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At the Interface
of Algebra and Statistics

A dissertation submitted to the Graduate Faculty in Mathematics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York

Contents

A Note to the Reader

SOME THINGS IN LIFE are too good not to share, and mathematics is one of those things. For this reason, *this dissertation was written with a wide audience in mind*. There is a great deal of exposition woven into the mathematics that provides intuition and motivation for the ideas. I've also sprinkled several "behind the scenes" snippets throughout, and alongside the propositions, lemmas, and corollaries there are *Takeaways* that summarize key ideas.[1] Several of these key ideas are introduced through simple examples that are placed before—not after—the theory they're meant to illustrate. And in a happy turn of events, there is a low entrance fee for following the mathematics. The main tools are linear algebra and basic probability theory, and I suspect you already have these in your toolbox. This brings us to the next point.

This thesis concerns the equation: **Algebra** + **Statistics** = **?** Said more carefully, this thesis stems from a desire to understand mathematical structure that has both algebraic and statistical properties. Here, "algebra" refers to the basic sense in which things come together to create something new. In an algebra, vectors can be multiplied together to create a new vector. Another word for this idea is *compositionality*, where small things assemble together to build a larger construction, and where knowledge of this larger construction comes through understanding the individual parts together with the rules for combining them. *But what if those rules are statistical?* What if the rule for multiplying vectors in an algebra is mediated by probability? Now we are at the interface of algebra and statistics, and one wonders what kind of mathematical structure is found there. To investigate it, we look for an example. Amazingly, we needn't look far. *It's right in front of us, carefully knitting together each word on this page*. That is, natural language—English, Greek, Tagalog,...—exhibits mathematical structure that is both algebraic and statistical. It's algebraic in that words come together to form larger expressions. The words *orange* and *fruit* can be concatenated to form *orange fruit*. But language is also statistical, as some expressions occur more often
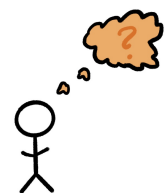
than others: *orange fruit* occurs more frequently than *orange idea*, and this contributes to the meanings of these expressions. The probability of reading or saying "orange fruit" is higher than the probability of "orange idea." But what *is* this mathematical structure? We look for a preliminary set of mathematical tools to start exploring it. To identify this toolbox, we search for a second example of where compositionality and statistics meet. Again we needn't look far. The world of quantum many body physics involves precisely these ideas. Small systems compose to form larger composite systems, and various properties of these quantum systems are driven by statistics. So that is where we begin. This thesis uses basic tools of quantum physics to understand compositional and statistical mathematical structure.

HERE'S A BRIEF WORD about the content itself. This work is ready-made to be digested in bits and pieces. Chapter 1 is the introduction and sets the layout of the land. You can read it, stop there, and have a good idea of what this work is about. But I hope you'll keep reading! Chapter 2 contains a series of tools and results from linear algebra called *quantum probability theory*, but I've included a number of expositional treats that may not be found in standard introductions to the subject. Importantly, I do not assume the reader has a background in physics; the examples and exposition are all anchored in the world of mathematics. Chapter 3 uses these tools to construct a mathematical machine, and with a clear understanding of the theory, we'll be able to "look under the hood" to see why it works. Chapter 4 describes an application with a concrete experiment that showcases the theory in action. The application falls under the genre of *unsupervised machine learning,* though the reader is not assumed to have familiarity with these words. The emphasis is placed on the underlying mathematics, and specialized language is introduced only when it helps to put the math in context.

Chapter 5 is largely independent from the rest of the text. The first four chapters illustrate the utility of a certain construction, which, as it turns out, arises in different areas of mathematics in different guises. The best way to see this is by lifting our feet off of the ground to get a clear, holistic view of the landscape. To do so, we'll use the language of category theory—a branch of mathematics whose *modus operandi* is identifying these kinds of sweeping connections. Chapter 5 assumes familiarity with the basics of category theory; I do not provide an introduction. Fortunately, no reader will be left behind—I've placed the tantalizing connection in simple terms in Chapter 1.

Let's begin.

Abstract

THIS THESIS TAKES inspiration from quantum physics to investigate mathematical structure that lies at the interface of algebra and statistics. The starting point is a passage from classical probability theory to quantum probability theory. The quantum version of a probability distribution is a density operator, the quantum version of marginalizing is an operation called the partial trace, and the quantum version of a marginal probability distribution is a reduced density operator. Every joint probability distribution on a finite set can be modeled as a rank one density operator. By applying the partial trace, we obtain reduced density operators whose diagonals recover classical marginal probabilities. In general, these reduced densities will have rank higher than one, and their eigenvalues and eigenvectors will contain extra information that encodes subsystem interactions governed by statistics. We decode this information—and show it is akin to conditional probability—and then investigate the extent to which the eigenvectors capture "concepts" inherent in the original joint distribution. The theory is then illustrated with an experiment. In particular, we show how to reconstruct a joint probability distribution on a set of data by gluing together the spectral information of reduced densities operating on small subsystems. The algorithm naturally leads to a tensor network model, which we test on the even-parity dataset. Turning to a more theoretical application, we also discuss a preliminary framework for modeling entailment and concept hierarchy in natural language—namely, by representing expressions in the language as densities. Finally, initial inspiration for this thesis comes from formal concept analysis, which finds many striking parallels with the linear algebra. The parallels are not coincidental, and a common blueprint is found in category theory. We close with an exposition on free (co)completions and how the free-forgetful adjunctions in which they arise strongly suggest that in certain categorical contexts, the "fixed points" of a morphism with its adjoint encode interesting information.

Acknowledgments

My time in graduate school can be characterized as a series of uniquely wonderful experiences, and this is largely due to the kindness, vision, and insight of my thesis advisor, John Terilla. I've deeply enjoyed working on and exploring the mathematics with John, and through his supervision, each year has been filled with more joy than the previous. He created *the* most perfect, vibrant environment in which I could thrive and has been a constant source of wholehearted support. I am immensely grateful.

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1

Introduction

The beauty of mathematics
only shows itself to more
patient followers.

Maryam Mirzakhani [Mir]

THIS THESIS FEATURES a passage from classical probability theory
to quantum probability theory by modeling probability distributions
with particular linear operators. We'll investigate the extent to which
the eigenvectors embody concepts inherent in the probability distri-
bution and use some experimental results as our guide. The linear
algebra is presented in Chapters 2 and 3, and the experimental con-
siderations are given in Chapter 4. Initial inspiration is drawn from
formal concept analysis, a mathematical framework that uses lattice
theory to identify concepts and concept hierarchies in data [DP02].
We give a brief introduction below. Think of this chapter as the pre-
lude to the main piece, which begins in Chapter 2.

1.1   Formal Concepts

A **formal concept** is the name given to a complete bipartite subgraph
of a particular bipartite graph. Intuitively, one views the two sets of
vertices as *objects* and *attributes*, and an edge indicates whether an
object possesses a certain attribute. A formal concept is thus a subset
A of objects and a subset B of attributes, with the property that every
object in A possesses all the attributes in B, and that each attribute
in B is possessed by all the objects in A. Typically, however, formal
concepts are defined in terms of finite sets and relations rather than
bipartite graphs. This set-theoretic definition mirrors a construction
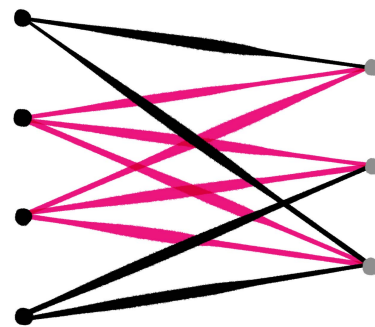that will reappear in the work to come, so let's describe it more care-
fully.

Figure 1.1: The subgraph in red is
complete bipartite. This is one way to
visualize a formal concept.

Let X and Y be finite sets and consider a function $R\colon X \times Y \to \{0,1\}$, which can be identified with a relation on, or equivalently a subset of, $X \times Y$. Intuitively, if X is a set of objects and Y is a set of attributes, then $R(x,y) = 1$ if and only if object x possesses attribute y. This relation determines a function a from X to the power set 2^Y of Y that associates to each element x the set of all elements in Y that relate to x. Likewise, there is a function $b\colon Y \to 2^X$ that associates to each element y the set of all elements in X that relate to it.

$$a(x) := \{y \in Y \mid R(x,y) = 1\} \qquad b(y) := \{x \in X \mid R(x,y) = 1\} \quad (1.1)$$

A similar assignment can be given to a subset $A \in 2^X$ by forming the set—call it $f(A)$—of all elements in Y that relate to *every* element in A. Think of this assignment as an *extension* of a. In other words, there is a natural inclusion $X \to 2^X$ that maps each x to the singleton set $\{x\}$, and the function a extends uniquely along this inclusion to give a function $f\colon 2^X \to 2^Y$ defined on each $A \in 2^X$ by

$$f(A) := \bigcap_{x \in A} a(x). \qquad (1.2)$$

Now is a good time to point out that there is additional structure lying around: Power sets are more than mere sets. They are **posets** (partially ordered sets) with subset containment providing the partial order. What's more, the function f preserves this structure in a way that is *order-reversing*: if $A' \subseteq A$ then $f(A) \subseteq f(A')$. To see this, it helps to think intuitively again: if $y \in f(A)$, then all objects in A—and in particular, those in A'—possess attribute y, and so $y \in f(A')$. It's possible, however, for the objects in A' to have a common attribute that is *not* shared by another object $x \in A \smallsetminus A'$. That is, there's no reason to expect an equality $f(A) = f(A')$ in general. So in the same way, the function b extends uniquely along the inclusion $Y \to 2^Y$ to give an order-reversing function $g\colon 2^Y \to 2^X$ defined on each $B \in 2^Y$ by

$$g(B) := \bigcap_{y \in B} b(y) \qquad (1.3)$$

which is the set containing all $x \in X$ that relate to all $y \in B$. Now observe that for any pair of subsets $A \in 2^X$ and $B \in 2^Y$,

$$A \subseteq g(B) \quad \text{if and only if} \quad B \subseteq f(A). \qquad (1.4)$$

The left-hand side states that the objects in A have all the attributes in B in common, though perhaps more. The right-hand side states that the attributes common to all objects in A are at least those in B. These are, of course, two ways of saying the same thing. Pairs (A, B) for which *equality* holds in both sides of (1.4) are given a special name.

Definition 1.1. Given finite sets X and Y and a function $R\colon X \times Y \to \{0,1\}$, a pair $(A, B) \in 2^X \times 2^Y$ is a **formal concept of** R if $f(A) = B$ and $g(B) = A$, where f and g are the functions defined above.

This definition admits a notion of concept hierarchy, as the set of all formal concepts of R is itself partially ordered. Define $(A', B') \leq (A, B)$ whenever $A' \subseteq A$ or equivalently whenever $B' \supseteq B$. Here is an example.

Example 1.1. Consider the sets

$$X = \{\text{orange, green, purple}\} \qquad Y = \{\text{fruit, vegetable}\}$$

and let $R\colon X \times Y \to \{0,1\}$ be the function defined by

$$R(\text{orange, fruit}) = 1$$
$$R(\text{green, fruit}) = 1$$
$$R(\text{purple, vegetable}) = 1$$

with $R(x, y) = 0$ for all other $(x, y) \in X \times Y$. This function can be represented by a 2×3 table with a 1 in the xyth entry if $R(x, y) = 1$ and with 0s elsewhere.

	orange	green	purple
fruit	1	1	0
vegetable	0	0	1

Table 1.1: The relation $R\colon X \times Y \to \{0,1\}$

In this example, the values of the function $a\colon X \to 2^Y$ defined in Equation (1.1) are as follows.

$$a(\text{orange}) = \{\text{fruit}\}$$
$$a(\text{green}) = \{\text{fruit}\}$$
$$a(\text{purple}) = \{\text{vegetable}\}$$

Notice that $a(\text{orange})$ can be read off from the nonzero entry in the first column of Table 1.1, while $a(\text{green})$ and $a(\text{purple})$ may be read off from the second and third columns. The values of the function $b\colon Y \to 2^X$ are similarly determined by the nonzero entries of the rows of the table.

$$b(\text{fruit}) = \{\text{orange, green}\}$$
$$b(\text{vegetable}) = \{\text{purple}\}$$

Given a and b, the functions $f\colon 2^X \rightleftarrows 2^Y \colon g$ are below.

BEHIND THE SCENES. In looking forward to language-inspired applications in Section 3.4 and Chapter 4, I've chosen the elements of X and Y be English words rather than generic x_i and y_j.

$$f\colon 2^X \longrightarrow 2^Y$$
$$\{\text{orange}\} \mapsto \{\text{fruit}\}$$
$$\{\text{green}\} \mapsto \{\text{fruit}\}$$
$$\{\text{purple}\} \mapsto \{\text{vegetable}\}$$
$$\{\text{orange, green}\} \mapsto \{\text{fruit}\}$$
$$\{\text{orange, purple}\} \mapsto \varnothing$$
$$\{\text{green, purple}\} \mapsto \varnothing$$
$$\{\text{orange, green, purple}\} \mapsto \varnothing$$

$$g\colon 2^Y \longrightarrow 2^X$$
$$\{\text{fruit}\} \mapsto \{\text{orange, green}\}$$
$$\{\text{vegetable}\} \mapsto \{\text{purple}\}$$
$$\{\text{fruit, vegetable}\} \mapsto \varnothing$$

A formal concept is a pair of subsets $(A, B) \in 2^X \times 2^Y$ so that $fA = B$ and $gB = A$. Looking at the assignments above, we find that there are two formal concepts: the pair {orange, green} and {fruit}, and the pair {purple} and {vegetable}.

({orange, green},{fruit})
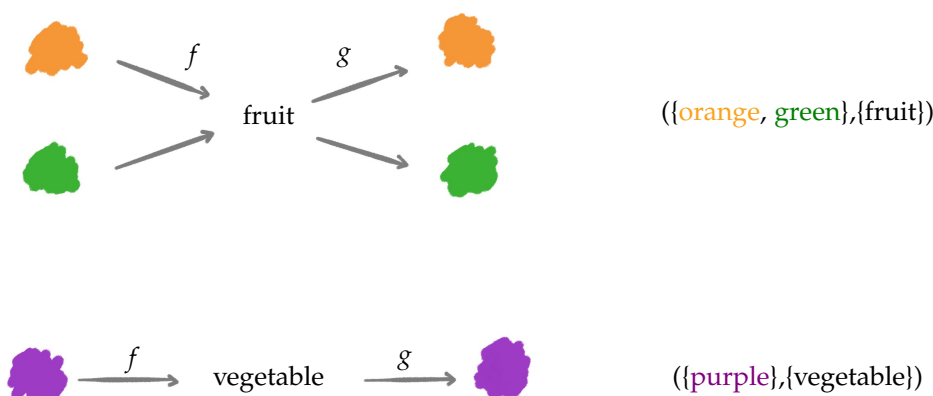
({purple},{vegetable})

The first formal concept is, perhaps, the concept of citrus fruits. The second formal concept is that of a purple vegetable. *There are plenty of these:* red cabbage, purple cauliflower, purple carrots, purple asparagus, endive, and eggplant—though that's technically a fruit!—to name a few.

As NOTED IN THE introduction, there is also a simple, graph theoretic way to understand formal concepts. In place of Table 1.1, the relation R may be represented as a bipartite graph. The sets X and Y provide the two sets of vertices, and there is an edge joining $x \in X$ and $y \in Y$ if and only if $R(x, y) = 1$.
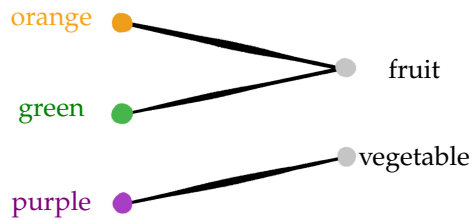
Formal concepts coincide with complete bipartite subgraphs. Indeed, this graph has two complete bipartite subgraphs—which happen to be disjoint in this example—and they correspond the two formal concepts listed above.

In general, formal concepts may also be identified with invariant subsets or "fixed points" of the composite functions fg and gf. Let Fixfg denote the set of all $B \in 2^Y$ satisfying $fg(B) = B$ and similarly for Fixgf. There are bijections

$$\text{formal concepts of } R \quad \cong \quad \text{Fix}fg \quad \cong \quad \text{Fix}gf.$$

If (A, B) is a formal concept, then B is a fixed point of fg, and A is a fixed point of gf:

$$f(gB) = fA = B \qquad g(fA) = gB = A.$$

Conversely, if $B \in \text{Fix}fg$, then (gB, B) is a formal concept, and if $A \in \text{Fix}gf$, then (A, fA) is also a formal concept. Let's summarize the discussion so far.

Takeaway 1. *Given finite sets X and Y, any function $R \colon X \times Y \to \{0, 1\}$ induces two functions $a \colon X \to 2^Y$ and $b \colon Y \to 2^X$ that lift to order-reversing functions f and g so that the following diagrams commute.*

$$
\begin{array}{ccc}
2^X \dashrightarrow^{f} 2^Y & \qquad & 2^Y \dashrightarrow^{g} 2^X \\
\uparrow \quad \nearrow_{a} & & \uparrow \quad \nearrow_{b} \\
X & & Y
\end{array}
$$

Moreover, f and g satisfy

$$A \subseteq g(B) \quad \textit{if and only if} \quad B \subseteq f(A),$$

for all $A \in 2^X$ and $B \in 2^Y$, and the invariant subsets of the compositions fg and gf are formal concepts. Moreover, there is a one-to-one correspondence between them.

The ideas here are an example of a construction that appears often throughout mathematics. The relationship between f and g as seen in (1.4) is closely related to the correspondence between groups

and fields in Galois theory and the correspondence between fundamental groups and covering spaces in algebraic topology. They are all instances of a general construction called a *Galois connection*, which is the name given to a pair of maps between posets that satisfy a property like that in (1.4). Galois connections themselves are examples of a more general construction known as an **adjunction** in category theory.[1] Indeed, the power set 2^X is, like any poset, a category whose objects are subsets of X and whose morphisms are provided by the partial order. The order-reversing functions f and g are contravariant functors, and the statement in (1.4) witnesses an adjunction $f\colon 2^X \rightleftarrows 2^Y \colon g$. As it turns out, pairs of adjoint functors on posets arise frequently in mathematics; the one we've discussed in this section is just a special case. Not coincidentally, the terms "adjunction" and "adjoint" arise from similarity with *adjoint linear maps*. (See Equation (1.5) in the margin.) In fact, when we exchange $\mathbb{C}$ for $\{0, 1\}$ in our discussion above, the summary in Takeaway 1 has a familiar linear algebraic version that leads to several key ideas for this thesis.

1.2 A Linear Algebraic Version

Let X and Y be finite sets as before, and consider a complex-valued function $M\colon X \times Y \to \mathbb{C}$. Let $\mathbb{C}^X$ denote the free complex vector space on X. For the moment, it will be helpful to think of vectors $v \in \mathbb{C}^X$ as functions $v\colon X \to \mathbb{C}$, just as a subset $A \in 2^X$ coincides with a function $A\colon X \to 2$. The function M gives rise to functions $\alpha\colon X \to \mathbb{C}^Y$ and $\beta\colon Y \to \mathbb{C}^X$. For each x the function $\alpha(x)\colon Y \to \mathbb{C}$ assigns $M(x, y)$ to each y. Likewise for each y define the function $\beta(y)\colon X \to \mathbb{C}$ to assign $\overline{M(x, y)}$ to each x. Now observe that there is a natural inclusion $X \to \mathbb{C}^X$ that associates to each x the function $v_x\colon X \to \mathbb{C}$ whose value $v_x(x')$ is 1 if $x' = x$ and is 0 otherwise. By the universal property of vector spaces, the function α uniquely extends along this inclusion to a linear map[2] $M\colon \mathbb{C}^X \to \mathbb{C}^Y$. The same letter M is used to denote this linear map since its matrix representation is precisely the function $M\colon X \times Y \to \mathbb{C}$ viewed as a $|Y| \times |X|$ matrix. In fact, $\alpha(x)$ is simply the xth column of M. In the same way, the function β extends to a linear map $M^\dagger\colon \mathbb{C}^Y \to \mathbb{C}^X$, and $\beta(y)$ is the (complex conjugate of the) yth row of M. Dagger notation is used since the matrix representing $M^\dagger$ is the conjugate transpose of M.

$$\begin{bmatrix} & | & \\ & \alpha(x) & \\ & | & \end{bmatrix} = M = \begin{bmatrix} & - & \beta(y) & - & \end{bmatrix}$$

---

[1] Given two categories C and D, a pair of functors $F\colon \mathsf{C} \to \mathsf{D}$ and $G\colon \mathsf{D} \to \mathsf{C}$ form an **adjunction** if

$$\mathrm{hom}_{\mathsf{C}}(FA, B) \cong \mathrm{hom}_{\mathsf{D}}(A, GB) \quad (1.5)$$

for all objects A in C and B in D. In other words, F and G are **adjoint functors** if the set of morphisms $FA \to B$ are in (natural) bijection with the set of morphisms $A \to GB$. Compare Equation (1.5) with Equation (1.6) to see where "adjoint" functors get their name.

[2] Said more informally, defining a linear map $\mathbb{C}^X \to \mathbb{C}^Y$ is as simple as specifying where the basis vectors go. That's what α is doing.

In other words, $M^\dagger \colon \mathbb{C}^Y \to \mathbb{C}^X$ is the linear adjoint of $M \colon \mathbb{C}^X \to \mathbb{C}^Y$ since for all $v \in \mathbb{C}^X$ and $w \in \mathbb{C}^Y$,

$$\langle Mv, w \rangle = \langle v, M^\dagger w \rangle. \tag{1.6}$$

"Fixed points" of the composite maps $M^\dagger M$ and $MM^\dagger$ are their eigenvectors, and we will show in Proposition 2.3 that there is a one-to-one correspondence between them[3]. Here's the takeaway of this discussion. Notice the similarity with Takeaway 1.

Takeaway 2. *Given finite sets X and Y, any function $M \colon X \times Y \to \mathbb{C}$ induces two functions $\alpha \colon X \to \mathbb{C}^Y$ and $\beta \colon Y \to \mathbb{C}^X$ that lift to linear maps M and $M^\dagger$ so that the following diagrams commute.*

$$
\begin{array}{ccc}
\mathbb{C}^X & \xdashrightarrow{M} & \mathbb{C}^Y \\
\uparrow & \nearrow{\scriptstyle \alpha} & \\
X & &
\end{array}
\qquad\qquad
\begin{array}{ccc}
\mathbb{C}^Y & \xdashrightarrow{M^\dagger} & \mathbb{C}^X \\
\uparrow & \nearrow{\scriptstyle \beta} & \\
Y & &
\end{array}
$$

Moreover, M and $M^\dagger$ satisfy

$$\langle Mv, w \rangle = \langle v, M^\dagger w \rangle$$

for all $v \in \mathbb{C}^X$ and $w \in \mathbb{C}^Y$, and the one-dimensional invariant subspaces of the compositions $M^\dagger M$ and $MM^\dagger$ correspond to their eigenvectors. Moreover, there is a one-to-one correspondence between them.

COMPARE THE LINEAR algebra in Takeaway 2 and Equation (1.6) with the set theory in Takeaway 1 and Statement (1.4). The similarities are unmistakable: a relation R is like a matrix M, the poset maps f, g are like the linear maps $M, M^\dagger$, and formal concepts are like eigenvectors. So we ask the natural question, *Do eigenvectors of $M^\dagger M$ and $MM^\dagger$ capture concepts inherent in the matrix M?* A main goal of this thesis is to show that the answer is "Yes." We further wish to understand the general construction for which the diagrams in Takeaways 1 and 2 are a special case. A first step in this direction is to notice that the diagrams are rather imprecise. Some of the arrows are functions, while others are functions that preserve structure.[4] It's not clear which *category* the mathematics is taking place in. A more careful treatment will clarify the situation. So another goal of this thesis is to shed light on the category theory underlying the two constructions discussed here.

1.3   Outline of Contents

Here's a preview of the ideas to come. First, for the applications we have in mind, a main focus will be on matrices $M \colon X \times Y \to \mathbb{C}$ with

[3] ...as long as M is "properly normalized" in a sense that the proposition makes precise.

[4] For instance, α is a function while M is a linear map. In fact, take a closer look at $\alpha \colon X \to \mathbb{C}^Y$. We've referred to α as a "function," but the domain and codomain of a function are *sets*. The domain of α is certainly a set, but its codomain is a set *equipped with* a vector space structure. So α is not well-typed. It would be better for us to say that α is "a function from X to the *underlying set* of the vector space $\mathbb{C}^Y$." Getting this right is more than pedantry. It plays an essential role in discovering why Takeaways 1 and 2 are so similar. As we'll see in Chapter 5, the answer is found in category theory.

the property that $\sum_{x,y}|M(x,y)|^2 = 1$; that is, the absolute square of the entries of M define a probability distribution on $X \times Y$. This matrix represents a linear map $\mathbb{C}^X \to \mathbb{C}^Y$, and so it can be identified with a unit vector in the tensor product $\mathbb{C}^X \otimes \mathbb{C}^Y$. Orthogonal projection onto this unit vector defines a certain type of linear operator known as a *density operator* or synonymously a *quantum state*. This operator induces two *reduced density operators*—one on $\mathbb{C}^X$ and one on $\mathbb{C}^Y$—whose matrix representations are precisely $M^\dagger M$ and $MM^\dagger$. If the ranks of these operators are greater than 1, then their eigenvectors will be shown to harness valuable information within the original quantum state, and this information will turn out to be useful in an applied setting. We will introduce all of these ideas from the ground up. Here's the path we'll take to do so.

CHAPTER TWO. We begin with preliminaries in Chapter 2. Section 2.1 motivates the linear algebra in the previous paragraph by presenting an elementary-yet-illuminating example that does not use the language of quantum mechanics. Section 2.2 then introduces *bra-ket* notation and *tensor network diagram* notation, which will be used throughout. We will hit the ground running in Sections 2.3, 2.4, and 2.5, which cover the basics of *density operators*, the *partial trace*, and *reduced density operators*. The main theme in this chapter is that density operators are the quantum version of probability distributions, reduced density operators are the quantum version of marginal probability, and the partial trace is the quantum version of marginalizing.

CHAPTER THREE. Armed with the prerequisites, we present the main contribution in Chapter 3. It is a procedure for modeling any joint probability distribution by a rank 1 density operator together with a decryption of the information carried in the eigenvalues and eigenvectors of its reduced density operators. The procedure is outlined in Section 3.1, and an extended illustration is given in Example 3.1. The example identifies a particularly simple scenario, namely that when the probability distribution being modeled is an *empirical* one, the reduced densities and their spectral information have simple combinatorial interpretations that can be read off visually from a graph representing the distribution. Section 3.2 explains this visual, combinatorial idea. The mathematics then branches off into a couple of directions. Section 3.3 revisits the connection with formal concept analysis with a more informed perspective, and Section 3.4 outlines a preliminary framework for modeling entailment and concept hierarchy using density operators.

CHAPTER FOUR. Chapter 4 is Chapter 3 in live action. We will discover that the spectral information of reduced densities of a *rank* 1 *density* can be pieced together to reconstruct the original state. We describe an algorithm for doing this, and along the way address a common puzzle in modeling probability distributions: Given a dataset of samples drawn from a possibly unknown probability distribution π, how might we use the samples to model a *new* probability distribution that estimates π, with the purpose of generating new data from it? Such models are called *generative models*. In Section 4.1 we'll show how the information stored in the eigenvectors and eigenvalues of reduced densities can be pieced together to build one of these models. The process is given by a deterministic algorithm that naturally leads to a *tensor network* presentation of the model. Because the algorithm and tools come from simple linear algebra, it's possible to predict how well the model will work, just given the number of samples used to build it. We will describe a concrete experiment on a dataset of even-parity bitstrings in Section 4.3. The application, algorithm, and experiment are work originally shared in [BST20].

CHAPTER FIVE. The last chapter reviews the mathematics of Chapters 1–4 from a high-level perspective. After distilling the essential ideas, it is apparent that the *fixed points of the composition of a map with its adjoint are interesting*. In the context of linear algebra, this refers to eigenvectors of reduced densities; in the context of sets and order theory, it refers to formal concepts. Both constructions are remarkably similar. In Chapter 5 we use the language of category theory to search for the reason for this similarity. As we'll see, both constructions arise from a free-forgetful adjunction. In Section 5.1 we'll recall the free-forgetful adjunction between the category of sets and the category of vector spaces. Special emphasis will be on the unit of the adjunction, which fits into a universal property that recovers Takeaway 2. In Section 5.2 we will remark on *free (co)completions* and their universal properties. Along the way, we'll comment on a number of striking analogies between category theory and linear algebra and a clear dictionary between the two. Section 5.3 then specializes the category theory to an *enrichment over truth values*, where a certain universal property will recover Takeaway 1. Know that Chapter 5 simply collects a number of known results into a single exposition with the purpose of calling attention to the similarity with our contributions in Chapters 1–4. Although we do not recover our linear algebraic constructions from the categorical blueprint, the pattern is crystal clear. We close in Section 5.4 with a remark on this.

2

Preliminaries

Networks transport classical
things like power, water, oil,
and cars. Tensor networks
transport linear algebraic
things like rank and
entanglement and should be
thought of as the quantum
analogy.

Shawn X. Cui et. al. [CFS$^+$15]

IN THIS CHAPTER we'll describe a passage from classical probability
to quantum probability by modeling any probability distribution π
as a pure quantum state; that is, a rank 1 density operator ρ. When
the state is entangled, the reduced density operators of ρ recover the
classical marginal probability distributions of π along their diago-
nals. Because the original state is entangled, the eigenvectors of the
reduced densities contain additional information from π, which we
see as conditional probability. The goal of this chapter is to present
these ideas from the ground up.

To begin, we think of density operators as the quantum version
of probability distributions, and of reduced density operators as the
quantum versions of marginal probability distributions. The opera-
tion that plays the role of marginalizing is called the partial trace. So
we give an overview of density operators in Section 2.3, of the par-
tial trace in Section 2.4, and of reduced density operators in Section
2.5. Know that these are basic constructions that may be found in
many excellent texts on quantum information theory and quantum
computing, such as [ASV02, NC00, Wat18, Wit18, Pre], though I've
included a number of expositional treats that may not be found in
standard introductions. Although the language of quantum mechan-
ics is used, the mathematics may appeal to a wider mathematical

audience with different applications in mind. So to help facilitate the transfer knowledge, Section 2.1 motivates this chapter with an elementary example that does not use the language of quantum mechanics. In the remaining sections, terminology is only introduced as needed. The opening example is followed by Section 2.2, which reviews bra-ket notation along with tensor network diagrams.

2.1 A Motivating Example

The best way to introduce the ideas in this chapter is through an example. The example in this section is remarkably elementary— understanding it requires no more than a few basic definitions from probability theory. Even so, it highlights interesting mathematics that is the keynote of this thesis.

2.1.1 Some Elementary Probability

Before the example, here's some basic terminology. A **probability distribution** (or simply, **distribution**) on a finite set S is a function $\pi\colon S \to \mathbb{R}$ satisfying

$$\sum_{s\in S} \pi(s) = 1, \qquad \pi(s) \geq 0 \text{ for all } s \in S.$$

If the elements of S are ordered so that $S = \{s_1,\ldots,s_n\}$, then a probability distribution may be written as a tuple $(\pi(s_1),\ldots,\pi(s_n))$ of nonnegative real numbers whose sum is 1. A **joint probability distribution** will refer to a probability distribution on a Cartesian product of finite sets; that is, a function $\pi\colon X \times Y \to \mathbb{R}$ satisfying

$$\sum_{(x,y)\in X\times Y} \pi(x,y) = 1.$$

Every joint distribution gives rise to **marginal probability distributions** by summing probabilities over one of the factors, sometimes referred to as "integrating out." So the marginal distribution $\pi_X\colon X \to \mathbb{R}$ on X and the marginal distribution $\pi_Y\colon Y \to \mathbb{R}$ on Y are defined by

$$\pi_X(x) = \sum_{y\in Y} \pi(x,y) \qquad \pi_Y(y) = \sum_{x\in X} \pi(x,y).$$

The process of marginalizing loses information. Informally, *marginal probability doesn't have memory.* Let's illustrate with an example. Suppose X and Y contain words from the English language.

$$X = \{\text{orange, green, purple}\} \qquad Y = \{\text{fruit, vegetable}\}$$

Consider the joint distribution on $X \times Y$ indicated in the 2×3 table below. For simplicity, suppose this distribution is an *empirical* one, so that for a fixed pair $(x, y) \in X \times Y$ the probability $\pi(x, y)$ is just the number of (x, y) divided by the total number of pairs.

	orange	green	purple
fruit	$\frac{1}{3}$	$\frac{1}{3}$	0
vegetable	0	0	$\frac{1}{3}$

So there are two kinds of food in three colors. You might imagine a very, very small corpus of text—a (rather dull) children's book, for instance—consisting of the three phrases

orange fruit   *green fruit*   *purple vegetable.*

Marginalizing provides a way to isolate and summarize the statistics of one feature at a time. For example, we can sum over Y to ignore food and only focus on colors alone. The resulting marginal probability distribution $\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ on X is computed by summing along the three columns of the table. In the same way, we can sum over X to ignore colors and obtain information about food alone. The resulting marginal probability distribution $\left(\frac{2}{3}, \frac{1}{3}\right)$ on Y is computed by summing across the two rows of the table.

$$\pi_X = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right) \qquad \longleftrightarrow \qquad \begin{matrix} \text{orange} \\ \text{green} \\ \text{purple} \end{matrix}$$

$$\pi_Y = \left(\frac{2}{3}, \frac{1}{3}\right) \qquad \longleftrightarrow \qquad \begin{matrix} \text{fruit} \\ \text{fruit} \\ \text{vegetable} \end{matrix}$$

Now it's apparent that marginal probability doesn't have memory.

- The marginal probability of *fruit* is $\frac{2}{3}$, though that number alone does not indicate that half of the fruits are orange and half are green.

- The marginal probability of *vegetable* is $\frac{1}{3}$, though that number alone does not indicate that all of the vegetables are purple.

So marginal probability is forgetful. It summarizes information and therefore leaves behind certain details from the joint distribution.

BUT THERE IS *another* way to compute marginal probability so that the information lost is in fact *not* lost but is readily available. Think of it as marginal probability with memory. We introduce it now.

fruit
fruit
vegetable

2.1.2   Marginal Probability With Memory

Here is a different way to compute marginal probabilities. Start with the same joint distribution on $X \times Y$. For reference, here it is again:

$$M = \begin{bmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} \end{bmatrix}$$

Some cosmetic changes have been made. First, the 2×3 table is now a 2×3 matrix, M. We may still think of the columns as being labeled by the colors *orange, green, purple*, and the rows as being labeled by *fruit* and *vegetable*. Also, square roots have been judiciously added. The reason will become clear soon. Now, without yet providing the reason *why*, let's consider the product of M with its (conjugate) transpose $M^\dagger$.

$$M^\dagger M = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix}$$

This matrix has several interesting features. First, it has three rows and three columns, which correspond to the three elements of the ordered set $X = \{\text{orange, green, purple}\}$. The ith diagonal entry can therefore be associated with the ith element of X. In particular, the diagonal entries of $M^\dagger M$ are precisely the marginal probabilities on X. So we turned the joint distribution into a matrix M and computed marginal probability as the diagonal of $M^\dagger M$.

	orange	green	purple
orange	$\frac{1}{3}$	$\frac{1}{3}$	0
green	$\frac{1}{3}$	$\frac{1}{3}$	0
purple	0	0	$\frac{1}{3}$

$\longleftrightarrow \qquad \pi_X = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$

But there's something else to notice. In addition to the diagonal entries, $M^\dagger M$ also contains non-zero off-diagonal entries. This guarantees that its *eigenvectors* are interesting.[1] Since $M^\dagger M$ is a rank 2 matrix, it has two eigenvectors. Not coincidentally, the set $Y = \{\text{fruit, vegetable}\}$ has two elements. Below are the two eigenvectors of $M^\dagger M$ along with a suggestive interpretation of their relation to the two elements of Y. In short, the squares of the entries of the

[1] If $M^\dagger M$ had *no* nonzero off diagonals, then its eigenvectors would correspond to the elements in X, which is not too interesting since we wouldn't have recovered anything new.

eigenvectors define conditional probability distributions on X.

$$
\begin{array}{cc}
\begin{array}{c}
\pi(\text{orange}|\text{fruit}) \\[1.2em]
\pi(\text{green}|\text{fruit}) \\[1.2em]
\pi(\text{purple}|\text{fruit})
\end{array}
\left[
\begin{array}{c}
\sqrt{\frac{1}{2}} \\[1em]
\sqrt{\frac{1}{2}} \\[1em]
0
\end{array}
\right]
&
\begin{array}{c}
\text{fruit} \longleftrightarrow
\end{array}
\quad
\begin{array}{c}
\text{orange fruit} \\
\text{green fruit}
\end{array}
\end{array}
$$

$$
\begin{array}{cc}
\begin{array}{c}
\pi(\text{orange}|\text{vegetable}) \\[1.2em]
\pi(\text{green}|\text{vegetable}) \\[1.2em]
\pi(\text{purple}|\text{vegetable})
\end{array}
\left[
\begin{array}{c}
0 \\[1em]
0 \\[1em]
1
\end{array}
\right]
&
\begin{array}{c}
\text{vegetable} \longleftrightarrow
\end{array}
\quad
\text{purple vegetable}
\end{array}
$$

Concretely, the squares of the entries of the first eigenvector define a probability distribution on X, conditioned on the first element of Y. For instance $\pi(\text{orange}|\text{fruit}) = \left(\sqrt{1/2}\right)^2 = 1/2$, which coincides with the fact that *half* the fruit are orange. Likewise, the squares of the entries of the second eigenvector define a probability distribution on X conditioned on the second element of Y. For example, $\pi(\text{purple}|\text{vegetable}) = 1$, which coincides with the fact that *all* of the vegetables are purple. So the eigenvectors of $M^\dagger M$ evidently capture **conditional probability**, which is precisely the information lost when marginalizing in the usual way as in Section 2.1.1. A similar phenomena happens for the matrix $MM^\dagger = \begin{bmatrix} 2/3 & 0 \\ 0 & 1/3 \end{bmatrix}$. Its diagonal recovers the marginal distribution $\pi_Y = \left(\frac{2}{3}, \frac{1}{3}\right)$ on Y, and the entries of its two eigenvectors have the interpretation of conditional probabilities.

So WE'VE PRESENTED a method to compute marginal probabilities in such a way that we have ready access to the information lost when marginalizing in the usual way. The general procedure, along with the theory behind it and the experimental results supporting it, are at the heart of this thesis. Here's the summary.

Main Procedure. Start with finite sets $X = \{x_1, \ldots, x_n\}$ and $Y = \{y_1, \ldots, y_m\}$ and a probability distribution $\pi \colon X \times Y \to \mathbb{R}$. Define an $m \times n$ matrix M whose ijth entry is the square root of the probability of (x_j, y_i).

$$
M_{ij} := \sqrt{\pi(x_j, y_i)}
$$

The diagonal of $M^\dagger M$ is the marginal probability distribution on X. The diagonal of $MM^\dagger$ is the marginal probability distribution on Y. Their eigenvectors capture information akin to conditional probability.

BEHIND THE SCENES. It might seem backwards to associate the ijth entry to the pair (x_j, y_i), but doing so means M corresponds to a linear map $\mathbb{C}^X \to \mathbb{C}^Y$, which is what we want. That is, for the application to come in Chapter 4, having $\mathbb{C}^Y$ as the target space will be important.

Think of the Main Procedure as being bottom-heavy. It takes no work to define M, and yet this simple passage from probabilities on a *set* to a linear map of *vector spaces* opens a floodgate of theory and applications. Understanding and exploiting the last sentence of the Main Procedure is the bulk of this thesis. The phrase "akin to" is particularly important. In special cases, the entries of the eigenvectors are conditional probabilities *on the nose*, as in our example. For more complicated M this won't be the case, but there is a very precise sense in which the information encoded by the eigenvectors is always conditional in nature. The precise statement will be given in Takeaway 3 and will be illustrated in Figure 2.2.

SETS | VECTOR SPACES

more structure here!
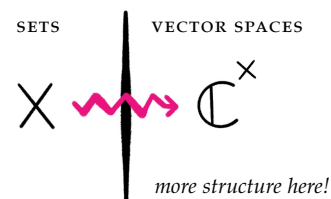
LET'S NOW PULL BACK the curtain and speak plainly. The mathematics here is **quantum probability theory**. Borrowing terminology that will be defined in Section 2.3, here's what's really going on.

- Every joint probability distribution on a finite set $\pi\colon X \times Y \to \mathbb{R}$ defines a rank 1 linear operator—called a **density operator** or synonymously a **pure quantum state**—on the tensor product of vector spaces $\mathbb{C}^X \otimes \mathbb{C}^Y$. *Density operators are the quantum version of probability distributions.*

  As we'll see in Section 2.3, there is more than one way to construct a rank 1 density operator from a joint probability distribution π. This thesis centers on a *very specific* rank 1 density, which will explain the phenomena observed in this section's motivating example. See Section 3.1.1 for the punchline.

- The rank 1 density operator gives rise to two **reduced density operators**, one on $\mathbb{C}^X$ and another on $\mathbb{C}^Y$. The matrices $M^\dagger M$ and $MM^\dagger$ in our example are representations of reduced density operators. *Reduced density operators are the quantum version of marginal probability distributions.*

- The eigenvalues and eigenvectors of these reduced density operators encode information about interactions between the $\mathbb{C}^X$ and $\mathbb{C}^Y$ subsystems, and we'll show that it is tantamount to conditional probability. More generally, the spectral information of reduced densities can be used to reconstruct a pure quantum state. When the state is that defined by a classical probability distribution, this ability to reconstruct suggests a new algorithm for reconstructing a classical joint probability distribution, which lends an application to data science. We will return to these points in Chapters 3 and 4.

