob) -> Ob:
        return old if isinstance(old, cls) else cls(str(old), z=0)

class Ty(monoidal.Ty, Ob):
    def __init__(self, objects=[]):
        monoidal.Ty.__init__(self, objects=map(Ob.upgrade, objects))

    l = property(lambda self: self.upgrade(Ty(*[x.l for x in self.objects[::-1]])))
    r = property(lambda self: self.upgrade(Ty(*[x.r for x in self.objects[::-1]])))
```

Example 1.4.6. We can check the axioms for objects in rigid categories hold on the nose.

```

x, y = Ty('x'), Ty('y')
assert Ty().l == Ty() == Ty().r
assert (x @ y).l == y.l @ x.l and (x @ y).r == y.r @ x.r
assert x.r.l == x == x.l.r

```

`rigid.Box` and `rigid.Ty` are implemented as subclasses of `cat.Box` and `monoidal.Ty` respectively, with `property` methods (i.e. attributes that are computed on the fly) `l` and `r` for the left and right adjoints. Thanks to the `upgrade` method, we do not need to override the `tensor` method inherited from `monoidal.Ty`. In turn, subclasses of `rigid.Ty` will not need to override `l` and `r`. Similarly, the `rigid.Diagram` class is a subclass of `monoidal.Diagram`, thanks to the `upgrade` we do not need to reimplement the identity, composition or tensor. `rigid.Box` is a subclass of `monoidal.Box` and `rigid.Diagram`, with `Box.upgrade = Diagram.upgrade`. `Cup` (`Cap`) is a subclass of `Box` initialised by a pair of types `x`, `y` such that `len(x) == len(y) == 1` `x == y.l` (`x.l == y`, respectively). The class methods `cups` and `caps` construct diagrams of nested cups and caps by induction, with `Cup` and `Cap` as a base case.

Listing 1.4.7. Implementation of the arrows of free rigid categories.

```

class Diagram(monoidal.Diagram):
    def transpose(self, left=True) -> Diagram:
        if left: ... # Symmetric to the right case.
        return self.caps(self.dom.r, self.dom) @ self.id(self.cod.r)\
            >> self.id(self.dom.r) @ self @ self.id(self.cod.r)\
            >> self.id(self.dom.r) @ self.cups(self.cod, self.cod.r)

class Box(monoidal.Box, Diagram):
    upgrade = Diagram.upgrade

class Cup(Box):
    def __init__(self, x: Ty, y: Ty):
        assert len(x) == 1 and x == y.l
        super().__init__("Cup({}, {})".format(x, y), x @ y, Ty())

class Cap(Box):
    def __init__(self, x: Ty, y: Ty):
        assert len(x) == 1 and x.l == y
        super().__init__("Cap({}, {})".format(x, y), Ty(), x @ y)

def nesting(box_factory):
    @classmethod
    def method(cls, x: Ty, y: Ty) -> Diagram:

```

```

if len(x) == 0: return cls.id(Ty())
if len(x) == 1: return box_factory(x, y)
head = box_factory(x[0], y[-1])
if head.dom: # We are nesting cups.
    return x[0] @ method(x[1:], y[:-1]) @ y[-1] >> head
return head >> x[0] @ method(x[1:], y[:-1]) @ y[-1]

```

```
Diagram.cups, Diagram.caps = nesting(Cup), nesting(Cap)
```

The *snake removal* algorithm listed below computes the normal form of diagrams in rigid categories. It is a concrete implementation of the abstract algorithm described in pictures by Dunn and Vicary [DV19, p. 2.12]. First, we implement a subroutine `follow_wire` takes a codomain node (given by the index `i` of its box and the index `j` of itself in the box's codomain) follows the wire till it finds either the domain of another box or the codomain of the diagram. When we follow a wire, we compute two lists of *obstructions*, the index of each box on its left and right. The `find_snake` function calls `follow_wire` for each `Cap` in the diagram until it finds one that is connected to a `Cup`, or returns `None` otherwise. A `Yankable` snake is given by the index of its cup and cap, the two lists of obstructions on each side and whether it is a left or right snake. `unsnake` applies `interchange` repeatedly to remove the obstructions, i.e. to make the cup and cap consecutive boxes in the diagram, then returns the diagram with the snake removed. Each snake removed reduces the length n of the diagram by 2, hence the `snake_removal` algorithm makes at most $n/2$ calls to `find_snake`. Finally, we call `monoidal.Diagram.normal_form` which takes at most cubic time. Finding a snake takes quadratic time (for each cap we need to follow the wire at each layer) as well as removing it (for each obstruction we make a linear number of calls to `interchange`). Thus, we can compute normal forms for diagrams in free rigid categories in cubic time. We conjecture that we can in fact solve the word problem (i.e. deciding whether two diagrams are equal) in quadratic time using the same reduction to planar map isomorphism as in theorem 1.2.19.

Listing 1.4.8. Outline of the snake removal algorithm.

