# First steps in a (linear) algebra of (quantum) functional programming

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#### INESC TEC & University of Minho (QuantaLab initiative)

Prelude

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Quantum folds?

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References

#### Context



- New initiative at Minho
- Quantum computing more and more on spot in the media
- Trying to address **quantum programming** from an **algebraic** (category-theoretical) perspective.
- Need to abstract from the physics level.

Acknowledgemen

References

#### Literature is vast!

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2011 (vintage year):
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The "bible", compiled by B. Coecke:
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"New Structures for Physics", Lect. Notes in Physics volume 813, 2011

The generic structures (monoidal categories) in which quantum physics are expressed in this book accommodate typed linear algebras in a natural way.



Acknowledgemen

References

#### Literature is vast!

2011 (vintage year):

The 10th Anniversary Edition of the "classic" by Nielsen and Chuang.

But there is more — Selinger's **qPL** (2004) etc etc

Literature is vast.

This includes previous WG2.1 work in this field, see e.g. Mu and Bird (2001).



#### Opportunities for QP

"Equation" a la Wirth:

(Quantum) Programs = (Quantum) Algorithms + (Quantum) Data Structures

Quantum algorithms based on elementary **components**, called **quantum gates**.

Classical bits generalize to quantum bits  $(\mathbf{qubits})$  — quantum data.



## What QP should (eventually) be

 $\ensuremath{\mathbf{QP}}$  expected to evolve and reach maturity as the other bodies of knowledge in programming, requiring

- a syntax
- a semantics
- a calculus

This enables **program calculation**, the *scientific method* applied to software.

E.g., the **FP calculus** derives one version of the *Fibonacci recurrence relation* (aside) from the other. fib 0 = 0fib 1 = 1fib (n+2) = fib (n+1) + fib n

fib n = let (x, y) = for loop (0, 1) n loop (x, y) = (y, x + y)in x

## Syntax, semantics, calculus (FP)

#### Syntax:

- Sequential composition  $(f \cdot g \text{ seen above})$
- Parallel composition (f v g) based on pairing (f v g) x = (f x, g x)
- Alternative composition [f, g] the dual of pairing
- Recursive solutions to equations involving the above.

Semantics, e.g. that of pairing

$$k = f \circ g \Leftrightarrow \begin{cases} fst \cdot k = f \\ snd \cdot k = g \end{cases}$$



(1)

#### Syntax, semantics, calculus (FP)

#### Calculus, e.g. fusion,

 $(f \circ g) \cdot h = (f \cdot h) \circ (g \cdot h)$ 

#### loss-less decomposition

 $k = (fst \cdot k) \lor (snd \cdot k)$ <sup>(2)</sup>

#### reflection

 $fst \circ snd = id \tag{3}$ 

pairwise equality

$$k \circ h = f \circ g \Leftrightarrow \begin{cases} k = f \\ h = g \end{cases}$$
(4)

and so on.

#### Does this hold in the quantum world?

Quantum computations are all **reversible**.

This is expressed in linear algebra by **unitary** matrices (more about this later)

Isomorphisms are unitary and many quantum gates are isos

Yesterday we have seen how **pairing** differs from functions in the case of stochastic matrices

With matrices in general, **products** have to do with **coproducts** and not with **pairing** — this leads to **biproducts**.

1.

#### **Biproducts**

1.

In LA **coproducts** correspond to putting matrices side by side (horizontally):

$$X = [M|N] \Leftrightarrow \begin{cases} X.i_1 = M \\ X.i_2 = N \end{cases} \qquad A \xrightarrow{q} A + B < 2 B \\ M \downarrow M \downarrow N \\ C \end{pmatrix}$$

Products correspond to putting matrices side by side vertically:



This is the basis of **block** operations in LA and leads to **direct sums**:  $M \oplus N = [i_1 \cdot M | i_2 \cdot N] = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix}.$  Prelude

Quantum folds?

#### Quantum gates

Let us briefly show how standard **quantum programming gates**, used in **quantum circuits** (Nielsen and Chuang, 2011), can be expressed in typed LA.