So the Main Procedure describes a particular passage from classical probability to quantum probability that defines special operators $M^\dagger M$ and $MM^\dagger$. The rest of this chapter is a careful walk-through of this passage. It is primarily a passage from *sets* to *functions on sets* (that is, to *vector spaces*), and the next section begins with some notational preliminaries. We'll introduce bra-ket notation as well as tensor network diagram notation, which is a clean way to visualize common objects and operations in linear algebra.

2.2   Notation

The passage from classical probability to quantum probability begins with the passage from sets to *functions on sets,* namely vector spaces, which have much richer structure than the sets themselves. Unless said otherwise, we will only consider finite sets and finite-dimensional vector spaces.

2.2.1   Bra-Ket Notation

Given a finite set S, the **free vector space** $V = \mathbb{C}^S$ **on** S consists of complex-valued functions on S, which is a **Hilbert space** with inner product

$$\langle v|w \rangle = \sum_{s \in S} \overline{v(s)} w(s).$$

We will sometimes denote $v(s)$ by v_s. The free vector space comes with a natural map from $S \to \mathbb{C}^S$, defined shortly. But first, to avoid confusion, it is helpful to use notation that distinguishes between an element $s \in S$ and its image in $\mathbb{C}^S$, which is a vector. The vector image of s is sometimes denoted with a boldface font $\mathbf{s}$ or an overset arrow $\overrightarrow{s}$. We'll use **bra and ket notation**, which is especially nice when dealing with inner products. For any $s \in S$, let $|s\rangle$ denote the function $S \to \mathbb{C}$ that sends $s \mapsto 1$ and $s' \mapsto 0$ for $s' \neq s$. The set $\{|s\rangle\}$ is a linearly independent orthonormal spanning set for V, and is sometimes called the **computational basis**. If an ordering is chosen on the set S, say $S = \{s_1 \ldots, s_n\}$, then $|s_i\rangle$ is identified with the ith standard basis vector in $\mathbb{C}^n$.

$$|s_i\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i\text{th entry}$$

This defines an isomorphism $\mathbb{C}^S \cong \mathbb{C}^n$. More generally we'll denote elements in V by **ket** notation $|v\rangle \in V$, which is just a linear combination of basis vectors $|s\rangle$. As an array, it is a column vector of complex numbers.

$$|v\rangle = \sum_{s \in S} v(s)|s\rangle = \begin{bmatrix} v(s_1) \\ \vdots \\ v(s_n) \end{bmatrix} \qquad v(s) \in \mathbb{C}$$

For any $|v\rangle \in V$, there is a linear functional in $V^* := \hom(V, \mathbb{C})$ whose value on $|v'\rangle \in V$ is the inner product $\langle v|v'\rangle$. We'll denote this

A **Hilbert space** is a vector space equipped with an inner product such that it is a *complete metric space* with respect to the metric induced by the inner product. If a vector space is finite dimensional, then the induced metric always has this property. So any finite-dimensional vector space with an inner product is a Hilbert space.

BEHIND THE SCENES. The notation $S \to \mathbb{C}^S$ is a bit sloppy: S is a set while $\mathbb{C}^S$ is a vector space. A mapping between different objects makes little mathematical sense. So by "a natural map $S \to \mathbb{C}^S$" I really mean a *function* from S to the *underlying set* of $\mathbb{C}^S$. This is much more than pedantry. Category theory gives a nice way to indicate this in the notation, and it will play a major role in Chapter 5.

The dual space $V^* = \hom(V, \mathbb{C})$ consists of all linear maps $V \to \mathbb{C}$.

linear functional by the **bra** notation $\langle v| \in V^*$.

$$V \xrightarrow{\ \langle v|\ } \mathbb{C}$$
$$|v'\rangle \longmapsto \langle v|v'\rangle$$

As an array with respect to the dual basis $\{\langle s|\}$, this is represented by the conjugate transpose of $|v\rangle$; that is $|v\rangle^\dagger = \langle v|$ and likewise $\langle v|^\dagger = |v\rangle$.

$$\langle v| = \sum_{s \in S} \overline{v(s)}\langle s| = \begin{bmatrix} \overline{v(s_1)} & \cdots & \overline{v(s_n)} \end{bmatrix} \qquad v(s) \in \mathbb{C}$$

Every linear functional in V^* is of the form $\langle v|$ for some $|v\rangle \in V$. So we have vectors $|v\rangle \in V$ and **covectors** $\langle v| \in V^*$ and the map

$$|v\rangle \longleftrightarrow \langle v|$$

defines a natural isomorphism between V and V^*. We have chosen to distinguish between vectors and covectors with bra and ket notation, but we will not give any special meaning to upper and lower indices. Given another vector space W, elements in the tensor product $V \otimes W$ will be denoted $|v\rangle \otimes |w\rangle$ or sometimes $|vw\rangle$, when $|v\rangle \in V$ and $|w\rangle \in W$. Further, the expression $|w\rangle\langle v|$ will be used for the tensor product $|w\rangle \otimes \langle v|$, which is an element of $W \otimes V^*$. It is naturally identified with the following map $V \to W$.

$$V \xrightarrow{\ |w\rangle\langle v|\ } W$$
$$|v'\rangle \longmapsto |w\rangle\langle v|v'\rangle$$

In particular, the expression $|v\rangle\langle v|$ is an element in $\mathrm{End}(V)$. Here, $\mathrm{End}(V)$ denotes the space of all linear operators on V, and in the presence of a basis is identified with $\dim(V) \times \dim(V)$ matrices. If $|\psi\rangle$ is a unit vector, then the operator $|\psi\rangle\langle\psi|$ is the orthogonal projection onto $|\psi\rangle$. It maps $|\psi\rangle$ to $|\psi\rangle$, and it maps every vector perpendicular to $|\psi\rangle$ to zero. To encourage fluency, Table 2.1 contains a dictionary summarizing the translation between bra-ket notation, the usual star notation, and array representations (column versus row vectors, and so on). Here are a few more helpful facts to know.

1. **The tensor product of vectors is the outer product of their column vector representations.** In other words,

$$|w\rangle \otimes |v\rangle = |w\rangle\langle v|. \tag{2.1}$$

To elaborate, recall that an element $|w\rangle\langle v|$ of the tensor product $W \otimes V^*$ corresponds to a linear map $V \to W$ as mentioned above. Under the identification $V \cong V^*$ it also corresponds to the element

I realize that bra-ket notation may not be familiar to all, but the concept behind it is not foreign to mathematics. In category theory, for instance, certain functors are commonly denoted by what they *do*, which is the idea behind bra-kets. Here's an example. Fix any set X and consider the functor F from the category Set of sets to itself whose assignment on a set Y is the Cartesian product $X \times Y$.

$$F(X) = X \times Y$$

In lieu of a generic "F," one usually denotes this assignment by the descriptive notation $X \times -$. The empty space tells us precisely what the functor does. Just stick any set Y in the blank spot to find out!

$$\mathsf{Set} \xrightarrow{\ X \times -\ } \mathsf{Set}$$
$$Y \longmapsto X \times Y$$

This is the same idea behind bra-ket notation. A bra $\langle v|$, which could also be written $\langle v|-\rangle$, is analogous to the symbol $X \times -$. The empty space tells us precisely what the linear map does. Just stick any vector v' in the blank spot to find out!

$$V \xrightarrow{\ \langle v|-\rangle\ } \mathbb{C}$$
$$v' \longmapsto \langle v|v'\rangle$$

Instead of carrying around $\langle v|-\rangle$, which feels a little lopsided, it's better to *declare* that vectors v' are denoted $|v'\rangle$ so that "sticking in a vector into the blank spot" simply corresponds to sandwiching the bra $\langle v|$ and the ket $|v'\rangle$ together.

	star	bra-ket	array
vector	v	$\lvert v \rangle$	$\begin{bmatrix} \vdots \end{bmatrix}$
covector	v^*	$\langle v \rvert$	$\begin{bmatrix} \cdots \end{bmatrix}$
element in $V \otimes W$	$v \otimes w$	$\lvert v \rangle \otimes \lvert w \rangle$	$\begin{bmatrix} \vdots \end{bmatrix} \otimes \begin{bmatrix} \vdots \end{bmatrix}$
inner product	$\langle v, w \rangle$	$\langle v \lvert w \rangle$	$\begin{bmatrix} \cdots \end{bmatrix} \begin{bmatrix} \vdots \end{bmatrix}$
linear map $V \to W$	$w \otimes v^*$	$\lvert w \rangle \langle v \rvert$	$\begin{bmatrix} \vdots \end{bmatrix} \begin{bmatrix} \cdots \end{bmatrix} \begin{bmatrix} \; \end{bmatrix}$
orthogonal projection	$\psi \otimes \psi^*$	$\lvert \psi \rangle \langle \psi \rvert$	$\begin{bmatrix} \vdots \end{bmatrix} \begin{bmatrix} \cdots \end{bmatrix}$

Table 2.1: A dictionary for translation between bra-ket notation and star notation.

$\lvert w \rangle \otimes \lvert v \rangle$ in $W \otimes V$. If bases are chosen for W and V then $\lvert w \rangle \otimes \lvert v \rangle$ is the $\dim(W) \times \dim(V)$ matrix obtained by multiplying the $\dim(W) \times 1$ column vector $\lvert w \rangle$ with the $1 \times \dim(V)$ row vector $\langle v \rvert$, which is Equation (2.1). This matrix product is called the **outer product** of $\lvert w \rangle$ and $\lvert v \rangle$.

Example 2.1. As a simple example, suppose

$$\lvert w \rangle = \begin{bmatrix} 1 \\ 2 \\ 3i \end{bmatrix} \qquad \lvert v \rangle = \begin{bmatrix} 4i \\ 5 \end{bmatrix}$$

Then the tensor product is a matrix

$$\lvert w \rangle \otimes \lvert v \rangle = \lvert w \rangle \langle v \rvert = \begin{bmatrix} 1 \\ 2 \\ 3i \end{bmatrix} \begin{bmatrix} -4i & 5 \end{bmatrix} = \begin{bmatrix} -4i & 5 \\ -8i & 10 \\ 12 & 15i \end{bmatrix}$$

called the *outer product* of $\lvert w \rangle$ and $\lvert v \rangle$.

Writing the vector $\lvert w \rangle \otimes \lvert v \rangle$ may be puzzling since we often think of vectors as *columns*. But there's no confusion here. The 3×2 matrix on the left may be effortlessly reshaped into a 6×1 vector, which we can also identify with the tensor product $\lvert w \rangle \otimes \lvert v \rangle$.

$$\lvert w \rangle \otimes \lvert v \rangle = \begin{bmatrix} -4i \\ 5 \\ -8i \\ 10 \\ 12 \\ 15i \end{bmatrix}$$

So whether we think of tensor products of vectors as linear maps $V \to W$ or as elements of $W \otimes V$ will determine whether we use a matrix representation or a column vector.

2. **The trace of the linear operator $\lvert v' \rangle \langle v \rvert$ is the inner product $\langle v \lvert v' \rangle$.** In other words,

$$\operatorname{tr} \lvert v' \rangle \langle v \rvert = \langle v \lvert v' \rangle$$

for any vectors $\lvert v \rangle, \lvert v' \rangle \in V$. Indeed, if $\{\lvert s \rangle\}$ is an orthonormal basis for V then the matrix representation of $\lvert v' \rangle \langle v \rvert$ is the outer

product

$$|v'\rangle\langle v| = \begin{bmatrix} \vdots \\ v'(s) \\ \vdots \end{bmatrix} \begin{bmatrix} \cdots & \overline{v(s)} & \cdots \end{bmatrix}$$

which has trace equal to $\sum_s \overline{v(s)}v'(s) = \langle v|v'\rangle$.

3. **An outer product of tensor products is the tensor product of outer products.** In other words, for any vectors $|v\rangle, |v'\rangle \in V$ and $|w\rangle, |w'\rangle \in W$, one has $|v\rangle \otimes |w\rangle\langle v'| \otimes \langle w'| = |v\rangle\langle v'| \otimes |w\rangle\langle w'|$. But this looks a bit confusing, so let's suppress the tensor product symbol and write $|vw\rangle := |v\rangle \otimes |w\rangle$. The claim is then

$$|vw\rangle\langle v'w'| = |v\rangle\langle v'| \otimes |w\rangle\langle w'|. \tag{2.2}$$

Observe that both the left- and the right-hand side are linear operators $V \otimes W \to V \otimes W$. To verify their equality, let's check that their assignments on basis vectors are the same. First, recall that if $f\colon A \to B$ and $f'\colon A' \to B'$ are linear maps, then their tensor product is a linear map $f \otimes f'\colon A \otimes A' \to B \otimes B'$ defined on any basis vector $|a\rangle \otimes |a'\rangle$ of $A \otimes A'$ by

$$(f \otimes f')|a\rangle \otimes |a'\rangle := f|a\rangle \otimes f|a'\rangle. \tag{2.3}$$

Now suppose $\{|s\rangle\}$ is a basis for V and $\{|t\rangle\}$ is a basis for W.

(left-hand side) The expression $|vw\rangle\langle v'w'|$ on the left-hand side of Equation (2.2) is the linear map sending the vector $|st\rangle$ to $|vw\rangle\langle v'w'|st\rangle$, where the inner product is equal to

$$\langle v'w'|st\rangle = ((\langle v'| \otimes \langle w'|)|s\rangle \otimes |t\rangle$$
$$= \langle v'|s\rangle\langle w'|t\rangle,$$

which follows from Equation (2.3) with $f = \langle v'|$ and $f' = \langle w'|$. So the image of $|st\rangle$ under the operator on the left-hand side of Equation (2.2) is

$$|vw\rangle \overbrace{\langle v'|s\rangle\langle w'|t\rangle}^{\text{a number}}.$$

(right-hand side) The image of any basis vector $|st\rangle$ under the right-hand side of (2.2) follows from a direct application of

Equation (2.3).

$$(|v\rangle\langle v'| \otimes |w\rangle\langle w'|)|s\rangle \otimes |t\rangle = |v\rangle\langle v'|s\rangle \otimes |w\rangle\langle w'|t\rangle$$
$$= |v\rangle \otimes |w\rangle\langle v'|s\rangle\langle w'|t\rangle$$
$$= |vw\rangle \overbrace{\langle v'|s\rangle\langle w'|t\rangle}^{\text{a number}}.$$

So we have equality as claimed.

Let's move on to another way to denote familiar tools in linear algebra, namely as *tensor network diagrams*, based on Roger Penrose's graphical notation [Pen71].

2.2.2   Tensor Network Diagrams

We'll start with some terminology. A **tensor of order** n is an n-dimensional array of (real or complex) numbers. Such an array represents a vector in, or a mapping between, tensor products of finite-dimensional vector spaces. A factorization of a tensor into smaller ones is called a **tensor network**. Every matrix factorization (singular value decomposition, QR decomposition, Cholesky decomposition, . . .) is an example.[2] More complicated factorizations of larger-dimensional tensors can be a notational chore to write down. Fortunately, there is a clean visual way to represent them—a **tensor network diagram**. In a tensor network diagram, an n-tensor is represented by a node, and each of the n vector spaces, or *dimensions*, is drawn as an edge incident to the node.

A scalar, for example, can be thought of as a zero-dimensional array—a point. It is a 0-tensor and corresponds to a node with no edges. A vector is a 1-tensor, a one-dimensional array, and hence corresponds to a node with one edge. A matrix is a 2-tensor and hence a node with two edges. A 3-tensor is a node with three edges and so on. The edges may be further decorated with indices to distinguish each dimension. For instance, to specify an $m \times n$ matrix M, one must specify all mn entries M_{ij}, where i indexes the number of rows and j indexes the number of columns of M.

a matrix M_{ij} is the diagram
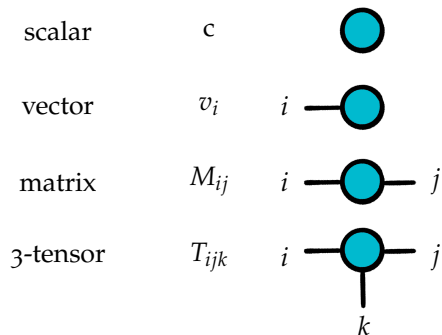
$$i \; \text{—}\!\bullet\!\text{—} \; j$$

One often thinks of "M_{ij}" not just as the ijth entry but also as a stand-in for all i, j entries at once, resulting in the full matrix M. In this same spirit we may drop the indices from the diagram and

Sometimes a "tensor of order n" is also called a "rank n tensor," though we will not use this expression. Rank already has a meaning in linear algebra!

[2] The expression "tensor product" might not come to mind when working with everyday matrices, but it should. Every linear map—and hence every matrix—corresponds to a vector in a tensor product of vector spaces. We'll say more about this in Section 2.5.

simply write ─◯─ as representing the linear map itself. More generally, we have the following diagrams.

scalar   c

vector v_i i ─◯

matrix M_{ij} i ─◯─ j

3-tensor T_{ijk} i ─◯─ j
                            |
                            k

Though these pictures might be new to some, I suspect the idea is familiar to all. When teaching students about functions, for instance, one often says, "A function is like a machine. You feed it an input, the machine does its job, and then it spits out the output." The accompanying picture is something like this:

in ─▢─ out

a function is a machine

This is an example of a tensor diagram, though we're now interested in *linear* functions. Think of the node as the linear mapping and think of the edges as the input (domain) and output (codomain) vector spaces. I prefer to draw the nodes as circles, rather than squares, though it doesn't matter.

─◯─

a matrix is a node

In this graphical notation, familiar notions have elegant pictures. Here is a brief showcase.

1. **Composition is tensor contraction**. Tensors can be composed along dimensions of matching indices, and tensor contraction corresponds to summing along this common index. Graphically, this corresponds to joining the corresponding edges between diagrams. For example, the product of two matrices

   M_{ij} N_{jk}

   i ─◯─ j j─◯─k

   is illustrated by "gluing" the two edges labeled j and then fusing the two nodes into a single node.

   $\sum_j M_{ij}N_{jk}$ $(MN)_{ik}$
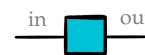
   i ─◯─◯─ k = i ─◯─ k
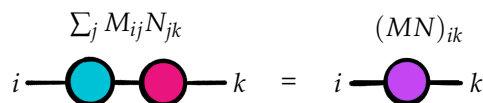
   The resulting diagram has two free indices, i and k, which indeed specify a new matrix. As another example, the product of a matrix M with a vector $|v\rangle$ results in another vector $M|v\rangle$, which is a node with one free edge.

   M $|v\rangle$ $M|v\rangle$

   ─◯─◯   =   ─◯
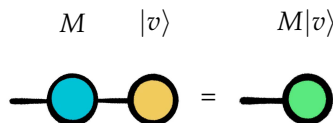
   To keep the picture clean, we've now dropped the indices. More generally, the composition of two or more tensors is represented by a cluster of nodes and edges where the contractions occur along edges with matching indices.

The diagram here illustrates another important point. There is great flexibility in how one chooses to orient the diagrams spatially. A vector, for instance, is characterized by the fact that it is *one node with one edge*. We will not imbue additional meaning to whether the edge is horizontal or vertical or otherwise. For example we take both —⬤ and ⬤ to represent the same vector.

2. **The shape of a node may convey additional meaning.** There is flexibility in the shapes used for nodes, as convention varies across the literature. This allows for creativity in how information can be conveyed through a diagram. When working with 2-tensors, for instance, we may wish to use a symmetric shape for symmetric matrices only. Then the dual mapping can be represented by reflecting its diagram,

symmetric   not symmetric

dual
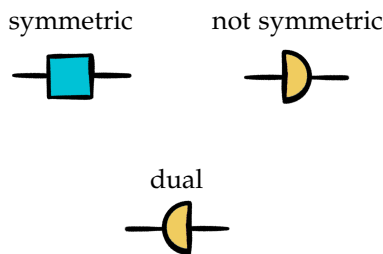
so that the symmetry is preserved in the notation.

$$M \qquad M^\dagger$$
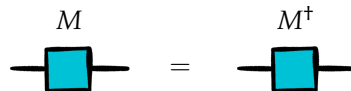
Another useful choice is to represent isometric embeddings as triangles:


An **isometric embedding** U is a linear map from a space V to a space W of larger dimension that preserves the lengths of vectors. Such a map satisfies $U^\dagger U = \mathrm{id}_V$ but $UU^\dagger \neq \mathrm{id}_W$. In words, projection of the large space W onto the embedded image $UV \subseteq W$ won't distort the vectors in V. This operation is the identity on

V. On the other hand, compressing W onto V necessarily loses information, so to speak. The asymmetry of the triangle serves as a visual reminder of this: the base (W) is larger than its tip (V).
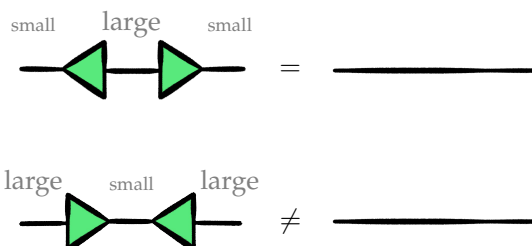
When $W = V$ and when U satisfies both equalities $UU^\dagger = U^\dagger U = \mathrm{id}_V$, then it is called a **unitary operator**. This illustrates another useful convention: the identity mapping is often represented as an edge with no node. Indeed, contraction with an identity leaves a tensor and its corresponding diagram unchanged.
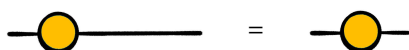
3. **Tensor decomposition is node decomposition.** The flexibility in choosing different node shapes provides useful pictures for tensor decomposition. For example, the singular value decomposition of a matrix $M = VDU^\dagger$ (see Section 2.5) can be illustrated as:
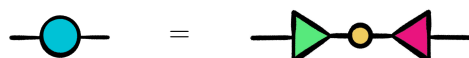
Here, U and V are unitary operators, hence isometries and hence triangles, while D is a diagonal operator drawn as a circle. More generally, tensor decomposition is the decomposition of one node into multiple nodes, while tensor composition is the fusion of multiple nodes into a single node.

*de*compose

compose
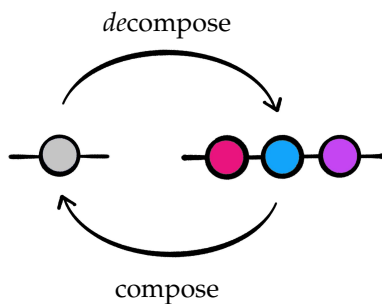
4. **Proofs have simple pictures**. Another feature of tensor diagram notation is the visual simplicity of proofs. Consider the trace of a matrix, for instance. It is the sum along a common index, and so the corresponding diagram is a loop:
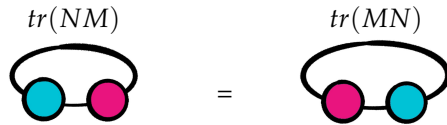
$$\sum_i M_{ii}$$

Note that a loop has no free indices, which is consistent with the idea that a scalar is a 0-tensor. Proving that the trace is invariant under cyclic permutations becomes as simple as sliding beads along a necklace.

$$tr(NM) \qquad tr(MN)$$

$$=$$

5. **Tensor products are illustrated by stacking in parallel**. The tensor product of vector spaces $V \otimes W$ is represented by two parallel edges, one associated to V and the other associated to W. An arbitrary vector $|\phi\rangle$ in this space is then drawn as a node with two parallel edges. If $|\phi\rangle = |v\rangle \otimes |w\rangle$ decomposes as the tensor product of two vectors $|v\rangle \in V$ and $|w\rangle \in W$, then we illustrate $|\phi\rangle$ by placing the diagrams for the vectors $|v\rangle$ and $|w\rangle$ side-by-side. Similarly, an arbitrary linear map between tensor products $h\colon V \otimes V' \to W \otimes W'$ is represented by a node with four edges, one for each space. If h decomposes as a tensor product $h = f \otimes f'$ for linear maps $f\colon V \to W$ and $f'\colon V' \to W'$, then the diagram for h is drawn as the diagrams for f and f' stacked side-by-side.[3]
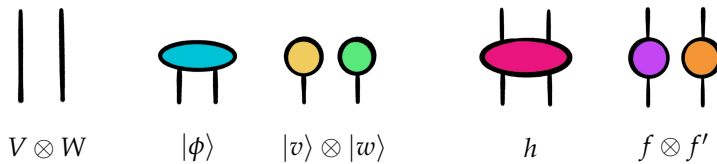
[3] Recall that $f \otimes f'\colon V \otimes V' \to W \otimes W'$ is the linear map defined in Equation (2.3).

$$V \otimes W \qquad |\phi\rangle \qquad |v\rangle \otimes |w\rangle \qquad h \qquad f \otimes f'$$

The diagram shown previously, for example, is a vector in the six-fold tensor product of vector spaces $V_1, V_2, \ldots, V_6$.

$$\in V_1 \otimes V_2 \otimes V_3 \otimes V_4 \otimes V_5 \otimes V_6$$

We've mentioned this particular orange diagram twice now. As it turns out, diagrams of this shape—a one-dimensional string of nodes with parallel edges sticking down—will resurface in a major way in Chapter 4. Understanding it further illustrates a main advantage to working with tensor networks, so let's say a few words about that now. Consider the N-fold tensor product of a d-dimensional vector space V. If $V = \mathbb{C}^X$ for some set $X = \{x_1, \ldots, x_d\}$, then the Cartesian product $X^N = \{(x_{i_1}, \ldots, x_{i_N}) \mid x_{i_k} \in X\}$ is a basis for the tensor product $V^{\otimes N} \cong \mathbb{C}^{X^N}$. So an arbitrary vector in $V^{\otimes N}$ is of the form

$$|\psi\rangle = \sum_{(x_{i_1}, \ldots, x_{i_N}) \in X^N} \psi_{i_1 i_2 \cdots i_N} |x_{i_1}\rangle \otimes |x_{i_2}\rangle \otimes \cdots \otimes |x_{i_N}\rangle.$$

To specify any vector $|\psi\rangle \in V^{\otimes N}$ we must therefore specify d^N numbers $\psi_{i_1 i_2 \cdots i_N}$. For large N, storing these numbers on a computer quickly becomes impractical. To make the situation manageable, one often looks for another vector in $V^{\otimes N}$ that is a good *approximation* to $|\psi\rangle$ and that can be specified using far fewer parameters. This is where tensor networks come in. For example, certain $|\psi\rangle$ are well-approximated by a **matrix product state** (MPS), also called a **tensor train**, which is a vector in $V^{\otimes N}$ whose coefficients $\psi_{i_1 i_2 \cdots i_N}$ are obtained as a product of just a few (relatively speaking) numbers. As a diagram, MPS are depicted as a string of 3-tensors, capped off with two matrices on the left and right. This is the diagram we saw above, with $N = 6$.
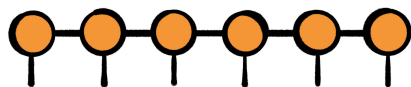
a matrix product state

For now, let's not worry about the precise definition of an MPS—we'll build one from scratch in Section 4.1.2. In the mean time, know that tensor networks come in many "flavors," and an MPS is one example. More generally, tensor networks are useful in modeling the states of quantum many body systems. Different systems have different properties, and some tensor networks are better than others at capturing those properties. For a brief sketch of widely-used tensor networks and main algorithms used to work with them, see the recent survey [Orú19]. For a more thorough introduction to tensor networks and their diagrammatic notation, see [Sto19, BC17, Orú14, BB17, Bia19, Pen71, RL19, Sch11] and other treatments.

WITH THESE NOTATIONAL preliminaries in hand, think back to the motivating example in Section 2.1.2. There we introduced an ad-

vantage of working with *density operators* in lieu of probability distributions, namely access to "marginal probability with memory." This advantage ultimately—and quite simply—arises from access to results and tools of linear algebra. Let's introduce this idea more formally now, starting with the definition of a density operator.

2.3 Density Operators

Definition 2.1. A **density operator**, or simply **density**, is a linear operator that is Hermitian, positive semidefinite, and has unit trace. A density operator is also called **quantum state**.

We think of density operators as the quantum version of probability distributions. The analogy is clear after unwinding the definition. Let's take a closer look at the three properties.

Hermitian operators are like real numbers. An operator $f \colon V \to V$ is **Hermitian** if $\langle fv|w \rangle = \langle v|fw \rangle$ for all $v, w \in V$. The matrix representation of a Hermitian operator is equal to its conjugate transpose $f = f^{\dagger}$, and the eigenvalues of Hermitian operators are always real. Analogously, probabilities are real numbers.

Positive semidefinite operators are like nonnegative numbers. An operator $f \colon V \to V$ is **positive semidefinite** if $\langle v|f|v \rangle \geq 0$ for all $v \in V$. Loosely speaking, if f is positive semidefinite, then the image of the vector $|v\rangle$ under f's transformation doesn't point in the "opposite" direction of $|v\rangle$. The eigenvalues of positive semidefinite operators are always nonnegative. Analogously, probabilities are nonnegative numbers.

The trace is a sum of numbers. The trace of an operator is the sum of the diagonal entries of a matrix representing it. The trace is also equal to the sum of the eigenvalues of the operator. A density operator has **trace equal to** 1. Analogously, probabilities sum to 1.

So density operators generalize probability distributions.

density operator	probability distribution
real eigenvalues	real numbers
nonnegative eigenvalues	nonnegative numbers
sum to 1	sum to 1

But more is true. Every density operator defines a classical probability distribution, and every classical probability defines a density operator.
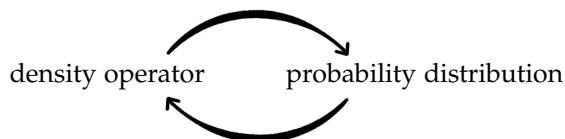
Let's understand the first claim first.

Every density on $\mathbb{C}^S$ defines a probability distribution on S.

Let S be a finite set. Any density operator $\rho\colon \mathbb{C}^S \to \mathbb{C}^S$ defines a probability distribution $\pi_\rho\colon S \to \mathbb{R}$ by the **Born rule**,

$$\pi_\rho(s) = \langle s|\rho|s\rangle \qquad s \in S. \tag{2.4}$$

The $\pi_\rho(s)$ are the diagonal entries of the matrix representation of ρ with respect to the basis $\{|s\rangle\}$. These values are real and nonnegative since ρ is Hermitian and positive semidefinite, and $\sum_s \pi_\rho(s) = 1$ since the trace of ρ is 1. So every density ρ on $\mathbb{C}^S$ does indeed define a probability distribution π_ρ on S. We can also go in the other direction, and in more than one way.

Every probability distribution on S defines densities on $\mathbb{C}^S$.

Suppose a probability distribution π on S is already given. Let's turn our attention to density operators ρ on $\mathbb{C}^S$ with the property that the Born distribution induced by ρ coincides with the given probability distribution π.

$$\pi = \pi_\rho \tag{2.5}$$

As it turns out, there are *multiple* ways to do this to build densities with this property. Below we share *two* such ways to define a density operator on $\mathbb{C}^S$ from a probability distribution on S so that Equation (2.5) is satisfied. These two ways can be thought of as two extremes in a range of options.

1. **Diagonal.** Given $\pi\colon S \to \mathbb{R}$ define $\rho_{\text{diag}} := \sum_{s\in S} \pi(s)|s\rangle\langle s|$. As a matrix, this is simply the operator with the probabilities $\pi(s)$ along its diagonal and zeros elsewhere.

$$\rho_{\text{diag}} = \begin{bmatrix} \pi(s_1) & & & \\ & \pi(s_2) & & \\ & & \ddots & \\ & & & \pi(s_n) \end{bmatrix}$$

$$\pi = \left(\tfrac{3}{5}, \tfrac{1}{5}, \tfrac{1}{5}\right) \quad \rightsquigarrow \quad \begin{bmatrix} \tfrac{3}{5} & 0 & 0 \\ 0 & \tfrac{1}{5} & 0 \\ 0 & 0 & \tfrac{1}{5} \end{bmatrix} = \rho_{\text{diag}}$$

   This is manifestly a density. It's symmetric with trace equal to 1, and for any vector $|v\rangle = \sum_{s\in S} v(s)|s\rangle$ the inner product $\langle v|\rho_{\text{diag}}|v\rangle$ is given by the sum $\sum_{s\in S} |v(s)|^2 \pi(s) \geq 0$, and so ρ_{diag} is positive

semidefinite. It's also straightforward to see that ρ_{diag} satisfies Equation (2.5). The diagonal operator has the probabilities on its diagonal! In short, any finite list of nonnegative real numbers that add up to 1 can be turned into a diagonal matrix, which is a density. Now let's give a second way to construct a density from π.

2. **Orthogonal Projection.** Given $\pi\colon S \to \mathbb{R}$ define a unit vector by taking the sum of all the elements in S and weighting each by the square root of its probability,

$$|\psi\rangle = \sum_{s \in S} \sqrt{\pi(s)}|s\rangle \qquad (2.6)$$

and consider the orthogonal projection onto the line spanned by it,

$$\rho_\pi := |\psi\rangle\langle\psi|. \qquad (2.7)$$

The operator ρ_π is Hermitian since for any vectors $|v\rangle, |w\rangle \in \mathbb{C}^S$, the inner product $\langle \rho_\pi v | w \rangle$ is $\langle v | \psi \rangle \langle \psi | w \rangle$, which is equal to $\langle v | \rho_\pi w \rangle$. The operator is also positive semidefinite since the inner product $\langle v | \psi \rangle \langle \psi | v \rangle = |\langle v | \psi \rangle|^2$ is nonnegative. Moreover the trace of ρ_π is $\langle \psi | \psi \rangle = 1$. Further, Equation (2.5) is satisfied as claimed:

$$\pi_{\rho_\pi}(s) = \langle s | \psi \rangle \langle \psi | s \rangle = \left(\sqrt{\pi(s)} \right)^2 = \pi(s).$$

As a matrix, ρ_π is computed as the outer product of $|\psi\rangle$ with itself.

$$\rho_\pi = \begin{bmatrix} \vdots \\ \sqrt{\pi(s)} \\ \vdots \end{bmatrix} \begin{bmatrix} \cdots & \sqrt{\pi(s)} & \cdots \end{bmatrix}$$

As a tensor network diagram, the covector $\langle\psi|$ is denoted by reflecting the diagram for $|\psi\rangle$, and we'll denote the picture for $\rho_\pi = |\psi\rangle\langle\psi|$ by stacking one on top of the other.

FOR MUCH OF this text, our main focus will be on the density operator $\rho_\pi = |\psi\rangle\langle\psi|$, which is orthogonal projection onto the vector

Remember the vector in Equation (2.6). It's the main character for the next three chapters!

$$\pi = \left(\frac{3}{5}, \frac{1}{5}, \frac{1}{5} \right) \rightsquigarrow \begin{bmatrix} \sqrt{\frac{3}{5}} \\ \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} \end{bmatrix} \begin{bmatrix} \sqrt{\frac{3}{5}} & \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{5}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{3}{5} & \frac{\sqrt{3}}{5} & \frac{\sqrt{3}}{5} \\ \frac{\sqrt{3}}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{\sqrt{3}}{5} & \frac{1}{5} & \frac{1}{5} \end{bmatrix} = \rho_\pi$$

defined in Equation (2.6). But think of diagonal operators and or-
thogonal projections as two extremes: ρ_{diag} has maximal rank while
ρ_π has rank 1. The language of quantum mechanics makes this more
precise.

Definition 2.2. A density operator ρ is called a **pure quantum state**
if its rank is equal to 1 and is called a **mixed quantum state** other-
wise. The degree of "mixedness" of a density is measured by its **von
Neumann entropy** $-\operatorname{tr}(\rho \ln \rho)$.

Let's spend some time on the terms just defined. First, as noted,
rank 1 densities are called *pure quantum states*. Unit vectors are also
referred to by this same name. The flexibility is understandable since
a unit vector may be identified with orthogonal projection onto the
line spanned by it. Knowing the projection operator is the same as
knowing the unit vector. Here's another way to see why a "state" is
an appropriate synonym for a vector. By definition, any unit vector
$|\psi\rangle = \sum_s \psi(s)|s\rangle$ in $\mathbb{C}^S$ has the property that $\sum_s |\psi(s)|^2 = 1$. So
its coordinates define a probability distribution on the set S: the
probability of $s \in S$ is $|\psi(s)|^2 = |\langle s|\psi\rangle|^2$. For this reason, the set S
can be thought of as representing some system, the internal states of
which are given by the probabilities $|\psi(s)|^2$. So we may occasionally
refer to $|\psi\rangle$ or $|\psi\rangle\langle\psi|$ as **the state of the system S.**

But what about densities not arising as projections-onto-lines? If
the rank of a density is larger than 1, then it is called a *mixed quantum
state.* This, too, is descriptive. As with every Hermitian operator, a
density ρ on $\mathbb{C}^S$ has a **spectral decomposition**. That is, there exists
an orthonormal set of eigenvectors $\{|e_1\rangle, \ldots, |e_r\rangle\}$ of ρ, where r is the
rank of ρ, so that

$$\rho = \sum_{i=1}^r \lambda_i |e_i\rangle\langle e_i|. \tag{2.8}$$

Each operator $|e_i\rangle\langle e_i|$ is orthogonal projection onto the line spanned
by the eigenvector $|e_i\rangle$, and so ρ is a *mixture* of pure states. As an
aside, notice that the eigenvalues λ_i of ρ are real (since ρ is Hermi-
tian), nonnegative (since ρ is positive semidefinite), and their sum
is 1 (since ρ has unit trace).[4] Therefore the λ_i are probabilities. Con-
cretely, they define a probability distribution on the set of eigenvec-
tors $\{|e_i\rangle\}$. What's more, each eigenvector *itself* defines a probability
distribution on the original set S. The probability of an element $s \in S$
is given by the Born rule $\langle s|e_i\rangle\langle e_i|s\rangle = |\langle s|e_i\rangle|^2$. Intuitively, just square
the modulus of the sth entry of the column vector $|e_i\rangle$. Since $|e_i\rangle$ is a
unit vector, the $|\langle s|e_i\rangle|^2$ are probabilities—they add up to 1.

[4] The trace is invariant under a change
of basis. So choosing the eigenvectors
$\{|e_i\rangle\}$ of ρ as a basis for its image,
the matrix representation of ρ has
its eigenvalues λ_i along the diagonal
and zeros elsewhere. The trace of that
matrix is $\lambda_1 + \cdots + \lambda_r = 1$.

Example 2.2. Suppose $S = \{s_1, s_2, s_3\}$ is a three-element set and

consider the following 3×3 density operator on $\mathbb{C}^S \cong \mathbb{C}^3$.

$$\rho = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix}$$

Its nonzero eigenvalues are $\lambda_1 = \frac{2}{3}$ and $\lambda_2 = \frac{1}{3}$ with corresponding eigenvectors

$$|e_1\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \qquad |e_2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

We've analyzed the spectral information of this matrix before. Recall the discussion of colors and fruits and vegetables in Section 2.1.2.

This has the following interpretation. With probability $\lambda_1 = \frac{2}{3}$ the state of the system S is $|e_1\rangle$, and with probability $\lambda_2 = \frac{1}{3}$ the state is $|e_2\rangle$. Moreover,

- When S is in the the state $|e_1\rangle$ then

  s_1 has probability $|\langle s_1|e_1\rangle|^2 = \left(\frac{1}{\sqrt{2}}\right) = \frac{1}{2}$,

  s_2 has probability $|\langle s_2|e_1\rangle|^2 = \left(\frac{1}{\sqrt{2}}\right) = \frac{1}{2}$,

  s_3 has probability $|\langle s_3|e_1\rangle|^2 = 0$.

- When S is in the state $|e_2\rangle$ then

  s_1 has probability $|\langle s_1|e_2\rangle|^2 = 0$,

  s_2 has probability $|\langle s_2|e_2\rangle|^2 = 0$,

  s_3 has probability $|\langle s_3|e_2\rangle|^2 = 1$.

In short, the probability associated to any element $s \in S$ is completely determined by one of the unit vectors $|e_i\rangle$. Think of the collection of these probabilities as a description of what's going on with the system S.

Before returning to the main text, let's say a few quick words about the third term in Definition 2.2. The *von Neumann entropy* $-\operatorname{tr}(\rho \ln \rho)$ of a density ρ coincides with the *Shannon entropy*[5] of the probability distribution defined by its eigenvalues $-\sum_{i=1}^{r} \lambda_i \ln \lambda_i$, where r is the rank of ρ. Think of entropy as a measure of uncertainty. For instance, when ρ is a mixed state, one thinks of the system (represented by the set) S as being in any one of the r states $|e_i\rangle$ with probability λ_i. This probabilistic uncertainty is captured by the entropy. In the extremal case when $r = 1$ so that ρ is a pure state, then it has only *one* eigenvector $|e\rangle$ and thus S can be in only one possible state. The probability that S is in that state is the eigenvalue $\lambda = 1$. The von Neumann entropy is then $1 \ln 1 = 0$, indicating the total lack of uncertainty.

[5] To see this, consider the spectral decomposition $\rho = UDU^\dagger$, where U is a unitary operator and D is a diagonal operator. Equivalently, write $\rho = \sum_i \lambda_i |e_i\rangle\langle e_i|$ where $|e_i\rangle$ are the columns of U and λ_i are the diagonals of D. Then since ρ is diagonalizable, we have that $\ln \rho = U \ln(D) U^\dagger$, where $\ln(D)$ is a diagonal matrix with $\ln \lambda_i$ on the diagonal,

$$\ln(D) = \begin{bmatrix} \ln \lambda_1 & & & \\ & \ln \lambda_2 & & \\ & & \ddots & \\ & & & \ln \lambda_r \end{bmatrix}$$

where r is the rank of ρ. Therefore $\rho \ln \rho = UD\ln(D)U^\dagger$ and so $-\operatorname{tr} \rho \ln \rho = -\sum_i \operatorname{tr}(|e_i\rangle\langle e_i|)\lambda_i \ln \lambda_i$.