```

Obstruction = tuple[list[int], list[int]]
Yankable = tuple[int, int, Obstruction, bool]

def follow_wire(self: Diagram, i: int, j: int) -> tuple[int, int, Obstruction]: ...
def find_snake(self: Diagram) -> Optional[Yankable]: ...
def unsnake(self: Diagram, yankable: Yankable) -> Diagram: ...
def snake_removal(self: Diagram) -> Diagram:

```



```

yankable = find_snake(diagram)
return snake_removal(unsake(diagram, yankable)) if yankable else diagram

Diagram.normal_form = lambda self:\
    monoidal.Diagram.normal_form(snake_removal(self))

```

Example 1.4.9. *We can check that the snake equations hold up to normal form.*

```

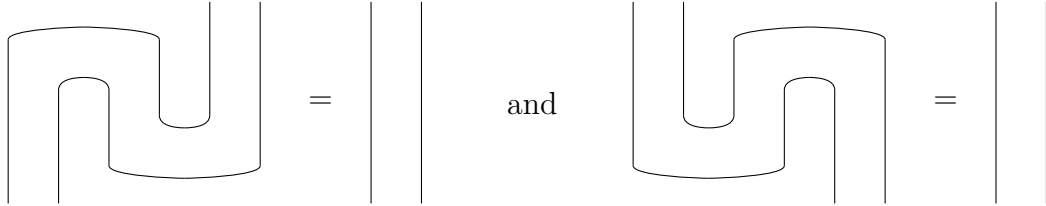
t = x @ y

left_snake = Diagram.id(t.l).transpose(left=False)
right_snake = Diagram.id(t).transpose(left=True)

assert left_snake.normal_form() == Diagram.id(t)\
    and right_snake.normal_form() == Diagram.id(t.l)

drawing.equation(
    drawing.Equation(left_snake, Diagram.id(t)),
    drawing.Equation(right_snake, Diagram.id(t.l)),
    symbol='and', space=2, draw_type_labels=False)

```



Example 1.4.10. *We can check that left and right transpose cancel up to normal form.*

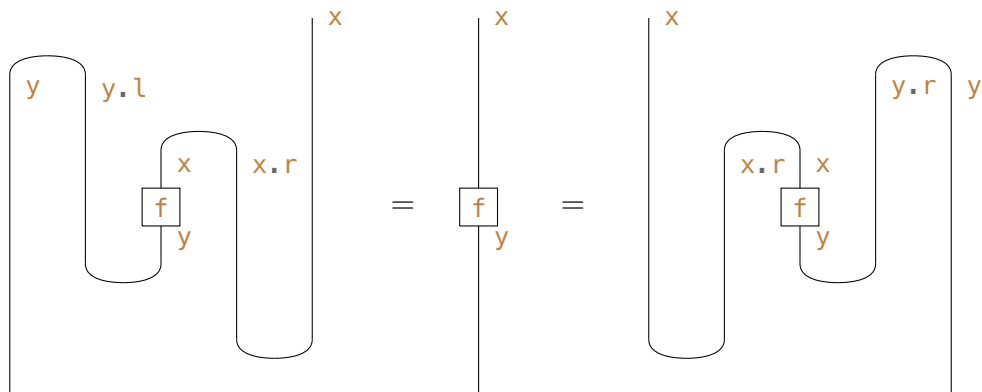
```

f = Box('f', x, y)

left_right_transpose = f.transpose(left=True).transpose(left=False)
right_left_transpose = f.transpose(left=False).transpose(left=True)

assert left_right_transpose.normal_form() == f == right_left_transpose.normal_form()
drawing.equation(left_right_transpose, f, right_left_transpose)

```



Listing 1.4.11. Implementation of **Circ** as a pivotal category.