They can be **decomposed** into polymorphic, elementary matrix categorial **units**.

Pairing (Khatri-Rao  $\nabla$  + Kronecker products  $\otimes$ )<sup>1</sup> is central to quantum data structuring.

Interestingly, **biproducts** can make quantum gates easier to understand and reason about, as I will briefly show.

<sup>&</sup>lt;sup>1</sup>The latter is defined by  $M \otimes N = (M \cdot fst) \lor (N \cdot snd)$ .

#### Quantum processing

**Quantum application** — like function application, the outcome of processing quantum data *s* by quantum gate *P* is given by  $P \cdot s$ :



**Qubits** — The smallest (useful) *A* is 2, the Booleans — so a (qu)bit  $2 < \frac{s}{b} = 1$  is always a vector of the form  $\begin{bmatrix} a \\ b \end{bmatrix}$ .

#### 'Ket' Notation — traditionally,

- $|0\rangle: 1 \to 2$  denotes the vector  $\begin{bmatrix} 1\\ 0 \end{bmatrix}$  which represents point  $\underline{0}$  (a bit holding 0).
- $|1\rangle: 1 \rightarrow 2$  denotes the vector  $\begin{bmatrix} 0\\1 \end{bmatrix}$  which represents point <u>1</u> (a bit holding 1).

## $|\phi angle$ notation

Since  $\begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ , the notation  $a |0\rangle + b |1\rangle$  is normally used to denote **qubit**  $\begin{bmatrix} a \\ b \end{bmatrix}$ .

A qubit  $2 < \frac{a |0\rangle + b |1\rangle}{1}$  expresses a quantum **superposition** of the two truth values.

Complex numbers  $a, b \in \mathbb{C}$  are called **amplitudes** and are such that  $a^2 + b^2 = 1$ .

Given two qubits  $1 \xrightarrow{u} 2$  and  $1 \xrightarrow{v} 2$ ,  $1 \xrightarrow{u^{\vee} v} 2 \times 2$  denotes their **pairing**.

This leads to an extension of the 'ket' notation (next slide).

## $|\phi\rangle$ notation and pairing

 $|0\rangle \, {\bf v} \, |1\rangle$ 

= { thinking functional helps }

 $\underline{0} \,\,^{\triangledown} \,\, \underline{1}$ 

= { constant functions }

(0,1)

- = { vector notation }
  - $\begin{bmatrix} 0\\1\\0\end{bmatrix}$

- $\{ extended `ket' notation \}$
- $|01\rangle$

=

## $|\phi\rangle$ notation and pairing

More generally, the qubit pairing  $(a |0\rangle + b |1\rangle) \circ (c |0\rangle + d |1\rangle)$  yields, once converted to vector notation

	$\left[\frac{a}{b}\right] \lor \left[\frac{c}{d}\right]$					
=	{ Khatri-Rao }					
	ac ad bc bd					
=	<pre>{ vector addition }</pre>					
	$\begin{bmatrix} \mathbf{ac} \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \mathbf{ad} \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \mathbf{bc} \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \mathbf{bd} \end{bmatrix}$					
that is, ac	$ 00\rangle + ad  01\rangle + bc  10\rangle + bd  11\rangle.$					

#### Qubit entanglement

The qubit pair

 $2 \times 2 \xleftarrow{\frac{|00\rangle + |01\rangle}{\sqrt{2}}} 1$ 

is a well-known example of **entaglement** – you get

 $\begin{aligned} & \textit{fst} \cdot \frac{|00\rangle + |01\rangle}{\sqrt{2}} = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \\ & \textit{snd} \cdot \frac{|00\rangle + |01\rangle}{\sqrt{2}} = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \end{aligned}$ 

but

$$\frac{|0\rangle+|1\rangle}{\sqrt{2}} \sqrt[]{} \frac{|0\rangle+|1\rangle}{\sqrt{2}} = 2 \times 2 \overset{\left(\frac{1}{2}\right)^{\circ}}{\checkmark} 1$$

is different from the original  $2 \times 2 \stackrel{|00\rangle+|01\rangle}{\checkmark} 1$  .