LET'S SUMMARIZE the discussion so far. Given a probability distribution $\pi\colon S \to \mathbb{R}$ we've described two ways to define a density on $\mathbb{C}^S$ so that the probabilities $\pi(s)$ are on the diagonal of ρ in the computational basis $\{|s\rangle\}$. One way to do this is by constructing the diagonal operator $\rho_{\text{diag}} = \sum_s \pi(s)|s\rangle\langle s|$, which is a maximal rank mixed state with von Neumann entropy equal to $-\sum_s \pi(s)\ln \pi(s)$. At the other extreme, the orthogonal projection operator $\rho_\pi = |\psi\rangle\langle\psi|$ is a pure state with zero von Neumann entropy, where $|\psi\rangle = \sum_s \sqrt{\pi(s)}|s\rangle$ is as defined in Equation (2.6). In the context of physics, classical probability distributions are almost always modeled by *diagonal* operators. In this work, however, we will always use the orthogonal projection operator ρ_π. The reason for this departure becomes clear when π is a *joint* probability distribution. As we'll soon see, the projection operator ρ_π reduces to smaller operators that harness valuable statistical information about π. The reduction process is the quantum version of marginalization, called the partial trace.

There are other ways to write π as a density, in addition to the two listed here. For instance, we could introduce a complex **phase** $e^{i\theta}$ for some $\theta \in \mathbb{R}$ into $|\psi\rangle$.

2.4   The Partial Trace

The partial trace is an operation in linear algebra that returns information about subsystems. Imagine, for instance, a system of many interacting "particles" or components. Given the state of this system, we may wish to know the state of a smaller subsystem—not in isolation, but rather—given that it interacts with its surrounding environment. The partial trace provides a way of zooming in and collecting such information. In quantum mechanics, *a system of interacting components* is modeled with the tensor product, and the state of the system is an operator on the space. So let's consider the tensor product of two finite-dimensional vector spaces $V \otimes W$. "Zooming in" to one component, say V, can be thought of as constructing a mapping from $V \otimes W$ to V. But it turns out that in general there *no* natural linear maps from a tensor product to each factor!

ZOOM

$$V \otimes W$$
no! .... no!
$$V \qquad\qquad\qquad W$$
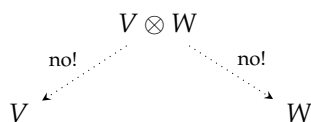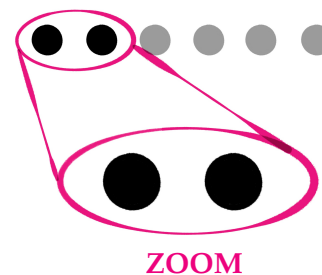
We might have in mind the mapping $|v\rangle \otimes |w\rangle \mapsto |v\rangle$, but that assignment is not linear. More concretely, the projection[6] $p\colon V \times W \to V$ defined by $(|v\rangle, |w\rangle) \mapsto |v\rangle$ is not bilinear,

[6] The **product** $V \times W$ is the vector space consisting of pairs $(|v\rangle, |w\rangle)$ where $|v\rangle \in V$ and $|w\rangle \in W$.

$$p(|v\rangle, |w\rangle + |z\rangle) = |v\rangle \neq 2|v\rangle = p(|v\rangle, |w\rangle) + p(|v\rangle, |z\rangle)$$

and so it does not extend to a linear map on the tensor product.

$$V \otimes W \xrightarrow{\text{no!}} V$$

$$V \times W \quad \nearrow p$$
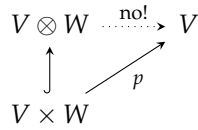
That's not to say there are *no* linear maps from a tensor product. There are plenty. If $\{|x\rangle\}$ is an orthonormal basis for V and if $\{|y\rangle\}$ is an orthonormal basis for W, then for each $|y\rangle$ there is a linear map $V \otimes W \to V$ given by $\mathrm{id}_V \otimes \langle y|$, which ma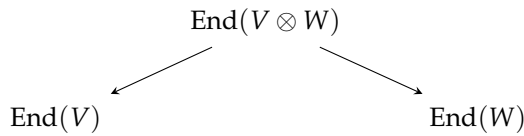ps any pair $|x\rangle \otimes |y'\rangle$ to $|x\rangle$ if $y' = y$ and to 0 otherwise. This assignment extends to a linear map, and yet it is not *natural* because it depends on the choice of $|y\rangle$. The point is there are generally no *naturally-defined linear maps* from a tensor product to each factor. However, there *are* natural linear maps after passing to endomorphisms of the spaces.

$$\mathrm{End}(V \otimes W)$$

$$\mathrm{End}(V) \qquad\qquad \mathrm{End}(W)$$

These natural maps are called **partial traces**. The formal definition first requires a lemma.

Lemma 2.1. *Given finite-dimensional vector spaces V and W there is an isomorphism*

$$\mathrm{End}(V \otimes W) \cong \mathrm{End}\, V \otimes \mathrm{End}\, W.$$

Proof. The proof quickly follows from the general fact that $\hom(A, B) \cong B \otimes A^*$ for finite-dimensional spaces A and B. In particular, we have cannonical isomorphisms

$$\begin{aligned}
\mathrm{End}(V \otimes W) &\cong (V \otimes W) \otimes (V \otimes W)^* \\
&\cong V \otimes W \otimes V^* \otimes W^* \\
&\cong V \otimes V^* \otimes W \otimes W^* \\
&\cong \mathrm{End}(V) \otimes \mathrm{End}(W).
\end{aligned}$$

$\square$

With this isomorphism in mind, here is the definition.

Definition 2.3. Given finite dimensional vector spaces V and W, there are two linear maps

$$\mathrm{End}(V \otimes W)$$

$$\xleftarrow{\mathrm{tr}_W} \qquad\qquad \xrightarrow{\mathrm{tr}_V}$$

$$\mathrm{End}(V) \qquad\qquad\qquad \mathrm{End}(W)$$
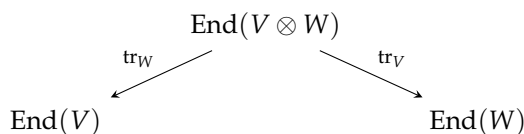
The diagram on the left refers to a defining property of the tensor product of vector spaces. The tensor product $V \otimes W$ is defined to be the vector space with the property that for any vector space Z and any bilinear map $f\colon V \times W \to Z$, there is a unique linear map $\hat{f}\colon V \otimes W \to Z$ so that $\hat{f}(|v\rangle \otimes |w\rangle) = f(v,w)$; that is, so that the following diagram commutes:

$$V \otimes W \xdashrightarrow{\hat{f}} Z$$

$$V \times W \quad \nearrow f$$
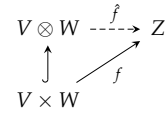
The inclusion $V \times W \hookrightarrow V \otimes W$ is the assignment $|(x,y)\rangle \mapsto |x\rangle \otimes |y\rangle$ whenever $\{|x\rangle\}$ is a basis for V and $\{|y\rangle\}$ is a basis for W. This is called the **universal property of the tensor product** $V \otimes W$.

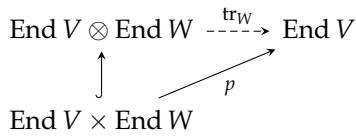Recall that $\mathrm{End}(V)$ denotes the vector space of linear operators $V \to V$.

The trace associates to a linear operator a number. The *partial* trace associates to a linear operator *another* linear operator.

defined for any $f \in \mathrm{End}(V)$ and $g \in \mathrm{End}(W)$ by

$$\mathrm{tr}_W(f \otimes g) := f\,\mathrm{tr}(g) \qquad \mathrm{tr}_V(f \otimes g) := g\,\mathrm{tr}(f).$$

These maps are called **partial traces**.

Notice why the partial trace repairs the lack of a natural linear map $V \otimes W \dashrightarrow V$. The assignment $\mathrm{End}(V) \otimes \mathrm{End}(W) \to \mathrm{End}(V)$ doesn't completely forget about W. Crucially, there is a trace of (that is, a bit of something left over from) W in the expression $\mathrm{tr}_W(f \otimes g) = f\,\mathrm{tr}(g)$, namely the value $\mathrm{tr}(g)$! The presence of the trace of g guarantees that the projection $p\colon \mathrm{End}\,V \times W \to \mathrm{End}\,V$ defined by $p(f,g) = f\,\mathrm{tr}\,g$ is bilinear and therefore lifts to give a linear map from the tensor product.

$$\mathrm{End}\,V \otimes \mathrm{End}\,W \xdashrightarrow{\ \mathrm{tr}_W\ } \mathrm{End}\,V$$
$$\uparrow \qquad \nearrow^{\ p}$$
$$\mathrm{End}\,V \times \mathrm{End}\,W$$

We also have explicit, basis-dependent expressions for the partial trace maps. Given orthonormal bases $\{|x_i\rangle\}$ for V and $\{|y_\alpha\rangle\}$ for W, any operator $f \in \mathrm{End}(V \otimes W)$ is of the form
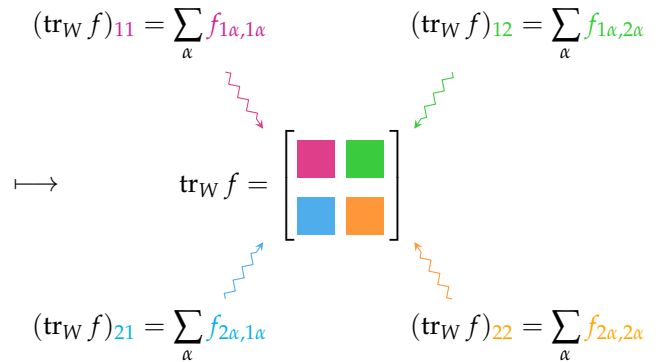
$$f = \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta}\,|x_i y_\alpha\rangle\langle x_j y_\beta|$$

and so

$$\mathrm{tr}_W f = \sum_{\substack{i,j \\ \alpha}} f_{i\alpha,j\alpha}\,|x_i\rangle\langle x_j| \qquad \mathrm{tr}_V f = \sum_{\substack{\alpha,\beta \\ i}} f_{i\alpha,i\beta}\,|y_\alpha\rangle\langle y_\beta|. \qquad (2.9)$$

Visually, the partial trace $\mathrm{tr}_W f$ is obtained by computing the trace of submatrices of the matrix representing f. Up to a reordering of the sets $\{|x_i\rangle\}$ and $\{|y_\alpha\rangle\}$, the partial trace $\mathrm{tr}_V f$ can be computed in a similar visual way.

To be explicit, the partial trace maps are obtained as the tensor product with the trace map and an identity.

$$\mathrm{tr}_W := \mathrm{id}_{\mathrm{End}(V)} \otimes \mathrm{tr}$$
$$\mathrm{tr}_V := \mathrm{tr} \otimes \mathrm{id}_{\mathrm{End}(W)}$$

So, for instance, we have

$$\mathrm{End}(V) \otimes \mathrm{End}(W)$$
$$\downarrow {\scriptstyle \mathrm{id}_{\mathrm{End}(V)} \otimes \mathrm{tr}}$$
$$\mathrm{End}(V) \otimes \mathbb{C}$$
$$\downarrow {\scriptstyle \cong}$$
$$\mathrm{End}(V)$$

Remember that $|x_i y_\alpha\rangle$ is shorthand for the tensor product $|x_i\rangle \otimes |y_\alpha\rangle$. Also notice that the sums in Equation (2.9) are analogous to the formula for the trace of a square matrix M,

$$\mathrm{tr}\,M = \sum_i M_{ii}.$$

In both cases, we sum over entries where the indices are the same. Since an operator f on a tensor product is specified by *four*, rather than two, indices $f_{i\alpha,j\beta}$, we can either sum over the common index $i = j$ or we can sum over the common index $\alpha = \beta$. Hence there are *two* partial trace maps.

$$f = \begin{bmatrix} f_{1\alpha,1\alpha} & f_{1\alpha,1\beta} & f_{1\alpha,1\gamma} & f_{1\alpha,2\alpha} & f_{1\alpha,2\beta} & f_{1\alpha,2\gamma} \\ f_{1\beta,1\alpha} & f_{1\beta,1\beta} & f_{1\beta,1\gamma} & f_{1\beta,2\alpha} & f_{1\beta,2\beta} & f_{1\beta,2\gamma} \\ f_{1\gamma,1\alpha} & f_{1\gamma,1\beta} & f_{1\gamma,1\gamma} & f_{1\gamma,2\alpha} & f_{1\gamma,2\beta} & f_{1\gamma,2\gamma} \\ \hline f_{2\alpha,1\alpha} & f_{2\alpha,1\beta} & f_{2\alpha,1\gamma} & f_{2\alpha,2\alpha} & f_{2\alpha,2\beta} & f_{2\alpha,2\gamma} \\ f_{2\beta,1\alpha} & f_{2\beta,1\beta} & f_{2\beta,1\gamma} & f_{2\beta,2\alpha} & f_{2\beta,2\beta} & f_{2\beta,2\gamma} \\ f_{2\gamma,1\alpha} & f_{2\gamma,1\beta} & f_{2\gamma,1\gamma} & f_{2\gamma,2\alpha} & f_{2\gamma,2\beta} & f_{2\gamma,2\gamma} \end{bmatrix} \longmapsto \mathrm{tr}_W f = \begin{bmatrix} \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \end{bmatrix}$$

$$(\mathrm{tr}_W f)_{11} = \sum_\alpha f_{1\alpha,1\alpha} \qquad (\mathrm{tr}_W f)_{12} = \sum_\alpha f_{1\alpha,2\alpha}$$

$$(\mathrm{tr}_W f)_{21} = \sum_\alpha f_{2\alpha,1\alpha} \qquad (\mathrm{tr}_W f)_{22} = \sum_\alpha f_{2\alpha,2\alpha}$$

Tensor network diagrams provide yet another way to visualize the partial trace. It corresponds to joining wires along a common index.

$\mathrm{tr}_W f$ $\mathrm{tr}_V f$
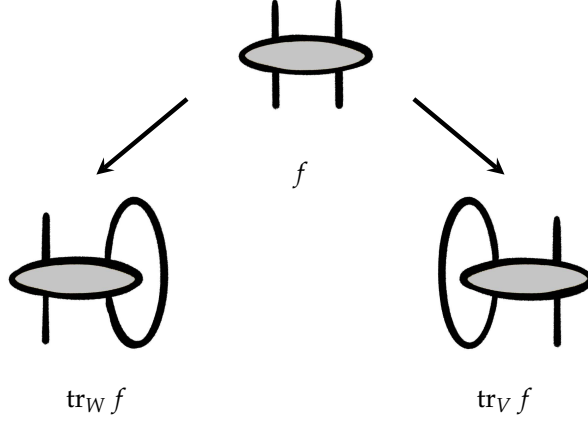
Importantly, the partial trace preserves several key properties of linear operators.

Lemma 2.2. *Let $f \in \mathrm{End}(V \otimes W)$.*

- *If f is Hermitian, then $\mathrm{tr}_W f$ and $\mathrm{tr}_V f$ are Hermitian.*

- *If f is positive semidefinite, then $\mathrm{tr}_W f$ and $\mathrm{tr}_V f$ are positive semidefinite.*

- *The traces of $\mathrm{tr}_W f$ and $\mathrm{tr}_V f$ are equal to the trace of f.*

Proof. The proof is an exercise in the definition. Let $\{|x_i\rangle\}$ be an orthonormal basis for V and let $\{|y_\alpha\rangle\}$ be an orthonormal basis for W. Let

$$f = \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta} |x_i y_\alpha\rangle \langle x_j y_\beta|$$

be any operator on $V \otimes W$, and let $f_V := \mathrm{tr}_W f$ be as in the left-hand side of Equation (2.9). If f is Hermitian, then

$$(f_V)_{ij} = \sum_\alpha f_{i\alpha,j\alpha} = \sum_\alpha \overline{f_{j\alpha,i\alpha}} = \overline{(f_V)_{ji}}$$

and so f_V is also Hermitian. If f is positive semidefinite then [7]

$$\sum_{\substack{i,\alpha \\ j,\beta}} \overline{\phi_{i\alpha}} \phi_{j\beta} f_{i\alpha,j\beta} \geq 0 \qquad \text{for any } \phi_{i\alpha}, \phi_{j\beta} \in \mathbb{C}.$$

So for any vector $|v\rangle = \sum_k v_k |x_k\rangle$ in V, the inner product $\langle v|f_V|v\rangle$ is the sum $\sum_{i,j,\alpha} \overline{v_i} v_j f_{i\alpha,j\alpha}$ which is nonnegative by the above assumption. Finally, the trace of f is $\sum_{i,\alpha} f_{i\alpha,i\alpha}$, which is also the trace of f_V. □

Equations (2.9) follow directly from the definition, but the computation is a good exercise in working with bra-kets. For instance, the fact that $|x_i y_\alpha\rangle\langle x_j y_\beta| = |x_i\rangle\langle x_j| \otimes |y_\alpha\rangle\langle y_\beta|$ as shown in Section 2.2.1 comes in handy. Here is the line-by-line derivation of $\mathrm{tr}_W f$.

$$\begin{aligned}
\mathrm{tr}_W f &= \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta} \, \mathrm{tr}_W |x_i y_\alpha\rangle\langle x_j y_\beta| \\
&= \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta} \, \mathrm{tr}_W (|x_i\rangle\langle x_j| \otimes |y_\alpha\rangle\langle y_\beta|) \\
&= \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta} |x_i\rangle\langle x_j| \otimes \mathrm{tr}\, |y_\alpha\rangle\langle y_\beta| \\
&= \sum_{\substack{i,\alpha \\ j,\beta}} f_{i\alpha,j\beta} |x_i\rangle\langle x_j| \otimes \langle y_\alpha|y_\beta\rangle \\
&= \sum_{\substack{i,j \\ \alpha}} f_{i\alpha,j\alpha} |x_i\rangle\langle x_j|.
\end{aligned}$$

The second-to-last line uses orthonormality: $\langle y_\alpha|y_\beta\rangle$ is 1 if $\beta = \alpha$ and is 0 otherwise.

[7] This is an expansion of the inner product $\langle \phi|f_V|\phi\rangle$, where $|\phi\rangle = \sum_{i,\alpha} \phi_{i\alpha}|x_i y_\alpha\rangle$ is any vector in $V \otimes W$.

By the lemma, we conclude that the partial trace maps density operators to density operators. This leads to the following definition.

Definition 2.4. If ρ is a density operator on $V \otimes W$, then

$$\rho_V := \mathrm{tr}_W \rho \qquad \text{and} \qquad \rho_W := \mathrm{tr}_V \rho$$

are called the **reduced density operators** associated to ρ.

Just as density operators are the quantum version of probability distributions, think of reduced density operators as the quantum version of marginal probability distributions, and think of the partial trace as the quantum version of marginalizing. This is more than an analogy. Reduced densities contain classical marginal probability distributions along their diagonals. This follows immediately from the Born rule, a fact summarized in the next proposition.

classical	quantum
probability distribution	density operator
marginal probability distribution	reduced density operator
marginalizing	partial trace

Proposition 2.1. *Let X and Y be finite sets, and let ρ be any density operator on $\mathbb{C}^X \otimes \mathbb{C}^Y$. Then*

$$\pi_{\rho_X} = (\pi_\rho)_X \qquad \text{and} \qquad \pi_{\rho_Y} = (\pi_\rho)_Y.$$

In other words, the probability distribution induced by the Born rule on ρ_X is the marginalization of the joint probability distribution induced by the Born rule on ρ, and similarly for ρ_Y.

Proof. As noted in Section 2.3, any density operator

$$\rho = \sum_{\substack{xy \\ x'y'}} \rho_{xy,x'y'} |xy\rangle\langle x'y'|$$

on $\mathbb{C}^X \otimes \mathbb{C}^Y$ defines a joint probability distribution $\pi_\rho \colon X \times Y \to \mathbb{R}$ by

$$\pi_\rho(x,y) := \langle xy|\rho|xy\rangle = \rho_{xy,xy},$$

where $|xy\rangle$ is shorthand for $|x\rangle \otimes |y\rangle$. The reduced density ρ_X is obtained by a sum over Y. In particular, its xx'th entry is

$$\langle x|\rho_X|x'\rangle = \sum_y \rho_{xy,x'y}.$$

Setting $x' = x$, the Born rule defines a probability distribution $\pi_{\rho_X} \colon X \to \mathbb{R}$ by

$$\pi_{\rho_X}(x) := \langle x|\rho_X|x\rangle = \sum_y \rho_{xy,xy} = \sum_y \pi_\rho(x,y) = (\pi_\rho)_X(x)$$

where $(\pi_\rho)_X \colon X \to \mathbb{R}$ is the marginal probability distribution obtained from π_ρ. □

This fact will be emphasized again in the next section. There, we'll consider the special case when ρ is a rank 1 density operator, namely projection onto the unit vector defined from a classical probability distribution π as in Equation (2.6). In the case when π is a *joint* distribution, the reduced densities of ρ will recover the marginal probabilities from π along their diagonals, and moreover their eigenvectors and eigenvalues will contain conditional probabilistic information. Before arriving at these results, here is one more general result about reduced densities [ASV02, Problem 11.2]. It features what's sometimes called a **Kraus representation** [Wat18] or **operator-sum decomposition** or representation [Pre, ASV02]. We won't need this Proposition until Section 3.4, but now is a good time to record it.

Proposition 2.2. *Let V and W be finite-dimensional Hilbert spaces and let ρ be any density operator on $V \otimes W$. For each $\alpha \in \{1, \ldots, \dim(W)\}$ and $i \in \{1, \ldots, \dim(V)\}$ there are linear maps*

$$
\begin{array}{ccc}
 & V \otimes W & \\
{}^{B_\alpha}\swarrow & & \searrow{}^{A_i} \\
V & & W
\end{array}
$$

such that the reduced densities can be written as

$$\rho_V = \sum_\alpha B_\alpha \rho B_\alpha^\dagger \qquad\qquad \rho_W = \sum_i A_i \rho A_i^\dagger$$

and which satisfy $\sum_\alpha B_\alpha^\dagger B_\alpha = \sum_i A_i^\dagger A_i = id_{V \otimes W}$.

Proof. The proof is an exercise in the definition and in bra-ket notation. We'll prove the claim for ρ_V. Let $\{|x_i\rangle\}$ be an orthonormal basis for V and let $\{|y_\alpha\rangle\}$ be an orthonormal basis for W. Define $B_\alpha = id_V \otimes \langle y_\alpha|$ to be projection onto a fixed vector. In other words,

$$B_\alpha(|x_j\rangle \otimes |y_\beta\rangle) = \begin{cases} |x_j\rangle & \text{if } \beta = \alpha \\ 0 & \text{otherwise} \end{cases}$$

The adjoint of B_α is tensoring with a fixed vector.

$$B_\alpha^\dagger|x\rangle = |x\rangle \otimes |y_\alpha\rangle.$$

Let's suggestively denote this mapping by $B_\alpha^\dagger = id_V \otimes |y_\alpha\rangle$. The goal is to show that the *ij*th entry of the operator $\sum_\gamma B_\gamma \rho B_\gamma^\dagger$ is equal to

$$\langle x_i| \sum_\gamma B_\gamma \rho B_\gamma^\dagger |x_j\rangle = \sum_\gamma \rho_{i\gamma,j\gamma}. \qquad\qquad (2.10)$$

Let us work on the inner product

$$\langle x_i| B_\gamma \rho B_\gamma^\dagger |x_j\rangle \qquad\qquad (2.11)$$

from right to left. First, $B_\gamma^\dagger |x_j\rangle = |x_j y_\gamma\rangle$ and so we're interested in the expression $\rho |x_j y_\gamma\rangle$ which, after expanding ρ in coordinates, is equal to

$$\rho |x_j y_\gamma\rangle = \sum_{\substack{i',\alpha \\ j',\beta}} \rho_{i'\alpha,j'\beta} |x_i y_\alpha\rangle \langle x_{j'} y_\beta | x_j y_\gamma\rangle = \sum_{i',\alpha} \rho_{i'\alpha,j\gamma} |x_i' y_\alpha\rangle.$$

The inner product in (2.11) is therefore

$$\sum_{i',\alpha} \rho_{i'\alpha,j\gamma} \langle x_i B_\gamma | x_{i'} y_\alpha\rangle = \sum_{i'} \rho_{i'\gamma,j\gamma} \langle x_i | x_{i'}\rangle = \rho_{i\gamma,i\gamma},$$

and summing over γ recovers Equation (2.10). Finally, a quick check shows that for any $|x_i\rangle$ and $|y_\beta\rangle$

$$\sum_\alpha B_\alpha^\dagger B_\alpha (|x_j\rangle \otimes |y_\beta\rangle) = B_\beta^\dagger |x_j\rangle = |x_j\rangle \otimes |y_\beta\rangle$$

and so $\sum_\alpha B_\alpha^\dagger B_\alpha = \mathrm{id}_{V \otimes W}$ as claimed. □

2.5   Reduced Densities of Pure Quantum States

Let's continue the discussion of reduced density operators, now focusing on reduced densities of rank 1 densities—pure quantum states. Reduced densities of these operators are especially interesting: they share the same spectrum, and they have particularly simple matrix representations. The goal of this section is to prove these two claims. The key is a simple fact about finite-dimensional vector spaces, namely that *every vector in $V \otimes W$ corresponds to a linear map $V \to W$.* There are a few ways to see this, some of which we've already covered.

An explicit isomorphism. We can describe an explicit pair of isomorphisms

$$V \otimes W \cong V^* \otimes W \cong \hom(V, W). \qquad (2.12)$$

Suppose $\{|x_1\rangle, \ldots, |x_n\rangle\}$ is a basis for V and $\{|y_1\rangle, \ldots, |y_m\rangle\}$ is basis for W. The first isomorphism is the identification of a vector with its dual $|x\rangle \leftrightarrow \langle x|$. For the second isomorphism, the assignment $\langle x| \otimes |y\rangle \mapsto |y\rangle\langle x|$ gives a map $V^* \otimes W \to \hom(V, W)$. Going in the other direction, any linear map $f \colon V \to W$ defines a vector $\sum_x \langle x| \otimes f|x\rangle$ in $V^* \otimes W$, and a quick check shows these assignments are linear inverses.

Bend the wires around. The isomorphism can be illustrated with tensor network diagrams by simply "sliding the wire around." To elaborate, recall that a vector in a tensor product of spaces $V \otimes W$ is drawn as a node with two parallel edges, one edge representing V and the other representing W. To distinguish between a vector

space and its dual, we may further decorate the edges with arrows. Let's say ⬇ represents the space V and ⬆ represents its dual V^*. Then to see that vectors in $V^* \otimes W$ correspond to vectors in $V \otimes W$ and hence linear maps $V \to W$, simply swap the first arrow and then slide the edge to the top.
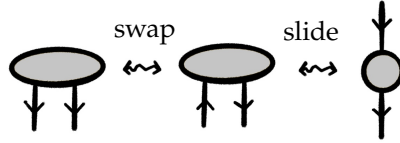
Assemble coefficients into a matrix. Another way to see the correspondence between vectors in $V \otimes W$ and linear maps $V \to W$ is to rearrange the coefficients of any vector in $V \otimes W$ into a matrix. This is the option to keep in mind. It's as simple as reshaping rectangles. Let $|\psi\rangle \in V \otimes W$ be any vector so that

$$|\psi\rangle = \sum_{x,y} \psi_{xy} |x\rangle \otimes |y\rangle,$$

and assemble the coefficients ψ_{xy} as the entries of an $m \times n$ matrix M. Informally, simply reshape the $nm \times 1$ column vector into a $m \times n$ rectangle.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} \quad \rightsquigarrow \quad \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

So suppose $|\psi\rangle \in V \otimes W$ is any vector and let M be the $\dim(W) \times \dim(V)$ matrix whose entries are the coefficients of $|\psi\rangle$ as just described. As with any matrix, M has a **singular value decomposition** (SVD) that is, a factorization of the form[8]

$$M = V\Sigma U^\dagger. \tag{2.13}$$

Here U is an $n \times n$ unitary matrix with columns $|u\rangle$ called the **right singular vectors** of M; and V is an $m \times m$ unitary matrix[9] with columns $|v\rangle$ called the **left singular vectors** of M; and Σ is an $n \times m$ matrix that, supposing $m \leq n$, is of the form $\Sigma = \left[\ D\ |\ 0\ \right]$ where D is a diagonal $m \times m$ matrix whose nonzero entries σ are the **singular values** of M, and here 0 denotes the $m \times (n - m)$ matrix of all zeros. Notice the last row of $U^\dagger$ makes no contribution to the matrix product $\Sigma U^\dagger$, since it is "zeroed out" by the submatrix of zeros in Σ. So the singular value decomposition of M may be rewritten as

$$M = VDU_0^\dagger \tag{2.14}$$

[8] *Proof.* Given any $m \times n$ matrix M, the matrix $M^\dagger M$ is Hermitian and therefore has a set of orthonormal eigenvectors $\{|u_1\rangle, \ldots, |u_n\rangle\}$ that form a basis for $\mathbb{C}^n$. The set of nonzero vectors $M|u_i\rangle$ is a basis for the image of M but may not form an orthonormal set. So for each $i = 1, \ldots, \mathrm{rank}(M)$ define $|v_i\rangle := M|u_i\rangle / \langle u_i | M^\dagger M | u_i\rangle = M|u_i\rangle / \sqrt{\lambda_i}$ where λ_i is the eigenvalue associated to $|u_i\rangle$. If $\mathrm{rank}(M) < m$ then extend this set to an orthonormal basis $\{|v_1\rangle, \ldots, |v_m\rangle\}$ for $\mathbb{C}^m$. Lastly define $\sigma_i := \sqrt{\lambda_i}$ and let Σ be the $m \times n$ matrix with the σ_i along its diagonal, let U be the $n \times n$ matrix whose columns are the $|u_i\rangle$, and let V be the $m \times m$ matrix whose columns are the $|v_i\rangle$.

[9] Let's not confuse the unitary operator V with the vector space V appearing on other pages. It's very common to use the letters V and Σ (or D) and U for the SVD of a matrix. I'm sticking to this convention, and the context should clarify which "V" we mean.

where $U_0^\dagger$ is the submatrix of U consisting of only the first m rows.

$$\begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix} = \begin{bmatrix} * & * \\ * & * \end{bmatrix} \begin{bmatrix} * & & 0 \\ & * & 0 \end{bmatrix} \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

$$M \qquad = \qquad V \qquad D \qquad\qquad U_0^\dagger$$

The matrix U_0 is no longer unitary, but it does satisfy $U_0 U_0^\dagger = \text{id}$, since its columns are orthonormal. So U_0 is a linear isometry, and we may[10] make use of this equality as well as $VV^\dagger = \text{id}$.

[10] And we will. See Figure 2.1.
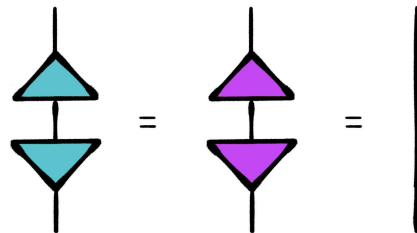
For simplicity let's always take the singular value decomposition of M to refer to the cleaned-up version in Equation (2.14), writing U in place of U_0. As tensor diagrams, we have the following picture.

As explained in Section 2.2.2, triangles are reserved for linear isometries.
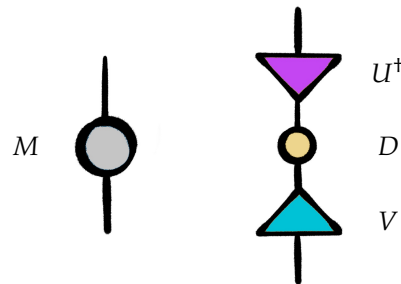
The next result follows immediately.

Lemma 2.3. *Let V and W be inner product spaces with $\dim V = n$ and $\dim W = m$ and suppose $m \leq n$. For any vector $|\psi\rangle \in V \otimes W$ there exist orthonormal vectors $|e_1\rangle, \ldots |e_m\rangle$ in V and $|f_1\rangle, \ldots, |f_m\rangle$ in W so that*

$$|\psi\rangle = \sum_{i=1}^{m} \sigma_i |f_i\rangle \otimes |e_i\rangle \tag{2.15}$$

for nonnegative, real σ_i.

Proof. Let $\{|x_1\rangle, \ldots, |x_n\rangle\}$ be any orthonormal basis for V and let $\{|y_1\rangle, \ldots, |y_m\rangle\}$ be any orthonormal basis for W so that

$$|\psi\rangle = \sum_{i,\alpha} \psi_{i\alpha} |x_i\rangle \otimes |y_\alpha\rangle.$$

Let M be the $m \times n$ matrix with αith entry $\psi_{i\alpha}$, and consider its singular value decomposition $M = VDU^\dagger$ where V is an $m \times m$ matrix with orthonormal columns $|f\rangle$, and U is an $n \times m$ matrix with orthonormal columns $|e\rangle$, and D is an $m \times m$ diagonal matrix with entries σ. Then $M = \sum_{i=1}^{m} \sigma_i |f_i\rangle\langle e_i|$, which defines the vector[11] in Equation (2.15). $\square$

[11] Recall the discussion in Section 2.2.1 about tensor products versus outer products.

To summarize, any vector $|\psi\rangle$ in $V \otimes W$ corresponds to a linear map $M\colon V \to W$, whose SVD produces orthonormal sets $\{|e\rangle\}$ in V and $\{|f\rangle\}$ in W so that the coefficients of $|\psi\rangle$ with respect to the basis $\{|e\rangle \otimes |f\rangle\}$ are the singular values of M. This alternate representation of $|\psi\rangle$ is called its **Schmidt decomposition**. We use this in the next proposition, which has important consequences in the pages to come.

Proposition 2.3. *Let V and W be finite-dimensional inner product spaces and let $|\psi\rangle \in V \otimes W$ be a unit vector. The reduced densities ρ_V and ρ_W of the orthogonal projection operator $\rho = |\psi\rangle\langle\psi|$ have the same eigenvalues, and there is a one-to-one correspondence between their eigenvectors.*

Proof. Let $|\psi\rangle = \sum_{i=1}^{m} \sigma_i |e_i\rangle \otimes |f_i\rangle$ be the Schmidt decomposition of $|\psi\rangle$, where m is the minimum of $\dim(W)$ and $\dim(V)$. Orthogonal projection onto $|\psi\rangle$ then has the following expression.

$$
\begin{aligned}
\rho &= |\psi\rangle\langle\psi| \\
&= \left(\sum_{i=1}^{m} \sigma_i |e_i\rangle \otimes |f_i\rangle \right) \left(\sum_{j=1}^{m} \sigma_j \langle f_j| \otimes \langle e_j| \right) \\
&= \sum_{i,j=1}^{m} \sigma_i \sigma_j |e_i\rangle\langle e_j| \otimes |f_i\rangle\langle f_j|.
\end{aligned}
$$

Tracing out W gives the reduced density operator $\rho_V = \mathrm{tr}_W \rho$, which is equal to

$$
\begin{aligned}
\mathrm{tr}_W \left(\sum_{i,j=1}^{m} \sigma_i \sigma_j |e_i\rangle\langle e_j| \otimes |f_i\rangle\langle f_j| \right) &= \sum_{i,j=1}^{m} \sigma_i \sigma_j |e_i\rangle\langle e_j| \cdot \mathrm{tr}(|f_i\rangle\langle f_j|) \\
&= \sum_{i,j=1}^{m} \sigma_i \sigma_j |e_i\rangle\langle e_j| \langle f_i | f_j\rangle \\
&= \sum_{i=1}^{m} \sigma_i^2 |e_i\rangle\langle e_i|. \qquad (2.16)
\end{aligned}
$$

Similarly, tracing out V from ρ gives the reduced density operator

$\rho_W = \text{tr}_V \rho$, which is equal to

$$\text{tr}_V \left(\sum_{i,j=1}^{m} \sigma_i \sigma_j |e_i\rangle \langle e_j| \otimes |f_i\rangle \langle f_j| \right) = \sum_{i,j=1}^{m} \sigma_i \sigma_j \, \text{tr}(|e_i\rangle \langle e_j|) \cdot |f_i\rangle \langle f_j|$$

$$= \sum_{i,j=1}^{m} \sigma_i \sigma_j \langle e_i | e_j \rangle |f_i\rangle \langle f_j|$$

$$= \sum_{i=1}^{m} \sigma_i^2 |f_i\rangle \langle f_i|. \tag{2.17}$$

As a result, for all i we have

$$\rho_V |e_i\rangle = \lambda_i |e_i\rangle \qquad \text{and} \qquad \rho_W |f_i\rangle = \lambda_i |f_i\rangle$$

where $\lambda_i = \sigma_i^2$. Therefore the reduced densities have the same spectrum, and there is a bijection between their sets of eigenvectors

$$|e_i\rangle \xleftrightarrow{\;\lambda_i\;} |f_i\rangle$$

which is provided by M and its linear adjoint,

$$M|e_i\rangle = \lambda_i |f_i\rangle \qquad M^\dagger |f_i\rangle = \lambda_i |e_i\rangle.$$

The two equalities above follow since $M = VDU^\dagger$ implies $MU = VD$ and $M^\dagger V = UD$. $\qquad\square$

So reduced densities of a pure quantum state $|\psi\rangle \langle \psi|$ share the same set of eigenvalues, and there is a bijection between their eigenvectors. Equations (2.16) and (2.17) of the proof give another important result, namely that the spectral decompositions of the reduced densities are

$$\rho_V = UD^2 U^\dagger \qquad \rho_W = VD^2 V^\dagger. \tag{2.18}$$

In other words, whenever M is the $\dim(W) \times \dim(V)$ matrix associated to a unit vector $|\psi\rangle \in V \otimes W$, the eigenvectors of $\text{tr}_W |\psi\rangle \langle \psi|$ and $\text{tr}_V |\psi\rangle \langle \psi|$ are the singular vectors of M, and their eigenvalues are the singular values of M. The following corollary is immediate.

Corollary 2.1. *Let V and W be finite-dimensional inner product spaces, let $|\psi\rangle \in V \otimes W$ be a unit vector, and let $\rho = |\psi\rangle \langle \psi|$ be orthogonal projection. There exists a matrix M so that the reduced densities of ρ are of the form*

$$\rho_V = M^\dagger M \qquad \rho_W = MM^\dagger \tag{2.19}$$

Proof. Let M be the $\dim(W) \times \dim(V)$ matrix associated to $|\psi\rangle$. If M has the singular value decomposition $M = VDU^\dagger$ then Equations (2.16) and (2.17) imply that $\rho_V = UD^2 U^\dagger$ and $\rho_W = VD^2 V^\dagger$, and so

$$M^\dagger M = (VDU^\dagger)^\dagger (VDU^\dagger)$$

$$= UD^\dagger V^\dagger VDU^\dagger$$

$$= UD^2 U^\dagger$$

$$= \rho_V$$

since $D^\dagger = D$ for a diagonal operator. Similarly,

$$MM^\dagger = (VDU^\dagger)(VDU^\dagger)^\dagger$$
$$= VD^\dagger U^\dagger UDV^\dagger$$
$$= VD^2V^\dagger$$
$$= \rho_W.$$

$\square$

Figure 2.1 captures this corollary in tensor diagram notation, where we have temporarily decorated the diagrams with arrows to show the flow of information.
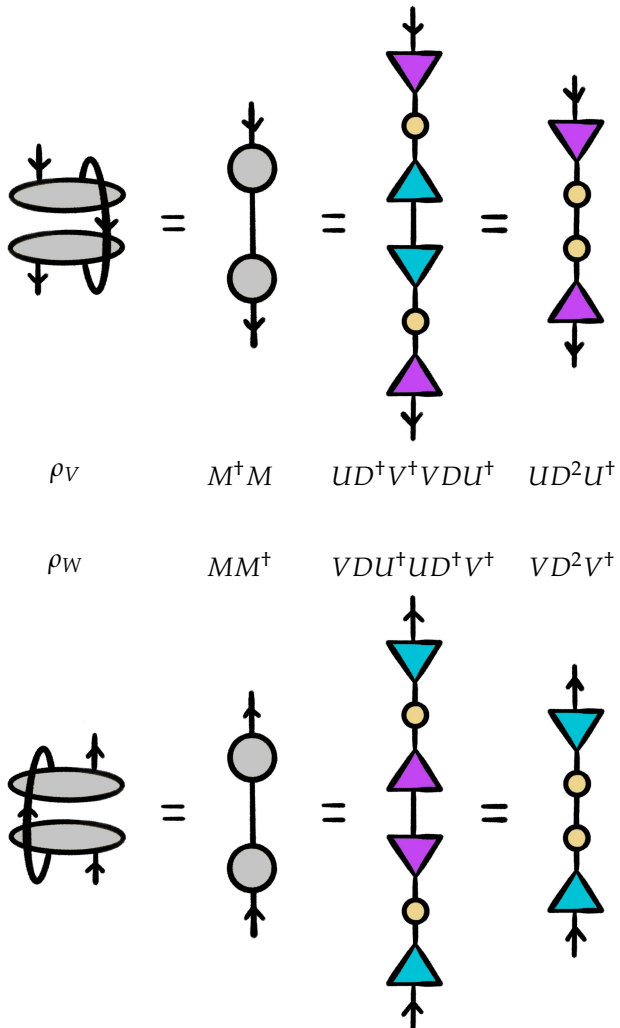

Figure 2.1: Understanding the decompositions $\rho_V = M^\dagger M = UD^2U^\dagger$ and $\rho_W = MM^\dagger = VD^2V^\dagger$ as tensor diagrams.