```

class Qubits(monoidal.Qubits, Ty):
    l = r = property(lambda self: self)

class Circuit(monoidal.Circuit, Diagram):
    cups = nesting(lambda _, _ : sqrt2 @ Ket(0, 0) >> H @ Id)
    caps = lambda x, y: Circuit.cups(x, y).dagger()

```

Example 1.4.12. *We can verify the teleportation protocol for two qubits.*

```

two_qubit_Bell_state = Circuit.cups(Qubits(2))
two_qubit_Bell_effect = Circuit.cups(Qubits(2))

assert (two_qubit_Bell_state @ Id @ Id >> Id @ Id @ two_qubit_Bell_effect).eval()\
    == (Id @ Id).eval()\
    == (Id @ Id @ two_qubit_Bell_state >> two_qubit_Bell_effect @ Id @ Id).eval()

```

`rigid.Functor` is implemented as a subclass of `monoidal.Functor` with the `__call__` method overridden. The image on types and on objects `x` with `x.z == 0` remains unchanged. The image on objects `x` with `x.z < 0` is defined by $F(x) = F(x.r).l$ and symmetrically for `x.z > 0`. Indeed, when defining a strict rigid functor we only need to define the image of basic types, the image of their iterated adjoints is completely determined. The only problem arises when the objects in the codomain do not have `l` and `r` attributes, such as the implementation of `Tensors` with `list[int]` as objects. In this case, we assume that the left and right adjoints are given by list reversal.

Listing 1.4.13. Implementation of strict rigid functors.

```

class Functor(monoidal.Functor):
    dom = cod = Category(Ty, Diagram)

    def __call__(self, other):
        if isinstance(other, Ty) or isinstance(other, Ob) and other.z == 0:
            return super().__call__(other)
        if isinstance(other, Ob):
            if not hasattr(self.cod.ob, 'l' if other.z < 0 else 'r'):
                return self(Ob(other.name, z=0))[:-1]
            return self(other.r).l if other.z < 0 else self(other.l).r
        if isinstance(other, Cup):
            return self.cod.ar.cups(self(other.dom[:1]), self(other.dom[1:]))
        if isinstance(other, Cap):
            return self.cod.ar.caps(self(other.dom[:1]), self(other.dom[1:]))
        return super().__call__(other)

```

Listing 1.4.14. Implementation of \mathbf{Tensor}_S as a pivotal category.

```
Tensor.cups = classmethod(lambda cls, x, y: cls(cls.id(x).inside, x + y, []))
Tensor.caps = classmethod(lambda cls, x, y: cls(cls.id(x).inside, [], x + y))
```

Example 1.4.15. We can check that \mathbf{Tensor}_S is indeed pivotal.

```
F = Functor(
    ob={x: 2, y: 3}, ar={f: [[1, 2, 3], [4, 5, 6]]}
    cod=Category(list[int], Tensor[int]))

assert F(left_snake) == F(Diagram.id(x)) == F(right_snake)
assert F(f.transpose(left=True)) == F(f).transpose() == F(f.transpose(left=False))

# Diagrammatic and algebraic transpose differ for tensors of order >= 2.
assert F(f @ f).transpose() != F((f @ f).transpose())
```

Free pivotal categories are defined in a similar way to free rigid categories, with the two-element field $\mathbb{Z}/2\mathbb{Z}$ instead of the integers \mathbb{Z} , i.e. simple types with adjunction numbers of the same parity are equal. Given a pivotal signature Σ with objects of the form $\Sigma_0 \times (\mathbb{Z}/2\mathbb{Z})$, the free pivotal category is the quotient $F^p(\Sigma) = F^r(\Sigma)/R$ of the free rigid category by the relation R equating the left and right transpose of the identity for each type. While the diagrams of free rigid categories can have snakes, those of free pivotal categories can have circles: we can compose $\cap(x) : 1 \rightarrow x^l \otimes x$ then $\cup(x^l) : x^l \otimes (x^l)^l = x^l \otimes x$ to form a scalar diagram called the *dimension* of the system x .

To the best of our knowledge, the word problem for pivotal categories is still open. When defining the normal form of pivotal diagrams, we would need to make a choice between the diagrams for left or right transpose of a box. Another solution is to add a new box $f^T : y^r \rightarrow x^r$ for the transpose of every box $f : x \rightarrow y$ in the signature, and set it as the normal form of both diagrams. We can add some asymmetry to the drawing of the box f , and draw f^T as its 180° degree rotation. If the category also has a dagger, we get a four-fold symmetry: the box, its dagger, its transpose and its dagger-transpose (also called its conjugate). This is still being developed by the DisCoPy community.

Listing 1.4.16. Implementation of free \dagger -pivotal categories.