Acknowledgemen

References

#### Quantum control

A well-known quantum gate is the Hadamard gate:

$$2 \stackrel{H}{\longleftarrow} 2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$$

Applying this gate to qubit  $u = a |0\rangle + b |1\rangle$ :



Calculation:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix} \cdot (\mathbf{a} |0\rangle + \mathbf{b} |1\rangle) = \frac{1}{\sqrt{2}} \left( \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} \right) = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{a} + \mathbf{b} \\ \mathbf{a} - \mathbf{b} \end{bmatrix} = \frac{\mathbf{a} + \mathbf{b}}{\sqrt{2}} |0\rangle + \frac{\mathbf{a} - \mathbf{b}}{\sqrt{2}} |1\rangle.$$

## Classic control (functional programming)

(Polymorphic) functional programming can play a nice role in quantum processing (perhaps not fully appreciated yet).

Think of the function swap (a, b) = (b, a), that is, the **isomorphism**:

 $A \times B \xrightarrow{swap} B \times A = snd \, \forall \, fst.$ 

For A = B = 2, this corresponds to the classical gate



=

References

#### SWAP Gates

Applied to a qubit pair it will yield:

$$\textit{swap} \cdot \left( \textit{a} \mid \! 00 \rangle + \textit{b} \mid \! 01 \rangle + \textit{c} \mid \! 10 \rangle + \textit{d} \mid \! 11 \rangle \right)$$

 $\{$  expand to vector notation  $\}$ 

swap 
$$\cdot$$
 (a  $\begin{bmatrix} 1\\0\\0\\0\end{bmatrix} + b \begin{bmatrix} 0\\1\\0\\0\end{bmatrix} + c \begin{bmatrix} 0\\0\\1\\0\end{bmatrix} + d \begin{bmatrix} 0\\0\\0\\1\end{bmatrix}$ )

$$= \{ swap = snd \lor fst ; vector addition \}$$
$$(snd \lor fst) \cdot \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

 $= \begin{cases} matrix-vector multiplication; then back to <math>|\phi\rangle$  notation }  $a |00\rangle + c |01\rangle + b |10\rangle + d |11\rangle \end{cases}$ 

#### The Fredkin gate

This is a 3-(qu)bit gate, also known as "controlled"-SWAP. Let us see why.

Untyped description:





As a function (pointwise) of type *fred* :  $2 \times (2 \times 2) \rightarrow 2 \times (2 \times 2)$ :

 $\begin{cases} fred (0, x) = (0, x) \\ fred (1, (b, c)) = (1, (c, b)) \end{cases}$ 

References

#### Back to elementary AoP

$$\begin{cases} fred \cdot (\underline{0} \circ id) = \underline{0} \circ id \\ fred \cdot (\underline{1} \circ id) = \underline{1} \circ swap \end{cases}$$

$$\Leftrightarrow \qquad \{ \text{ coproducts } \} \\ fred \cdot \underline{[0} \circ id | \underline{1} \circ id] = \underline{[0} \circ id | \underline{1} \circ swap] \\ \Leftrightarrow \qquad \{ \underline{1} \cdot swap = \underline{1} \text{ and so on } \} \\ fred \cdot \alpha = \alpha \cdot (id \oplus swap) \\ \Leftrightarrow \qquad \{ \text{ introduce } C = (id \oplus) \} \\ fred \cdot \alpha = \alpha \cdot C \ swap \end{cases}$$

that is,  $\alpha$  translates *fred*kin into *C*ontrolled *swap*.

Acknowledgemen

References

(5)

(6)

(7)

#### The $\alpha$ -isomorphism

The above is a faithful transformation

fred  $\leftarrow \alpha$  C swap

because it relies on parametric isomorphism

 $\alpha : \mathbf{A} + \mathbf{A} \to 2 \times \mathbf{A}$  $\alpha = [\underline{0} \lor id | \underline{1} \lor id])$ 

that (by the exchange law) can also be written  $\alpha = [0|1] \lor [id|id]$ 

with natural property:

 $\alpha \cdot (M \oplus M) = (id \otimes M) \cdot \alpha$ 

For free we obtain that *fred* is an **isomorphism** too.