So we get a lot of mileage out of the singular value decomposition. Reduced densities of pure states have the same eigenvalues, they have the same number of eigenvectors, which are the singular vectors of a matrix M, and moreover their matrix representations are obtained as the composition of M with its linear adjoint. Here's yet another result staring right at us: The original density operator $\rho = |\psi\rangle\langle\psi|$ can be reconstructed from its reduced densities ρ_V and ρ_W. In other words, if we have $\rho_V = UD^2U^\dagger$ and $\rho_W = VD^2V^\dagger$, then we can "pick out" V and D and U and compose them to obtain $M = VDU^\dagger$ whose entries can be reassembled into the vector $|\psi\rangle$, as illustrated in Figure 2.2. This may seem obvious, but imagine a scenario in which one does not have full access to the quantum state $\rho = |\psi\rangle\langle\psi|$. Perhaps the system described by ρ is too complicated to know precisely, or too large to store on a computer. It's often easier to estimate the eigenvectors of ρ_V and ρ_W—which are operators on a smaller, and hence more manageable, subsystem—perhaps discard those eigenvectors corresponding to the smallest eigenvalues, and then use this approximate spectral information to reconstruct the ρ. This is precisely the approach we take in the machine learning problem of Chapter 4. This section has collected a number of important tools. Here's the takeaway.

Takeaway 3. *Let $|\psi\rangle \in V \otimes W$ be a unit vector and consider the orthogonal projection operator $\rho = |\psi\rangle\langle\psi|$. Then*

1. *the reduced density operators ρ_V and ρ_W have the same spectrum, and there is a one-to-one correspondence between their eigenvectors. (Proposition 2.3)*

Moreover, if $M = VDU^\dagger$ is the singular value decomposition of the $\dim(W) \times \dim(V)$ matrix corresponding to $|\psi\rangle$ then

2. *the columns of U are the eigenvectors of ρ_V, the columns of V are the eigenvectors of ρ_W, and the squares of the diagonal entries of D are their common eigenvalues. (Equation 2.18)*

3. *The reduced densities are obtained as the product of M with its linear adjoint; that is, $\rho_V = M^\dagger M$ and $\rho_W = MM^\dagger$. (Corollary 2.1)*

4. *The original density ρ may be reconstructed from the spectral decompositions of its reduced densities ρ_V and ρ_W. (Figure 2.2)*

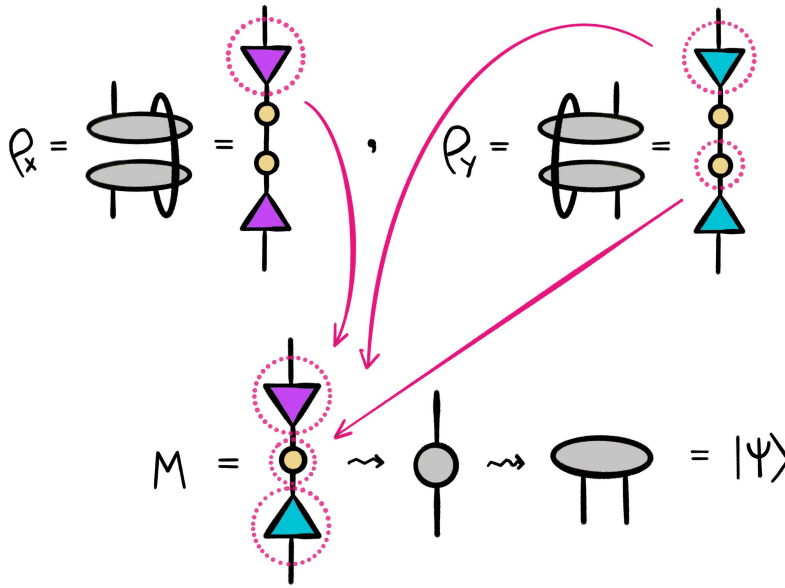While on the topic of reduced densities, let's say a few brief words about the mathematics of entanglement.

Figure 2.2: Reconstructing $|\psi\rangle$ from the eigenvectors of ρ_V and ρ_W and their common eigenvalues.

2.5.1 Entanglement

In Section 2.3 it was noted that density operators come in different types—mixed and pure—the difference being measured by von Neumann entropy, all notions being mediated by rank. Like "pure" versus "mixed," the notion of *entanglement* is also related to rank, and the partial trace plays a key role.

Definition 2.5. A rank 1 density operator is called an **entangled quantum state** if the rank of its reduced densities is greater than 1, and it is not entangled otherwise.

A related notion is that of entropy. The **entanglement entropy** of a rank 1 density is defined to be the Shannon entropy of the probability distribution defined by the (common) eigenvalues of its reduced densities, $-\sum_i \lambda_i \ln \lambda_i$. The entanglement entropy is zero precisely when the rank of the reduced densities is 1; that is, when there's only one eigenvalue $\lambda = 1$. There's an equivalent characterization of entanglement to know about. Let $|\psi\rangle \in V \otimes W$ be any unit vector and suppose $\rho = |\psi\rangle\langle\psi|$ is the pure state given by orthogonal projection onto $|\psi\rangle$. Then ρ is *not* an entangled state—that is, its reduced densities have rank 1—if and only if[12] $|\psi\rangle$ is of the form $|\psi\rangle = |v\rangle \otimes |w\rangle$ for some $|v\rangle \in V$ and $|w\rangle \in W$. Sometimes vectors of this form are called **simple tensors**. The following proposition draws a simple connection between classical independence and the absence of entanglement.

The use of "the" as in "the rank of its reduced densities..." is justified by Proposition 2.3. The reduced densities of a pure state always have the same rank!

[12] *Proof.* If $|\psi\rangle = |v\rangle \otimes |w\rangle$ for unit vectors $|v\rangle \in V$ and $|w\rangle \in W$ then the reduced densities of $|\psi\rangle\langle\psi|$ are orthogonal projection onto $|v\rangle$ and $|w\rangle$, respectively, which both have rank 1. Conversely, suppose $|\psi\rangle$ does not decompose as a simple tensor. Say, for example, $|\psi\rangle = |v\rangle \otimes |w\rangle + |v'\rangle \otimes |w'\rangle$ where $|v'\rangle$ is not a scalar multiple of $|v\rangle$ and $|w'\rangle$ is not a scalar multiple of $|w\rangle$. Then $\rho_V = |v\rangle\langle v| + |v'\rangle\langle v'|$, which has rank 2, and similarly for ρ_W.

Proposition 2.4. *Let X and Y be finite sets. If a joint probability distribution $\pi\colon X \times Y \to \mathbb{R}$ satisfies*

$$\pi(x,y) = \pi_X(x)\pi_Y(y)$$

for all $x \in X$ and $y \in Y$, then the orthogonal projection $\rho_\pi = |\psi\rangle\langle\psi|$ is not entangled, where $|\psi\rangle = \sum_{x,y} \sqrt{\pi(x,y)}|xy\rangle$. Conversely, suppose $|a\rangle \in \mathbb{C}^X$ and $|b\rangle \in \mathbb{C}^Y$ are unit vectors and consider the orthogonal projection $\rho = |ab\rangle\langle ab|$. Then the Born distribution induced by ρ satisfies[13]

$$\pi_\rho(x,y) = \pi_{\rho_X}(x)\pi_{\rho_Y}(y)$$

where $\rho_X = \mathrm{tr}_Y\,\rho$ and $\rho_Y = \mathrm{tr}_X\,\rho$.

[13] Equivalently, by Propostion 2.1, we may express this in terms of the marginal distributions obtained from π_ρ; that is,

$$\pi_\rho(x,y) = (\pi_\rho)_X(x)(\pi_\rho)_Y(y).$$

Proof. If a joint distribution satisfies $\pi(x,y) = \pi_X(x)\pi_Y(y)$, then the matrix representation for the reduced density $\rho_X = \mathrm{tr}_Y\,\rho_\pi$ is given by

$$\rho_X = \sum_y \sqrt{\pi(x,y)\pi(x',y)} = \sqrt{\pi_X(x)\pi_X(x')}\sum_y \pi_Y(y) = \sqrt{\pi_X(x)\pi_X(x')}$$

which shows that $\rho_X = \mathrm{tr}_Y\,\rho_\pi$ is orthogonal projection onto the vector $\sum_x \sqrt{\pi_X(x)}|x\rangle$. The reduced density ρ_Y is obtained as a similar rank 1 projection, and so ρ_π not entangled. Conversely, consider the density $\rho = |ab\rangle\langle ab|$ for unit vectors $|a\rangle \in \mathbb{C}^X$ and $|b\rangle \in \mathbb{C}^Y$. The Born distribution $\pi_\rho\colon X \times Y \to \mathbb{R}$ induced by ρ is defined on any pair $(x,y) \in X \times Y$ by

$$\begin{aligned}
\pi_\rho(x,y) &= \langle xy|ab\rangle\langle ab|xy\rangle \\
&= \langle x|a\rangle\langle y|b\rangle\langle a|x\rangle\langle b|y\rangle \\
&= |\langle a|x\rangle|^2|\langle b|y\rangle|^2 \\
&= \pi_{\rho_X}(x)\pi_{\rho_Y}(y).
\end{aligned}$$

$\square$

EITHER WAY we think about it, let's be careful not to gloss over a couple of points. First, *entanglement is only defined for density operators on a tensor product.* So if someone were to ask, "Is my state ρ on the inner product space H entangled?" the best response would be a question, "Has a tensor decomposition been chosen for H?" The point is that a state is said to be entangled *with respect to* a chosen decomposition $H \cong V \otimes W$. Second, *we've only defined entanglement entropy for pure states.* If the rank of a density operator is greater than 1, then its reduced densities may not have the same spectrum or the same rank, in which case the notion of entanglement entropy is not well-defined.

For the work to come it will helpful to keep in mind this connection between *entanglement* and the *rank of reduced densities.* In fact, this will help to understand certain aspects of the application in Chapter 4. Since the mathematics is fresh in our mind, let's take a quick behind-the-scenes look at the role that rank will play in the pages to come.

BEHIND THE SCENES. Suppose $|\psi\rangle \in V \otimes W$ is a unit vector whose matrix has singular value decomposition $VDU^\dagger$. In some cases (for instance, when searching for an optimal approximation to $|\psi\rangle$) it is advantageous to drop—that is, set equal to zero—those singular values that are smaller than some desired threshold. This truncation means we drop the corresponding eigenvectors of the reduced densities of $|\psi\rangle\langle\psi|$, which therefore lowers the rank of the operators and hence decreases the entanglement associated to $|\psi\rangle$. In tensor network diagram notation, this idea has the following illustration.
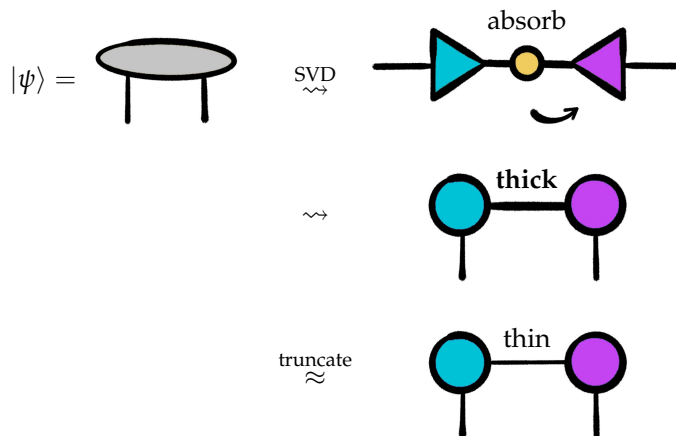

In the second line, the matrix D has been absorbed into $U^\dagger$ simply to keep the diagram clean. We've also drawn circles in lieu of triangles to suggest a connection with *matrix product states.* (More on that below.) So the blue tensor is V and the purple tensor is $DU^\dagger$. In the third line, we imagine dropping the smallest singular values. By doing so, the range of $U^\dagger$ becomes a smaller-dimensional space, which is represented by a thinner edge. We won't use a thick-edge/thin-edge convention going forward, but we introduce it here to share intuition. Think of this *truncated SVD* as a technique for decreasing the flow of information. Intuitively, a thick edge (a large-dimensional space) allows more information to pass between the subsystems than does a thin edge (a small-dimensional space). Of course, *no* information can pass between them if there's *no* edge; that is, if $|\psi\rangle$ factors as a product (a "simple tensor") of two vectors. This brings to mind the descriptive quote at the beginning of this chapter, taken from the

illuminating quantum max-flow/min-cut result of [CFS$^+$15].

> Networks transport classical things like power, water, oil, and cars.
> Tensor networks transport linear algebraic things like rank and entan-
> glement and should be thought of as the quantum analogy.

So we think of information about the two subsystems as being trans-
ported across the vector space represented by the edge joining the
two nodes. How *much* information can flow is determined by the
dimension of that space, which is the rank of the operators.
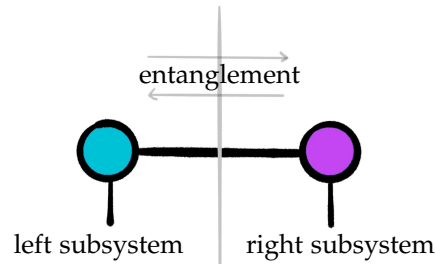
Think of the paradigm described here as a mini-version of how a
matrix product state—introduced in Section 2.2.2—is formed. In
general, one may start with a vector in a tensor product of *many*
vector spaces, $|\psi\rangle \in V^{\otimes N}$. Any such vector corresponds to a linear
map $V^{\otimes k} \to V^{\otimes N-k}$ for each $k < N$. A truncated SVD of that map
gives us access to the most dominant eigenvectors of reduced density
operators. One can imagine iteratively harnessing those eigenvectors
for each k into a tensor network with N nodes. The SVD illustrated
above is a special case of this idea.
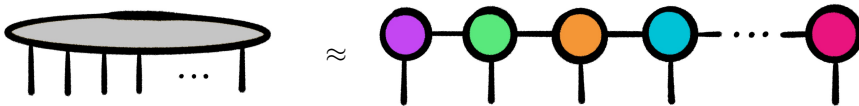
In fact, *any* $|\psi\rangle$ can be factored *exactly* by an MPS, just as any matrix
can be factored *exactly* by an SVD. (This is more than an analogy. It's
a corollary.) But not all $|\psi\rangle$ can be approximated *well* after dropping
the lowest singular values at each step. That is, not all states $|\psi\rangle$ can
be modeled well by a *low rank, low entanglement* tensor. The applica-
tion we describe in Chapter 4 applies to those $|\psi\rangle$ which do satisfy
this hypothesis. But we'll cross that bridge when we get to it. Here's
the takeaway for this brief discussion.

Takeaway 4. *A density operator ρ on an inner product space H is called*

- *a **pure state** if the rank of ρ is 1. If H further decomposes as $H \cong V \otimes W$ then ρ is said to be*

    1. ***entangled** if the rank of its reduced densities is greater than 1*

    2. ***not entangled** if the rank of its reduced densities is equal to 1,*

- *a **mixed state** if the rank of ρ is greater than 1.*

IN THE NEXT chapter, we use the preliminaries accumulated in this chapter to revisit the idea that density operators on a tensor product are the quantum version of joint probability distributions, that their reduced density operators are the quantum version of marginal distributions, and that the partial trace is the quantum version of marginalizing. This analogy crystallizes when the density operator is orthogonal projection onto a vector $|\psi\rangle$ that arises from a classical probability distribution as in Equation (2.6). We describe the details next.

3
A Passage from Classical to Quantum Probability

There does however seem to
be some undefinable sense
that a certain piece of
mathematics is "on to
something," that it is a piece
of a larger puzzle waiting to
be explored further.

Terence Tao [Tao07]

IN THIS CHAPTER, we carefully outline the main procedure of this
thesis by repackaging the theory in Chapter 2. The starting ingre-
dient is any classical joint probability distribution π, which defines
a particular unit vector $|\psi\rangle$. The main advantage of $|\psi\rangle$ is that the
spectral information of the reduced density operators of the rank 1
density $|\psi\rangle\langle\psi|$ organizes and encodes useful statistical information
from the original distribution π. Think of the technique outlined here
as a general recipe that can be applied to any finite set—so in particu-
lar, any *dataset*. (We will revisit this applied perspective in Chapter 4.)
The procedure can be systematically described in a series of six steps.

1. Start with any probability distribution π on $X \times Y$.

2. Represent the elements of X and Y as orthonormal basis vectors.

3. Form the unit vector $|\psi\rangle = \sum_{x,y} \sqrt{\pi(x,y)}|x\rangle \otimes |y\rangle$ in $\mathbb{C}^X \otimes \mathbb{C}^Y$.

4. Form the density operator $\rho = |\psi\rangle\langle\psi|$.

5. Compute the reduced density operators ρ_X and ρ_Y from ρ.

6. Decode their spectral information.

In Section 3.1 we will expand on each step in Section 3.1 and will il-
lustrate with a simple example afterwards. The example will bring to

light an especially simple scenario: when π is an *empirical* probability distribution, then the reduced densities of $|\psi\rangle\langle\psi|$ can be computed from simple combinatorics of a bipartite graph associated to π. This will be explained in Section 3.2. In Section 3.3 we will revist the connection with formal concept analysis that was introduced early on in Section 1.1. This chapter will close in Section 3.4 with some preliminary remarks on how this framework paves the way for modeling entailment and concept hierarchy in language using density operators.

3.1   Reduced Densities from Classical Probability Distributions

In this section, we will put the theory explaining the main procedure upfront and will illustrate with Example 3.1 afterwards. The example will rederive the elementary results in Section 2.1.2 using the language of quantum probabillity, thus explaining mathematics presented there. Here is the procedure for modeling any probability distribution as a pure quantum state and for decoding the information therein.

1. Start with a joint probability distribution.

Let X and Y be any finite sets and let $\pi\colon X \times Y \to \mathbb{R}$ be any probability distribution. Here we strongly emphasize the word *any*. Although our language is borrowed from quantum mechanics, it is not necessary to assume that π has any quantum-like interpretation or properties.

2. Represent the elements as orthonormal vectors.

Choose an ordering the sets X and Y, say $X = \{x_1, \ldots, x_n\}$ and $Y = \{y_1, \ldots, y_m\}$, and represent each element $x_i \in X$ as the ith standard basis vector $|x_i\rangle \in \mathbb{C}^X \cong \mathbb{C}^n$, and identify each element $y_\alpha \in Y$ with the αth standard basis vector $|y_\alpha\rangle \in \mathbb{C}^Y \cong \mathbb{C}^m$. Also consider the tensor product $\mathbb{C}^{X \times Y} \cong \mathbb{C}^X \otimes \mathbb{C}^Y$ which is the *nm*-dimensional vector space whose bases are the tensor products $|x_i\rangle \otimes |y_\alpha\rangle$.

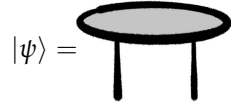The passage $x_i \mapsto |x_i\rangle$ might be called a "one-hot encoding."

The isomorphism $\mathbb{C}^{X \times Y} \cong \mathbb{C}^X \otimes \mathbb{C}^Y$ is given by $|(x,y)\rangle \longleftrightarrow |x\rangle \otimes |y\rangle$.

3. Form the unit vector $|\psi\rangle$ defined in Equation (2.6).

To define the vector $|\psi\rangle$ in Equation (2.6) we began with a set S. Here $S = X \times Y$ and so $|\psi\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$ is the sum of all elements in $X \times Y$ weighted by the square roots of their probabilities.

$$|\psi\rangle = \sum_{i,\alpha} \sqrt{\pi(x_i, y_\alpha)}|x_i\rangle \otimes |y_\alpha\rangle \qquad (3.1)$$

As a tensor diagram, $|\psi\rangle$ is a node with two parallel edges.
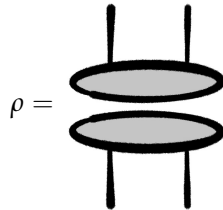
$$|\psi\rangle = \text{}$$

4. Form the orthogonal projection operator $|\psi\rangle\langle\psi|$.

Now we form the rank 1 density operator associated to $|\psi\rangle$ as in Equation (2.7). Computing $\rho = |\psi\rangle\langle\psi|$ explicitly, one has
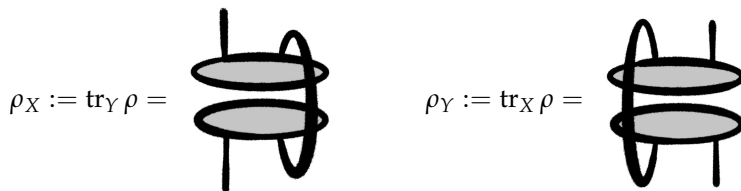
$$\rho = |\psi\rangle\langle\psi|$$

$$= \left(\sum_{i,\alpha}\sqrt{\pi(x_i,y_\alpha)}|x_i\rangle\otimes|y_\beta\rangle\right)\left(\sum_{j,\beta}\sqrt{\pi(x_j,y_\beta)}\langle x_j|\otimes\langle y_\beta|\right)$$

$$= \sum_{\substack{i,\alpha\\j,\beta}}\sqrt{\pi(x_i,y_\alpha)\pi(x_j,y_\beta)}|x_i\rangle\langle x_j|\otimes|y_\alpha\rangle\langle y_\beta|.$$

Although the density ρ carries no more information than $|\psi\rangle$ does, working with a linear operator allows us to call on the partial trace. This is the next step.

$$\rho = \text{}$$

5. Compute the reduced density operators associated to $|\psi\rangle\langle\psi|$.

Let's use the notation $\text{tr}_Y := \text{tr}_{\mathbb{C}^Y}$ and $\text{tr}_X := \text{tr}_{\mathbb{C}^X}$ and consider the reduced density operators associated to $\rho = |\psi\rangle\langle\psi|$,

$$\rho_X := \text{tr}_Y\rho = \qquad\qquad \rho_Y := \text{tr}_X\rho =$$

We have are two ways to compute the reduced densities explicitly.[1] The first is to recall from Corollary 2.1 that there exists a matrix M so that

$$\rho_X = M^\dagger M \qquad \rho_Y = MM^\dagger.$$

[1] In fact, we have at least *four*. In addition to the two described here, there is also the operator sum decomposition in Proposition 2.2, as well as the combinatorial description given in Section 3.2 below.

The matrix M is precisely the vector $|\psi\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$ viewed as a linear map $\mathbb{C}^X \to \mathbb{C}^Y$. Explicitly, the entries of M are the square roots of the probabilities,

$$M_{\alpha i} := \sqrt{\pi(x_i, y_\alpha)}.$$

The second option is to apply the partial trace directly. Carefully understanding the latter is particularly helpful for understanding the theory, so let's proceed by this route. Applying the partial trace to ρ, the reduced density operator $\rho_X : \mathbb{C}^X \to \mathbb{C}^X$ has the following expression.

$$
\begin{aligned}
\rho_X &= \operatorname{tr}_Y |\psi\rangle\langle\psi| \\
&= \sum_{\substack{i,\alpha \\ j,\beta}} \sqrt{\pi(x_i, y_\alpha)\pi(x_j, y_\beta)}\, \operatorname{tr}_Y(|x_i\rangle\langle x_j| \otimes |y_\alpha\rangle\langle y_\beta|) \\
&= \sum_{\substack{i,\alpha \\ j,\beta}} \sqrt{\pi(x_i, y_\alpha)\pi(x_j, y_\beta)}\, |x_i\rangle\langle x_j| \cdot \operatorname{tr} |y_\alpha\rangle\langle y_\beta| \\
&= \sum_{\substack{i,j \\ \alpha}} \sqrt{\pi(x_i, y_\alpha)\pi(x_j, y_\alpha)}\, |x_i\rangle\langle x_j|
\end{aligned}
$$

$$
\rho_X = \begin{bmatrix} \pi_X(x_1) & & & * \\ & \pi_X(x_2) & & \\ & & \ddots & \\ * & & & \pi_X(x_n) \end{bmatrix}
$$

The last line follows since $\operatorname{tr} |y_\alpha\rangle\langle y_\beta| = \langle y_\alpha | y_\beta\rangle$ which is 1 if $\alpha = \beta$ and is zero otherwise. The ijth entry of the operator ρ_X is therefore

$$(\rho_X)_{ij} = \sum_\alpha \sqrt{\pi(x_i, y_\alpha)\pi(x_j, y_\alpha)}. \tag{3.2}$$

Notice that the ith diagonal entry is $(\rho_X)_{ii} = \sum_\alpha \pi(x_i, y_\alpha) = \pi_X(x_i)$, and so ρ_X recovers the classical marginal probability distribution $\pi_X : X \to \mathbb{R}$ along its diagonal. The off-diagonals of ρ_X are also interesting. To explain, let's first adopt the following language.

Definition 3.1. Given a pair $(x, y) \in X \times Y$, call the element x the **prefix** of the pair and call the element y the **suffix** of the pair.

Using this terminology, we are thinking of ρ_X as an operator on the prefix subsystem. Its ijth off-diagonal entry then has a simple iterpretation—*it measures the extent to which prefixes x_i and x_j share common suffixes in Y.* Indeed, the ijth off-diagonal of ρ_X is zero precisely when either $\pi(x_i, y) = 0$ or $\pi(x_j, y) = 0$ for all y; that is, when x_i and x_j share no common suffixes in Y. On the other hand, the ijth entry receives a positive contribution for each suffix y for which the probabilities of being paired with x_i and x_j are nonzero. In much the same way, the reduced density operator on the suffix subsystem $\rho_Y : \mathbb{C}^Y \to \mathbb{C}^Y$ is given by,

$$\rho_Y = \sum_{\substack{\alpha,\beta \\ i}} \sqrt{\pi(x_i, y_\alpha)\pi(x_i, y_\beta)}\, |y_\alpha\rangle\langle y_\beta|. \tag{3.3}$$

The $\alpha\beta$th entry of the operator ρ_Y is therefore

$$(\rho_Y)_{\alpha\beta} = \sum_i \sqrt{\pi(x_i, y_\alpha)\pi(x_i, y_\beta)}. \qquad (3.4)$$

$$\rho_Y = \begin{bmatrix} \pi_Y(y_1) & & & & * \\ & \pi_Y(y_2) & & & \\ & & \ddots & & \\ * & & & & \pi_Y(y_m) \end{bmatrix}$$

In particular, the αth diagonal entry is $(\rho_Y)_{\alpha\alpha} = \sum_i \pi(x_i, y_\alpha) = \pi_Y(y_\alpha)$, and so we recover the classical marginal probability distribution $\pi_Y \colon Y \to \mathbb{R}$ along the diagonal of ρ_Y. Moreover, the $\alpha\beta$th off-diagonal entry measures the extent to which y_α and y_β share common prefixes in X.

So THE REDUCED densities ρ_X and ρ_Y recover classical marginal probabilities along their diagonal. For this reason, we think of the reduced densities of $|\psi\rangle\langle\psi|$ as the *quantum version of marginal probability distributions*, and we think of the partial trace as the *quantum version of marginalizing.* In general, the reduced densities will also have nonzero off-diagonal entries. These off diagonals encode information about subsystem interactions. From Equation 3.2, for instance, it is evident that the ijth off-diagonal of ρ_X "knows" something about the complementary subsystem Y. This fact clearly distinguishes ρ_X and ρ_Y from their classical counterparts π_X and π_Y, where all knowledge of the complementary subsystem is completely *lost* when marginalizing. On the other hand, it is preserved when "marginalizing" with the partial trace. The preserved information is manifest in the nonzero off-diagonal entries of the reduced densities, the existence of which guarantees that ρ_X and ρ_Y will have interesting eigenvectors and eigenvalues. This spectral information therefore harnesses the subsystem interactions in a clean and organized fashion. Understanding this is the next and final step. But first, let us emphasize that the mathematics just described depends on our choice of $\rho = |\psi\rangle\langle\psi|$ as orthogonal projection. If instead the original density was chosen to be the diagonal operator $\rho_{\text{diag}} = \sum_{i,\alpha} \pi(x_i, y_\alpha)|x_i y_\alpha\rangle\langle x_i y_\alpha|$, then its reduced densities would *themselves* be diagonal operators, with the marginal distributions along their diagonals and zeros elsewhere. The absence of off-diagonal entries would give us no information about subsystem interactions, and the eigenvectors of the reduced densities would simply recover the basis vectors $|x_i\rangle$ and $|y_\alpha\rangle$. This is the reason we prefer to model the joint distribution π as a pure state $|\psi\rangle\langle\psi|$ rather than a diagonal operator. Now, let's close with the last step.

6. Decode the spectral information.

The reduced density operators ρ_X and ρ_Y of $\rho = |\psi\rangle\langle\psi|$ recover the classical marginal distributions along their diagonals, and they contain extra information on their off-diagonals. We've interpreted this

extra information as a measure of subsystem interactions, but there
is a more principled way to both *understand* this information and to
harness it. Indeed, the off diagonal entries directly contribute to the
eigenvalues and eigenvectors of the reduced densities. To understand
this, recall from Proposition 2.3 that the reduced densities share the
same eigenvalues λ_i and there is a bijection between their sets of
eigenvectors $\{|e_i\rangle\} \leftrightarrow \{|f_i\rangle\}$. So we write their spectral decomposi-
tions as

$$\rho_X = \sum_{i=1}^{m} \lambda_i |e_i\rangle\langle e_i| \qquad \rho_Y = \sum_{i=1}^{m} \lambda_i |f_i\rangle\langle f_i|.$$

This leads to the following paradigm.

> With probability λ_i the prefix subsystem will be in the state defined
> by the ith eigenvector $|e_i\rangle$ of ρ_X, and the suffix subsystem will be
> in the state defined by the ith eigenvector $|f_i\rangle$ of ρ_Y. Here's what
> this means.

- Since the eigenvector $|e_i\rangle = \sum_{x \in X} e_i(x)|x\rangle$ may be written as a
  linear combination of the basis vectors $|x\rangle \in \mathbb{C}^X$, we obtain a
  probability distribution on the set of prefixes X. When the prefix
  subsystem is in the state $|e_i\rangle$, the probability of a prefix $x \in X$ is
 $\langle x|e_i\rangle|^2 = |e_i(x)|^2$.

- Likewise, the eigenvector $|f_i\rangle = \sum_{y \in Y} f_i(y)|y\rangle$ may be written as a
  linear combination of the basis vectors $|y\rangle \in \mathbb{C}^Y$. This defines a
  probability distribution on the set of suffixes Y. So when the suffix
  subsystem is in the state $|f_i\rangle$, the probability of a suffix $y \in Y$ is
  $|\langle y|f_i\rangle|^2 = |f_i(y)|^2$.

This shows how to make sense of the individual eigenvectors and
eigenvalues. But we may also wish to place this information in a
broader context. Mathematically speaking, what really *is* the infor-
mation being encoded in the eigenvectors and eigenvalues of these
reduced densities? The answer is simple. *It must be akin to conditional
probability.* The reason for this conclusion is found in a remark given
towards the end of Section 2.5. Recall from Figure 2.2 of that section
that the original state $|\psi\rangle = \sum_{x,y} \sqrt{\pi(x,y)}|x\rangle \otimes |y\rangle$ may be fully re-
constructed from the eigenvectors and eigenvalues of the reduced
densities of $\rho = |\psi\rangle\langle\psi|$. Quite crucially, an analogous reconstruc-
tion *does not exist* in classical probability theory. Consider the familiar
equation relating joint probability with marginals and conditionals.

$$\pi(x,y) = \pi(x|y)\pi_Y(y) \tag{3.5}$$

It is not possible to reconstruct the joint distribution given the marginal
distributions π_X and π_Y alone. Conditional probability is needed as
well. But this is not the case in the quantum version, where the state

Now is an opportune time to think
back to the discussion on entanglement
in Section 2.5.1. As noted there, the
notion of entanglement is defined by
the (common) rank of the reduced
densities ρ_X and ρ_Y. Now it's hopefully
clear why rank and entanglement go
hand-in-hand. Knowing something
about the prefix subsystem X—namely,
that its state is $|e_i\rangle$—gives immediate
knowledge about the suffix subsystem
Y—namely, that its state is $|f_i\rangle$—and
vice versa.
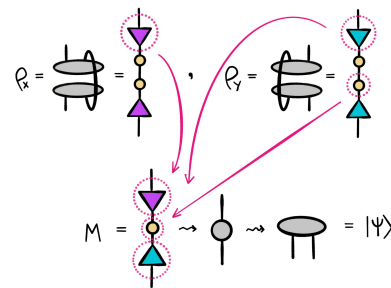
$\rho = |\psi\rangle\langle\psi|$—and hence π itself!—*can* be fully reconstructed from the spectral decompositions of the reduced densities ρ_X and ρ_Y. Therefore since ρ_X and ρ_Y contain the classical marginals along their diagonals *as well as* extra information in their off diagonals, the extra information must account for conditional probability, which is the information lost in the classical process of marginalizing. Let's illustrate the ideas so far with an extended example.

3.1.1   The Motivating Example, Revisited

We'll now walk through each of the six steps of the main procedure, this time illustrating each step with an elementary example.

Example 3.1. We will revisit the opening example in Section 2.1. There we began with a small toy corpus of text consisting of the following three phrases.

> orange fruit   green fruit   purple vegetable

Let's identify these phrases with a subset T of the Cartesian product of the ordered sets $X = \{\text{orange, green, purple}\}$ and $Y = \{\text{fruit, vegetable}\}$. The phrase xy corresponds to the pair $(x, y) \in X \times Y$. Now we're in position to take the first step.

1. Start with a joint probability distribution.

Consider the joint probability distribution $\pi\colon X \times Y \to \mathbb{R}$ defined by

$$\pi(\text{orange, fruit}) = 1/3$$
$$\pi(\text{green, fruit}) = 1/3$$
$$\pi(\text{purple, vegetable}) = 1/3$$

with $\pi(x, y) = 0$ for all other pairs $(x, y) \in X \times Y$. As an aside, notice this probability distribution is an empirical one. The probability of a pair (x, y) is simply the number of times it appears in the set T, divided by the size of T. Let's move on to the next step.

The equation that is analogous to $\pi(x, y) = \pi(x|y)\pi_Y(y)$ is essentially the singular value decomposition

$$M = VDU^\dagger,$$

where M is the matrix associated to $|\psi\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$. In especially simple cases, the eigenvectors of ρ_X and ρ_Y (equivalently, the columns of U and V) will define conditional probabilities on the nose. For instance, suppose $M\colon \mathbb{C}^X \to \mathbb{C}^Y$ has exactly one nonzero probability in each column, then look at its singular value decomposition.

BEHIND THE SCENES. Thinking ahead to Chapter 4, the letter T stands for "training set."

In Section 2.1 the joint distribution π was depicted as a 2×3 table.

	orange	green	purple
fruit	$\frac{1}{3}$	$\frac{1}{3}$	0
vegetable	0	0	$\frac{1}{3}$

2. Represent the elements as orthonormal vectors.

The elements of $X = \{$orange, green, purple$\}$ and $Y = \{$fruit, vegetable$\}$ correspond to the following standard basis vectors in $\mathbb{C}^X \cong \mathbb{C}^3$ and in $\mathbb{C}^Y \cong \mathbb{C}^2$.

$$|\text{orange}\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad |\text{green}\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad |\text{purple}\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$|\text{fruit}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |\text{vegetable}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Moreover, for each $x \in X$ and $y \in Y$ the tensor product $|x\rangle \otimes |y\rangle$ is computed as an outer product. This gives a basis for the space $\mathbb{C}^X \otimes \mathbb{C}^Y$. For example, $|\text{orange}\rangle \otimes |\text{fruit}\rangle$ is given by the product of their vector representations.

$$|\text{orange}\rangle \otimes |\text{fruit}\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

After stacking the two columns, this 3×2 matrix reshapes as the column vector $\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^\top$. Representations of the vectors $|\text{green}\rangle \otimes |\text{fruit}\rangle$ and $|\text{purple}\rangle \otimes |\text{vegetable}\rangle$ are obtained similarly, and so the three phrases in the subset $T \subseteq X \times Y$ correspond to the following three vectors in $\mathbb{C}^X \otimes \mathbb{C}^Y$.

$$|\text{orange}\rangle \otimes |\text{fruit}\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^\top$$

$$|\text{green}\rangle \otimes |\text{fruit}\rangle = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}^\top$$

$$|\text{purple}\rangle \otimes |\text{vegetable}\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}^\top$$

3. Form the unit vector defined in Equation (2.6).

The unit vector defined by the joint probability distribution π is a weighted sum of the three phrases in T.

$$|\psi\rangle = \tfrac{1}{\sqrt{3}}(|\text{orange}\rangle \otimes |\text{fruit}\rangle + |\text{green}\rangle \otimes |\text{fruit}\rangle + |\text{purple}\rangle \otimes |\text{vegetable}\rangle)$$

By identifying each term with its vector representation, we may represent $|\psi\rangle$ with the 6×1 column vector,

$$|\psi\rangle = \begin{bmatrix} \tfrac{1}{\sqrt{3}} & \tfrac{1}{\sqrt{3}} & 0 & 0 & 0 & \tfrac{1}{\sqrt{3}} \end{bmatrix}^\top.$$

4. Form the orthogonal projection operator $|\psi\rangle\langle\psi|$.

The explicit expression for orthogonal projection onto $|\psi\rangle\langle\psi|$ consists of nine terms.

$$|\psi\rangle\langle\psi| = \frac{1}{3}(|\text{orange}\rangle\langle\text{orange}| \otimes |\text{fruit}\rangle\langle\text{fruit}| + |\text{orange}\rangle\langle\text{green}| \otimes |\text{fruit}\rangle\langle\text{vegetable}| + \cdots)$$

As written, it looks rather messy. It will be easier to read if we organize the terms into an array. Let's also adopt the following abbreviations.

$$o = \text{orange} \quad g = \text{green} \quad p = \text{purple} \quad F = \text{fruit} \quad V = \text{vegetable}$$

Then the pure state $|\psi\rangle\langle\psi|$ is as follows.

$$|\psi\rangle\langle\psi| = \frac{1}{3}\begin{pmatrix} |o\rangle\langle o| \otimes |F\rangle\langle F| & + & |o\rangle\langle g| \otimes |F\rangle\langle F| & + & |o\rangle\langle p| \otimes |F\rangle\langle V| \\ |g\rangle\langle o| \otimes |F\rangle\langle F| & + & |g\rangle\langle g| \otimes |F\rangle\langle F| & + & |g\rangle\langle p| \otimes |F\rangle\langle V| \\ |p\rangle\langle o| \otimes |V\rangle\langle F| & + & |p\rangle\langle g| \otimes |V\rangle\langle F| & + & |p\rangle\langle p| \otimes |V\rangle\langle V| \end{pmatrix} \tag{3.6}$$

As an array, $|\psi\rangle\langle\psi|$ is computed as an outer product that results in a 6×6 matrix.

$$|\psi\rangle\langle\psi| = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \end{bmatrix}$$

5. Compute the reduced density operators associated to $|\psi\rangle\langle\psi|$.

Let's now compute the density operators ρ_X and ρ_Y by applying the partial trace to the projection operator in Equation (3.6) above.

$$\rho_X = \text{tr}_Y |\psi\rangle\langle\psi| \qquad \rho_Y = \text{tr}_X |\psi\rangle\langle\psi|$$

The idea is to compute $\text{tr}_Y(|x_i\rangle\langle x_j| \otimes |y_\alpha\rangle\langle y_\beta|) = |x_i\rangle\langle x_j|\langle y_\alpha|y_\beta\rangle$ for each of the nine terms and add the result. Notice that only terms with $y_\alpha = y_\beta$ lend a contribution since $\langle y_\alpha|y_\beta\rangle = 0$ whenever $\alpha \neq \beta$. So the partial trace collects only those elements x_i and x_j that have common suffixes.[2] For example, among the three phrases

orange fruit   green fruit   purple vegetable

the prefixes *orange* and *green* have exactly one shared suffix, namely *fruit*, and so the partial trace returns $\text{tr}_Y(|o\rangle\langle g| \otimes |F\rangle\langle F|) = |o\rangle\langle g|\langle F|F\rangle$

[2] BEHIND THE SCENES. This is the reason we choose to represent elements $x \in X$ and $y \in Y$ as orthonormal vectors, as opposed to some other representation. Otherwise this particular interpretation of the partial trace would not hold.

which is $|o\rangle\langle g|$ since $\langle F|F\rangle = 1$. On the other hand, the words *orange* and *purple* have different suffixes, and so the partial trace returns $\text{tr}_Y(|o\rangle\langle p| \otimes |F\rangle\langle V|) = |o\rangle\langle p|\langle F|V\rangle$ which is 0 since $\langle F|V\rangle = 0$. Proceeding this way for each term comprising $|\psi\rangle\langle\psi|$, the reduced density ρ_X is as follows.

$$\rho_X = \text{tr}_Y |\psi\rangle\langle\psi| = \frac{1}{3}\begin{pmatrix} |o\rangle\langle o| \otimes \langle F|F\rangle & + & |o\rangle\langle g| \otimes \langle F|F\rangle & + & |o\rangle\langle p| \otimes \langle\cancel{F|V}\rangle \\ |g\rangle\langle o| \otimes \langle F|F\rangle & + & |g\rangle\langle g| \otimes \langle F|F\rangle & + & |g\rangle\langle p| \otimes \langle\cancel{F|V}\rangle \\ |p\rangle\langle o| \otimes \langle\cancel{V|F}\rangle & + & |p\rangle\langle g| \otimes \langle\cancel{V|F}\rangle & + & |p\rangle\langle p| \otimes \langle V|V\rangle \end{pmatrix}$$

$$= \frac{1}{3}(|o\rangle\langle o| + |o\rangle\langle g| + |g\rangle\langle o| + |g\rangle\langle g| + |p\rangle\langle p|)$$

Each of the five operators in the previous line is computed as an outer product of standard basis vectors, so they have simple matrix representations,

$$|o\rangle\langle o| = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad |p\rangle\langle p| = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$|g\rangle\langle g| = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad |o\rangle\langle g| = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and so on. Therefore ρ_X has the following matrix representation.

$$\rho_X = \begin{array}{c} \\ o \\ g \\ p \end{array} \begin{array}{cc} \begin{array}{ccc} o & g & p \end{array} & \\ \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} & \frac{1}{3} \end{array} \qquad (3.7)$$

Notice the factor of $\frac{1}{3}$ on the right, which ensures that ρ_X has unit trace. What's more, the diagonal of ρ_X is the classical marginal probability distribution $\pi_X = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ on X. Momentarily ignoring the normalization factor, we verify that the entries of ρ_X have a combinatorial interpretation.