```
class Ob(rigid.Ob):
    l = r = property(lambda self: self.upgrade(Ob(self.name, (self.z + 1) % 2)))

class Ty(rigid.Ty, Ob):
```

```

def __init__(self, objects=[]):
    rigid.Ty.__init__(self, objects=map(Ob.upgrade, objects))

class Diagram(rigid.Diagram): pass

class Box(rigid.Box, Diagram):
    upgrade = Diagram.upgrade

class Cup(rigid.Cup, Box):
    def dagger(self):
        return Cap(self.dom[0], self.dom[1])

class Cap(rigid.Cap, Box):
    def dagger(self):
        return Cup(self.cod[0], self.cod[1])

Diagram.cups, Diagram.caps = nesting(Cup), nesting(Cap)

class Functor(rigid.Functor):
    dom = cod = Category(Ty, Diagram)

```

1.4.3 Braided categories & wire crossing

With rigid and pivotal categories, we have removed the assumption that diagrams are progressive: we can bend wires. With braided and symmetric monoidal categories, we now remove the planarity assumption: wires can cross.

A monoidal category C is *braided* when it comes with a natural isomorphism $B(x, y) : x \otimes y \rightarrow y \otimes x$ (and its inverse B^{-1}) drawn as a wire for x crossing under (over) a wire y and subject to the following *hexagon equations*:

- $B(x, y \otimes z) = B(x, y) \otimes z \circ y \otimes B(x, z),$

$$\begin{array}{c}
 \begin{array}{c} x \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} y \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} z \\ \downarrow \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} y \otimes z \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} x \\ \downarrow \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} y \otimes z \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} z \\ \downarrow \\ \text{---} \end{array}
 \end{array}
 =
 \begin{array}{c}
 \begin{array}{c} x \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} y \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} z \\ \downarrow \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} y \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} x \\ \downarrow \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} z \\ \downarrow \\ \text{---} \end{array} \begin{array}{c} x \\ \downarrow \\ \text{---} \end{array}
 \end{array}$$

- $B(x \otimes y, z) = x \otimes B(y, z) \circ B(x, z) \otimes y$

$$\begin{array}{c}
 \begin{array}{c}
 \begin{array}{c} x & y \end{array} \\
 \text{---} \\
 \begin{array}{c} x \otimes y \end{array} \\
 \text{---} \\
 \begin{array}{c} z \end{array} \\
 \text{---} \\
 \begin{array}{c} x \otimes y \end{array} \\
 \text{---} \\
 \begin{array}{c} x & y \end{array}
 \end{array}
 =
 \begin{array}{c}
 \begin{array}{c} x & y \end{array} \\
 \text{---} \\
 \begin{array}{c} z \end{array} \\
 \text{---} \\
 \begin{array}{c} z \end{array} \\
 \text{---} \\
 \begin{array}{c} x \end{array}
 \end{array}
 \end{array}$$

which owe their name to the shape of the corresponding commutative diagrams when C is non-strict monoidal. The hexagon equations may be taken as an inductive definition: the braiding $B(x, 1)$ of an object with the unit 1 is the identity, and we can decompose the braiding $B(x, y \otimes z)$ of an object with a tensor in terms of two simpler braids $B(x, y)$ and $B(x, z)$. Thus, we can take the data for a braided category to be that of a foo-monoidal category together with a pair of functions $B, B^{-1} : C_0 \times C_0 \rightarrow C_1$ which send a pair of generating objects to their braiding and its inverse. Once we have specified the braids of generating objects, the braids of any type (i.e. list of objects) is uniquely determined. A monoidal functor $F : C \rightarrow D$ between two braided categories C and D is braided when $F(B(x, y)) = B(F(x), F(y))$. Thus, we get a category **BraidCat** with a forgetful functor $U : \mathbf{BraidCat} \rightarrow \mathbf{MonSig}$, we now describe its left adjoint.

Given a monoidal signature Σ , the free braided category is a quotient $F^B(\Sigma) = F(\Sigma^B)/R$ of the free monoidal category generated by $\Sigma^B = \Sigma \cup B \cup B^{-1}$ for the braiding $B(x, y) : x \otimes y \rightarrow y \otimes x$ and its inverse $B^{-1}(x, y) : y \otimes x \rightarrow x \otimes y$ for each pair of generating objects $x, y \in \Sigma_0$. The relation R is given by the following axioms for a natural isomorphism:

