Introduction to Quantum Programming and Semantics

Week 2: Categories, Hilbert spaces

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Categorical semantics

Want:

- Compositionality: $[F; G] = [G] \circ [F]$
- Concurrency: $[F \par G] = [F] \otimes [G]$
- Recursion: $[F(X)] = [F]([X])$

Where can $[F; K]$ live:

- $\lambda$-calculus
- partially ordered sets
- categories

Instantiate in different categories:

- Isolate differences between quantum and classical behaviour
- Apply quantum thinking to other settings
Categorical semantics

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Instantiate in different categories:

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Category theory is a way of thinking more than deep theorems

“The essential virtue of category theory is as a discipline for making definitions, the programmer’s main task in life.”
– D. E. Rydeheard

“Good general theory does not search for the maximum generality, but for the right generality.”
– S. Mac Lane
Categories

Categories consist of

- objects $A, B, C, \ldots$
- morphisms $A \xrightarrow{f} B$ going between objects
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Examples:

- physical systems, physical processes governing them
- data types, algorithms manipulating them
- algebraic/geometric structures, structure-preserving functions
- logical propositions, implications between them
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Ignore all structure of objects, focus relationships between objects

“Morphisms are more important than objects”
Categories

A category $\mathbf{C}$ consists of the following data:

- a collection $\text{Ob}(\mathbf{C})$ of objects
- for every pair of objects $A$ and $B$, a collection $\mathbf{C}(A, B)$ of morphisms, with $f \in \mathbf{C}(A, B)$ written $A \xrightarrow{f} B$
- for all morphisms $A \xrightarrow{f} B$ and $B \xrightarrow{g} C$ a composite $A \xrightarrow{g \circ f} C$
- for every object $A$ an identity morphism $A \xrightarrow{id_A} A$

such that:

- associativity: $h \circ (g \circ f) = (h \circ g) \circ f$
- identity: $\text{id}_B \circ f = f = f \circ \text{id}_A$
Sets and functions

The category \textbf{Set} of sets and functions:

- \textit{objects} are sets \(A, B, C, \ldots\)
- \textit{morphisms} are functions \(f, g, h, \ldots\)
- \textit{composition} of \(A \xrightarrow{f} B\) and \(B \xrightarrow{g} C\) is the function \(g \circ f : a \mapsto g(f(a))\)
- \textit{the identity morphism} on \(A\) is the function \(\text{id}_A : a \mapsto a\)
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Think of a function $A \xrightarrow{f} B$ dynamically, as indicating how elements of $A$ can evolve into elements of $B$

\[ A \xrightarrow{f} B \]
Relations

Given sets $A$ and $B$, a relation $A \stackrel{R}{\to} B$ is a subset $R \subseteq A \times B$.

Nondeterministic: an element of $A$ can relate to more than one element of $B$, or to none.
Composition of relations

Suppose we have a pair of head-to-tail relations:

\[
\begin{align*}
A & \xrightarrow{R} B \\
B & \xrightarrow{S} C
\end{align*}
\]
Composition of relations

Suppose we have a pair of head-to-tail relations:

\[ A \xrightarrow{R} B \]

\[ B \xrightarrow{S} C \]

Then our interpretation gives a natural notion of composition:

\[ A \xrightarrow{S \circ R} C \]
Relations as matrices

We can write relations as (0,1)-valued matrices:

\[
A \xrightarrow{R} B
\]

\[
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 1 & 1 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

Composition of relations is then ordinary matrix multiplication, with logical disjunction (OR) and conjunction (AND) for + and \( \times \).
Sets and relations

The category **Rel** of sets and relations:

- **objects** are sets $A, B, C, \ldots$;
- **morphisms** are relations $R \subseteq A \times B$, with $(a, b) \in R$ written $aRb$;
- **composition** $A \xrightarrow{R} B \xrightarrow{S} C$ is \((a, c) \in A \times C \mid \exists b \in B: aRb, bSc\); 
- **the identity morphism** on $A$ is \{(a, a) \in A \times A \mid a \in A\}.
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- \textit{the identity morphism} on \( A \) is \( \{(a, a) \in A \times A \mid a \in A\} \).

It seems like \textbf{Rel} should be a lot like \textbf{Set}, but we will discover it behaves a lot more like \textbf{Hilb}.