Off diagonals count shared suffixes. The ijth off-diagonal entry of ρ_X counts the number of times the prefixes x_i and x_j share a common suffix in Y. For instance, *orange* and *green* have exactly one shared suffix—*fruit*—and the corresponding off-diagonal entries are 1. On the other hand, *purple* shares no common suffixes with either *orange* or *green*, and the corresponding off-diagonal entries are zero.

Diagonals count occurrences. The ith diagonal entry counts the number of times x_i appears in the set T. *Orange, green,* and *purple* each appear once, and so the diagonals are each 1.

Let's now compute the reduced density operator $\rho_Y = \text{tr}_X |\psi\rangle\langle\psi| \colon \mathbb{C}^Y \to \mathbb{C}^Y$, which can be understood similarly. When tracing out $\mathbb{C}^X$ from the nine terms of $|\psi\rangle\langle\psi|$, only terms with $x_i = x_j$ will lend a contribution since $\text{tr}_X(|x_i\rangle\langle x_j| \otimes |y_\alpha\rangle\langle y_\beta|) = \langle x_i | x_j\rangle |y_\alpha\rangle\langle y_\beta|$ and $\langle x_i | x_j\rangle = 0$ whenever $i \neq j$. Therefore the reduced density ρ_Y is as follows.

$$
\rho_Y = \text{tr}_X |\psi\rangle\langle\psi| = \frac{1}{3}
\begin{pmatrix}
\langle o|o\rangle \otimes |F\rangle\langle F| & + & \cancel{\langle o|g\rangle} \otimes |F\rangle\langle F| & + & \cancel{\langle o|p\rangle} \otimes |F\rangle\langle V| \\
\cancel{\langle g|o\rangle} \otimes |F\rangle\langle F| & + & \langle g|g\rangle \otimes |F\rangle\langle F| & + & \cancel{\langle g|p\rangle} \otimes |F\rangle\langle V| \\
\cancel{\langle p|o\rangle} \otimes |V\rangle\langle F| & + & \cancel{\langle p|g\rangle} \otimes |V\rangle\langle F| & + & \langle p|p\rangle \otimes |V\rangle\langle V|
\end{pmatrix}
$$

$$
= \frac{1}{3} \left(|F\rangle\langle F| + |F\rangle\langle F| + |V\rangle\langle V| \right)
$$

Each operator in the previous line is computed as an outer product of standard basis vectors, so they have simple matrix representations.

$$
|F\rangle\langle F| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}
\qquad
|V\rangle\langle V| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}
$$

Therefore ρ_Y has the following matrix representation.

$$
\rho_Y = \begin{array}{c} \\ F \\ V \end{array}
\begin{array}{c} F \quad V \\ \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \end{array} \frac{1}{3}
\tag{3.8}
$$

Notice the factor of $\frac{1}{3}$ on the right, which ensures that ρ_Y has unit trace. Moreover the diagonal of ρ_Y is the classical marginal probability distribution $\pi_Y = \left(\frac{2}{3}, \frac{1}{3}\right)$. Ignoring the normalization factor for the moment, we verify that the entries of ρ_Y have a combinatorial interpretation.

Off diagonals count shared prefixes. The $\alpha\beta$th off-diagonal entry counts the number of times the suffixes y_α and y_β share a common prefix. In this example, *fruit* and *vegetable* are never described by the same color, and so both off diagonals are zero.

Diagonals count occurrences. The αth diagonal entry counts the number of times y_α appears in the corpus. *Fruit* appears twice, and the corresponding entry is 2. *Vegetable* appears once, and the corresponding entry is 1.

So the reduced densities ρ_X and ρ_Y recover classical marginal probability along their diagonals, but they also carry additional information about interactions between the prefix and suffix subsystems. This information is harnessed neatly in their eigenvectors and eigenvalues. Decoding this information is the final step.

As an aside, by Corollary 2.1, the reduced densities may also be computed as a product of a matrix with its transpose. The vector $|\psi\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$ computed in Step 3 corresponds to the following matrix, which represents a linear map $\mathbb{C}^X \to \mathbb{C}^Y$.

$$
M = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \leftrightsquigarrow |\psi\rangle
$$

The product of M with its adjoint gives us the reduced density operators of ρ.

$$
M^\dagger M = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix} = \rho_X
$$

$$
MM^\dagger = \begin{bmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{bmatrix} = \rho_Y
$$

Either way, we've now recovered the matrices presented early on in the motivating example of Section 2.1.2.
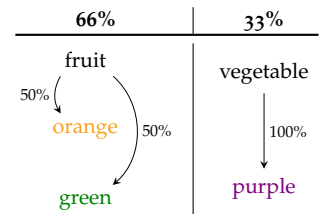
6. Decode the spectral information.

Lastly, we decode the spectral information of the two reduced densities. Here are their eigenvalues and eigenvectors.

	eigenvectors of ρ_X	eigenvectors of ρ_Y
$\lambda_1 = \frac{2}{3}$	$\lvert e_1 \rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \begin{matrix} o \\ g \\ p \end{matrix}$	$\lvert f_1 \rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{matrix} F \\ V \end{matrix}$
$\lambda_2 = \frac{1}{3}$	$\lvert e_2 \rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \begin{matrix} o \\ g \\ p \end{matrix}$	$\lvert f_2 \rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{matrix} F \\ V \end{matrix}$
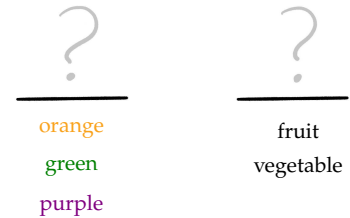
This has the following interpretation.

- With probability $\lambda_1 = \frac{2}{3}$, the state of prefix subsystem is given by $\lvert e_1 \rangle$, and the state of the suffix subsystem is given by $\lvert f_1 \rangle$. The absolute squares of the entries of $\lvert e_1 \rangle$ define a probability distribution on X. For instance, the probability of the prefixes *orange* and *green* are both $\lvert \langle e_1 \vert \text{orange} \rangle \rvert^2 = \lvert \langle e_1 \vert \text{green} \rangle \rvert^2 = \frac{1}{2}$, which are conditional probabilities given that the suffix of a phrase is *fruit*. Likewise, the absolute squares of the entries of $\lvert f_1 \rangle$ define a probability distribution on Y. For instance, the probability of the suffix *fruit* is $\lvert \langle f_1 \vert \text{fruit} \rangle \rvert^2 = 1$, which is a conditional probability given that the prefix of a phrase is either *orange* or *green*.

- With probability $\lambda_2 = \frac{1}{3}$, the state of the prefix subsystem given by $\lvert e_2 \rangle$, and the state of the suffix subsystem is given by $\lvert f_2 \rangle$. The entries of $\lvert e_2 \rangle$ define a probability distribution on X. The probability of the prefix *purple* is $\lvert \langle e_2 \vert \text{purple} \rangle \rvert^2 = 1$, which is the probability of the prefix of a phrase being purple given that the suffix is *vegetable*. Likewise, the entries of $\lvert f_2 \rangle$ define a probability distribution on Y. The probability of the suffix *vegetable* is $\lvert \langle f_2 \vert \text{vegetable} \rangle \rvert^2 = 1$, which is a conditional probability given that the prefix of a phrase is *purple*.

THIS EXAMPLE CONCLUDES a description of the main passage from classical to quantum probability $\pi \mapsto \lvert \psi \rangle \langle \psi \rvert$. The punchline is that the eigenvalues and eigenvectors of the reduced densities of $\lvert \psi \rangle \langle \psi \rvert$ recover classical marginal probabilities and also harness extra information that is akin to conditional probability. For the application to come, it will be good to know about an especially simple case that

Compare this to Example 2.2, which was essentially this example without context.

makes the theory even more interpretable. If the initial joint proba-
bility distribution $\pi\colon X \times Y \to \mathbb{R}$ is an empirical one, then it may be
represented as a bipartite graph, and the entries of the reduced densi-
ties may be read off from the combinatorics of the graph. We will rely
on this combinatorial understanding in the application of Chapter 4,
so let's collect the ideas here.

3.2 Reduced Densities from Empirical Distributions

We now take a quick look at the main procedure of Section 3.1 in the
special case when the joint probability distribution is an empirical
one. As before, let X and Y be finite sets and now choose a subset
$T \subseteq X \times Y$. This defines an empirical distribution $\hat{\pi}\colon X \times Y \to \mathbb{R}$ by

$$\hat{\pi}(x,y) = \begin{cases} \frac{1}{|T|} & \text{if } (x,y) \in T \\ 0 & \text{otherwise.} \end{cases}$$

This probability distribution may be illustrated as a weighted bipar-
tite graph. The sets X and Y provide the two sets of vertices, and
an edge connecting $x \in X$ and $y \in Y$ is labeled by the probability
$\hat{\pi}(x,y)$. To keep the graph clean, let's omit the edge between x and y
whenever $\hat{\pi}(x,y) = 0$ and let's always leave off the weights, knowing
that the probability associated to any edge is simply 1 divided by the
total number of edges in the graph.
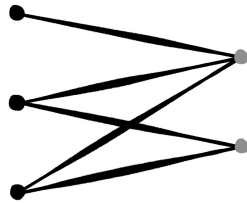
The distribution $\hat{\pi}$ then defines the unit vector as in Equation (3.1).

$$|\psi\rangle = \frac{1}{\sqrt{|T|}} \sum_{(x_i, y_\alpha) \in T} |x_i\rangle \otimes |y_\alpha\rangle \tag{3.9}$$

In this case, the entries of the reduced density matrices associated to
$|\psi\rangle\langle\psi|$ have especially clean, combinatorial interpretations. En route
to understanding this, define the following nonnegative integers.

$$d(x_i, x_j) := |\{y \in Y \mid (x_i, y) \in T \text{ and } (x_j, y) \in T\}|$$

$$d(y_\alpha, y_\beta) := |\{x \in X \mid (x, y_\alpha) \in T \text{ and } (x, y_\beta) \in T\}|$$

In words, $d(x_i, x_j)$ is the number of suffixes that x_i and x_j have in
common in T. In terms of the graph associated to $\hat{\pi}$, it is the number

of paths of length two between x_i and x_j. If $i = j$, then $d(x_i, x_i)$ is simply the degree of vertex x_i. Likewise, $d(y_\alpha, y_\beta)$ is the number prefixes that y_α and y_β have in common in T. It is also the number of paths of length two between y_α and y_β in the graph associated to $\hat{\pi}$. If $\alpha = \beta$ then $d(y_\alpha, y_\alpha)$ is the degree of vertex y_α. In this simple setup, the entries of the reduced density operators as defined in Equations (3.2) and (3.4) specialize to

$$(\rho_X)_{ij} = \frac{d(x_i, x_j)}{|T|} \qquad (3.10)$$

$$(\rho_Y)_{\alpha\beta} = \frac{d(y_\alpha, y_\beta)}{|T|}. \qquad (3.11)$$

As a result, we have the following general combinatorial interpretation of the reduced densities, as seen in Example 3.1.

Off diagonals count shared prefixes. Up to the normalizing factor $1/|T|$, the ijth off-diagonal entry of ρ_X counts the number of times x_i and x_j share a common suffix in T. The $\alpha\beta$th off diagonal entry of ρ_Y counts the number of times y_α and y_β share a common prefix in T.

Diagonals count occurrences. Up to the normalizing factor $1/|T|$, the ith diagonal of ρ_X counts the number of times x_i occurs as a prefix in T. The αth diagonal entry of ρ_Y counts the number of times y_α appears as a suffix in T.

The upshot is that the entries of the reduced densities obtained from an empirical distribution may be read off rather quickly—just look at the graph. We will use this tactic when peering into the application of Chapter 4, happily following Gromov's advice, "If you don't understand, count!" [Gro19].

Example 3.2. Suppose X is a set with three elements and Y is a set with two elements and consider the following graph with 5 edges.
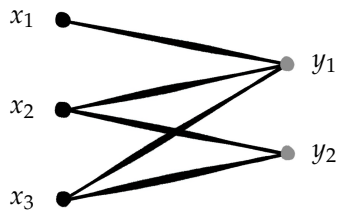

Let $T \subseteq X \times Y$ be the set consisting of all pairs (x, y) for which there is an edge joining x and y. Then the reduced densities of the state

$$|\psi\rangle = \frac{1}{\sqrt{5}} \sum_{(x_i,y_\alpha)\in T} |x_i\rangle \otimes |y_\alpha\rangle \text{ associated to this graph are}$$

$$\rho_X = \begin{array}{c} \\ x_1 \\ x_2 \\ \\ x_3 \end{array} \begin{array}{ccc} x_1 & x_2 & x_3 \\ \left[\begin{array}{ccc} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{array}\right. \end{array}\begin{array}{c} \\ \\ \left] \frac{1}{5} \right. \\ \\ \end{array} \qquad \rho_Y = \begin{array}{c} \\ y_1 \\ y_2 \end{array} \begin{array}{cc} y_1 & y_2 \\ \left[\begin{array}{cc} 3 & 2 \\ 2 & 2 \end{array}\right] \frac{1}{5} \end{array}$$

To see this, take a look at ρ_Y, for the moment. Ignoring the factor of $\frac{1}{5}$, the diagonal entries 3 and 2 are the degrees of the vertices in Y.


$$\begin{bmatrix} 3 & 2 \\ 2 & 2 \end{bmatrix}$$
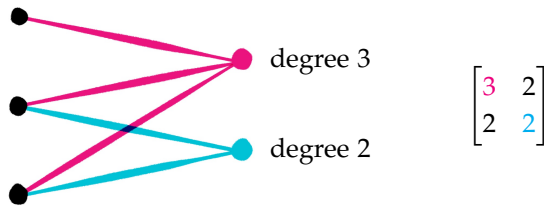
degree 3

degree 2

The off-diagonal entry of ρ_Y is 2, which is the number of paths of length two that connect the elements of Y.

degree 2

degree 2

$$\begin{bmatrix} 3 & 2 \\ 2 & 2 \end{bmatrix}$$
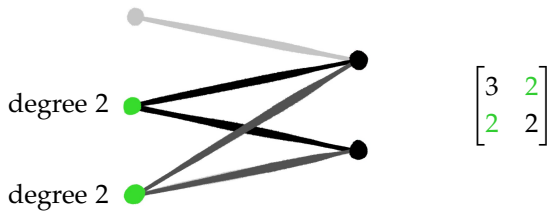
The entries for ρ_X are understood just as easily. Ignoring the factor of $\frac{1}{5}$, the diagonal entries $1,2,2$ are the degrees of the vertices in X.

degree 1

degree 2

degree 2

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{bmatrix}$$
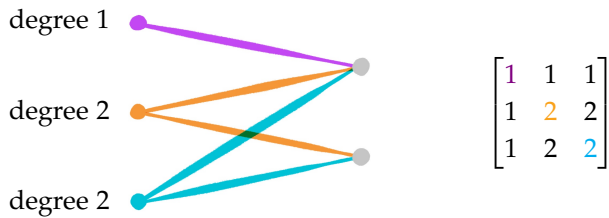
The off diagonals of ρ_X are 1 and 1 and 2. The first off diagonal counts the single path of length two that joins x_1 and x_2.

degree 2

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{bmatrix}$$
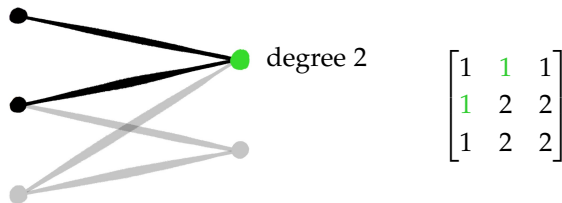
The third off diagonal counts the two paths of length two that join x_2 and x_3.

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{bmatrix}$$
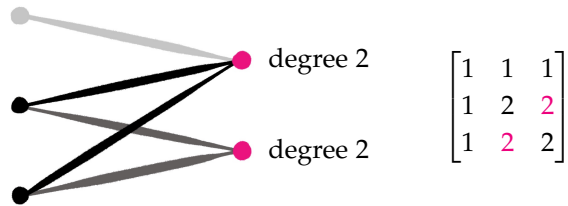
The second off diagonal counts the single path of length two that joins x_1 and x_3. You can imagine the picture.

With these combinatorial interpretations in mind, notice that Example 3.1 can be greatly simplified.

Example 3.3. The joint distribution on the toy corpus introduced in Example 3.1 is an empirical one. With $X = \{\text{orange, green, purple}\}$ and $Y = \{\text{fruit, vegetable}\}$ the example corpus corresponds to the following subset $T \subseteq X \times Y$.

$$T = \{(\text{orange, fruit}), (\text{green, fruit}), (\text{purple, vegetable})\}$$

As a graph, the empirical distribution $\hat{\pi}$ consists of three edges that are each weighted by $\frac{1}{3}$.
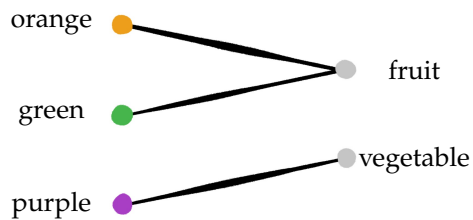
Now recall the reduced density operators $\rho_X = \text{tr}_Y |\psi\rangle\langle\psi|$ and $\rho_Y = \text{tr}_X |\psi\rangle\langle\psi|$ derived in Example 3.1.

$$\rho_X = \begin{array}{c} \\ o \\ g \\ p \end{array} \begin{array}{c} o \quad g \quad p \\ \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{array} \frac{1}{3} \qquad \rho_Y = \begin{array}{c} \\ F \\ V \end{array} \begin{array}{c} F \quad V \\ \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \end{array} \frac{1}{3}$$

Observe that the diagonals of ρ_X are the degrees of the three vertices $x \in X$, and the off-diagonals count paths of length two. For instance, the *orange-green* and *green-orange* off-diagonal entries are both 1, as there is a single path of length two joining those vertices. On the other hand, there is *no* path of length two joining *purple* to any other

vertex in X. This accounts for all entries in ρ_X that are zero. The diagonals of ρ_Y are likewise the degrees of the vertices $y \in Y$. Both off-diagonals are zero since *fruit* and *vegetable* have no prefixes in common. Equivalently, there is not path of length two between *fruit* and *vegetable*.

By now, we've covered a lot of information. The following takeaway summarizes the discussion.

Takeaway 5. *Given finite sets X and Y, any joint probability distribution $\pi: X \times Y \to \mathbb{R}$ defines a unit vector in $\mathbb{C}^X \otimes \mathbb{C}^Y$ whose coefficients are the square roots of the probabilities*

$$|\psi\rangle = \sum_{(x,y) \in X \times Y} \sqrt{\pi(x,y)} |x\rangle \otimes |y\rangle.$$

Orthogonal projection onto this unit vector defines a density operator $\rho = |\psi\rangle\langle\psi|$ whose reduced densities ρ_X and ρ_Y have the following properties.

- *The classical marginal probability distribution $\pi_X: X \to \mathbb{R}$ is contained along the diagonal of ρ_X.*

$$(\rho_X)_{ii} = \sum_\alpha \pi(x_i, y_\alpha) = \pi_X(x_i)$$

- *The classical marginal probability distribution $\pi_Y: Y \to \mathbb{R}$ is contained along the diagonal of ρ_Y.*

$$(\rho_Y)_{\alpha\alpha} = \sum_i \pi(x_i, y_\alpha) = \pi_Y(y_\alpha)$$

- *The reduced densities ρ_X and ρ_Y generally have nonzero off-diagonal entries that encode extra information about subsystem interactions.*

$$(\rho_X)_{ij} = \sum_\alpha \sqrt{\pi(x_i, y_\alpha)\pi(x_j, y_\alpha)}$$

$$(\rho_Y)_{\alpha\beta} = \sum_i \sqrt{\pi(x_i, y_\alpha)\pi(x_i, y_\beta)}$$

  This information contributes to the eigenvalues and eigenvectors of ρ_X and ρ_Y, and it is akin to conditional probability.

- *When π is an empirical probability distribution, the matrix entries of ρ_X and ρ_Y have simple, combinatorial interpretations that can be read off from a bipartite graph associated to π. In particular, the off-diagonal entries count the number of shared suffixes and prefixes.*

AT THIS POINT, the theory branches off into a few directions.

An application. Now that we understand the information stored in reduced densities, we may return to the idea of reconstructing a pure quantum state from its reduced densities. In practice, how does one use information about smaller subsystems and their interactions to recover knowledge about a larger whole? As we'll see in Chapter 4, the answer is exploited in a well-known procedure in physics—*the density matrix renormalization group* (DMRG) procedure [Sch11, Whi92]. As it turns out, this ability to reconstruct a quantum state is immensely useful for tackling a familiar puzzle in an applied setting: Given some data generated by an unknown probability distribution, what is a good algorithm for building a *model* of that distribution with the goal of generating new data from it? In Chapter 4, we will share one such algorithm inspired by DMRG. It successively builds one of these so-called *generative models* entirely from eigenvectors of reduced density operators.

A link with formal concepts. The graph-theoretic approach for understanding reduced densities described in Section 3.2 is directly connected with the graph-theoretical presentation of formal concepts introduced in Chapter 1. Indeed, the observant reader will notice that the eigenvectors of the reduced densities that we computed in Example 3.1 actually *recovered* the formal concepts in Example 1.1! In fact, more is true—Example 3.1 recovered the classical formal concepts and further *enriched* them with probabilities. We will spell this out more carefully below in Section 3.3.

A framework for entailment. So far, we've only discussed probability distributions on a Cartesian product of two sets X and Y. The results of this section still hold if X and Y each decompose as products of smaller sets. In other words, the theory holds for larger systems where the initial joint probability distribution is over a set of sequences of any fixed length. As we'll show in Section 3.4, every sequence (and any subsequence) can be represented by a density operator on a multi-partite system obtained from the state $|\psi\rangle$ of Equation (3.1). The set of density operators on any given space form a partially-ordered set, and so there is a natural way to compare sequences based on the statistics encoded by the densities. When those sequences consist of *words* in a natural language, this paves the way for modeling entailment and hierarchy.

Each of these points is worth expanding upon a little more. Below in Section 3.3 we'll say more about the intriguing connection between eigenvectors and formal concepts. In Section 3.4 we will expand on the theory behind modeling entailment. In Chapter 4, we will outline an algorithm that produces a generative model using the

mathematics of this chapter. All three endeavors may be thought of as "corollaries" to the main ideas presented in Sections 3.1–3.2.

3.3   Eigenvectors versus Formal Concepts

Turning back a few pages to the formal concept construction in Example 1.1 is now encouraged. There we started with the same finite sets that we had in Example 3.1, namely $X = \{\text{orange, green, purple}\}$ and $Y = \{\text{fruit, vegetable}\}$. The remaining ingredients in each example are completely analogous to each other. In Example 1.1 we started with a function $R \colon X \times Y \to \{0,1\}$, indicated by this table:

	orange	green	purple
fruit	1	1	0
vegetable	0	0	1

In Example 3.1 we started with a probability distribution $\pi \colon X \times Y \to \mathbb{R}$, indicated by this table:

	orange	green	purple
fruit	$\frac{1}{3}$	$\frac{1}{3}$	0
vegetable	0	0	$\frac{1}{3}$

Both R and π were then visualized as the same bipartite graph.
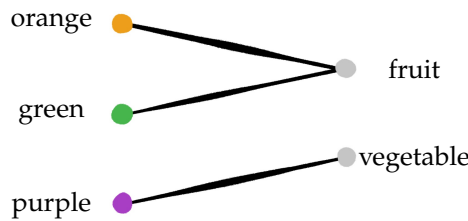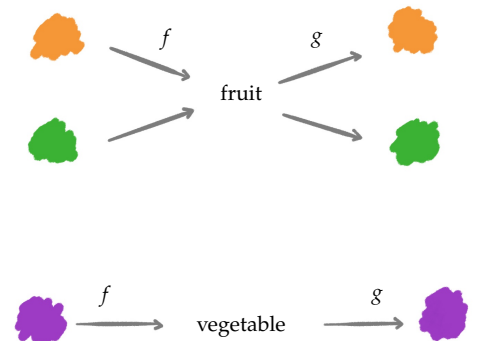

Using this graph in Example 1.1, we first obtained a pair maps between power sets $f \colon 2^X \rightleftarrows 2^Y \colon g$, and the fixed points of fg and gf gave two formal concepts.

$$(\{\text{orange, green}\}, \{\text{fruit}\})$$

$$(\{\text{purple}\}, \{\text{vegetable}\})$$

Using the same graph in Example 3.1, we also obtained a pair of maps between vector spaces $M \colon \mathbb{C}^X \rightleftarrows \mathbb{C}^Y \colon M^\dagger$, and the fixed points of $MM^\dagger$ and $M^\dagger M$ gave two pairs of eigenvectors, $\{|e_1\rangle, |f_1\rangle\}$

and $\{|e_2\rangle, |f_2\rangle\}$, where each pair is further "tagged" with an eigen-value.

$$\{|e_1\rangle, |f_1\rangle\} = \left\{ \frac{1}{\sqrt{2}} \left(|\text{orange}\rangle + |\text{green}\rangle \right), |\text{fruit}\rangle \right\} \qquad \lambda_1 = \frac{2}{3}$$

$$\{|e_2\rangle, |f_2\rangle\} = \{|\text{purple}\rangle, |\text{vegetable}\rangle\} \qquad \lambda_2 = \frac{1}{3}$$

These sets of eigenvectors are clearly a statistically-enriched version of the formal concepts. But the analogy goes deeper. Recall from Equation (1.1) that f and g are defined as lifts of the following functions $a\colon X \to 2^Y$ and $b\colon Y \to 2^X$.

$$X \xrightarrow{\quad a \quad} 2^Y$$
$$x \longmapsto a(x) := \{y \in Y \mid R(x,y) = 1\}$$

$$Y \xrightarrow{\quad b \quad} 2^X$$
$$y \longmapsto b(y) := \{x \in X \mid R(x,y) = 1\}$$
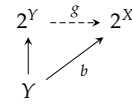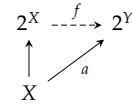
The subset $a(x)$ can be identified with the xth column of the table (or $\{0,1\}$-valued matrix) associated to R, and the subset $b(y)$ can be identified with the yth row. Analogously, there are functions $\alpha\colon X \to \mathbb{C}^Y$ and $\beta\colon Y \to \mathbb{C}^X$ that lift to give the linear maps M and $M^\dagger$. Recall from Proposition 2.2 that for each $i = 1, \ldots, |X|$ there is a map $A_i \in \hom(\mathbb{C}^X \otimes \mathbb{C}^Y, \mathbb{C}^Y)$ defined by $A_i := \langle x_i| \otimes \mathrm{id}_{\mathbb{C}^Y}$. So when $|\psi\rangle = \sum_{x,y} \sqrt{\pi(x,y)}|x\rangle \otimes |y\rangle$ is the state associated to π, "evaluation at $|\psi\rangle$" defines a function

$$X \xrightarrow{\quad \alpha \quad} \mathbb{C}^Y$$
$$x_i \longmapsto A_i|\psi\rangle$$

Note that $A_i|\psi\rangle \in \mathbb{C}^Y$ is the ith column of M. By the universal property of vector spaces, α *lifts* to a linear map $\mathbb{C}^X \to \mathbb{C}^Y$, which is precisely M. In the same way, for each $\alpha = 1, \ldots, |Y|$ there is a map $B_\alpha \in \hom(\mathbb{C}^X \otimes \mathbb{C}^Y, \mathbb{C}^X)$ so that evaluation at $|\psi\rangle$ defines a function

$$Y \xrightarrow{\quad \beta \quad} \mathbb{C}^X$$
$$y_\alpha \longmapsto B_\alpha|\psi\rangle$$
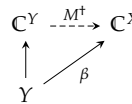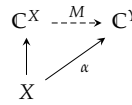
where $B_\alpha|\psi\rangle \in \mathbb{C}^X$ is the αth row of M. Up to complex conjugation, β lifts to the linear adjoint $M^\dagger\colon \mathbb{C}^Y \to \mathbb{C}^X$.

SO THE PARALLELS between formal concepts and eigenvectors of reduced densities are striking. Even so, we may **not** conclude that they always coincide, or that the linear algebra always recovers the set theory. In fact, *this is only true when the relation R satisfies the property*

that its bipartite graph is a disjoint union of complete bipartite subgraphs, or "clusters." Then one expects that the eigenvectors of the reduced densities derived from the uniform probability distribution defined by the graph *will* coincide with classical formal concepts, and each formal concept or pair of eigenvectors corresponds to a cluster. (The verification is a straightforward, though perhaps tedious, exercise in arithmetic.) So it's very easy to find an example where formal concepts and eigenvectors don't coincide. Consider the following graph, for instance, which contains four edges instead of three.
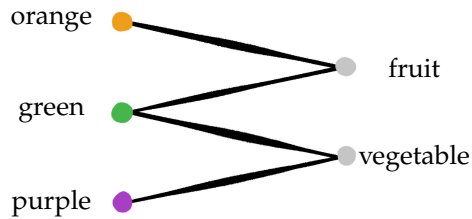
It defines the following uniform probability distribution on $X \times Y$.

	orange	green	purple
fruit	$\frac{1}{4}$	$\frac{1}{4}$	0
vegetable	0	$\frac{1}{4}$	$\frac{1}{4}$

By replacing each "$\frac{1}{4}$" with a "1," this table also defines a relation $R \subset X \times Y$, which—as can be quickly verified—has the following three formal concepts.

$$(\{\text{orange, green}\}, \{\text{fruit}\})$$

$$(\{\text{green, purple}\}, \{\text{vegetable}\})$$

$$(\{\text{green}\}, \{\text{fruit, vegetable}\})$$

On the other hand, there are only *two* pairs of eigenvectors from $MM^\dagger$ and $M^\dagger M$, where $M = \frac{1}{\sqrt{4}} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$. Here they are, together with their associated eigenvalues.

$$\left\{ \tfrac{1}{\sqrt{6}} (|\text{orange}\rangle + |\text{green}\rangle + |\text{purple}\rangle) \ , \ \tfrac{1}{\sqrt{2}}(|\text{fruit}\rangle + |\text{vegetable}\rangle) \right\} \qquad \lambda_1 = \tfrac{3}{4}$$

$$\left\{ \tfrac{1}{\sqrt{2}}(|\text{orange}\rangle - |\text{purple}\rangle) \ , \ \tfrac{1}{\sqrt{2}}(|\text{fruit}\rangle - |\text{vegetable}\rangle) \right\} \qquad \lambda_2 = \tfrac{1}{4}$$

So in this simple example, the two notions—eigenvectors and formal concepts—diverge. (And notice the negatives!)

LET'S CLOSE THIS SECTION with two remarks. First, although eigenvectors and formal concepts don't always coincide, we've taken time

to discuss the connection between them because we think it is interesting, if not tantalizing. Second, there *is* a sense in which the two notions are clearly related. But to see this we must lift our feet off the ground and view the situation from the perspective of category theory. Chapter 5 is fully devoted to this endeavor. In the mean time, let's now turn our attention to another "corollary" of the theory of Section 3.2, namely modeling entailment with density operators.

3.4   Modeling Entailment with Densities

In some settings, the spectral information of reduced densities of pure states may serve as a proxy for "meaning." Let's think in the context of language, for instance. To understand something about the meaning of the word *orange*, it's helpful to know how often the word occurs in the language as well as the *context* in which it appears. From a mathematical perspective, this idea is not unfamiliar. The Yoneda lemma in category theory informally says that a mathematical object is completely determined by the network of relationships it shares with other objects of its kind. In the same way, think of the meaning of a word as being captured by the network of all expressions that the word fits into *along with* with the statistics of those occurences.

The Yoneda lemma brings to mind the oft-cited quote by linguist John Firth: "You shall know a word by the company it keeps." [Fir57] I like to think of this as the Yoneda Lemma for Language.
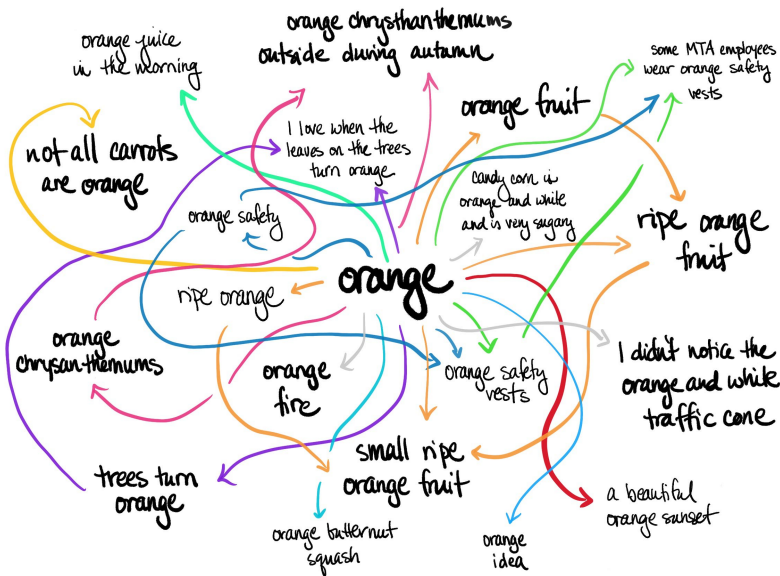
As it turns out, density operators provide a natural framework for capturing this very idea. The goal of this section is to show that a word such as *orange* naturally unravels as a weighted sum of all expressions containing that word, where the weights are conditional probabilities. More precisely, we'll see that any word or expression

can be assigned a density, and the density for *orange* decomposes as a weighted sum of densities, one for each expression containing *orange*. One might think of this as a *Yoneda-enriched spectral decomposition*, which will give a clear candidate for modeling entailment and concept hierarchy using a simple poset structure on densities.
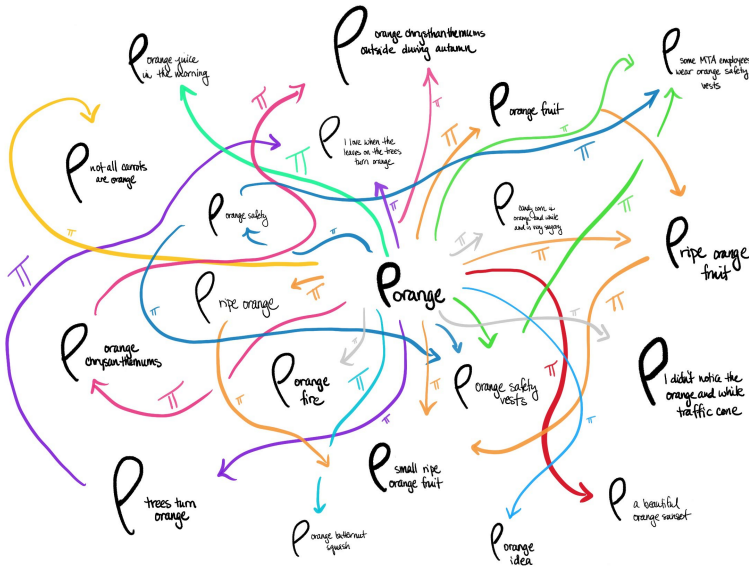
The ideas in this section are the results of joint work with Yiannis Vlassopoulos, in which we further investigate entailment and concept hierarchy in language. The simple example in Section 3.4.1 is meant to spark the reader's interest for the extended theory appearing in a forthcoming paper [BV20]. Notably, Section 3.4.1's passage from words to densities, such as orange $\mapsto \rho_{\text{orange}}$, will be derived differently in [BV20], and the latter greatly expands upon the general theory of Section 3.4.2. We hope the simple ideas here will whet your appetite for much more to come. Further connections between language modeling and tensor networks may be found in [PTV17, PV17]. Others have also explored a density matrix model for entailment using the Lowener order. The authors in [BCLM16] present one such framework based on the category theoretical approach of [CSC10]. We may view the work below as an instantiation of the theory presented there. In particular, conditional probabilities present themselves as a natural candidate for entailment strength, and we are using statistics as a proxy for grammar.

WITH THIS INTRODUCTION in mind, let us now describe how these ideas connect with the mathematics described in Section 3.1. As noted then, the starting ingredient is always a probability distribution on a finite set $\pi\colon S \to \mathbb{R}$. When S decomposes as an N-fold Cartesian

product of a finite set A, say $S = A \times A \cdots \times A$, we may think of elements $s \in S$ as sequences of symbols from the "alphabet" A. The elements of A may be thought of as individual characters or words or phrases in a language so that concatenations of them are longer expressions; S contains all those of length N. The distribution π then captures something of the statistics in the language built from A, and the vector $|\psi\rangle = \sum_s \sqrt{\pi(s)}|s\rangle$ is the state of the language. As we will show below, knowledge of this state then gives an easy way to compare words and expressions from A. For example, the mathematics will give us a natural way to compare something that is "orange" with something that is "small, ripe" and "orange," and to see that the latter is a specific case of the former. The key tool for making these kinds of comparisons is a passage from *words* to *reduced density operators*.

Concretely, we aim to show that expressions from the alphabet A can be represented by reduced density operators obtained from the orthogonal projection operator $|\psi\rangle\langle\psi|$. These densities can then be compared to one another using a simple partial order. Given positive semidefinite operators σ and τ on the same space, one has $\sigma \geq \tau$ if and only if $\sigma - \tau$ is positive semidefinite. This is called the **Loewner order** on positive semidefinite operators, and it defines a partial order on the set of densities operating on a fixed space.

Here's the outline for this section. In Section 3.4.1, we'll show that words and phrases, say *orange* and *small ripe orange*, have density matrix representations, ρ_{orange} and $\rho_{\text{small ripe orange}}$. Then we'll use Proposition 2.2 to show that the density for a given word, say ρ_{orange}, decomposes as a weighted sum of densities corresponding to all expressions containing that word. Finally we'll show that this decomposition naturally gives a way to model entailment between various expressions using the Loewner order. In particular, we'll see that conditional probabilities from π provide a natural measure of entailment strength:

$$\rho_{\text{orange}} \geq \pi(\text{small ripe orange} \mid \text{orange})\rho_{\text{small ripe orange}} \qquad (3.12)$$

Because the ideas here are relatively new, we will put an elementary example up front and derive the above inequality. Afterwards we'll describe the general theory in Section 3.4.2.

3.4.1   An Extended Example

In previous examples, we have worked with a toy corpus of text containing three phrases of length two: *orange fruit, green fruit, purple vegetable*. In this example we will start with a different set of phrases that are a little longer. Suppose we have the following toy corpus of

text containing five phrases of length four.

small ripe orange fruit   large rotten green vegetable
large ripe orange vegetable   small ripe orange vegetable
small rotten orange fruit

Let's now follow the procedure outlined in Section 3.1 to obtain a
probability distribution that can be modeled by a quantum state $|\psi\rangle$.
As a first step, consider the following ordered sets.

$$A := \{\text{small, large}\} \qquad C := \{\text{orange, green}\}$$
$$B := \{\text{ripe, rotten}\} \qquad Y := \{\text{fruit, vegetable}\}$$

Let $X = A \times B \times C$ so that elements in X are **prefixes** and elements
in Y are **suffixes.** Identify each of the five phrases xy in the corpus
with its corresponding sequence (x, y) and let $T \subseteq X \times Y$ be the
set consisting of these pairs. This defines a probability distribution
$\hat{\pi} \colon X \times Y \to \mathbb{R}$ by

$$\hat{\pi}(x, y) = \begin{cases} \frac{1}{5} & \text{if } (x, y) \in T \\ 0 & \text{if } (x, y) \notin T. \end{cases}$$

Now define $|\psi\rangle$ to be the unit vector obtained as the sum of all se-
quences in T weighted by the square roots of their probabilities.
Observe that $|\psi\rangle$ lies in the tensor product $\mathbb{C}^A \otimes \mathbb{C}^B \otimes \mathbb{C}^C \otimes \mathbb{C}^Y$ where
each factor is isomorphic to $\mathbb{C}^2$.

$$|\psi\rangle = \sum_{x,y} \sqrt{\hat{\pi}(x, y)} |x\rangle \otimes |y\rangle$$

$$= \sum_{a,b,c,y} \sqrt{\hat{\pi}(a, b, c, y)} |a\rangle \otimes |b\rangle \otimes |c\rangle \otimes |y\rangle$$

$$= \frac{1}{\sqrt{5}} \begin{pmatrix} |\text{small}\rangle & \otimes & |\text{ripe}\rangle & \otimes & |\text{orange}\rangle & \otimes & |\text{fruit}\rangle & + \\ |\text{small}\rangle & \otimes & |\text{rotten}\rangle & \otimes & |\text{orange}\rangle & \otimes & |\text{fruit}\rangle & + \\ |\text{large}\rangle & \otimes & |\text{ripe}\rangle & \otimes & |\text{orange}\rangle & \otimes & |\text{vegetable}\rangle & + \\ |\text{large}\rangle & \otimes & |\text{rotten}\rangle & \otimes & |\text{green}\rangle & \otimes & |\text{vegetable}\rangle & + \\ |\text{small}\rangle & \otimes & |\text{ripe}\rangle & \otimes & |\text{orange}\rangle & \otimes & |\text{vegetable}\rangle & \end{pmatrix}$$

As a tensor diagram, $|\psi\rangle$ is a node with four parallel edges, the first
three representing $\mathbb{C}^X$ and the fourth representing $\mathbb{C}^Y$.

$$|\psi\rangle =$$

With $|\psi\rangle$ in hand, our next goal is to compute the reduced density
operator on the suffix subsystem $\rho_Y = \text{tr}_X |\psi\rangle\langle\psi|$. There are a few

ways to do this, but let us refer to Proposition 2.2, which states that ρ_Y decomposes as a sum of projection operators,

$$\rho_Y = \sum_{x \in X} A_x |\psi\rangle\langle\psi| A_x^\dagger \tag{3.13}$$

where each $A_x \colon \mathbb{C}^X \otimes \mathbb{C}^Y \to \mathbb{C}^Y$ is defined by $A_x := \langle x| \otimes \mathrm{id}_{\mathbb{C}^Y}$. That is, for any prefix-suffix pair $(x', y) \in X \times Y$ we have that $A_x(|x'\rangle \otimes |y\rangle) = \langle x|x'\rangle |y\rangle$ which is equal to $|y\rangle$ if $x' = x$ and is equal to 0 otherwise. So each term in Equation (3.13) involves a vector of the form

$$A_x |\psi\rangle = \sum_y \sqrt{\hat{\pi}(x, y)} |y\rangle \tag{3.14}$$

$$= \sqrt{\hat{\pi}(x, \text{fruit})} |\text{fruit}\rangle + \sqrt{\hat{\pi}(x, \text{vegetable})} |\text{vegetable}\rangle.$$

Notice that the vector $A_x |\psi\rangle$ is the xth column of the matrix representation of the linear map $M \colon \mathbb{C}^X \to \mathbb{C}^Y$ associated to $|\psi\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$, whose yxth entry is the probability $M_{yx} = \sqrt{\pi(x, y)}$. Equation (3.13) says that ρ_Y decomposes as the *sum of projections onto each of these columns.* This is a point worth emphasizing. Every density operator has a spectral decomposition and therefore decomposes as a sum of projection operators onto the spaces spanned by its eigenvectors. But Equation (3.13) is giving us *a completely different* decomposition into projections, namely one onto each column of M. To get a better feel for this, let's write down the matrix M explicitly. To do so we first need to choose an ordering on the set $X = \{x_1, x_2, \ldots, x_8\}$. Let's choose ordering below.