- $B(x, y) \circ B^{-1}(x, y) = \text{id}(x \otimes y) = B^{-1}(x, y) \circ B(x, y),$

$$\begin{array}{c}
 \begin{array}{c} x & y \\ \text{---} \\ y & x \\ \text{---} \\ x & y \end{array}
 =
 \begin{array}{c} x & y \\ | & | \\ | & | \\ | & | \end{array}
 =
 \begin{array}{c} y & x \\ \text{---} \\ x & y \\ \text{---} \\ y & x \end{array}
 \end{array}$$

- $f \otimes x \circ B(b, x) = B(a, x) \circ x \otimes f$ and $x \otimes f \circ B(x, b) = B(x, a) \circ f \otimes x.$

$$\begin{array}{c}
 \begin{array}{c} a & x \\ \boxed{f} & \\ b & \\ \text{---} \\ x & b \end{array}
 =
 \begin{array}{c} a & x \\ \text{---} \\ x & a \\ \boxed{f} & \\ & b \end{array}
 \quad
 \begin{array}{c} x & a \\ \text{---} \\ \boxed{f} & \\ b & \\ \text{---} \\ b & x \end{array}
 =
 \begin{array}{c} x & a \\ \text{---} \\ a & x \\ \boxed{f} & \\ & b \end{array}
 \end{array}$$

for all generating objects $x, y \in \Sigma_0$ and boxes (including braidings) $f : a \rightarrow b$ in Σ^B . From B being an isomorphism on generating objects, we can prove it is

self-inverse on any type by induction. Similarly, from B being natural on the left and right for each box, we can prove by induction that it is in fact natural for any diagram. Note that the naturality axiom holds for boxes with domains and codomains of arbitrary length. In particular, it holds for $f = B(y, z)$ in which case we get the following Yang-Baxter equation:

$$\begin{array}{c}
 \begin{array}{|c|} \hline x \\ \hline \end{array} \begin{array}{|c|} \hline y \\ \hline \end{array} \begin{array}{|c|} \hline z \\ \hline \end{array} \\
 \begin{array}{|c|} \hline z \\ \hline \end{array} \begin{array}{|c|} \hline x \\ \hline \end{array} \begin{array}{|c|} \hline y \\ \hline \end{array} \\
 \begin{array}{|c|} \hline y \\ \hline \end{array} \begin{array}{|c|} \hline x \\ \hline \end{array}
 \end{array} = \begin{array}{c}
 \begin{array}{|c|} \hline x \\ \hline \end{array} \begin{array}{|c|} \hline y \\ \hline \end{array} \begin{array}{|c|} \hline z \\ \hline \end{array} \\
 \begin{array}{|c|} \hline y \\ \hline \end{array} \begin{array}{|c|} \hline x \\ \hline \end{array} \begin{array}{|c|} \hline z \\ \hline \end{array} \\
 \begin{array}{|c|} \hline z \\ \hline \end{array} \begin{array}{|c|} \hline y \\ \hline \end{array} \begin{array}{|c|} \hline x \\ \hline \end{array}
 \end{array}$$

It also holds for any scalar $f : 1 \rightarrow 1$, which allows to pass them through a wire:

$$\boxed{f} \begin{array}{|c|} \hline x \\ \hline \end{array} = \begin{array}{|c|} \hline x \\ \hline \end{array} \boxed{f}$$

A braided category C is *symmetric* if the braiding B is its own inverse $B = B^{-1} = S$, in this case it is called a *swap* and drawn as the intersection of two wires. A symmetric functor is a braided functor between symmetric categories. A \dagger -braided category is a braided category with a dagger structure, such that the braidings are unitaries, i.e. their inverse is also their dagger. A \dagger -symmetric category is a \dagger -braided category that is also symmetric.

Remark 1.4.17. *The arrows of the free symmetric PRO (i.e. with one generating object x) with no generating boxes (i.e. only swaps) are called permutations, the arrows of the free braided PRO with no boxes are called braids. Both are groupoids, i.e. all their arrows are isomorphisms, which also implies that they are \dagger -braided. For every $n \in \mathbb{N}$, the arrows $f : x^n \rightarrow x^n$ in the free symmetric (braided) PRO are the elements of the n -th symmetric group S_n (braid group B_n).*

DisCoPy implements free \dagger -symmetric (\dagger -braided) categories with a class `Swap` (`Braid`) initialised by types of length one and a class method `swap` (`braid`) for types of arbitrary length. The method `simplify` cancels every braid followed by its inverse. We also override the `interchange` method to implement the naturality axioms: we can interchange a box through a braid¹.

Listing 1.4.18. Implementation of free \dagger -braided and \dagger -symmetric categories.

```

class Diagram(monoidal.Diagram):
    def simplify(self):

```

¹As of today, this is only implemented for boxes with domain and codomain of length one.