While \textbf{Set} is a setting for classical physics, and \textbf{Hilb} is a setting for quantum physics, \textbf{Rel} is somewhere in the middle.
Diagrams

Helps to draw diagrams, indicating how morphisms compose

Diagram commutes if every path from object to another is equal

Two ways to speak about equality of composite morphisms: algebraic equations, and commuting diagrams.
Terminology

For morphism $A \xrightarrow{f} B$

- $A$ is its domain
- $B$ is its codomain
- $f$ is endomorphism if $A = B$
- $f$ is isomorphism if $f^{-1} \circ f = \text{id}_A$, $f \circ f^{-1} = \text{id}_B$ for some $B \xleftarrow{f^{-1}} A$
- $A$ and $B$ are isomorphic ($A \simeq B$) if there is isomorphism $A \rightarrow B$
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If a morphism has an inverse, it is unique:

$$g = g \circ \text{id} = g \circ (f \circ g') = (g \circ f) \circ g' = \text{id} \circ g' = g'$$
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A groupoid is a category where every morphism is an isomorphism.
Graphical notation

Draw object $A$ as:

It’s just a line. Think of it as a picture of the identity morphism $A \xrightarrow{id_A} A$. Remember: morphisms are more important than objects.
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\[
\begin{array}{c}
A \\
\end{array}
\]

It’s just a line. Think of it as a picture of the identity morphism \( A \xrightarrow{id_A} A \). Remember: morphisms are more important than objects.

Draw morphism \( A \xrightarrow{f} B \) as:

\[
\begin{array}{c}
B \\
\end{array} \xrightarrow{f} \begin{array}{c}
A \\
\end{array}
\]
Graphical notation

Draw composition of $A \xrightarrow{f} B$ and $B \xrightarrow{g} C$ as:
Graphical notation

Identity law and associativity law become:

\[
\begin{align*}
  B & \quad = \quad B \\
  f & \quad id_B \\
  A & \quad = \quad \quad = \quad A \\
  A & \quad = \quad \quad = \quad A
\end{align*}
\]

\[
\begin{align*}
  D & \quad = \quad D \\
  h & \quad g \\
  C & \quad = \quad B \\
  B & \quad = \quad f \\
  A & \quad = \quad \quad = \quad A
\end{align*}
\]

This one-dimensional representation is familiar; we usually draw it horizontally, and call it algebra. The graphical calculus 'absorbs' the axioms of a category.
Graphical notation

Identity law and associativity law become:

This *one-dimensional* representation is familiar; we usually draw it horizontally, and call it algebra. The graphical calculus ‘absorbs’ the axioms of a category.
Functors

Morphisms are more important than objects: what about categories themselves? Given categories $\mathbf{C}$ and $\mathbf{D}$, a functor $F: \mathbf{C} \to \mathbf{D}$ is:

- for each object $A \in \text{Ob}(\mathbf{C})$, an object $F(A) \in \text{Ob}(\mathbf{D})$
- for each morphism $A \xrightarrow{f} B$ in $\mathbf{C}$, a morphism $F(A) \xrightarrow{F(f)} F(B)$ in $\mathbf{D}$ such that structure is preserved:
  - $F(g \circ f) = F(g) \circ F(f)$ for morphisms $A \xrightarrow{f} B \xrightarrow{g} C$ in $\mathbf{C}$
  - $F(\text{id}_A) = \text{id}_{F(A)}$ for objects $A$ in $\mathbf{C}$
Functors

Morphisms are more important than objects: what about categories themselves? Given categories \( C \) and \( D \), a functor \( F: C \to D \) is:

- for each object \( A \in \text{Ob}(C) \), an object \( F(A) \in \text{Ob}(D) \)
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  - \( F(g \circ f) = F(g) \circ F(f) \) for morphisms \( A \xrightarrow{f} B \xrightarrow{g} C \) in \( C \)
  - \( F(\text{id}_A) = \text{id}_{F(A)} \) for objects \( A \) in \( C \)

It is:

- **full** when \( f \mapsto F(f) \) are surjections \( C(A, B) \to D(F(A), F(B)) \)
- **faithful** when \( f \mapsto F(f) \) are injections \( C(A, B) \to D(F(A), F(B)) \)
- **essentially surjective on objects** each \( B \in \text{Ob}(D) \) is isomorphic to \( F(A) \) for some \( A \in \text{Ob}(C) \)
- **equivalence** when full, faithful, essentially surjective on objects
Natural transformations

Given functors $F, G : \mathcal{C} \to \mathcal{D}$, a natural transformation $\zeta : F \Rightarrow G$ assigns to every object $A$ in $\mathcal{C}$ of a morphism $F(A) \xrightarrow{\zeta_A} G(A)$ in $\mathcal{D}$, such that for every morphism $A \xrightarrow{f} B$ in $\mathcal{C}$:

\[
\begin{array}{ccc}
F(A) & \xrightarrow{\zeta_A} & G(A) \\
\downarrow F(f) & & \downarrow G(f) \\
F(B) & \xrightarrow{\zeta_B} & G(B)
\end{array}
\]

If every component $\zeta_A$ is an isomorphism then $\zeta$ is called a natural isomorphism, and $F$ and $G$ are said to be naturally isomorphic.
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If every component $\zeta_A$ is an isomorphism then $\zeta$ is called a natural isomorphism, and $F$ and $G$ are said to be naturally isomorphic.