$x_1 = (\textbf{small}, \textbf{ripe}, \textbf{orange})$ $x_5 = (\text{small}, \text{ripe}, \text{green})$

$x_2 = (\textbf{large}, \textbf{ripe}, \textbf{orange})$ $x_6 = (\text{large}, \text{ripe}, \text{green})$

$x_3 = (\textbf{small}, \textbf{rotten}, \textbf{orange})$ $x_7 = (\text{small}, \text{rotten}, \text{green})$

$x_4 = (\text{large}, \text{rotten}, \text{orange})$ $x_8 = (\textbf{large}, \textbf{rotten}, \textbf{green})$

Of these eight sequences, recall that only *four* of them appear as prefixes in T, namely x_1, x_2, x_3 and x_8, indicated in boldface above. Notably, x_1 appears in T twice. With this ordering, the matrix M associated to $|\psi\rangle$ has the probability $\sqrt{\hat{\pi}(x_i, y_\alpha)}$ as the αith entry.
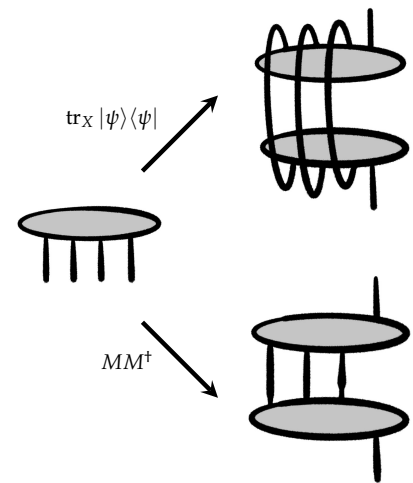
$$M = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Each of the eight columns correspond to one of the prefixes $x_i \in X$, and each of two rows correspond to one of the suffixes $y_\alpha \in Y$. There is a $1/\sqrt{5}$ in the αith entry if and only if $(x_i, y_\alpha) \in T$. Here's a

The linear map M associated to $|\psi\rangle$ has the following diagram,
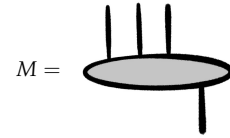
and the equation $\rho_Y = \mathrm{tr}_X |\psi\rangle\langle\psi| = MM^\dagger$ has the following picture:

The sum decomposition in Equation (3.13) gives yet *another* expression for ρ_Y. It doesn't have a standard tensor diagram representation, but we will illustrate it as below.
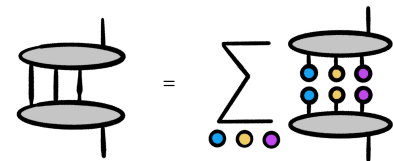
In symbols,

$$\rho_Y = \sum_{(a,b,c) \in A \times B \times C} M|abc\rangle\langle abc|M^\dagger$$

where we are using the fact that $A_i |\psi\rangle = M|x_i\rangle$ for each i, as remarked in the main text.

decorated version of the matrix,

$$
M = \begin{array}{c} \\ y_1 \\ y_2 \end{array}
\begin{array}{c}
\begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \end{array} \\
\left[\begin{array}{cccccccc}
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1
\end{array} \right]
\end{array} \frac{1}{\sqrt{5}}
$$

or more elaborately,

	ripe		rotten		ripe		rotten	
	small	large	small	large	small	large	small	large
fruit	1	0	1	0	0	0	0	0
vegetable	1	1	0	0	0	0	0	1

$$
M = \qquad\qquad \underbrace{\qquad\qquad\qquad}_{\text{orange}} \qquad \underbrace{\qquad\qquad\qquad}_{\text{green}} \qquad \frac{1}{\sqrt{5}}
$$

Now we may quickly verify the claim that $A_i|\psi\rangle$ is the ith column of M. Recall that the natural map $Y \to \mathbb{C}^Y$ represents suffixes as standard basis vectors, $|\text{fruit}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|\text{vegetable}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Then Equation (3.14) implies that

$$
A_1|\psi\rangle = \tfrac{1}{\sqrt{5}}(|\text{fruit}\rangle + |\text{vegetable}\rangle) = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}
$$

$$
A_2|\psi\rangle = \tfrac{1}{\sqrt{5}}|\text{vegetable}\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}
$$

$$
A_3|\psi\rangle = \tfrac{1}{\sqrt{5}}|\text{fruit}\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 0 \end{bmatrix}
$$

$$
A_8|\psi\rangle = \tfrac{1}{\sqrt{5}}|\text{vegetable}\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}
$$

and $A_i|\psi\rangle = 0$ for any prefix x_i that is not in T. So indeed $A_i|\psi\rangle$ is the ith column of M. Equivalently, we have that $A_i|\psi\rangle = M|x_i\rangle$. So thinking of M as a linear map between the prefix and suffix subsystems, M maps every prefix in T onto its suffix. For example, $M|x_2\rangle = M|\text{large ripe orange}\rangle = \tfrac{1}{\sqrt{5}}|\text{vegetable}\rangle$. Also observe that two prefixes have the same image under M whenever they share the same suffix in T. For instance, the vectors $|x_2\rangle$ and $|x_8\rangle$ both map to $\tfrac{1}{\sqrt{5}}|\text{vegetable}\rangle$ since the prefixes *large ripe orange* and *large rotten green* both have *vegetable* as a suffix. The upshot is that Equation (3.13) gives a decomposition of ρ_Y as a sum of projections onto these

vectors. Explicitly,

$$\rho_Y = A_1|\psi\rangle\langle\psi|A_1^\dagger + A_2|\psi\rangle\langle\psi|A_2^\dagger + A_3|\psi\rangle\langle\psi|A_3^\dagger + A_8|\psi\rangle\langle\psi|A_8^\dagger$$

$$= \frac{1}{5}\left(\begin{bmatrix}1\\1\end{bmatrix}\begin{bmatrix}1 & 1\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} + \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix}\right)$$

$$= \frac{1}{5}\left(\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} + \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}\right)$$

$$= \frac{1}{5}\begin{bmatrix}2 & 1\\1 & 3\end{bmatrix}.$$

$x_1 = $ (small, ripe, orange)
$x_2 = $ (large, ripe, orange)
$x_3 = $ (small, rotten, orange)
$x_8 = $ (large, rotten, green)

Notice the diagonals of ρ_Y count the number of occurrences of *fruit* and *vegetable* in the corpus, while the off-diagonal entry counts the number of shared prefixes. This is consistent with the combinatorial claims of Section 3.2. In any case, the path for defining a density matrix representation for sequences is now clear. For each prefix $x_i \in T$ define the **unnormalized reduced density operator** associated to x_i to be

$$\hat{\rho}_{x_i} = A_i|\psi\rangle\langle\psi|A_i^\dagger$$

As a projection operator, $\hat{\rho}_{x_i}$ is positive semidefinite and Hermitian, though it does not have unit trace. Should we want a properly normalized density operator, simply divide $\hat{\rho}_{x_i}$ by its trace, which is the marginal probability of x_i:
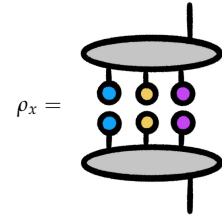
$$\rho_{x_i} := \frac{1}{\hat{\pi}_X(x_i)}\hat{\rho}_{x_i}$$

To see this latter claim, recall that $A_i|\psi\rangle = \sum_y \sqrt{\hat{\pi}(x_i,y)}|y\rangle$ and so $A_i|\psi\rangle\langle\psi|A_i^\dagger = \sum_{y,y'} \sqrt{\hat{\pi}(x_i,y)\hat{\pi}(x_i,y')}|y\rangle\langle y'|$ which has trace equal to $\sum_y \hat{\pi}(x_i,y) = \hat{\pi}_X(x_i)$, where $\hat{\pi}_X \colon X \to \mathbb{R}$ is the marginal distribution obtained from $\hat{\pi} \colon X \times Y \to \mathbb{R}$. In the above example we obtain the following properly normalized reduced densities associated to each prefix,

If $x_i = (a, b, c)$ so that $|abc\rangle = $

then $\hat{\rho}_{x_i}$ is projection onto $A_i|\psi\rangle = M|abc\rangle$ which has the following picture.

$\rho_x = $

$$\rho_{x_1} = \rho_{\text{small ripe orange}} = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} \qquad \rho_{x_3} = \rho_{\text{small rotten orange}} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$$

$$\rho_{x_2} = \rho_{\text{large ripe orange}} = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} \qquad \rho_{x_8} = \rho_{\text{large rotten green}} = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}$$

$\hat{\pi}_X(x_1) = 2/5$
$\hat{\pi}_X(x_2) = 1/5$
$\hat{\pi}_X(x_3) = 1/5$
$\hat{\pi}_X(x_8) = 1/5$

while the *unnormalized* densities $\hat{\rho}_{x_i}$ are the four matrices whose sum is ρ_Y, as shown above. To summarize, every prefix x_i in T corresponds to a (normalized or unnormalized) density operator identified with one of the projections that sum to ρ_Y.

Notice, however, that some sequences x_i contain the same words. For instance, x_1, x_2, and x_3 are all phrases that contain the word *orange*. Intuitively, the sum $\hat{\rho}_{x_1} + \hat{\rho}_{x_2} + \hat{\rho}_{x_3}$ of all unnormalized densities containing *orange* should be defined as the unnormalized density $\hat{\rho}_{\text{orange}}$ associated to *orange* itself, and similarly for $\hat{\rho}_{\text{green}}$.

$$\rho_Y = \overbrace{A_1|\psi\rangle\langle\psi|A_1^\dagger + A_2|\psi\rangle\langle\psi|A_2^\dagger + A_3|\psi\rangle\langle\psi|A_3^\dagger}^{\hat{\rho}_{\text{orange}}} \quad + \quad \overbrace{A_8|\psi\rangle\langle\psi|A_8^\dagger}^{\hat{\rho}_{\text{green}}}$$

As tensor diagrams, this equation is
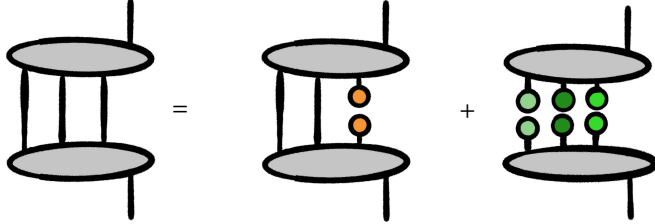
where $|\text{orange}\rangle = $ and $|\text{green}\rangle = $. Now for $\hat{\rho}_{\text{orange}}$ to have unit trace, we must divide by the marginal probability $\hat{\pi}_C(\text{orange}) = 4/5$. So let's make this a definition.[3]

$$\rho_{\text{orange}} := \frac{1}{\hat{\pi}_C(\text{orange})}\hat{\rho}_{\text{orange}}$$

$$= \frac{1}{\hat{\pi}_C(\text{orange})}(\hat{\rho}_{x_1} + \hat{\rho}_{x_2} + \hat{\rho}_{x_3})$$

$$= \frac{1}{4}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

In fact, this suggests a nicer way to write the result:

$$\rho_{\text{orange}} = \frac{1}{\pi_C(\text{orange})}\sum_{i=1,2,3}\hat{\rho}_{x_i}$$

$$= \sum_{i=1,2,3}\frac{\pi_X(x_i)}{\pi_C(\text{orange})}\frac{\hat{\rho}_{x_i}}{\pi_X(x_i)}$$

$$= \sum_{i=1,2,3}\pi(x_i \mid \text{orange})\rho_{x_i}.$$

Consequently, for any $i \in \{1,2,3\}$ we have the inequality

$$\rho_{\text{orange}} \geq \pi(x_i|\text{orange})\rho_{x_i}$$

since their difference is a sum of positive semidefinite operators weighted by nonnegative numbers. Setting $i = 1$ we have now recovered Inequality (3.12), as was the goal:

$$\rho_{\text{orange}} \geq \pi(\text{small ripe orange} \mid \text{orange})\rho_{\text{small ripe orange}}.$$

You might wonder why the tensor network diagram for $\hat{\rho}_{\text{green}}$ isn't the following:
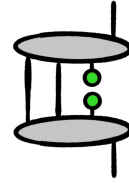
In fact, it *is*. The two edges connecting the gray nodes imply a sum over prefixes x_i that contain the word "green." But there is only *one* such prefix, namely x_8, and so $\hat{\rho}_{\text{green}}$ is comprised of the single term $A_8|\psi\rangle\langle\psi|A_8^\dagger$, which is projection onto the vector $A_8|\psi\rangle$. That projection operator is the diagram illustrated in the main text.

[3] Here I am expanding the Cartesian product $X = A \times B \times C$ to recall that our original joint distribution is on the four-fold Cartesian product $\hat{\pi} \colon A \times B \times C \times Y \to \mathbb{C}$, which defines a marginal distribution $\pi_C \colon C \to \mathbb{R}$. A quick check shows that the trace of $\hat{\rho}_{\text{orange}} := \hat{\rho}_{x_1} + \hat{\rho}_{x_2} + \hat{\rho}_{x_3}$ is computed as $\sum_{a,b,y}\hat{\pi}(a, b, \text{orange}, y)$, which is the marginal probability $\pi_C(\text{orange})$.

In a similar vein, we can easily sum over those tuples $x_i = (a, b, c) \in A \times B \times C$ with $b = ripe$ as well as $c = orange$ to obtain the unnormalized density associated to the expression *ripe orange*,

$$\hat{\rho}_{\text{ripe orange}} := A_1 |\psi\rangle \langle \psi| A_1^\dagger + A_2 |\psi\rangle \langle \psi| A_2^\dagger = \frac{1}{5} \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}.$$

The difference $\hat{\rho}_{\text{orange}} - \hat{\rho}_{\text{ripe orange}} = \frac{1}{5} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \geq 0$ is a positive operator and therefore we have $\hat{\rho}_{\text{orange}} \geq \hat{\rho}_{\text{ripe orange}} \geq \hat{\rho}_{\text{small ripe orange}}$, which pairs well with the intuition that *ripe orange* is a more specific instance of something that is *orange* but is more general than something that is *small ripe orange*.

$$\hat{\rho}_{\text{orange}} \qquad\qquad \hat{\rho}_{\text{ripe orange}} \qquad\qquad \hat{\rho}_{\text{small ripe orange}}$$
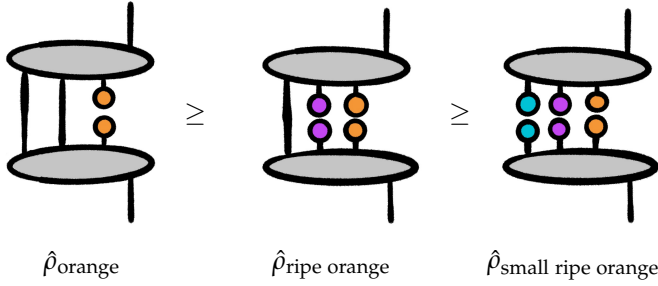
To SUMMARIZE, the reduced density associated to the word *orange* decomposes as a weighted sum of densities, one associated to each expression that contains the word orange. Crucially, the weights are naturally found to be conditional probabilities and may be thought of measuring the strength of entailment.

3.4.2   The General Idea

This extended example illustrates the general idea, which we summarize briefly here. For any finite set A, consider a subset of prefix-suffix pairs $T \subseteq X \times Y$ with $X = A^{N-1} = A \times \cdots \times A$ and $Y = A$. This defines an empirical probability distribution $\hat{\pi} \colon X \times Y \to \mathbb{R}$ and therefore a state $|\psi\rangle = \frac{1}{\sqrt{|T|}} \sum_{(x,y) \in T} |x\rangle \otimes |y\rangle \in \mathbb{C}^X \otimes \mathbb{C}^Y$. Choose an ordering on the set of prefixes, say $X = \{x_1, \ldots, x_n\}$. Then each prefix x_i corresponds to an *unnormalized reduced density operator*

$$\hat{\rho}_{x_i} := M |x_i\rangle \langle x_i| M^\dagger$$

where $M \colon \mathbb{C}^X \to \mathbb{C}^Y$ is the linear map associated to $|\psi\rangle$. (Equivalently, $\hat{\rho}_{x_i} := A_i |\psi\rangle \langle \psi| A_i^\dagger$ where A_i is as in Proposition 2.2.) To obtain the properly normalized reduced density associated to x_i, simply divide by its marginal probability,

$$\rho_{x_i} := \frac{1}{\hat{\pi}_X(x_i)} \hat{\rho}_{x_i}.$$

By Proposition 2.2 the reduced density operator ρ_Y on the suffix subsystem decomposes as a sum of these unnormalized projections,

$$\rho_Y = \sum_i \hat{\rho}_{x_i}.$$

By summing over a *subset* of the indices i, we can obtain a reduced density associated to various subsequences in X. For instance, let $X(a)$ denote the set of all sequences x_i that contain $a \in A$ as the *last* entry. Then we define the *unnormalized reduced density operator associated to a* to be

$$\hat{\rho}_a = \sum_{x \in X(a)} \hat{\rho}_x$$

This is not a density as its trace is the marginal probability $\hat{\pi}(a) < 1$, so we normalize by dividing by the marginal probability of a and obtain the *reduced density operator associated to a*,

$$\rho_a := \frac{1}{\hat{\pi}(a)} \hat{\rho}_a$$
$$= \sum_{x \in X(a)} \frac{1}{\hat{\pi}(a)} \hat{\rho}_x$$
$$= \sum_{x \in X(a)} \frac{\hat{\pi}(x)}{\hat{\pi}(a)} \frac{1}{\hat{\pi}(x)} \hat{\rho}_x$$
$$= \sum_{x \in X(a)} \pi(x \mid a)\rho_x.$$

As the last line shows, $\rho_a \geq \pi(x|a)\rho_x$ for any prefix x. We may think of this as witnessing the fact that x is an expression containing a, thereby being a *refinement* of a. There's nothing special about a being the *last* term in $x = (a_1, \ldots, a)$, nor is there anything special about a being a singleton. Using the ideas here, one could associate a density ρ_s to *any* subsequence s of any length in X, and one can obtain a similar "unraveling" of ρ_s into a weighted sum of all expressions that contain s. Some care must be taken in *where s* occurs, but we won't provide the details here.

To emphasize a point mentioned earlier, any density such as ρ_a can be written as a weighted sum of projections onto its eigenvectors, where the weights are eigenvalues. The decomposition for ρ_a shown here is similar yet different. It is still a weighted sum of projections, but now the projections are onto vectors associated with each expression containing the word "a," and the weights are conditional probabilities. For this reason, we might think of $\rho_a = \sum_{x \in X(a)} \pi(x|a)\rho_x$ as a probabilistically enriched spectral decomposition of ρ_a.
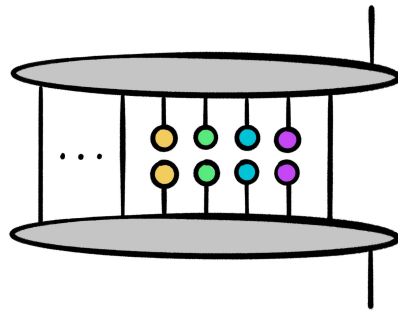
4

An Application and an Experiment

Language is a
one-dimensional painting.

Yiannis Vlassopoulos [Vla19]

THIS CHAPTER HIGHLIGHTS an application of the mathematics in
Chapters 2 and 3. As we've seen, any probability distribution on a
finite set can be represented as a rank 1 density operator—a pure
quantum state. We've described this idea in detail, and so we now
anticipate the question, "Why bother?" That ism why go through
the trouble of passing from basic probability to (possibly ultra large-
dimensional) vector spaces, densities, and reduced densities? The
answer is hidden in plain sight in Figure 2.2. That is, understanding
how to piece together the eigenvectors of reduced densities to recon-
struct a quantum state suggests a *new* algorithm for reconstructing a
classical joint probability distribution—namely by putting together
smaller pieces of it in a highly principled way that knows something
about how those pieces interact.

   We share such a reconstruction algorithm below and illustrate it by
performing an experiment on a well-known dataset. But first, to help
put this application in a larger context, let's consider the following
question. Suppose we have a set of data drawn from an unknown
probability distribution π. How might we use these samples to de-
fine a *new* probability distribution that estimates π, with the goal
of generating new data from it? Here are a couple of examples to
illustrate.

   Bitstrings. Suppose our data points are bitstrings—sequences of
   0s and 1s—all of length 16, for example. There are $2^{16} = 65,536$
   such strings, but suppose we only have a small fraction of them
   that were drawn from some distribution π. We may or may not
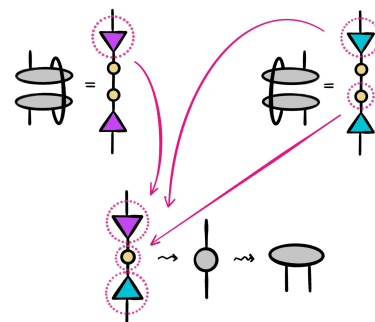
know what π is, but either way we'd like to use the statistics of the samples we *do* have in order to estimate π. With the estimation in hand, we can then generate new bitstrings by sampling from the estimated distribution.

Natural language. Suppose our data points are meaningful sentences; that is, sequences of words from the English alphabet, say. There are many of possibilities, of course, but suppose we only have a small fraction of samples. There is some probability distribution on natural language—the probability of the phrase "orange fruit" is higher than the probability of "orange idea"—though we don't know it, exactly. But we might like to use the data we *do* have to estimate the probability distribution on language in order to generate new, plausible text.

In both of these examples, the data are sequential, meaning they are sequences of symbols from some alphabet. The second example is a case of statistical language modeling. Both examples are instances of *generative modeling*—the task of modeling probabilities with the goal of generating data. This falls under the wider genre of *unsupervised machine learning.*

IN THIS CHAPTER we will illustrate how the extra information stored in the eigenvectors of reduced densities of a pure entangled state form the building blocks of a generative model. Here's the big-picture idea. The passage from classical to quantum probability outlined in Chapter 3 gives a straightforward recipe for modeling any finite dataset T as a quantum state $|\psi\rangle$, as long as the elements of T are sequences; that is, as long as T is a subset of a Cartesian product of finite sets. Further supposing the elements $s \in T$ are samples generated from a (possibly unknown) probability distribution π, the dataset T defines an empirical probability distribution $\hat{\pi}$. Think of $\hat{\pi}$ as a rough approximation to the *true* distribution π. As we know from Chapter 3, the empirical distribution $\hat{\pi}$ can be modeled by a unit vector $|\psi\rangle$ so that the probabilities are the coefficients, $\hat{\pi}(s) = |\langle s|\psi\rangle|^2$. The machine learning problem is to find an algorithm that takes in $|\psi\rangle$ and outputs a *new* unit vector, call it $|\psi_{\mathrm{MPS}}\rangle$, so that the resulting probabilities $|\langle s|\psi_{\mathrm{MPS}}\rangle|^2$ are close to the true probabilities $\pi(s)$, for which the $\hat{\pi}(s)$ were merely an approximation. This new vector $|\psi_{\mathrm{MPS}}\rangle$ is the desired generative model.

This is how the mathematics of Chapter 3 arises in an applied setting. In this chapter, we'll give the bird's-eye view of the ideas. The first thing to know is that *there exists* an algorithm that successfully accomplishes the task just described. It is motivated by and built from the mathematics of Chapters 2–3. More formally, it is inspired

start with $|\psi\rangle$

finish with $|\psi_{\mathrm{MPS}}\rangle$
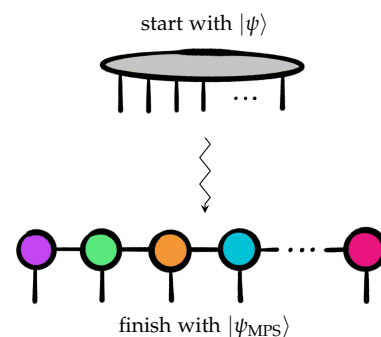
by the *density matrix renormalization group* procedure—a procedure used in physics to construct the ground state of a Hamiltonian operator [Sch11, Whi92]. Here, we use it to reconstruct a joint probability distribution modeled as a quantum state. The algorithm we share is deterministic and requires only simple tools from linear algebra. As a result, it's possible to predict just how *well* the algorithm will work given only the number of samples in the training set T. What's more, the vector $|\psi_{\mathrm{MPS}}\rangle$ turns out to be an example of a tensor network known as an MPS (see Section 2.2.2). We wish to keep the focus on the theory-side-of-things, so rather than giving a detailed description of the algorithm, we will only share the main highlights. We'll then close with a few words about an experiment that tests it. As we'll soon see, the procedure to build $|\psi_{\mathrm{MPS}}\rangle$ is like a machine that reaps what we've sown in $|\psi\rangle$: it sweeps across the training samples, builds reduced density operators from them, and glues their eigenvectors together to form a sequence of tensors that become $|\psi_{\mathrm{MPS}}\rangle$. Readers are referred to our joint work with Stoudenmire and Terilla in [BST20] for any details omitted here.

Although we are using the tools and language of quantum physics, it is *not* necessary that the set or probability distribution being modeled have any interpretation of being quantum. But see Sidenote 2 in Section 4.1.2 for a remark about *which* probability distributions the algorithm is intended.

4.1 Building a Generative Model

To build the model $|\psi_{\mathrm{MPS}}\rangle$ we first need a training set T and an initial probability distribution $\hat{\pi}$. We choose T to be a set of even-parity bitstrings of length $N > 2$, and will let $\hat{\pi}$ be the probability distribution uniformly concentrated on that set. Let's describe this more carefully.

4.1.1 Initial Inputs

Begin with the finite set $A = \{0, 1\}$ and consider the N-fold Cartesian product $A^N = A \times \cdots \times A$, which coincides with the set of all bitstrings of length N. Later in an experiment, we will ultimately take $N = 16$, but let's be flexible with this number. In a few examples we'll suppose $N = 5$ for simplicity. Now observe that bitstrings of length N always come in two "flavors" based on their parity— even or odd. A bitstring $s \in A^N$ is called **even** if it has an even number of 1s, and it is called **odd** if it has an odd number of 1s. Let $E_N := \{s \in A^N \mid s \text{ is even}\}$ be the set of even bitstrings; let $O_N := \{s \in A^N \mid s \text{ is odd}\}$ be the set of odd bitstrings. So $00110 \in E_5$ while $00111 \in O_5$. Observe that $A^N = E_N \cup O_N$ and that $|E_N| = |O_N| = 2^{N-1}$. Now suppose $T \subseteq E_N$ is a subset of N_T even-parity bitstrings, for some number $N_T \leq 2^{N-1}$. This defines an empirical

BEHIND THE SCENES. Think of the set A as an alphabet for some language, and think of A^N as the set of all possible "phrases" (of length N) in that language. The word *all* is important. Not every phrase will be a valid expression in the language. Indeed, not every concatenation of words in English produces a meaningful sentence. Here we are defining *meaningfulness* to be based on probability. A phrase is meaningless if, essentially, the probability of it appearing in the language is zero, and it's meaningful otherwise. In this bitstring example, we are therefore declaring even-parity bitstrings to be the only meaningful expressions in this simple langauge of 0s and 1s.

probability distribution $\hat{\pi} \colon A^N \to \mathbb{R}$ by

$$\hat{\pi}(s) = \begin{cases} \frac{1}{N_T} & \text{if } s \in T, \\ 0 & \text{otherwise.} \end{cases}$$

Think of $\hat{\pi}$ as a rough approximation of the "true" probability distribution $\pi \colon A^N \to \mathbb{R}$ uniformly concentrated on the set of all even bitstrings, where $\pi(s) = 1/2^{N-1}$ if s is even and $\pi(s) = 0$ otherwise. In a real-world application, we would likely not know or have access to the target distribution π (suppose the elements of A were English words scraped from the Internet, for instance), and so the goal is to find a model for it. Of course we *do* know π exactly in this toy example, but let us suppose that we *don't* for the sake of illustrating the idea.

Then the first step in finding a model for π is the passage from sets to vector spaces outlined in Chapter 3. In particular, we start by representing the empirical distribution $\hat{\pi}$ as a pure quantum state. To do this, begin by letting $V = \mathbb{C}^A \cong \mathbb{C}^2$ be the two-dimensional vector space with basis vectors $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ so that every sequence $s \in T$ corresponds to a vector in $|s\rangle \in V^{\otimes N} \cong \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$. For example the sequence $00101 \in E_5$ maps to the basis vector $|0\rangle \otimes |0\rangle \otimes |1\rangle \otimes |0\rangle \otimes |1\rangle \in V^{\otimes 5}$. The probability distribution $\hat{\pi}$ therefore defines a unit vector in $V^{\otimes N}$ as the sum of all samples in T weighted by the square roots of their probabilities,

$$|\psi\rangle = \frac{1}{\sqrt{N_T}} \sum_{s \in T} |s\rangle. \tag{4.1}$$

The tensor network diagram for $|\psi\rangle$ is the following.

This vector serves as input for the algorithm that outputs a new vector $|\psi_{\text{MPS}}\rangle \in V^{\otimes N}$. As explained in the introduction, $|\psi_{\text{MPS}}\rangle$ will have the property that its coefficients define a probability distribution on A^N which is closer to the distribution for which $\hat{\pi}$ was merely an approximation; that is, $|\psi_{\text{MPS}}\rangle$ will satisfy the property that $|\langle s|\psi_{MPS}\rangle|^2 \approx \pi(s) = 1/2^{N-1}$ for all even bitstrings s. We also mentioned that $|\psi_{\text{MPS}}\rangle$ will turn out to be an MPS, which is a particular tensor network factorization of $|\psi\rangle$. Think of this as the higher-dimensional analogue to approximating a matrix by a truncated SVD. We won't need the details, but interested readers may see the references in Section 2.2.2 for more on MPS. In any case, the procedure to build $|\psi_{\text{MPS}}\rangle$ consists of N steps where the task in step

k is to construct the kth tensor of $|\psi_{\text{MPS}}\rangle$. Conveniently, we already wrote the instruction manual in Chapter 3. In step k we will define a reduced density operator whose eigenvectors assemble into the kth tensor of $|\psi_{\text{MPS}}\rangle$. Even better, the procedure is an inductive one. Steps $3, \ldots, N-1$ are all nearly identical to step 2.
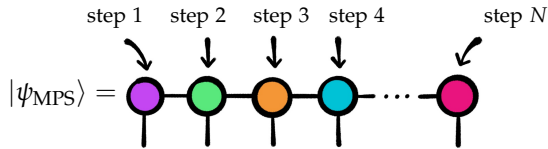
Figure 4.1: Building $|\psi_{\text{MPS}}\rangle$ by constructing each tensor individually

To streamline the discussion, we will only explain steps 1 and 2, being sure to share examples and intuition along the way. This abridged approach will equip interested readers to read through the original work in [BST20], which contains all of the details that we omit. So let's now proceed to describe the construction of the first two tensors of $|\psi_{\text{MPS}}\rangle$ in Figure 4.1.

4.1.2   A Bird's-Eye View

The first step is mostly a formality. Define the first tensor comprising $|\psi_{\text{MPS}}\rangle$ to be the identity operator id_V on $V = \mathbb{C}^2$. As an array, it is simply the 2×2 identity matrix, $\underline{}\bullet\underline{} = \left[\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right]$. The second step is much more interesting.

Step 2: Apply the Recipe in Chapter 3.

Let's now build the second tensor of $|\psi_{\text{MPS}}\rangle$ in Figure 4.1. Doing so requires a few steps. First, we start by "modifying" $|\psi\rangle$ by composing the first edge with the identity operator. Call this vector $|\psi_2\rangle$.
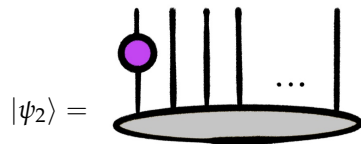
Here's how to understand $|\psi_2\rangle$ more carefully. Start with $|\psi\rangle \in V^{\otimes N}$ and reshape it into a linear map $M\colon V \to V^{\otimes N-1}$. Then precompose this map with the identity operator $M\,\text{id}_V\colon V \to V^{\otimes N-1}$ and reshape it back into a vector in $V^{\otimes N}$. This is the vector we're calling $|\psi_2\rangle$. See Figure 4.2.

$$|\psi\rangle = \quad\quad\quad\quad\quad\quad\quad\quad\quad = M$$

$$M\,\mathrm{id}_V = \quad\quad\quad\quad\quad\quad\quad\quad = |\psi_2\rangle$$

Figure 4.2: Obtaining the vector $|\psi_2\rangle$ from $|\psi\rangle$

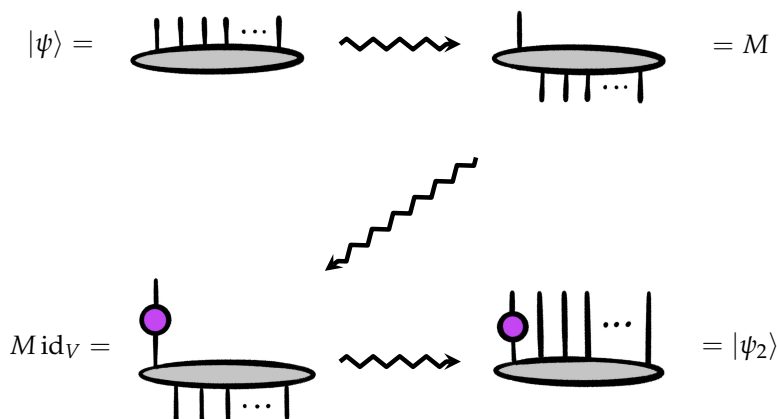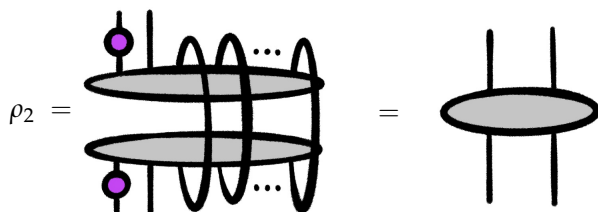Of course $|\psi_2\rangle = |\psi\rangle$ since composition with the identity changes nothing, but we have belabored this point because another version of it will appear soon. In any case, we are now in familiar territory. Consider the orthogonal projection operator $|\psi_2\rangle\langle\psi_2|\colon V^{\otimes N} \to V^{\otimes N}$ and apply the partial trace to the last $N-2$ factors.[1] This gives a reduced density operator $\rho_2 := \mathrm{tr}_{V^{\otimes N-2}}|\psi_2\rangle\langle\psi_2|\colon V \otimes V \to V \otimes V$.


$$\rho_2 = \quad\quad\quad\quad\quad =$$

Since ρ_2 is a density, it has a spectral decomposition $\rho_2 = UDU^\dagger$. The matrix D is 4×4 diagonal containing the eigenvalues of ρ_2, and U is a 4×4 unitary operator with the four eigenvectors of ρ_2 as its columns. In general ρ_2 will be full rank, but for reasons explained in Sidenotes 1 and 2 let us *drop* the eigenvectors associated to the two smallest eigenvalues.[2] Use the same letter U to denote the resulting 4×2 matrix. If W is the span of these top two eigenvectors, then we have a linear isometry $U\colon W \to V \otimes V$ whose adjoint is $U^\dagger\colon V \otimes V \to W$. Note that the 2×2 diagonal containing the two largest eigenvalues of ρ_2—let's also call it D—is an isomorphism of W.

[1] BEHIND THE SCENES. The reason we choose to trace out the last $N-2$ factors, as opposed to some other number, is due to an important practical point: We're dealing with high-dimensional linear algebra! The state $|\psi\rangle$ lives in a space that grows exponentially in N and orthogonal projection onto it is an operator on this space. Fully realizing it and trying to find a direct approximation won't be feasible. This motivates the use of *reduced* densities. Indeed, it's more manageable to work with operators on smaller subsystems, which can then give us knowledge of the whole. To do this, we are exploiting the fact that our data are *sequences*, which naturally gives us a way to subdivide the system into smaller ones.

[2] Resuming the conversation in Sidenote 1, we are forcing our reduced density to operate on a subsystem that is two-dimensional. (Example 4.1 will shed light on why the number *two* was chosen.) To borrow language from Section 2.5.1, the algorithm assumes $|\psi\rangle$ has low entanglement properties. To borrow language from machine learning, this is our *model hypothesis*.

The reason we keep the rank *low* is due to a hypothesis that is more philosophical than mathematical. It is the idea that data systems that arise in nature are not random but rather have underlying structure. For instance, natural language is not comprised of random sequences of characters—words have meaning! So the algorithm being described gives a way to summarize information in a structured dataset. In particular, the eigenvalues of ρ_2 stratify the importance of information in the subsystem on which it operators. By choosing to keep only the largest eigenvalues, we have control over how fine-tuned our summaries will be. For instance, dropping the smaller eigenvalues is akin to getting rid of sampling errors and thereby extracting the inherent meaning and structure beneath. As we'll see in Section 4.3, this allows one to learn interesting probability distributions extremely well from a remarkably small amount of samples.
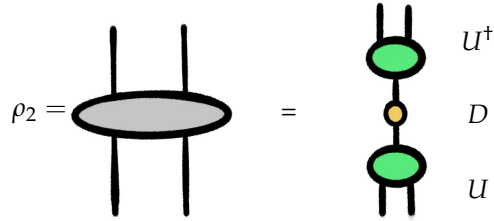
Now here's the point of step 2: we take U to be the *second* tensor comprising $|\psi_{\mathrm{MPS}}\rangle$.
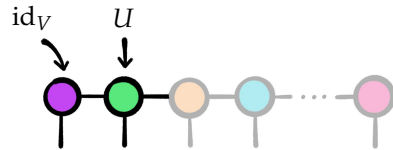
$$
\begin{array}{ccc}
V \otimes V & \xrightarrow{\rho_2} & V \otimes V \\
U^\dagger \downarrow & & \uparrow U \\
W & \xrightarrow{\;\;D\;\;} & W
\end{array}
$$

To understand what this means, think back to the initial vector $|\psi_2\rangle \in V^{\otimes N}$. We may define a *new* vector $|\psi_3\rangle$ by composing U with the first two edges of $|\psi_2\rangle$.
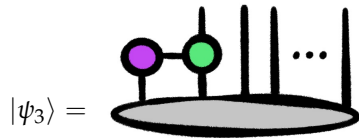
Said more carefully, start with $|\psi_2\rangle$ and view it as a linear mapping $M_2\colon V^{\otimes 2} \to V^{\otimes N-2}$, then precompose this mapping with U, then reshape the resulting composition $M_2 U\colon W \to V^{\otimes N-2}$ into the vector $|\psi_3\rangle \in W \otimes V^{\otimes N-2}$. See Figure 4.3.
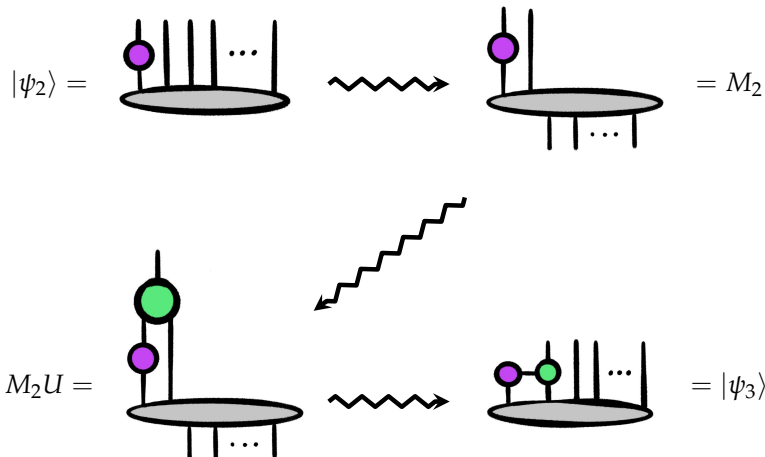
Figure 4.3: Obtaining the vector $|\psi_3\rangle$ from $|\psi_2\rangle$

Now you can see the MPS starting to form within the diagram associated to $|\psi_3\rangle$. This concludes step 2 of the algorithm.