```

    for i, (x, f, _) , (y, g, _) in enumerate(zip(self.layers, self.layers[1:])):
        if x == y and isinstance(f, Braid) and f == g[::-1]:
            layers = self.layers[:i] + self.layers[i + 2:]
            return simplify(self.upgrade(Diagram(self.dom, self.cod, layers)))
    return self

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

class Box(monoidal.Box, Diagram):
    upgrade = Diagram.upgrade

class Braid(Box):
    def __init__(self, x: Ty, y: Ty, is_dagger=False):
        assert len(x) == len(y) == 1
        super().__init__("Braid({}, {})".format(x, y), x @ y, y @ x, is_dagger)

    def dagger(self): return Braid(self.dom[1], self.dom[0], not self.is_dagger)

class Swap(Braid):
    def __init__(self, x: Ty, y: Ty):
        super().__init__(x, y); self.name = self.name.replace("Braid", "Swap")

    def dagger(self): return Swap(self.dom[1], self.dom[0])

def hexagon(box_factory) -> Callable:
    @classmethod
    def method(cls, x: Ty, y: Ty) -> Diagram:
        if len(x) == 0: return cls.id(y)
        if len(x) == 1:
            if len(y) == 1: return box_factory(x[0], y[0])
            return method(cls, x, y[:1]) @ cls.id(y[1:]) \
                >> cls.id(y[1:]) @ method(cls, x, y[1:]) # left hexagon equation.
        return cls.id(x[:1]) @ method(cls, x[1:], y) \
            >> method(cls, x[:1], y) @ cls.id(x[1:]) # right hexagon equation.
    return method

Diagram.braid, Diagram.swap = hexagon(Braid), hexagon(Swap)

class Functor(monoidal.Functor):
    def __call__(self, other):
        if isinstance(other, Swap):
            return self.cod.ar.swap(self(other[0]), self(other[1]))
        if isinstance(other, Braid) and not other.is_dagger:
            return self.cod.ar.braid(self(other[0]), self(other[1]))

```

```
return super().__call__(other)
```

Example 1.4.19. *We can check the hexagon equations hold on the nose.*

```
x, y, z = map(Ty, "xyz")
```

```
assert Diagram.braid(x, y @ z) == Braid(x, y) @ z >> y @ Braid(x, z)
assert Diagram.braid(x @ y, z) == x @ Braid(y, z) >> Braid(x, z) @ y
```

*We can check that **Braid** is an isomorphism up to a **simplify** call.*

```
assert (Diagram.braid(x, y @ z) >> Diagram.braid(x, y @ z)[::-1]).simplify()\
== Diagram.id(x @ y @ z)\
== (Diagram.braid(x, y @ z)[::-1] >> Diagram.braid(x, y @ z)).simplify()
```

*We can check that both **Braid** and its inverse are natural by calling **interchange**.*

```
a, b = Ty('a'), Ty('b')
f = Box('f', a, b)
```

```
assert (f @ x >> Braid(b, x)).interchange(0) == Braid(a, x) >> x @ f
assert (x @ f >> Braid(x, b)).interchange(0) == Braid(x, a) >> f @ x
```

```
assert (f @ x >> Braid(x, b)[::-1]).interchange(0) == Braid(x, a)[::-1] >> x @ f
assert (x @ f >> Braid(b, x)[::-1]).interchange(0) == Braid(a, x)[::-1] >> f @ x
```

Listing 1.4.20. Implementation of **Pyth** and **Tensor_S** as symmetric categories.

```
def function_swap(x: list[type], y: list[type]) -> Function:
    def inside(*xs):
        assert len(xs) == len(x + y)
        return untuple(xs[len(x):] + xs[:len(x)])
    return Function(inside, dom=x + y, cod=y + x)
```

```
Function.swap = Function.braid = function_swap
```

```
@classmethod
```

```
def tensor_swap(cls, x: list[int], y: list[int]) -> Tensor:
    inside = [(i0, j0) == (i1, j1)
               for j0 in range(product(y)) for i0 in range(product(x))]
    for i1 in range(product(x)) for j1 in range(product(y))]
    return cls(inside, dom=x + y, cod=y + x)
```

```
Tensor.swap = Tensor.braid = tensor_swaps
```

Example 1.4.21. We can check the axioms for symmetric categories hold in **Tensor_S** and **Pyth**.