A functor $F : \textbf{C} \rightarrow \textbf{D}$ is an equivalence if and only if there is a functor $G : \textbf{D} \rightarrow \textbf{C}$ and natural isomorphisms $G \circ F \simeq \text{id}_\textbf{C}$ and $F \circ G \simeq \text{id}_\textbf{D}$. 

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**Products**

Given objects $A$ and $B$, a **product** is:

- an object $A \times B$
- morphisms $A \times B \xrightarrow{p_A} A$ and $A \times B \xrightarrow{p_B} B$

such that any two morphisms $X \xrightarrow{f} A$ and $X \xrightarrow{g} B$ allow a unique morphism $(f/g) : X \to A \times B$ with $p_A \circ (f/g) = f$ and $p_B \circ (f/g) = g$

**Universal property:** $A \times B$ is universal way to put $A$ and $B$ together
Vector spaces

Set $V$ with element $0$, functions $+: V \times V \rightarrow V$, and $\cdot: \mathbb{C} \times V \rightarrow V$

- **additive associativity**: $u + (v + w) = (u + v) + w$;
- **additive commutativity**: $u + v = v + u$;
- **additive unit**: $v + 0 = v$;
- **additive inverses**: there exists a $-v \in V$ such that $v + (-v) = 0$;
- **additive distributivity**: $a \cdot (u + v) = (a \cdot u) + (a \cdot v)$
- **scalar unit**: $1 \cdot v = v$;
- **scalar distributivity**: $(a + b) \cdot v = (a \cdot v) + (b \cdot v)$;
- **scalar compatibility**: $a \cdot (b \cdot v) = (ab) \cdot v$.

Example: $\mathbb{C}^n$
Function $f: V \rightarrow W$ is **linear** when

$$f(v + w) = f(v) + f(w)$$

$$f(a \cdot v) = a \cdot f(v)$$

Vector spaces and linear maps form a category $\textbf{Vect}$
Bases and matrices

- Vectors \( \{e_i\} \) form basis when any vector \( v \) takes the form \( v = \sum_i v_i e_i \) for \( v_i \in \mathbb{C} \) in precisely one way.

- Any vector space has a basis
  any two bases have the same cardinality: dimension

- Finite-dimensional vector spaces and linear maps form a category \( \text{FVect} \)
Bases and matrices

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- Finite-dimensional vector spaces and linear maps
  form a category \( \mathbf{FVect} \)

- Given bases \( \{d_i\} \) and \( \{e_j\} \), linear map \( V \xrightarrow{f} W \) gives matrix \( f(d_i)_j \),
  and vice versa

- There is a category \( \mathbf{Mat}_\mathbb{C} \) of natural numbers and matrices
  There is an equivalence \( \mathbf{Mat}_\mathbb{C} \to \mathbf{FVect} \) given by \( n \mapsto \mathbb{C}^n \)
Hilbert spaces

Vector space $H$ with inner product $\langle -| - \rangle : H \times H \to \mathbb{C}$ such that

- **conjugate-symmetric**: $\langle v|w \rangle = \langle w|v \rangle^*$

- **linear** in second argument:
  $\langle v|a \cdot w \rangle = a \cdot \langle v|w \rangle$ and $\langle u|v + w \rangle = \langle u|v \rangle + \langle u|w \rangle$

- **positive definite**: $\langle v|v \rangle \geq 0$ with equality iff $v = 0$

- **complete** in the norm $\|v\| = \sqrt{\langle v|v \rangle}$
  (if $\sum_{i=1}^{\infty} \|v_i\| < \infty$ then $\lim_{n} \|v - \sum_{i=1}^{n} v_i\| = 0$ for some $v$)
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Linear $f : H \to K$ is **bounded** when $\|f(v)\| \leq \|f\| \cdot \|v\|$ for some $\|f\| \in \mathbb{R}$

Hilbert spaces and bounded linear maps form category **Hilb**
Finite-dimensional Hilbert spaces form category **FHilb**
Dual space

- Basis is **orthogonal** when \( \langle e_i | e_j \rangle = 0 \) for \( i \neq j \); **orthonormal** if \( \langle e_i | e_i \rangle = 1 \)

- Bounded \( H \xrightarrow{f} K \) has **adjoint** \( K \xrightarrow{f^\dagger} H \) with \( \langle f(v) | w \rangle = \langle v | f^\dagger(w) \rangle \) (conjugate transpose matrix)

- Given \( v \in H \), its **ket** \( \mathbb{C} \xrightarrow{|v\rangle} H \) is \( z \mapsto zv \); **bra** \( H \xrightarrow{\langle v|} \mathbb{C} \) is \( w \mapsto \langle v | w \rangle \)

- Dual Hilbert space \( H^* \) is \( \textbf{Hilb}(H, \mathbb{C}) \)
Categories: objects and (more importantly) morphisms

Examples: sets and functions, sets and relations, vector spaces and linear functions, Hilbert spaces and bounded linear functions

Isomorphic objects: behave the same

Functors: ‘morphisms between categories’

Equivalent categories: behave the same

Products: combine objects universally