PERHAPS NOW YOU have an idea of what step 3 will be. The similarities between Figure 4.2 and Figure 4.3 suggest the pattern. Let's quickly make the connection. Step 3 starts with the vector $|\psi_3\rangle$. The first two "sites" of $|\psi_3\rangle\langle\psi_3|$ remain untouched while the partial trace is applied to the remaining sites. This gives a reduced density operator ρ_3, whose spectral decomposition is $\rho_3 = U_3 D_3 U_3^\dagger$
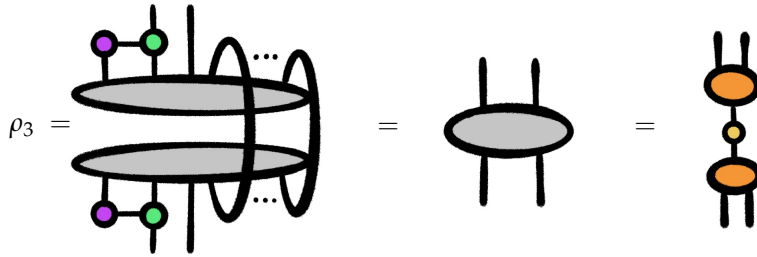
We take U_3 to be the 4×2 array whose two columns are the two eigenvectors of ρ_3 associated to its two largest eigenvalues. This forms the third tensor of $|\psi_{\mathrm{MPS}}\rangle$. It also tells us how to define the vector $|\psi_4\rangle$ that initiates step 4, which leads to U_4, and so on. See Figure 4.4.
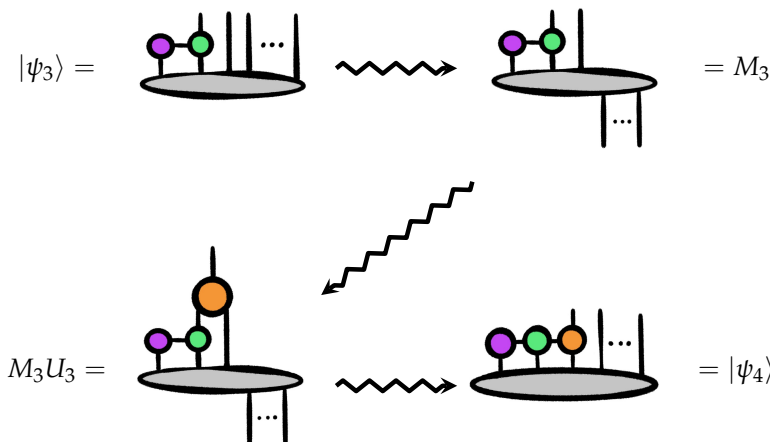
Figure 4.4: Obtaining the vector $|\psi_4\rangle$ from $|\psi_3\rangle$

Continuing the pattern at each step, the upshot is that the arrays of eigenvectors $U = U_2, U_3, \ldots, U_N$ assemble into the desired vector $|\psi_{\mathrm{MPS}}\rangle$.
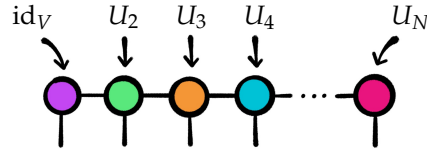
The claim is that $|\psi_{\text{MPS}}\rangle$ has the property that the distribution induced by the Born rule is close to the true uniform distribution on even-parity bitstrings, $|\langle s|\psi MPS\rangle|^2 \approx 1/2^{N-1}$, for which the empirical probabilities $\hat{\pi}(s) = 1/N_T$ were merely an approximation. Let's now discuss the intuition for *why* this is so, and then we'll report experimental results that illustrate the claim.

4.2 Intuition: Why Does This Work?

Intuition is gained through an example. Let's take a closer inspection at the eigenvectors of the reduced density operator ρ_2 obtained in step 2 by working with a simple example.

Example 4.1. Fix $N = 5$ and suppose the training set contains the *entire* set of even-parity bitstrings, $T = E_N$. The goal for this example is to compute the eigenvectors of ρ_2 explicitly. So first we'll need to find the matrix representation of ρ_2. To do so, recall that the procedure described in Section 4.1.2 distinguished between the first two bits of a sample, and the remaining $N - 2$ bits. In light of this, let's think of every even-parity bitstring $s \in T$ as a prefix-suffix pair $s = (x, y)$, where $x \in A^2$ is a bitstring of length 2 and $y \in A^3$ is a bitstring of length 3. Since s must have even parity, $(x, y) \in T$ if and only if x and y both have the same parity. There is a nice way to represent T visually—it corresponds to a bipartite graph. The sets of prefixes and suffixes define the two sets of vertices, and there is an edge joining x and y if and only if their concatenation xy is even. For example, the training set $T = E_5$ is illustrated by the following graph.
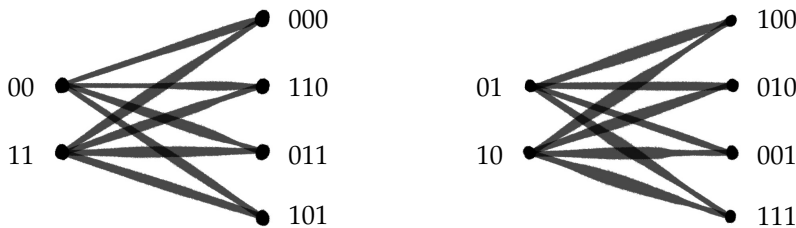
The graph has two disconnected components because there is no sample (x, y) in T where x and y have different parity. For example, there is no edge joining 00 and 111. So the left component of the graph contains all *even-even* prefix-suffix pairs, while the right

component contains all *odd-odd* prefix-suffix pairs. Now recall from Section 3.2 that the entries of reduced density operators defined by such a graph may be read off directly *from* the graph. To be clear, ρ_2 is an operator on the prefix subsystem $V \otimes V$, a four-dimensional space whose bases are the four bitstrings of length two, $|00\rangle, |11\rangle, |01\rangle$ and $|01\rangle$. As a 4×4 matrix, the rows and columns of ρ_2 correspond to these four prefixes. Choosing the ordering $A^2 = \{00, 11, 01, 10\}$ we may write ρ_2 as

$$\rho_2 \;=\; \begin{array}{c c} & \begin{array}{cccc} {\scriptstyle 00} & {\scriptstyle 11} & {\scriptstyle 01} & {\scriptstyle 10} \end{array} \\ \begin{array}{c} {\scriptstyle 00} \\ {\scriptstyle 11} \\ {\scriptstyle 01} \\ {\scriptstyle 10} \end{array} & \begin{bmatrix} \deg 00 & s_e & 0 & 0 \\ s_e & \deg 11 & 0 & 0 \\ 0 & 0 & \deg 01 & s_o \\ 0 & 0 & s_o & \deg 10 \end{bmatrix} \end{array} \frac{1}{2^4} \;=\; \frac{1}{2^4} \begin{bmatrix} 4 & 4 & 0 & 0 \\ 4 & 4 & 0 & 0 \\ 0 & 0 & 4 & 4 \\ 0 & 0 & 4 & 4 \end{bmatrix}$$

The diagonal entries are the degrees of the four prefixes. The off diagonal s_e is the number of suffixes that the even prefixes 00 and 11 have in common. It is also the number of paths of length two that join 00 and 11, and is equivalently the number of suffixes with degree 2 in the graph's left component. The off-diagonal s_o is likewise the number of suffixes that the odd prefixes 01 and 10 have in common, which is the number of paths of length two that join 01 and 10, which also is the number of degree two suffixes in the graph's right component. The matrix is normalized by the total number of edges in the graph, 2^4, which guarantees that ρ_2 has trace 1. So the nonzero entries of ρ_2 are all equal to $4/2^4$. It is therefore a rank 2 operator, and each nonzero 2×2 block contributes one eigenvalue and one eigenvector. Both eigenvalues are $\frac{1}{2}$. The eigenvector from the first block is the normalized sum of even-parity bitstrings of length 2, let's call it $|E_2\rangle$.

$$|E_2\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix}^\top$$

The second eigenvector is the normalized sum of odd-parity bitstrings of length 2, let's call it $|O_2\rangle$.

$$|O_2\rangle = \frac{|01\rangle + |01\rangle}{\sqrt{2}} = \begin{bmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}^\top$$

These two eigenvectors capture the two "concepts" that exist in our simple bitstring language—evenness and oddness! Moreover, they are precisely the two[3] columns in the matrix U obtained in the spec-

BEHIND THE SCENES. By choosing the ordering $A^2 = \{00, 11, 01, 10\}$ I am associating the ith element to the ith standard basis vector in $\mathbb{C}^2 \otimes \mathbb{C}^2 \cong \mathbb{C}^4$. So $|00\rangle := \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^\top$ and $|11\rangle := \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^\top$ and so on. This does not match with the convention that $|ab\rangle = |a\rangle \otimes |b\rangle$ since, for instance, $|11\rangle$ would be $|1\rangle \otimes |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ which gives $\begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^\top$. We've temporarily suspended this convention and are sticking with the choice above for the purpose of sharing intuition. With this choice, the two blocks in ρ_2 correspond to the two components of the graph, which is nice!

[3] We refer to "the two" columns since D is really a 4×4 diagonal, but the third and fourth diagonal entries are both 0, and so the third and fourth columns of U are "zeroed out."

tral decomposition of $\rho_2 = UDU^\dagger$.

$$\rho_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

To gain further intuition, let's turn our attention to the adjoint of U. Let W denote the two-dimensional space spanned by $|E_2\rangle$ and $|O_2\rangle$ and observe that the linear mapping $U^\dagger \colon V \otimes V \to W$ acts as a "summarizer." It maps each prefix onto its parity.

$$U^\dagger |00\rangle = \tfrac{1}{\sqrt{2}}|0\rangle \quad \text{(even)} \qquad U^\dagger |01\rangle = \tfrac{1}{\sqrt{2}}|1\rangle \quad \text{(odd)}$$

$$U^\dagger |11\rangle = \tfrac{1}{\sqrt{2}}|0\rangle \quad \text{(even)} \qquad U^\dagger |10\rangle = \tfrac{1}{\sqrt{2}}|1\rangle \quad \text{(odd)}$$

The essential observation is two-fold:

First, $|00\rangle$ and $|11\rangle$ have the same image under $U^\dagger$. *This captures the idea that* 00 *and* 11 *always share the same suffixes in the dataset* T, namely those with even parity.

Likewise, $|01\rangle$ and $|10\rangle$ also have the same image under $U^\dagger$. *This captures the fact that* 01 *and* 10 *always share the same suffixes in* T, namely those with odd parity.

The point is that $U^\dagger$ summarizes the prefixes while knowing information about which suffixes they can be paired with. This feature is precisely that which was emphasized in Chapter 3: *Eigenvectors of reduced densities of pure entangled states capture information about complementary subsystems.*[4] It's precisely this information that's lost when marginalizing to subsystems in the classical way—recall Takeaway 5 and the motivating example in Section 2.1.2.

Let us take this a step further by making the connection with tensor network diagrams. Note that the 2×4 matrix representing $U^\dagger \colon V \otimes V \to W$ can be reshaped into a $2 \times 2 \times 2$ tensor of order three, which is essentially $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$ stacked next to $\frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$. Schematically, we have this picture.

[4] There's a second half to this statement, namely that *the information stored in the eigenvectors can be pieced together to reconstruct the full state.* We will circle back to this point at the end of the chapter.
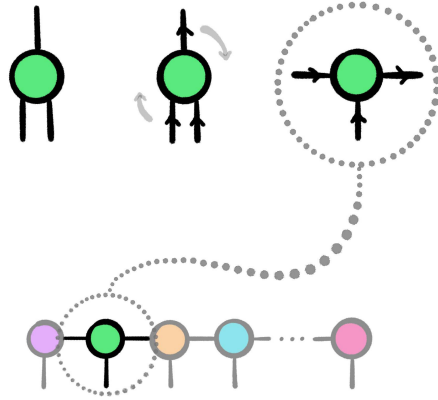
In this way, we can envision the green tensor as a machine. It receives a pair of incoming bits and outputs the parity of their concatenation.[5] In fact, the remaining tensors comprising $|\psi_{\text{MPS}}\rangle$ all behave in the same way.

THIS EXAMPLE ILLUSTRATES the general idea. A typical dataset T will not include all of the bitstrings in E_N, and so ρ_2 will likely be full rank. Fortunately, we can still understand its matrix entries explicitly in terms of a graph, and we still collect its top two eigenvectors $|E_2'\rangle$ and $|O_2'\rangle$ associated to its two largest eigenvalues. Concretely, we may write the reduced density ρ_2 as

$$\rho_2 = \frac{1}{N_T} \begin{bmatrix} d_1 & s_e & 0 & 0 \\ s_3 & d_2 & 0 & 0 \\ 0 & 0 & d_3 & s_o \\ 0 & 0 & s_o & d_4 \end{bmatrix}$$

As a simple example with $N = 5$, the graph below is associated to a seven-sample set.

The number of training samples $N_T = |T|$ is the total number of edges in the graph, and the matrix entries are nonnegative integers that have combinatorial interpretations. The diagonal entries count degrees of prefixes, and the off-diagonals count the number of paths of length two in each component of the graph.
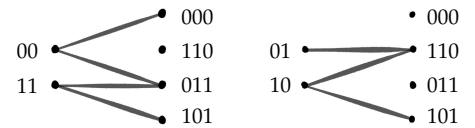
When $|\psi\rangle \in V^{\otimes 5}$ is the weighted sum of these seven samples, the resulting reduced density on the prefix subsystem is

$$\rho_2 = \text{tr}_{V^{\otimes 3}} |\psi\rangle\langle\psi| = \frac{1}{7} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

d_1 is the degree of 00	s_e is the number of suffixes that
d_2 is the degree of 11	00 and 11 have in common
d_3 is the degree of 01	s_o is the number of suffixes that
d_4 is the degree of 10	01 and 10 have in common

The two eigenvectors $|E_2'\rangle$ and $|O_2'\rangle$ associated to the two largest eigenvalues of ρ_2 therefore have explicit expressions in terms of the graph's information. Concretely, we may write $|E_2'\rangle = \begin{bmatrix} \cos\theta & \sin\theta & 0 & 0 \end{bmatrix}^\top$ and $|O_2'\rangle = \begin{bmatrix} 0 & 0 & \cos\phi & \sin\phi \end{bmatrix}^\top$ where θ and ϕ are angles defined explicitly in terms of the combinatorics of the graph.[6] In the trun-

cated spectral decomposition $\rho_2 = UDU^\dagger$, the 2×4 matrix $U^\dagger$ has $|E_2'\rangle$ and $|O_2'\rangle$ as its two rows. It therefore acts as an *imperfect* summarizer. The error—or deviation from perfection—is measured by the values θ and ϕ. For instance, if $\theta = \phi = \pi/4$, then we recover the ideal eigenvectors $|E_2'\rangle = |E_2\rangle$ and $|O_2'\rangle = |O_2\rangle$, and in that case $U^\dagger$ is a perfect summarizer as in Example 4.1.

As it turns out, *every* tensor comprising $|\psi_{\text{MPS}}\rangle$ (with the minor exception of the first and last[7]) behaves like the summarizer described here. That is, at step k we collect a tensor U_k built from eigenvectors $|E_k'\rangle$ and $|O_k'\rangle$ whose entries are determined by angles θ_k and ϕ_k that are read off explicitly from the combinatorics of a bipartite graph associated to the training set T. With this, we have a theoretical understanding of $|\psi_{\text{MPS}}\rangle$ both at a low level—the tensors can be understood entry-wise—and at a high level—the tensors are eigenvectors of reduced densities, which harness prefix-suffix interactions.

As a closing remark, know that Example 4.1 showcased the *idealized* scenario where each tensor is a perfect summarizer. When this happens (that is, when every $U_k^\dagger$ maps a small bitstring onto its parity) one finds that $|\psi_{\text{MPS}}\rangle$ is *equal* to the normalized sum of all even bitstrings of length N,

$$|E_N\rangle = \frac{1}{\sqrt{2^{N-1}}} \sum_{s \text{ even}} |s\rangle.$$

This is the this best-case scenario, for the probability of any even bitstring s is given by $|\langle s|\psi_{\text{MPS}}\rangle|^2 = |\langle s|E_N\rangle|^2 = 1/2^{N-1}$, which is the target probability $\pi(s)$ identified at the opening of this section. Situations that are less than ideal will not have equality $|\psi_{\text{MPS}}\rangle \neq |E_N\rangle$, but the inner product $\langle E_N|\psi_{\text{MPS}}\rangle$ (or some expression involving it) serves a measure of how close the model $|\psi_{\text{MPS}}\rangle$ is to the goal $|E_N\rangle$. As a teaser, here's a summary of an experiment that illustrates this.

4.3   The Experiment

As a concrete experiment, we worked with bitstrings of length $N = 16$. We built a theoretical vector $|\psi_{\text{MPS}}\rangle$ as described in Section 4.1.2 and compared it to an *experimental* version built with the algorithm using the ITensor library [Lib]; the code is available on Github.[8] For a fixed fraction $0 < f \leq 0.2$, the experimental model was built by running the algorithm on ten different datasets T, each containing $N_T = f2^{N-1}$ bitstrings of length 16. We then compared the resulting vector $|\psi_{\text{MPS}}\rangle$ with the target vector $|E_N\rangle$ by computing

[7] The first tensor is the identity map, as we previously described. To understand the last tensor, recall the procedure described in Section 4.1.2, and observe that the final vector $|\psi_N\rangle$ can be reshaped into a map between a 2-dimensional space (the span of the top two eigenvectors of ρ_{N-1}) and another 2-dimensional space, $V \cong \mathbb{C}^A$. We take this mapping to be the final MPS tensor.

$$|\psi_N\rangle =$$
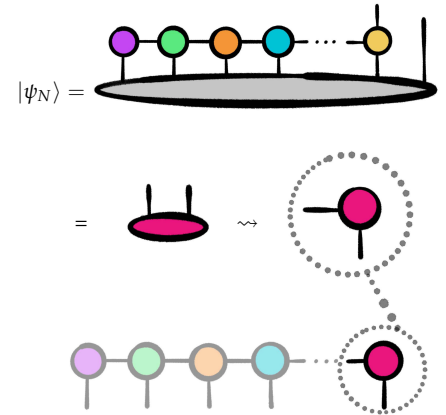
the Bhattacharyya distance[9] between them. The x-axis in Figure 4.5 is the range of fractions $0 < f \leq 0.2$, and the Bhattacharyya distances are plotted vertically. Figure 4.6 gives a zoomed-in look for $.15 \leq f \leq 0.2$. In both figures, each black dot represents one of these values, and the pink curve is their experimental average. The green curve is our theoretical prediction using the mathematics described above.[10]

[9] The Bhattacharyya distance is a measure between two probability distributions, computed as the negative log of their "inner product." That is, suppose $p, q \colon S \to \mathbb{R}$ are probability distributions on a finite set S. The **Bhattacharyya distance** between them is $d_B(p,q) := -\ln\left(\sum_s \sqrt{p(s)q(s)}\right)$. When $p(s) = |\langle s|\psi_{\mathrm{MPS}}\rangle|^2$ and $q(s) = |\langle s|E_N\rangle|^2$ then $d_B(p,q) = -\ln\langle\psi_{\mathrm{MPS}}|E_N\rangle$.

[10] Obtaining the green curve is not an elementary calculation, and the story behind it is quite interesting. It involves understanding the entries of a number of reduced densities, $\rho_3, \rho_4, \ldots, \rho_N$, similar to the one shown in Example 4.1. As it turns out, this task is rather complicated, so instead of calculating the entries *exactly*, we instead find estimates for their expected values. The angles θ_k and ϕ_k that were mentioned in the main text play a role in finding these values. These expected entries then contribute to the expected eigenvectors of the operators, and these eigenvectors are used to find the green curve.

Figure 4.5: The experimental average (pink) and theoretical prediction (green).
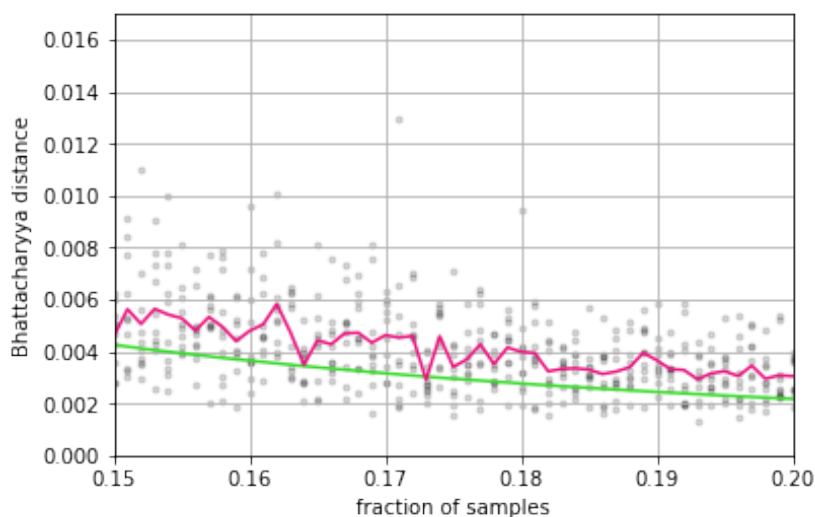
Figure 4.6: Taking a closer look for $.15 \leq f \leq 0.2$.

Notice that experiment (pink) and theory (green) go hand-in-hand, as the two curves grow closer together at the end. Hence we can predict how good the model $|\psi_{\text{MPS}}\rangle$ will be just given the fraction f of samples used to train it. The plots tend *downward* as one would expect: the more samples used, the better the model will be. Remarkably, the model does quite well training with just 2.5%! In other words, with just a small fraction of training samples, the model state $|\psi_{\text{MPS}}\rangle$ is quite close to the true state $|E_N\rangle$.

THIS EXPERIMENT IS THUS an instantiation of the theory illustrated in Figure 2.2 and summarized in Takeaway 3 of Chapter 2. Succinctly put, the eigenvectors of reduced densities harness interactions between small subsystems (here, prefix-suffix subsystems), and this information can be pieced together to reconstruct the state (or a close approximation of it) of the full system. Here's the takeaway.

Takeaway 6. *Reduced densities of pure entangled states harness information about interactions between subsystems. When those subsystems are sequences (that is, a one-dimensional string of "particles"), knowledge about the state of a subsystem and its complement can be pieced together to reconstruct the state of the whole.*

5
Fixed Points, Categorically

When you see the same
beautiful idea pop up
everywhere, you begin to
think that it is pointing to
some deeper truth you haven't
yet grasped.

Francis Su [Su20]

CHAPTER 1 MOTIVATED the investigation of eigenvectors of reduced
densities by drawing an analogy with formal concepts—an analogy
that was revisited in Section 3.3. This chapter aims to put that anal-
ogy on firmer categorical ground. To do so, we will introduce a *third*
construction—a categorical one—that is parallel to both formal con-
cepts and eigenvectors. The category theory will specialize to give
formal concepts in a certain case. It will not specialize to the linear
algebra, but there is a clear, common categorical thread connecting
them, which will be discussed at the end of the chapter.

This chapter assumes familiarity with
the basics of category theory (cate-
gories, functors, natural transforma-
tions, (co)limits, and adjunctions),
though I'll occasionally provide extra
commentary for interested readers.
For thorough introductions, see [Rie17,
Lei14, Awo10, Lan13, Spi14, FS19].
For a lighter treatment of the basics
of category theory, see the articles on
Math3ma, under the "Category Theory"
tag [Bra].

Here is an overview of the ideas to come. We will consider three
familiar mathematical objects: a vector space with basis set X, the
power set of a set X, and the category of presheaves on a small cate-
gory C.

$$\mathbb{C}^X \qquad 2^X \qquad \mathsf{Set}^{\mathsf{C^{op}}}$$

These three objects are related in that all are "free" in a sense that
can be made precise. Moreover, all three fit into a construction that is
strikingly similar to that featured in Chapter 1. To recall, any matrix
M corresponds to a function $M\colon X \times Y \to \mathbb{C}$ where X and Y are finite
sets. The matrix represents a linear map $M\colon \mathbb{C}^X \to \mathbb{C}^Y$, which has an
adjoint going in the other direction $M^\dagger\colon \mathbb{C}^Y \to \mathbb{C}^X$. The eigenvectors
of $M^\dagger M$ and $MM^\dagger$ capture interesting information about the values
$M(i,j)$, especially when they determine a probability distribution on

$X \times Y$. Interestingly, a nearly identical story holds when the complex numbers $\mathbb{C}$ are exchanged for the poset 2 of *truth values* (which we define later) or for the category Set. In this chapter we will carefully unwind this claim.

We start in Section 5.1 by recalling the universal property of a free vector space on a set and will use it to recast the elementary linear algebra of Section 1.2 in a categorical light. Section 5.2 discusses another free object with a very similar universal property: the free (co)completion of a category. Unwinding the theory, one finds a number of strong analogies with linear algebra and a clear dictionary between the two worlds. In particular, we will see that categorical version of a matrix $M\colon X \times Y \to \mathbb{C}$ is a functor $R\colon \mathsf{C}^{\mathrm{op}} \times \mathsf{D} \to \mathsf{Set}$; the categorical version of adjoint linear maps $\mathbb{C}^X \rightleftarrows \mathbb{C}^Y$ is an adjunction between (co)presheaf categories $\mathsf{Set}^{\mathsf{C}^{\mathrm{op}}} \rightleftarrows (\mathsf{Set}^{\mathsf{D}})^{\mathrm{op}}$; and the categorical version of eigenvectors is a generalized *Isbell completion*. Section 5.3 specializes this to the setting of *enriched category theory* by replacing Set with the poset (category) of truth values 2. A functor is then a relation $R\colon X \times Y \to 2$; the free (co)completion of a set, viewed as a discrete category, is the free join/meet semilattice on that set; the adjunction between (co)presheaf categories becomes an adjunction of join/meet-preserving maps $2^{X^{\mathrm{op}}} \rightleftarrows (2^Y)^{\mathrm{op}}$; and the generalized Isbell completion gives formal concepts.

Recall that an **adjunction** consists of a pair of functors $F\colon \mathsf{C} \rightleftarrows \mathsf{D} \colon G$ such that there is a natural isomorphism of hom sets

$$\mathsf{C}(Fc, d) \cong \mathsf{D}(c, Gd)$$

for all objects c in C and d in D. Equivalently, an adjunction consists of functors F and G together with natural transformations $\eta\colon \mathrm{id}_{\mathsf{C}} \Rightarrow GF$, called the **unit**, and $\epsilon\colon FG \Rightarrow \mathrm{id}_{\mathsf{D}}$, called the **counit**, such that the following diagrams commute

$$
\begin{array}{ccc}
F \xrightarrow{F \circ \eta} FGF & \quad & G \xrightarrow{\eta \circ G} GFG \\
{\scriptstyle \mathrm{id}_F} \searrow \;\; \big\downarrow{\scriptstyle \epsilon \circ F} & \quad & {\scriptstyle \mathrm{id}_G} \searrow \;\; \big\downarrow{\scriptstyle G \circ \epsilon} \\
F & \quad & G
\end{array}
$$

Here $F \circ \eta$ denotes the natural transformation whose components are of the form $F(\eta_c)\colon F(c) \to FGF(c)$, for each object c in C, and similarly for the others.

Section 5.1	**Section 5.2**	**Section 5.3**
LINEAR ALGEBRA	CATEGORY THEORY	ENRICHED CATEGORY THEORY
eigenvectors of reduced densities	generalized Isbell completion	formal concepts

Sections 5.1, 5.2, and 5.3 are meant to feel repetitious. All three are essentially the same story told in different contexts, the motif being that *fixed points of the composition of a morphism with its "adjoint" are interesting.* Section 5.4 closes with a remark on the category theory that summarizes this. Here's a quick note on notation. As seen already, sans serif is used for categories C. Also $\mathsf{C}(c, c')$ is used to denote the hom set of morphisms from an object c to an object c' in C. Given categories C and D, a pair of adjoint functors will be denoted by $F\colon \mathsf{C} \rightleftarrows \mathsf{D}\colon G$ or by $F \dashv G$.

5.1   Revisiting Eigenvectors

The motivating construction was already presented in Section 1.2, but think of that as the appetizer. In this section, we revisit the elementary linear algebra, this time being mindful of the category theory

behind the scenes. To start, let Vect be the category of complex vector spaces and linear transformations, and let Set be the category of sets and functions. There is a free-forgetful adjunction

$$U\colon \mathsf{Vect} \rightleftarrows \mathsf{Set}\colon F.$$

The functor $U\colon \mathsf{Vect} \to \mathsf{Set}$ associates to any vector space V its underlying set UV. The functor $F\colon \mathsf{Set} \to \mathsf{Vect}$ associates to a set X the free vector space FX on X. It is "free" in that the unit natural transformation $\eta\colon \mathrm{id}_{\mathsf{Set}} \Longrightarrow UF$ of this adjunction fits into the following familiar universal property.

Universal Property for Vector Spaces. The *free vector space on a set* X is a vector space FX with the property that for any vector space W and for any function $f\colon X \to UW$ there is a unique linear map $\hat{f}\colon FX \to W$ so that the following diagram commutes

$$
\begin{array}{ccc}
UFX & \xdashrightarrow{\;U\hat{f}\;} & UW \\
{\scriptstyle \eta_X}\big\uparrow & \nearrow & \\
X & \raise6pt{\scriptstyle f} &
\end{array}
$$

Concretely, FX is the vector space whose basis is X. A vector in FX is then a complex-valued function v on X with the property that $v(x) \neq 0$ for finitely many $x \in X$. The formal sum

$$|v\rangle := \sum_x v(x)x \tag{5.1}$$

is then guaranteed to be finite and may be thought of as the vector $|v\rangle$. If X is finite, then vectors in FX may be identified with *all* functions from X. In either case, the function η_X associates to an element $x \in X$ the independent basis vector $|x\rangle$, and the space FX is sometimes denoted $\mathbb{C}^X$. On any vector $|v\rangle = \sum_x v(x)|x\rangle$ in FX the unique lift of any function $f\colon X \to UW$ is defined by

$$\hat{f}|v\rangle = \sum_x v(x)f(x). \tag{5.2}$$

Oftentimes, the Us are omitted from the diagram and one sees the following.

$$
\begin{array}{ccc}
\mathbb{C}^X & \xdashrightarrow{\;\hat{f}\;} & W \\
{\scriptstyle \eta_X}\big\uparrow & \nearrow & \\
X & \raise6pt{\scriptstyle f} &
\end{array}
$$

But this is not the best practice. The above diagram is not in the correct—or in any!—category. For example, the domain of $f\colon X \to W$ is a set while its codomain is a vector space. The diagrams in Takeaway 2 also suffered from this ambiguity. Going forward, let's avoid

this imprecision. Instead we'll always have in mind the adjunction $U\colon \mathsf{Vect} \rightleftarrows \mathsf{Set}\colon F$ and insert a "U" where appropriate. Let's also avoid writing "$FX = \mathbb{C}^X$." As noted earlier, vectors in FX may be identified with finitely supported functions $X \to \mathbb{C}$, which explains the convenient exponential notation $\mathbb{C}^X$. But we must be careful. The phrase "a function $X \to \mathbb{C}$" has the same problem mentioned above. On one hand, X is a set; on the other hand, $\mathbb{C}$ is a vector space. An arrow $X \to \mathbb{C}$ is not a morphism in any category, and the exponential $\mathbb{C}^X$ of a vector space by a set is not an object in any category. Rather, here's the better observation: the *underlying set* of the free vector space on X coincides with functions $X \to U\mathbb{C}$. This is summarized in the following takeaway.

Takeaway 7. *Given the free-forgetful adjunction $U\colon \mathsf{Vect} \rightleftarrows \mathsf{Set}\colon F$, the free vector space FX on a set X has the property that*

$$UFX = U\mathbb{C}^X, \tag{5.3}$$

where $U\mathbb{C}^X$ denotes the set of "finite" functions $X \to U\mathbb{C}$, which is all function if X is finite or finitely-supported functions otherwise. In short, the adjunction $F \dashv U$ has the property that there is a special object in Vect, namely $\mathbb{C}$, such that all free vector spaces are, in some sense, built up from it.

Now we are close to rediscovering Takeaway 2 in Chapter 1. Suppose X and Y are finite sets and consider any function $M\colon X \times Y \to U\mathbb{C}$. The category of sets is Cartesian closed, and so we have a product-hom adjunction and hence the following bijections.

$$\mathsf{Set}(X, U\mathbb{C}^Y) \qquad \cong \qquad \mathsf{Set}(X \times Y, U\mathbb{C}) \qquad \cong \qquad \mathsf{Set}(Y, U\mathbb{C}^X)$$
$$\alpha \longleftarrow\!\!\dashv M \vdash\!\!\longrightarrow \beta$$

Under this adjunction, the function $\alpha\colon X \to U\mathbb{C}^Y$ is defined on each $x \in X$ by $\alpha x(y) = M(x, y)$. Likewise define the function $\beta\colon Y \to U\mathbb{C}^X$ on each $y \in Y$ by $\beta y(x) = \overline{M(x, y)}$. By the universal property for vector spaces, α lifts uniquely to a linear map $M\colon FX \to FY$, and β lifts uniquely to a linear map $M^\dagger\colon FY \to FX$ so that the following diagrams commute.

> A category C is called **Cartesian closed** if for every pair of objects x and z there is an object z^x in C so that for all objects y there is a natural bijection
>
> $$\mathsf{C}(x \times y, z) \cong \mathsf{C}(y, z^x)$$
>
> The object z^x is called the **internal hom** and should be thought of as a C's worth of morphisms from x to z.

$$
\begin{array}{cc}
\begin{array}{c}
U\mathbb{C}^X \xdashrightarrow{UM} U\mathbb{C}^Y \\
\uparrow \quad \nearrow{\scriptstyle \alpha} \\
X
\end{array}
&
\begin{array}{c}
U\mathbb{C}^Y \xdashrightarrow{UM^\dagger} U\mathbb{C}^X \\
\uparrow \quad \nearrow{\scriptstyle \beta} \\
Y
\end{array}
\end{array}
\tag{5.4}
$$

What's more, M and $M^\dagger$ are linear adjoints so that

$$\langle Mv, w \rangle = \langle v, M^\dagger w \rangle \qquad \text{for all } v \in FX \text{ and } w \in FY. \tag{5.5}$$

If we drop the "Us" from the diagrams, then we recover the contents of Takeaway 2. When the function $M\colon X \times Y \to U\mathbb{C}$ further satisfies the condition that $\sum_{x,y} |M(x,y)|^2 = 1$, then it represents a pure quantum state in $FX \otimes FY$, and we've shown in detail in Chapter 3 that the eigenvectors of the reduced density operators $MM^\dagger$ and $M^\dagger M$ harness valuable information from that state.

These ideas, though elementary, set the stage for the remainder of this chapter. Here are the key points to have in mind. We started with the free-forgetful adjunction $U\colon \text{Vect} \rightleftarrows \text{Set}\colon F$ and observed that Vect contains a special object, namely $\mathbb{C}$, with the property that the free space FX on a set X always "looks like" functions from X to $U\mathbb{C}$. As a result, every function $X \times Y \to U\mathbb{C}$ gives rise to a pair of adjoint maps $M\colon FX \rightleftarrows FY\colon M^\dagger$, whose composites $M^\dagger M$ and $MM^\dagger$ have interesting fixed points.[1] This very same template will reappear in Section 5.2 and again in Section 5.3. More precisely, the idea that "fixed points of a map with its adjoint are interesting" is strikingly similar to a known scenario in category theory—there is nearly a word-for-word analogy between the two. Even better, the categorical version recovers the formal concept construction in Section 1.1 as a special case. Let's discuss this category theory now.

[1] That is, they have interesting *eigenvectors*. So we may restate our claim is, "The one-dimensional invariant subspaces of $M^\dagger M$ and $MM^\dagger$ are interesting."

5.2   Free (Co)Completions

To construct the free vector space on a set X, we added all formal sums of elements in X. Category theory generalizes sums through **colimits**, and it generalizes multiplication through **limits**. We refer to any basic text for the formal definitions [Rie17]. But here are three *informal* things to know.

1. **Intuition.** Colimits and limits subsume many constructions in mathematics. Unions of sets and joins in a poset are two examples of colimits. Cartesian products of sets and meets in a poset are two examples of limits. Informally, colimits have a "glue-y" feel to them, whereas limits have an "equation-y" feel to them.

2. **Vocabulary.** One always takes the (co)limit *of* something. That "something" is a **diagram** in a category C, which is synonymous with a functor whose codomain is C. The diagram is called **small** if the domain of the functor is a small category. (See the next bullet.) A category is called **cocomplete** if it contains colimits of all small diagrams; it is called **complete** if it contains limits of all small diagrams.

3. **More Vocabulary.** A category is called **small** if the morphisms of the category form a set. It is called **locally small** if the morphisms

between any two objects form a set. As an example, the category
with two objects and a single nonidentity arrow $\bullet \rightarrow \bullet$ is small
and hence locally small, whereas Set is locally small but not small.

As IN THE LINEAR algebra of Section 5.1, the starting ingredient
for this section is an adjunction. Let CAT denote the category whose
objects are locally small categories and whose morphisms are func-
tors. Let CocompCAT denote the category of locally small cocomplete
categories and cocontinuous functors between them.[2] Both CAT and
CocompCAT are actually 2-categories; that is, there are morphisms
(natural transformations) between the morphisms (functors). There is
a free-forgetful "adjunction" between these 2-categories.

$$U \colon \mathsf{CocompCAT} \rightleftharpoons \mathsf{CAT} \colon F.$$

The functor $U \colon \mathsf{CocompCAT} \rightarrow \mathsf{CAT}$ associates to any locally small
cocomplete category D its underlying category $U\mathsf{D}$. The functor
$F \colon \mathsf{CAT} \rightarrow \mathsf{CocompCAT}$ associates to a locally small category C the
free cocomplete category $F\mathsf{C}$ on C. The setup here isn't quite an
adjunction in the usual sense, as 2-categorical considerations pre-
vent it from being so. Instead, it is called a **biadjunction**, which is
the appropriate notion of adjunctions in this higher-categorical set-
ting. But here's the main idea for us: just as every set gives rise to a
free vector space, so every category C gives rise to a free cocomplete
category $F\mathsf{C}$ [DL07, KL00, nLa20c]. Crucially, $F\mathsf{C}$ is free in that unit
$\eta \colon \mathrm{id}_{\mathsf{CAT}} \implies UF$ of the biadjunction has the following universal
property.

Universal Property for the Free Cocompletion of a Category. The
free cocompletion of a category C is a cocomplete category $F\mathsf{C}$ with the
property that for any other cocomplete category D and for any func-
tor $f \colon \mathsf{C} \rightarrow U\mathsf{D}$, there is a unique cocontinuous functor $\hat{f} \colon F\mathsf{C} \rightarrow \mathsf{D}$ so
that the following diagram commutes up to natural isomorphism.

$$U F\mathsf{C} \xdashrightarrow{U\hat{f}} U\mathsf{D}$$
$$\eta_{\mathsf{C}} \uparrow \quad \nearrow f$$
$$\mathsf{C}$$

Let's unwind this statement. First, the category $F\mathsf{C}$ has a familiar
construction. If C is small, then its free cocompletion is the category
of all contravariant functors from C to Set, also called **presheaves**
[DL07]. It is typically written as[3]

$$F\mathsf{C} = \mathsf{Set}^{\mathsf{C}^{\mathrm{op}}}.$$

If the category C is *not* small, then the construction of $F\mathsf{C}$ needs a mi-
nor adjustment, which will be explained shortly. But first, know that

[2] A functor is said to be **cocontinuous** if
it takes colimits to colimits.

[3] Every category C has an **opposite cat-
egory** C^{op} whose objects are the same
as the objects in C. A morphism $c \rightarrow c'$
in C^{op} is defined to be a morphism
$c' \rightarrow c$ in C. As a result, for any cate-
gory D, a contravariant functor $\mathsf{C} \rightarrow \mathsf{D}$
is a functor $\mathsf{C}^{\mathrm{op}} \rightarrow \mathsf{D}$.

the unit $\eta_C \colon C \to UFC$ of the biadjunction is the **Yoneda embedding** $c \mapsto C(-,c)$. Oftentimes the "U"s are omitted from the diagram and one typically sees

$$
\begin{array}{ccc}
\mathsf{Set}^{C^{\mathrm{op}}} & \dashrightarrow^{\hat{f}} & D \\
\eta_C \uparrow & \nearrow{f} & \\
C & &
\end{array}
$$

But let's be careful to insert a "U" where appropriate. In particular— and for reasons explained below—it's better not to write "$FC = \mathsf{Set}^{C^{\mathrm{op}}}$," even though the notation may be familiar. We will suggest a better observation in Takeaway 8 later on.

Now, how are we to understand the free cocompletion FC when C is a locally small (possibly large) category? Size issues prevent the presheaf category from being its free cocompletion, so a minor adjustment must be made. To motivate the idea, it will help to think back to the familiar linear algebra of Section 5.1. Recall that the free vector space on a set X does not coincide with *all* functions $X \to UC$ but rather only those functions with finite support. In a completely analogous way, if C is not small, then its free cocompletion does not coincide with *all* functors $C^{\mathrm{op}} \to \mathsf{Set}$ but rather only those functors that are "finite," or more precisely, **small**. (Intuitively, a presheaf is said to be small if it can be written as a small colimit of representable functors.) For a precise definition and a thorough treatment of these ideas see [DL07].