```
F = Functor(
    ob={a: 2, b: 3, x: 4, y: 5, z: 6},
    ar={f: [[1-2j, 3+4j]]},
    cod=Category(list[int], Tensor[complex]))

assert F(f @ x >> Swap(b, x)) == F(Swap(a, x) >> x @ f)
assert F(x @ f >> Swap(x, b)) == F(Swap(x, a) >> f @ x)
assert F(Diagram.swap(x, y @ z) >> Diagram.swap(y @ z, x)) == Tensor.id(F(x @ y @ z))

G = Functor(
    ob={a: complex, b: real, x: int, y: bool, z: str},
    ar={f: lambda z: abs(z) ** 2},
    cod=Category(list[type], Function))

assert G(swap_twice)(42, True, "meaning of life") == (42, True, "meaning of life")
assert G(f @ x >> Swap(b, x))(1j, 2) == G(Swap(a, x) >> x @ f)(1j, 2) == (2, f(1j))
assert G(x @ f >> Swap(x, b))(2, 1j) == G(Swap(x, a) >> f @ x)(2, 1j) == (f(1j), 2)
```

Remark 1.4.22. Note that the naturality axioms in **Pyth** hold only for its subcategory of pure functions, as we will see in section 1.5 **Pyth** is in fact a symmetric premonoidal category. This is also the case for **Tensor_S** when the rig \mathbb{S} is non-commutative.

A *compact closed category* is one that is both rigid and symmetric, which implies that it is also pivotal, a \dagger -compact closed category is both \dagger -pivotal and \dagger -symmetric. The arrows of free \dagger -compact closed categories (i.e. equivalence classes of diagrams with cups, caps and swaps) are also called *tensor networks*, a graphical equivalent to *Einstein notation* and *abstract index notation*, first introduced by Penrose [Pen71]. Unlike the computer scientists however, physicists tend to identify the diagram (syntax) with its image under some interpretation functor to the category of tensors (semantics).

A *tortile category*, also called a *ribbon category*¹, is a braided, pivotal category which furthermore satisfies the following *untwisting* equation:

¹Here again we take a *strict* definition, where the twist is an identity rather than an isomorphism. In a non-strict tortile category, the wires would be drawn as ribbons, i.e. two wires side by side. The twist isomorphism would be drawn as the two wires being braided twice. In a strict tortile category, the ribbon has no width thus the twist is invisible.

The scalars of the free tortile category with no boxes (i.e. equivalence classes of diagrams with only cups, caps and braids) are called *links* in general and *knots* when they are connected. Untwisting, the self-inverse equation and the Yang-Baxter equation (i.e. naturality with respect to braids) are called the three *Reidemeister moves*, they completely characterise the continuous deformations of circles embedded in three-dimensional space [Rei13].

The *unknotting problem* (given a knot, can it be untied, i.e. continuously deformed to a circle?) is a candidate NP-intermediate problem: it is decidable [Hak61] and in NP [Lac15], but there is neither a proof of it being NP-complete nor a polynomial-time algorithm. Delpeuch and Vicary [DV21] proved that the word problem for free braided categories is unknotting-hard. Hence, there is little hope of finding a simple polynomial-time algorithm for computing normal forms of braided diagrams. It is not known whether it is even decidable.

The word problem for free symmetric categories reduces to the *graph isomorphism problem* [PSV21], another potential NP-intermediate problem. The word problem for free compact closed categories also reduces to graph isomorphism [Sel07]. To the best of our knowledge, it is not known whether they are graph-isomorphism-hard, i.e. whether there is a reduction the other around that sends any graph to a diagram with swaps (and cups and caps) so that graphs are isomorphic if and only their diagrams are equal. Thus, there could be a simple polynomial-time algorithm for computing normal forms of diagrams in symmetric and compact closed categories. In any case, DisCoPy does not implement any normal forms for diagrams with braids yet.

Of course, we can also enrich rigid and braided categories in commutative monoids, i.e. we can take formal sums of diagrams with cups, caps and braids in the same way as any other box. We can also define bubbles and draw them in the same way as for monoidal diagrams.

Example 1.4.23. *We can define knot polynomials such as the Kauffman bracket using pivotal functors into a category where braids are defined as a weighted sum of diagrams.*

```

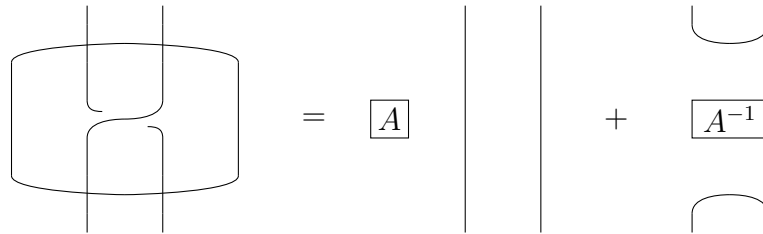
x = pivotal.Ty('$x$')
A, A.inverse = Box('$A$', Ty(), Ty()), Box('$A^{-1}$', Ty(), Ty())

class Polynomial(pivotal.Diagram):
    def braid(x, y):
        assert x == y and len(x) == len(y) == 1
        return (A @ x @ y) + (Cup(x, y) >> A.inverse >> Cap(x, y))

Kauffman = Functor(
    ob={x: x}, ar={}, cod=Category(pivotal.Ty, Polynomial))

drawing.equation(Braid(x, x).bubble(), Kauffman(Braid(x, x)))

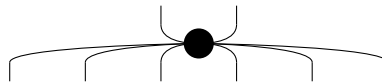
```



1.4.4 Hypergraph categories & wire splitting

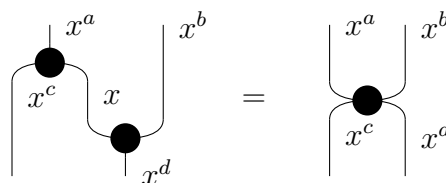
With compact closed and tortile categories, we have removed both the progressivity and the planarity assumptions: wires can bend and cross. With *hypergraph categories* now remove the assumption that diagrams are graphs, i.e. wires can split and merge, they need not be homeomorphic to an open interval.

The data for a hypergraph category is that of a symmetric category together with a *spider* (non-natural) transformation $\mathbf{spider}_{a,b}(x) : x^a \rightarrow x^b$ for every pair of natural numbers $a, b \in \mathbb{N}$. Spiders owe their name to their arachnomorphic drawing, for example $\mathbf{spider}_{2,6}$ is drawn as a node (the head) and its wires (the eight legs of the spider, two of them menacing us):



The axioms for hypergraph categories are the following *spider fusion*, *(co)-commutativity* and *coherence* equations:

- $\mathbf{spider}_{a,c+1}(x) \otimes x^b \circ x^c \otimes \mathbf{spider}_{1+c,d}(x) = \mathbf{spider}_{a+b,c+d}(x)$



- $\mathbf{spider}_{a+b,c+d}(x) \circ S(x^c, x^d) = \mathbf{spider}_{a+b,c+d}(x) = S(x^a, x^b) \circ \mathbf{spider}_{a+b,c+d}(x),$

- $\mathbf{spider}_{a,b}(1) = \text{id}(1)$ and $\mathbf{spider}_{1,2}(x \otimes y) = \mathbf{spider}_{1,2}(x) \otimes \mathbf{spider}_{1,2}(y) \circ x \otimes S(x, y) \otimes y.$

A hypergraph functor is a symmetric functor $F : C \rightarrow D$ between hypergraph categories such that $F \circ \mathbf{spider}_{a,b} = \mathbf{spider}_{a,b} \circ F$, thus we get a category **HypCat**. A \dagger -hypergraph category is both a \dagger -symmetric category and a hypergraph category such that $\dagger \circ \mathbf{spider}_{m,n} = \mathbf{spider}_{n,m} \circ \dagger$. A \dagger -hypergraph functor is both a hypergraph functor and a dagger functor.

The (co)commutativity axioms say that we can swap the legs of spiders.

Finally, the coherence axioms give us an inductive definition of spiders for composite types: the spiders of the unit are the identity, the spiders of a tensor $x \otimes y$ are given by tensoring the spiders for x and y then swapping their legs to match the types. The first coherence axiom would be drawn as the equality of two empty diagrams, we can draw the second with non-free-on-objects diagrams, i.e. with explicit equality boxes.

Thus, we can take the data for a free-on-objects hypergraph category C to be that of a monoidal category together with a function $\mathbf{spider}_{a,b} : C_0 \rightarrow C_1$. Once we fix the spiders for generating objects, the spiders for any type (i.e. list of objects) is fixed.

WTF

1.5 A premonoidal approach

1.5.1 Abstract premonoidal categories

1.5.2 Concrete premonoidal categories

1.5.3 Free premonoidal categories

1.5.4 The state construction

1.6 Related & future work

1.6.1 Graph-based data structures

1.6.2 Higher-dimensional diagrams

2

Quantum natural language processing

- 2.1** Natural language processing with diagrams
- 2.2** Classical-quantum processes with diagrams
- 2.3** QNLP models
- 2.4** Learning functors
- 2.5** Future work

3

Diagrammatic differentiation

3.1 Dual numbers

3.2 Dual diagrams

3.3 Dual circuits

3.4 Gradients & bubbles

3.5 Future work

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