Continuing to unwind the universal property, how should we understand the unique cocontinuous extension $\hat{f}$ along the Yoneda embedding? To aid intuition, we draw another comparison with linear algebra. Recall from the universal property for vector spaces that any function on a set X lifts to a linear map on the free vector space on X that agrees with the function on basis elements in X. Simply put, the lift is a *linear extension* of the function. In a completely analogous way, the universal property above says that any functor $f \colon C \to UD$ has a "cocontinuous extension" $\hat{f} \colon FC \to D$ that agrees with f on **representable functors**, which are very much like basis vectors of the presheaf category $\mathsf{Set}^{C^{\mathrm{op}}}$. More formally, *any presheaf* $V \colon C^{\mathrm{op}} \to \mathsf{Set}$ *is a colimit of representable functors*, which are functors of the form $C(-,c) \colon C^{\mathrm{op}} \to \mathsf{Set}$ for some object c in C [Rie17, Theorem 6.5.8], [Lei14, Theorem 6.2.17]. There are a few ways to express this statement notationally. Here's one way that uses notation that we have not defined, but which is very suggestive [Lor15, Proposition 2.2.1].[4] For any presheaf V, one has

$$
V \cong \int^{c \in C} C(-,c) \cdot Vc, \tag{5.6}
$$

"The representables are the prime numbers of presheaves." [Lei14]

[4] See also [nLa20a, Proposition 2.2] and [nLa20c, Section 2].

and the lift $\hat{f}$ in the universal property is then defined by

$$\hat{f}V := \int^{c \in \mathsf{C}} fc \cdot Vc. \qquad (5.7)$$

The integral $\int^{c \in \mathsf{C}}$ is a type of a colimit called a *coend*. The dot $\cdot$ is called a *copower*, and the expression $\mathsf{C}(-, c) \cdot Xc$ denotes the Xc-indexed coproduct of the hom-functor $\mathsf{C}(-, c)$ with itself, and similarly for $fc \cdot Vc$. The particulars are not needed here, but we mention this simply to point out the similarities between Equation (5.6) and Equation (5.1),

$$|v\rangle = \sum_{x \in X} v(x)|x\rangle \quad \bigg| \quad V \cong \int^{c \in \mathsf{C}} \mathsf{C}(-, c) \cdot Vc$$

and between Equation (5.2) and Equation (5.7).

$$\hat{f}|v\rangle = \sum_{x \in X} v(x)f(x) \quad \bigg| \quad \hat{f}V = \int^{c \in \mathsf{C}} fc \cdot Vc$$

The analogy is clear: presheaves are *like* vectors, representable functors are *like* basis vectors, colimits are *like* sums, cocontinuous functors are *like* linear maps, and so on.[5]

IN SUMMARY, the free cocompletion $F\mathsf{C}$ of a category C is very much like the free vector space FX on a set X. As suggested above, it's better not to use the notation "$F\mathsf{C} = \mathsf{Set}^{\mathsf{C}^{op}}$." The category Set has many nice properties, one of them being that it is cocomplete. Since an arbitrary category C may *not* be cocomplete, an arrow $\mathsf{C}^{op} \to \mathsf{Set}$ is not well-typed. Instead, it's better to say that a presheaf is a functor from C^{op} to the *underlying category* of the cocomplete category Set, and that the *underlying category* of the free cocompletion $F\mathsf{C}$ coincides with these presheaves. This is summarized in the takeaway below. Compare it with the linear algebra in Takeaway 7.

Takeaway 8. *Given the free-forgetful biadjunction $U\colon \mathsf{CocompCAT} \rightleftarrows \mathsf{CAT}\colon F$, the free cocompletion $F\mathsf{C}$ of a category C has the property that*

$$UF\mathsf{C} = U\mathsf{Set}^{\mathsf{C}^{op}}, \qquad (5.8)$$

where $U\mathsf{Set}^{\mathsf{C}^{op}}$ denotes the category of "small" presheaves $\mathsf{C}^{op} \to U\mathsf{Set}$, namely all presheaves if C is small or small presheaves otherwise. In short, the adjunction $F \dashv U$ has the property that there is a special object in $\mathsf{CocompCAT}$, namely Set, such that all free cocomplete categories are, in some sense, built up from it.

As expected, there is a dual discussion obtained by "reversing all the arrows." It's worth mentioning briefly. Let $\mathsf{CompCAT}$ denote the

[5] Here's yet another analogy. If M is an $n \times m$ matrix and N is an $m \times p$ matrix, then MN is an $n \times p$ matrix whose ijth entry is obtained by "tracing out" a common index $\sum_k M_{ik}N_{kj}$. The categorical version of a matrix $X \times Y \to U\mathsf{C}$ is a *profunctor*, which is the name given to a functor of the form $\mathsf{C}^{op} \times \mathsf{D} \to \mathsf{Set}$. The composition of two profuctors $F\colon \mathsf{C}^{op} \times \mathsf{D} \to \mathsf{Set}$ and $G\colon \mathsf{D}^{op} \times \mathsf{E} \to \mathsf{Set}$ is given by a coend, which is a colimit over the common index $FG = \int^{d \in \mathsf{D}} F(-, d) \times G(d, -)$. More generally, one could imagine composing profunctors several variables, which brings to mind tensor contraction. I first learned of this analogy from [Kis].

2-category of locally small complete categories, continuous functors,[6] and natural transformations between them. There is a free-forgetful biadjunction

$$U\colon \mathsf{CompCAT} \rightleftarrows \mathsf{CAT} \colon \bar{F}.$$

The functor $U\colon \mathsf{CompCAT} \to \mathsf{CAT}$ associates to any complete category C its underlying category $U\mathsf{C}$. The functor $\bar{F}\colon \mathsf{CAT} \to \mathsf{CompCAT}$ associates to a category C the **free complete category** $\bar{F}\mathsf{C}$ on C. It is free in that the unit $\eta\colon \operatorname{id}_{\mathsf{CAT}} \Longrightarrow U\bar{F}$ of this biadjunction satisfies the following universal property.

Universal Property for the Free Completion of a Category. The *free completion of a category* C is a complete category $\bar{F}\mathsf{C}$ with the property that for any complete category D and for any functor $g\colon \mathsf{C} \to U\mathsf{D}$, there is a unique continuous functor $\hat{g}\colon \bar{F} \to \mathsf{D}$ so that the following diagram commutes up to natural isomorphism.

$$
\begin{array}{ccc}
U\bar{F}\mathsf{C} & \overset{U\hat{g}}{\dashrightarrow} & U\mathsf{D} \\[4pt]
{\scriptstyle \eta_{\mathsf{C}}}\big\uparrow & \nearrow{\scriptstyle g} & \\[4pt]
\mathsf{C} & &
\end{array}
$$

The free completion $\bar{F}\mathsf{C}$ is constructed as[7] the opposite category of *co*presheaves on C, typically denoted $(\mathsf{Set}^{\mathsf{C}})^{\mathrm{op}}$. So $\bar{F}\mathsf{C}$ is the category whose objects are (small) functors $f\colon \mathsf{C} \to U\mathsf{Set}$, and where a morphism between copresheaves $f \to f'$ is a natural transformation going in the other direction $f' \Longrightarrow f$. In particular, when C is a small category $\bar{F}\mathsf{C}$ coincides with *all* copresheaves $\mathsf{C} \to U\mathsf{Set}$. In either case, the free completion of C has the property that

$$U\bar{F}\mathsf{C} = (U\mathsf{Set}^{\mathsf{C}})^{\mathrm{op}},$$

where the right-hand side is the category of small (and thus all when C is small) functors $\mathsf{C} \to U\mathsf{Set}$. The functor $\eta_{\mathsf{C}}\colon \mathsf{C} \to U\bar{F}\mathsf{C}$ in the universal property is the *dual* Yoneda embedding that sends an object $c \in \mathsf{C}$ to its representable functor $\mathsf{C}(c, -)$, and the unique continuous extension $\hat{g}$ is defined dually to the unique cocontinuous extension in Equation (5.7).

THERE IS QUITE a bit of heavy machinery here, but we won't need to work with it explicitly. We mentioned it simply to call attention to the fact that *there exists* well-developed theory that connects with familiar ideas in linear algebra and—as we'll see in the next section—formal concept analysis. En route to making this connection clearer, let us close with one final remark. Suppose C is a small category. We have the following two observations.

The free cocomplete category $F\mathsf{C}$ is not only cocomplete, it is also complete.

The free complete category $\bar{F}C$ is not only complete, it is also cocomplete.

The reason behind both statements is simple. The category of (contravariant) functors $C \to U$Set inherits (co)completion from Set, which is both complete and cocomplete. The (co)limit of any diagram of functors $C^{op} \to$ Set is obtained by evaluating them pointwise and then computing the (co)limit in Set. This is analogous to how the set of functions from a set $X \to \mathbb{C}$ inherits a vector space structure from $\mathbb{C}$ by pointwise evaluation. These simple observations lead to our final analogy with linear algebra.[8]

Let D be a small category. Any functor $M\colon C^{op} \times D \to U$Set gives rise to functors A and B on each factor,

$$\text{Cat}(C^{op}, U\text{Set}^D) \longleftarrow \text{Cat}(C^{op} \times D, U\text{Set}) \longrightarrow \text{Cat}(D, U\text{Set}^{C^{op}})$$
$$A \longleftarrow\!\shortmid \; M \; \longmapsto B$$

Notice that functors $C^{op} \to U$Set^D on the left-hand side are in bijection with functors $C \to (U$Set$^D)^{op}$. Under this correspondence, the functor $A\colon C \to (U$Set$^D)^{op}$ obtained from M is defined on an object c in C by $Ac(d) = M(c,d)$ for each object d in D. Likewise the functor $B\colon D \to U$Set$^{C^{op}}$ is defined on each d by $Bd(c) = M(c,d)$. By the universal property for free cocompletions, A lifts uniquely to a cocontinuous functor $M^*\colon FC \to \bar{F}D$, and by the universal property for free completions, B lifts uniquely to a continuous functor $M_*\colon \bar{F}D \to FC$ so that the following diagrams commute,

$$
\begin{array}{ccc}
U\text{Set}^{C^{op}} \xdashrightarrow{\ UM^*\ } (U\text{Set}^D)^{op} & \qquad & (U\text{Set}^D)^{op} \xdashrightarrow{\ UM_*\ } U\text{Set}^{C^{op}} \\
\big\uparrow \quad\nearrow_{A} & & \big\uparrow \quad\nearrow_{B} \\
\mathsf{C} & & \mathsf{D}
\end{array}
$$

$$\text{(5.9)}$$

See the excellent exposition in [Wil13b] for explicit expressions for M^* and M_* in the enriched setting, and compare this with the analogous discussion in Section 5.1 leading up to the two diagrams in (5.4). The climax here is that the functors M^* and M_* are adjoints. That is, there is a natural isomorphism $(\text{Set}^D)^{op}(M^*V, W) \cong \text{Set}^{C^{op}}(V, M_*W)$ for all presheaves V and copresheaves W. Here we have lifted our self-imposed ban on writing $FC = \text{Set}^{C^{op}}$ to call attention to the "op" on the left-hand side of the isomorphism. A morphism $M^*V \to W$ in $(\text{Set}^D)^{op}$ is a morphism $W \to M^*V$ in Set^D, and so we may rewrite the correspondence as

$$\text{Set}^D(W, M^*V) \cong \text{Set}^{C^{op}}(V, M_*W).$$

The functors M_* and M^* are thus said to be **mutually right adjoints** that come with "unit" natural transformations $\eta\colon \text{id} \implies M_*M^*$

and $\epsilon\colon \mathrm{id} \implies M_*M^*$ [Rie17, Definition 4.3.1], and their invariant
subcategories, or "fixed points," now arise as the topic of interest.
Let $\mathrm{Fix}(M_*M^*)$ be the category whose objects are objects c in C such
that the unit $\eta_c\colon c \xrightarrow{\cong} M_*M^*c$ is an isomorphism. Likewise, let
$\mathrm{Fix}(M^*M_*)$ denote the category hose objects are objects d in D so that
$\epsilon_d\colon d \xrightarrow{\cong} M^*M_*d$ is an isomorphism. There is an equivalence of
categories[9]

$$\mathrm{Fix}(M_*M^*) \cong \mathrm{Fix}(M^*M_*)$$

and their objects are called the **nucleus** of M. When $\mathsf{D} = \mathsf{C}$ and
$M\colon \mathsf{C}^{\mathrm{op}} \times \mathsf{C} \to \mathsf{Set}$ is the hom-functor $\mathsf{C}(-,-)$, the adjunction
$M^* \dashv M_*$ is called the **Isbell adjunction** or Isbell conjugation, and
its nucleus is called the **Isbell completion** of C. If Set is further re-
placed by the category 2 of truth values (defined in the next section)
and the category C is a poset P, then this recovers the **Dedekind
MacNeille completion of** P. If $P = \mathbb{Q}$ with the usual ordering,
then the Isbell completion gives the completion of $\mathbb{Q}$ by Dedekind
cuts. If instead of replacing Set by 2, we were to replace it with
$[0,\infty]$ with an appropriate categorical structure, this recovers the
tight span of a metric space. For more on these constructions see
[Wil15, Pav12, Isb66, Law86, Ell17, Wil13c]. By now we've covered a
lot of information in a small amount of space. Here's the takeaway.

Takeaway 9. *Given small categories* C *and* D, *any functor* $M\colon \mathsf{C}^{\mathrm{op}} \times \mathsf{D} \to$
$U\mathsf{Set}$ *induces two functors* $A\colon \mathsf{C} \to U\mathsf{Set}^{\mathsf{C}^{\mathrm{op}}}$ *and* $B\colon \mathsf{D} \to (U\mathsf{Set}^{\mathsf{D}})^{\mathrm{op}}$ *that
lift to a cocontinuous functor* M^* *and a continuous functor* M_* *so that the
following diagrams commute.*

$$\tag{5.10}$$

Moreover M^* *and* M_* *satisfy*

$$\mathsf{Set}^{\mathsf{D}}(W, M^*V) \cong \mathsf{Set}^{\mathsf{C}^{\mathrm{op}}}(V, M_*W)$$

for all presheaves V *in* $\mathsf{Set}^{\mathsf{C}^{\mathrm{op}}}$ *and copresheaves* W *in* $\mathsf{Set}^{\mathsf{D}}$, *and the invari-
ant subcategories of the compositions* M_*M^* *and* M^*M_* *are the nucleus of
M, and there is an equivalence between them.*

Take note of the unmistakable similarity with the linear alge-
bra in Takeaway 2, shown in the margin for convenience. In one
case, a function $M\colon X \times Y \to U\mathbb{C}$ defines a pair of linear adjoints
$M\colon \mathbb{C}^X \rightleftarrows \mathbb{C}^Y\colon M^\dagger$, and the eigenvectors of $M^\dagger M$ and $MM^\dagger$ we've
discussed at length in Chapters 3 and 4. In another case, a func-
tor $M\colon \mathsf{C}^{\mathrm{op}} \times \mathsf{D} \to U\mathsf{Set}$ defines a pair of categorical adjoints

[9] This is a standard exercise. Every
adjunction restricts to an equivalence of
categories in this way.

Takeaway 2. *Given finite sets X and Y,
any function $M\colon X \times Y \to \mathbb{C}$ induces two
functions $\alpha\colon X \to \mathbb{C}^Y$ and $\beta\colon Y \to \mathbb{C}^X$
that lift to linear maps M and $M^\dagger$ so that
the following diagrams commute.*

Moreover, M and $M^\dagger$ satisfy

$$\langle Mv, w\rangle = \langle v, M^\dagger w\rangle$$

*for all $v \in \mathbb{C}^X$ and $w \in \mathbb{C}^Y$, and the
one-dimensional invariant subspaces of
the compositions $M^\dagger M$ and $MM^\dagger$ are
their eigenvectors. Moreover, there is a
one-to-one correspondence between them.*

$M^*\colon \mathsf{Set}^{\mathbb{C}^{\mathrm{op}}} \rightleftarrows (\mathsf{Set}^D)^{\mathrm{op}}\colon M_*$, and the one-dimensional invariant subspaces of $M_* M^*$ and $M^* M_*$ are a known construction. Naturally, one is left wondering whether the dictionary between the category theory and linear algebra is more than a coincidence. Is it? Towards an answer, here's something to know. The category theory in this section may be promoted to an *enriched* version. In other words, (co)presheaves and (co)completions have an analogous version when Set is replaced by any other symmetric monoidal closed category $\mathcal{V}$ that is both complete and cocomplete. This is a part of **enriched category theory**, which stems from the idea that a set of morphisms in a category may actually be another object in that category.[10]

In view of this, it might seem desirable to ask that $\mathbb{C}$ be an enriching category, so that the linear algebra in Section 5.1 is subsumed by the category theory in this section. But despite the many parallels, it is not known—to my knowledge—whether $\mathbb{C}$ may be viewed as a symmetric monoidal category which is also closed, complete, and cocomplete, so that one recovers the basic constructions in linear algebra as a special case. But perhaps one shouldn't expect this anyway. Colimits, for instance, are "a remarkable enhancement of the concept of addition" [Bae20], and freely adding linear algebraic *structure* is different than freely adding limits and colimits, which are closer to *property-like structures* [nLa20b, Section 4]. But all is not lost. Although linear algebra does not appear to be a special case of enriched category theory, it turns out that the formal concept construction discussed in Sections 1.1 and 3.3 *is*. This is explained in the next section.

Let us give a quick preview of the ideas. If Set is replaced by the poset (category) of *truth values*, then free (co)completions reduce to familiar constructions in order theory. Briefly, any set X can be viewed as a discrete category—the objects are the elements in X and there are no nonidentity morphisms. The free cocompletion of X coincides with the **free join semilattice** on X, and the free completion of X coincides with the **free meet semilattice** on X. Moreover, there is an adjunction between these two semilattices, and the invariant subsets of the adjoint maps are formal concepts. Because the enriched category theory reduces constructions that are both elementary and familiar, we will not introduce, use, or assume familiarity with the language of enriched category theory. Instead, we will only give a somewhat abridged, unenriched presentation with the simple goal of sharing the big-picture ideas. Readers are referred to [Law73, Wil14, Wil15, Ell17, Kel82] for more details. So while there is no claim that eigenvectors of reduced density operators are the fixed points of functors between (co)presheaf categories, it *is* true of formal concepts. Understanding this will then shed light on the category theory that

[10] For example, the *set* of linear operators is itself a *vector space*, the *set* of continuous functions is itself a *topological space*, and so on.

does unite eigenvectors, generalized Isbell completions, and formal concepts.

5.3 Revisiting Formal Concepts

The present goal is specialize the category theory of Section 5.2 with the aim of rederiving the definition of a formal concept given in Section 1.1. Perhaps not obvious at first, this section is essentially a repeat of Section 5.2 but with Set replaced by "2." This will be explained soon. For now the starting point is, as before, an adjunction.

Let Join denote the category of join semilattices and join-preserving functions. A **join semilattice** is a set P with a partial order $\leq$ such that the join (the least upper bound) of any nonempty finite subset of P exists. A function between join semilattices $f \colon P \to Q$ is said to **preserve joins** if $f(p \vee p') = fp \vee fp'$ for all $p, p' \in P$. Any join-preserving function automatically respects the partial order.[11] This information can also be expressed in the language of category theory. Every poset P is a category. Objects are the elements p, p' of P, and a hom set $P(p, p')$ contains exactly one morphism $p \to p'$ if and only if $p \leq p'$. The colimit of any diagram in P is the join of the elements, if it exists. So "P is a cocomplete category" is synonymous with "P is a joint semilattice." An order-preserving function between posets is a functor, and a join-preserving function between join semilattices is a cocontinuous functor.[12] We won't need this perspective now, but being aware of it may be helpful in interpreting some of the results to come. We will, however, need the following fact. There is a free-forgetful adjunction

$$U \colon \mathsf{Join} \rightleftarrows \mathsf{Set} \colon F.$$

The functor $U \colon \mathsf{Join} \to \mathsf{Set}$ forgets partial orders and hence joins, and it associates to any join semilattice P its underlying set UP. The functor $F \colon \mathsf{Set} \to \mathsf{Join}$ associates to a set X the free join semilattice FX on X. It is free in that the unit natural transformation $\eta \colon \mathrm{id}_{\mathsf{Set}} \implies UF$ of this adjunction satisfies the following universal property.

Universal Property for Free Join Semilattices. The *free join semilattice on a set X* is a join semilattice FX with the property that for any join semilattice P and for any function $f \colon X \to UP$ there is a unique join-preserving function $\hat{f} \colon FX \to P$ so that the following diagram commutes.

$$
\begin{array}{ccc}
UFX & \xrightarrow{\ U\hat{f}\ } & UP \\
{\scriptstyle \eta_X}\Big\uparrow & \nearrow {\scriptstyle f} & \\
X & &
\end{array}
$$

[11] Note that $p = p \vee p'$ if and only if $p' \leq p$, so if f is join-preserving and if $p' \leq p$, then $fp = f(p \vee p') = fp \vee fp'$, which implies $fp' \leq fp$.

[12] There's a dual version to this. The *limit* of any diagram in P is the *meet* (the greatest lower bound) of the elements, if it exists. So P is a **meet semilattice** precisely when it is a complete category. A meet-preserving function between meet semilattices is a continuous functor.

For any $A \in FX$ the unique lift in Equation (5.7) specializes in this context to give

$$\hat{f}A := \bigvee_{x \in A} fx. \qquad (5.11)$$

Concretely, FX is the poset consisting of all finite subsets of X ordered by inclusion. The join of finite subsets $A, B \subseteq X$ is their union $A \vee B := A \cup B$. The function η_X associates to an element $x \in X$ the singleton set $\{x\}$, and verifying that $\hat{f}$ preserves joins is a simple check. Elements in FX may be identified with finitely-supported functions from X to the two-element set $\{0, 1\}$. When X is finite this coincides with *all* functions from X. Either way, it may be tempting to write "$FX = 2^X$," but let's resist the urge for the same reason we resist writing $\mathbb{C}^X$ and $\mathsf{Set}^{\mathsf{Cop}}$. That is, just as the complex numbers $\mathbb{C}$ and the category Set are special objects in Vect and CAT, respectively, so "2" is a special object in Join. We take a brief interlude to discuss this.

As a technical aside, we are including the emptyset in FX, and so it may be referred to as the free *bounded* join semilattice on X since $\varnothing \leq A$ for every subset A of X.

5.3.1   Interlude: 2, Categorically

Start with the definition

$$2 := \{0 \leq 1\}.$$

So 2 is a poset. In fact, it is a join semilattice. For all elements a and b in 2, their join $a \vee b$ exists:

$$0 \vee 0 = 0 \qquad 0 \vee 1 = 1 \vee 0 = 1 \vee 1 = 1.$$

So 2 is an object in Join, and its underlying set is $U2 = \{0, 1\}$. In fact, there's more: 2 is also a **meet semilattice**. For all elements a and b in 2, their meet $a \wedge b$ exists:

$$0 \wedge 0 = 0 \wedge 1 = 1 \wedge 0 = 0 \qquad 1 \wedge 1 = 1.$$

So 2 is also an object in Meet, which is the category of meet semilattices and meet-preserving maps between them. Think of the elements of 2 as representing **truth values** with 0 as false and 1 as true, and think of meets as logical "and" and of joins as "or." This pairs well with the intuition that a relation $R \subseteq X \times Y$ defines any function $R \colon X \times Y \to U2$, which provides a "yes or no" answer to the question, "Are x and y related?" As with any poset, 2 is also a category. It has two objects with a single nonidentity morphism between them.

That 2 is both a join and a meet semilattice is completely analogous to the fact that Set is both cocomplete and complete.

$$0 \longrightarrow 1$$
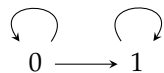
Think of the arrow $0 \to 1$ as logical entailment. In this way, 2 is quite rich in the eyes of category theory: it is symmetric monoidal (the

monoidal product is "and") and it is closed[13] (the internal hom is implication). It is also both complete and cocomplete, for in any poset, the limit of any diagram is—if it exists—the meet of the elements in the diagram, and the colimit of any diagram is—if it exists—the join of the elements. So every meet (join) semilattice is a complete (cocomplete) category. In short, 2 it is an excellent example of a category that one can "do enriched category theory in." Though interesting, we omit the details. The enriched constructions ultimately recover familiar constructions in order theory, and the latter is sufficient for our goals. But, as a quick aside, here's the main idea connecting the two:

> A subset $A \subseteq X$ is completely determined by its characteristic function $\bar{A} \colon X \to U2$ defined by $\bar{A}x = 1$ if and only if $x \in A$.

In other words, knowing a subset A is the same thing as knowing the truth value of the question "Is $x \in A$?" for every $x \in X$. Enriched category theory capitalizes on this. It's worth digressing a little more to understand just how. There is a precise sense in which every poset P is enriched (a word that we still haven't, and won't, define) over the category 2. Here's the basic idea. Rather than considering a hom-*set* $P(p, p')$, which contains a single element $p \to p'$ if and only if $p \leq p'$, one instead considers an *object* $2(p, p')$ in 2, which is thought of as a hom-*truth value*. The truth value answers the question "Is $p \leq p'$?" with 1 when the answer is yes and with 0 when the answer is no. As an example, if P is the free join semilattice on a set X, then for any finite subsets $A, B \subseteq X$, the truth value between them indicates whether or not B contains A.

$$2(A, B) = \begin{cases} 1 & \text{if } A \subseteq B \\ 0 & \text{otherwise.} \end{cases} \tag{5.12}$$

Since A and B ultimately correspond to functions $\bar{A}, \bar{B} \colon X \to U2$, the hom-object $2(A, B)$ arises from pointwise evaluation.

$$2(\bar{A}, \bar{B}) = \begin{cases} 1 & \text{if } \bar{A}x \leq \bar{B}x \text{ for all } x \in X \\ 0 & \text{otherwise} \end{cases} \tag{5.13}$$

So just as the dominance of B in $A \subseteq B$ is indicated by a truth value $2(A, B)$, so the dominance of Bx in $Ax \leq Bx$ is also indicated by a truth value, which we can denote by $[Ax, Bx]$. More precisely, 2 can be equipped with a pairing $[-, -] \colon 2 \times 2 \to 2$ called the **internal hom of 2**. Continuing to borrow the language of category theory, functions $\bar{A}, \bar{B} \colon X \to U2$ are examples of **enriched presheaves**,[14] and the existence of a hom truth value $2(\bar{A}, \bar{B})$ between them is the first step in discovering that FX is a **category enriched over** 2.

[13] Informally, a category is **closed** if the morphisms between any two objects form another *object* in that category. That object is called an *internal hom.*

[14] More generally, a presheaf on any poset P is simply an order-reversing function $P^{\text{op}} \to 2$, where P^{op} is the poset obtained by reversing the order on P. A finite set X is an example of a poset with $x \leq x'$ if and only if $x = x'$. In this way, $X^{\text{op}} = X$ and thus a presheaf $X^{\text{op}} \to 2$ is nothing more than a function $X \to U2$.

After working through the details, it turns out that *the free join semilattice FX is quite literally the free cocompletion of X*, in a precise, enriched sense; that the join in Equation (5.11) corresponds to a presheaf (i.e. a truth-valued function) analogous to Equation (5.7); and that the inclusion $\eta_X\colon X \to UFX$ sending an element to its singleton set $\{x\}$ is ultimately an enrichment of the Yoneda embedding. For more on enrichment over truth values, see Lawvere's classic [Law73] as well as the informal article [Wil14] and the PhD thesis [Ell17, Appendix A]. For more on enriched category theory in general, see [Rie14, Kel82]. To summarize, the purpose of this digression is simply to call attention to analogous constructions

$$\mathbb{C}^X \qquad \mathsf{Set}^{\mathsf{C}^{\mathrm{op}}} \qquad \mathcal{V}^{\mathsf{C}^{\mathrm{op}}} \qquad 2^X$$

for a finite set X and small category C. Here $\mathcal{V}$ is a sufficiently nice category that can replace Set in the constructions in Section 5.2. Crucially, 2 is an example of such a $\mathcal{V}$, and this chapter is essentially a repeat of Section 5.2 in this truth-enriched setting.

End of Interlude 5.3.1.

This is a good time to summarize the takeaway of the discussion so far. Compare the following with Takeaways 7 and 8.

Takeaway 10. *Given the free-forgetful adjunction $U\colon$ Join $\rightleftarrows$ Set$\colon F$, the free join semilattice FX on a set X has the property that*

$$UFX = U2^X, \tag{5.14}$$

where $U2^X$ denotes the set of finitely-supported functions (and hence all functions if X is finite) $X \to U2$. To emphasize, the adjunction $F \dashv U$ has the property that there is a special object in Join*, namely 2, such that all join semilattices are, in some sense, built up from it.*

As expected, there is a dual discussion obtained by "reversing all the arrows." In Section 5.2 this led to the free completion of a category. It specializes in this context to the *free meet semilattice of a set*. Explicitly, there is a free-forgetful adjunction

$$U\colon \mathsf{Meet} \rightleftarrows \mathsf{Set}\colon \bar{F}$$

where Meet is the category of meet semilattices and meet-preserving functions. It is free in that the unit $\eta\colon \mathrm{id}_{\mathsf{Set}} \implies U\bar{F}$ of this adjunction satisfies the following universal property.

Universal Property for Free Meet Semilattices. The *free meet semilattice on a set X is a meet semilattice $\bar{F}X$ such that for any meet semilattice P and for any function $g\colon X \to UP$ there is a unique

meet-preserving function $\hat{g}\colon \bar{F}X \to P$ so that the following diagram commutes.

$$UX̄ \xrightarrow{\;U\hat{g}\;} UP$$

$$\begin{array}{c} U\bar{F}X \xrightarrow{\;U\hat{g}\;} UP \\ \eta_X \uparrow \quad \nearrow{g} \\ X \end{array}$$

Explicitly, for any $B \in \bar{F}X$ the unique lift is given by

$$\hat{g}B := \bigwedge_{x \in B} gx. \qquad (5.15)$$

The free meet semilattice on X is constructed as the *opposite* of its free join semilattice.

$$\bar{F}X = (FX)^{\text{op}} \qquad (5.16)$$

In other words, $\bar{F}X$ consists of all finite subsets of X with the superset order, rather than inclusion. The meet of subsets $A, B \subseteq X$ in $\bar{F}$ is therefore their union $A \wedge B := A \cup B$. The elements of $\bar{F}X$ may be identified with the set $U2^Y$ of all finitely-supported functions $Y \to U2$; that is,

$$U\bar{F}Y = U2^Y = UFY.$$

The unit of the adjunction $\eta_X\colon X \to U\bar{F}X$ is again the inclusion of an element $x \in X$ to the singleton set $\{x\}$. A quick calculation verifies that $(FX)^{\text{op}}$ does indeed satisfy the universal property and that the map given in Equation (5.15) preserves meets,[15] meaning that $\hat{g}(A \cup B) = \hat{g}A \cap \hat{g}B$.

LET'S TAKE INVENTORY of the results so far.

- Subsets $X \to U2$ of a finite set X are like functors $\mathsf{C}^{\text{op}} \to \mathsf{Set}$ on a small category C. In fact, one finds they are *truth-enriched* functors.

- Free join (meet) semilattices are like free cocompletions (completions). In fact, they are *truth-enriched* (co)completions.

- The inclusion $x \mapsto \{x\}$ is like the Yoneda embedding $c \mapsto \mathsf{C}(-, c)$. In fact, it arises from the *truth-enriched* Yoneda embedding.

In light of this dictionary, the following may come as no surprise. Recall from Section 5.2 that the free cocompletion of C was also *complete*, and that its free completion was also *cocomplete*. This led to the nice diagrams in Takeaway 9. The truth-enriched version has the same feature.

The free join semilattice FX on X is also a meet semilattice.

The free meet semilattice $(FX)^{\text{op}}$ on X is also a join semilattice.

[15] Note that any meet-preserving map $(FY)^{\text{op}} \to P$ is automatically order-*reversing*. This follows from the fact that $A \cup B = B$ if and only if $A \subseteq B$ and that $p \wedge p' = p'$ if and only $p' \leq p$, for all $p, p' \in P$ and $A, B \in FY$.

The meet of subsets in FX is their intersection, and the join of subsets in $(FX)^{\mathrm{op}}$ is also their intersection. These two facts go hand-in-hand in the following consideration. Let X and Y be finite sets and consider any function $R\colon X \times Y \to U2$. The category of sets is Cartesian closed, and so we have a product-hom adjunction and hence the following bijections.

$$\mathsf{Set}(X, U2^Y) \qquad \cong \qquad \mathsf{Set}(X \times Y, U2) \qquad \cong \qquad \mathsf{Set}(Y, U2^X)$$
$$a \longleftarrow\!\!\mid R \mid\!\longrightarrow b$$

Under this adjunction, the function $a\colon X \to U2^Y$ is defined on each $x \in X$ by

$$ax(y) = \begin{cases} 1 & \text{if } R(x,y) = 1 \\ 0 & \text{if } R(x,y) = 0, \end{cases} \qquad (5.17)$$

and the function $b\colon Y \to U2^X$ is defined similarly. By the universal properties for free join and meet semilattices, a lifts uniquely to a join-preserving function $f\colon FX \to (FY)^{\mathrm{op}}$, while b lifts uniquely to a meet-preserving function $g\colon (FY)^{\mathrm{op}} \to FX$ so that the following diagrams commute:

$$\begin{array}{ccc} U2^X \xdashrightarrow{Uf} U2^Y & \qquad & U2^Y \xdashrightarrow{Ug} U2^X \\ \uparrow \quad \nearrow{}_{a} & & \uparrow \quad \nearrow{}_{b} \\ X & & Y \end{array} \qquad (5.18)$$

Explicitly, for any $A \subseteq X$ and $B \subseteq Y$,

$$fA = \bigcap_{x \in A} ax \qquad \text{and} \qquad gB = \bigcap_{y \in B} by$$

which recovers Equations (1.2) and (1.3) in Chapter 1. Compare this with the analogous discussion in Section 5.2 leading up to the two diagrams in (5.9). As was the case then, the climax is that f and g form a categorical adjunction—order-reversing functions are contravariant functors!—and so there is a bijection $(FY)^{\mathrm{op}}(fA, B) \cong FX(A, gB)$ for all $A \in FX$ and $B \in FY$. This is the same as having a bijection

$$FY(B, fA) \cong FX(A, gB)$$

which is equivalent to the original claim in (1.4) that

$$B \subseteq fA \quad \text{if and only if} \quad A \subseteq gB.$$

A **formal concept** is defined to be a pair of sets (A, B) for which equality holds. As noted in Chapter 1, such pairs coincide with fixed points of the compositions fg and gf and, to borrow the language of Section 5.2, is the *nucleus* of R.

THE PAST THREE sections have featured a single construction that resurfaces in different contexts. We've briefly mentioned the *Isbell completion* of a small category C, which is the nucleus of the hom functor $C(-,-)\colon C^{op} \times C \to U\mathsf{Set}$. When Set is replaced by 2 and when C is a poset P, then the nucleus of $P(-,-)\colon P^{op} \times P \to U2$ is the *Dedekind MacNeille completion of P*. The Isbell completion has a generalization when considering *any* functor $M\colon C^{op} \times D \to U\mathsf{Set}$ for any small category D. When Set is replaced by 2 and when $C = X$ and $D = Y$ are sets (viewed as discrete posets) then the nucleus of the relation $R := M\colon X \times Y \to U2$ contains the formal concepts of R. By way of analogy, this thesis has replaced 2 by the complex numbers $\mathbb{C}$ to study the "nucleus" of the matrix $M\colon X \times Y \to U\mathbb{C}$, in the special case when the values $|M(x,y)|^2$ define a probability distribution. In the next section, we close with a brief comment on the shared blueprint behind these constructions.

One notable difference between the linear algebra and the other constructions is that eigenvectors come with *eigenvalues*. This is absent from the categorical version of the story, and so it could be interesting to generalize the Isbell completion yet further to allow for "eigenvalues of profunctors."

5.4 A Special Adjunction

Let's now zoom back a bit and summarize the overarching theme of Sections 5.1, 5.2, and 5.3. Each begins with an adjunction $U\colon C \rightleftarrows D\colon F$ where the category C contains a special object—call it E—with the property that UFX "looks like" morphisms $X \to UE$ for every object X in D. Then for any objects X and Y in D, a morphism $X \times Y \to UE$ induces two morphisms $X \to UFX$ and $Y \to UFY$ which have universal lifts $FX \to FY$ and $FY \to FX$ in C, which are adjoints in some sense. In each case, "fixed points" of the composition of these adjoint maps are interesting. More concretely,

- When the adjunction is $U\colon \mathsf{Vect} \rightleftarrows \mathsf{Set}\colon F$, the special object is $\mathbb{C}$. The universal lifts $FX \rightleftarrows FY$ are linear maps, and their one-dimensional invariant subspaces are **eigenvectors**.

- When the biadjunction is $U\colon (\mathsf{Co})\mathsf{compCAT} \rightleftarrows \mathsf{CAT}\colon F$, the special object is Set. The universal lifts $FC \rightleftarrows FD$ are (co)continuous functors, and their invariant subcategories are **nuclei**.

- When the adjunction is $U\colon \mathsf{Join}/\mathsf{Meet} \rightleftarrows \mathsf{Set}\colon F$, the special object is 2. The universal lifts $FX \rightleftarrows (FY)^{op}$ are join/meet-preserving functions, and their invariant subsets are **formal concepts**.

Modulo colimits versus limits, let us point out an interesting blueprint.

5.4.1 A Blueprint

Let D be a category with binary products, let C be any category, let $U\colon C \to D$ be a **faithful functor** and consider an adjunction

$U\colon \mathsf{C} \rightleftarrows \mathsf{D}\colon F$ with the following property: There exists an object E in C such that for each object X in D there exists an object UE^X in D together with an **evaluation morphism**

$$\mathrm{eval}\colon UE^X \times X \to UE$$

that is **exponential**; that is, for any object $Y \in \mathsf{D}$ and any morphism $M\colon Y \times X \to UE$ there is a unique morphism $m\colon Y \to UE^X$ so that the following diagram commutes

$$
\begin{array}{ccc}
Y \times X & \xrightarrow{\ M\ } & UE \\
{\scriptstyle m \times \mathrm{id}_X} \downarrow & \nearrow & \\
UE^X \times X & {\scriptstyle \mathrm{eval}} &
\end{array}
$$

In other words, there is a bijection

$$\mathsf{D}(X \times Y, UE) \cong \mathsf{D}(Y, UE^X). \tag{5.19}$$

Moreover assume that

$$UFX \cong UE^X \qquad \text{for every } X \in \mathsf{D}. \tag{5.20}$$

To understand this better, let's further suppose that D has a terminal object I. Then under the bijection in Equation (5.19),

$$\mathsf{D}(I, UE^X) \cong \mathsf{D}(X \times I, UE) \cong \mathsf{D}(X, UE)$$

An object I in a category D is called **terminal** if for every object d in D there is exactly one morphism $d \to I$.

Therefore UE^X may be identified with morphisms $X \to UE$ in D. The unit natural transformation $i\colon \mathrm{id}_\mathsf{D} \implies UF$ of the adjunction $U\colon \mathsf{C} \rightleftarrows \mathsf{D}\colon F$ satisfies a universal property.

Universal Property of the Unit. For any object C in C and any morphism $f\colon X \to UC$ in D, there is a unique morphism $\hat{f}\colon FX \to C$ in C so that the diagram commutes.

$$
\begin{array}{ccc}
UFX & \dashrightarrow{\ U\hat{f}\ } & UC \\
{\scriptstyle i} \uparrow & \nearrow & \\
X & {\scriptstyle f} &
\end{array}
$$

In the special case when $C = FY$ for some object Y in D, morphisms $X \to UFY$ in D correspond to morphisms $FX \to FY$ in C,

$$\mathsf{C}(FX, FY) \cong \mathsf{D}(X, UE^Y). \tag{5.21}$$

Here's the diagram:

$$
\begin{array}{ccc}
UE^X & \dashrightarrow{\ U\hat{f}\ } & UE^Y \\
{\scriptstyle i} \uparrow & \nearrow & \\
X & {\scriptstyle f} &
\end{array}
$$

Compare this diagram with Diagrams 5.4, 5.10, and 5.18 where the special object E is C, Set, and $\mathsf{2}$, respectively.

By exchanging X and Y there is also a bijection

$$\mathsf{C}(FY, FX) \cong \mathsf{D}(Y, UE^X) \qquad\qquad (5.22)$$

Now a priori, there's no relationship between $\mathsf{C}(FX, FY)$ and $\mathsf{C}(FY, FX)$. But in fact they are isomorphic because UE^X is exponential, as in Isomorphism (5.19). Explicitly,

$$\mathsf{C}(FX, FY) \overset{\text{by (5.21)}}{\cong} \mathsf{D}(X, UE^Y)$$

$$\overset{\text{by (5.19)}}{\cong} \mathsf{D}(X \times Y, UE)$$

$$\overset{\text{by (5.19)}}{\cong} \mathsf{D}(Y, UE^X)$$

$$\overset{\text{by (5.22)}}{\cong} \mathsf{C}(FY, FX).$$

As a result, morphisms $X \times Y \to UE$ in D correspond to morphisms $FX \rightleftarrows FY$ in C, and it is apparent that the "fixed points" of the composite morphisms carry interesting information encoded in $X \times Y \to UE$.

Conclusion

In this thesis, we set out to understand mathematical structure that has both algebraic and statistical properties, and basic tools from quantum probability theory have played a key role. In approaching the interface of algebra and statistics, we've seen that the eigenvalues and eigenvectors of reduced densities of a particular pure quantum state harness algebraic and statistical information in a highly principled way. In a further attempt to understand the marriage of these ideas, we think back to the density matrix model for entailment sketched in Section 3.4. As it turns out, the way in which algebra and statistics meet in that setting is not incompatible with the categorical perspectives in Chapter 5. This will be expanded on in the forthcoming paper [BV20], which is part of an ongoing, promising investigation into this mathematical structure.

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