#### The $\alpha$ -isomorphism

The translation from a pair-wise description of the Fredkin gate to a copair-wise one is so useful that we define, for every  $M: 2 \times A \rightarrow B$ , the corresponding  $M': A + A \rightarrow B$  defined by

$$M' = M \cdot \alpha \tag{8}$$

This transform has a number of immediate properties:

$$(M \circ N)' = M' \circ N' \tag{9}$$

$$id' = \alpha \tag{10}$$

$$fst' = ! \oplus ! \tag{11}$$

$$xor' = [id|\neg] \tag{13}$$

an so on.

## The CNOT gate

Think now of implementing *xor* :  $2 \times 2 \rightarrow 2$  defined by

xor (0, a) = a $xor (1, a) = \neg a$ 

Clearly, this gate is not **injective** — e.g. *xor* (0,0) = xor (1,1) — and therefore not **reversible**.

The laws of quantum physics give no hope for non-reversible computations, so how can such an important classical gate be incorporated in quantum circuits?

The trick is to add a "garbage" bit to the output, which becomes type  $2 \times 2$  making room for a reversible computation:

 $xor_{-}(a,b) = (a,xor(a,b))$ 

How can we be sure this is reversible (isomorphism)?

Acknowledgemen

References

## Easy (indirect) calculation

xor\_′ { definition }  $(fst \lor xor)'$ { laws given }  $(! \oplus !) \lor [id | \neg]$  $\{ ! \forall M = M \text{ etc } \}$ =  $[i_1|i_2 \cdot \neg]$ { coproducts }  $id \oplus \neg$ { defined above } =  $C \neg$ 

Because  $\alpha$  is an isomorphism, f is **injective** iff  $f' = f \cdot \alpha$  is so.

So the calculation on the left is an indirect way of proving that *fst* is a **constant complement** of *xor* (Matsuda et al., 2007).

No need for **pointwise** arguments!

## Toffoli gate (CCNOT)

#### Diagram:



As a functional program:

 $toffoli: (2 \times 2) \times 2 \rightarrow (2 \times 2) \times 2$  $toffoli ((1,1), c) = ((1,1), \neg c)$ toffoli ((a,b), c) = ((a,b), c)

the same as

toffoli  $((a, b), c) = ((a, b), xor (a \land b, c))$ 

A very useful gate, cf.

toffoli  $((a, 1), c) = ((a, 1), xor \ a \ c)$  — implements xor toffoli  $((a, b), 0) = ((a, b), a \land b)$  — implements  $\land$ toffoli  $((1, 1), c) = ((1, 1), \neg c)$  — implements  $\neg$ 

## Toffoli gate

Pointfree *toffoli*, as a linear algebra expression:

 $toffoli : (2 \times 2) \times 2 \rightarrow (2 \times 2) \times 2$  $toffoli = fst \lor (xor \cdot (\land \otimes id))$ (14)

Again note how far the "useful part" of toffoli

$$xor \cdot (\wedge \otimes id) = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

is from being a  $\ensuremath{\textit{reversible}}$  computation, as all quantum gates should be.

The trick will be the same — pair with constant complement (fst  $\vee$  \_).

In general, functional pairing always increases injectivity because

 $(f \circ g)^{\circ} \cdot (f \circ g) = (f^{\circ} \cdot f) \times (g^{\circ} \cdot g)$ (15)

and  $f^{\circ} \cdot f$  (the kernel of f) measures the injectivity of f.

## Toffoli gate

Altogether, for A = 2 in the type of  $\alpha$ :



Calculations (omitted for brevity) will derive, from the diagram above,

$$X = id \oplus (id \oplus \neg) = C (C \neg))$$



where  $2 \xrightarrow{\neg} 2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$  — a much simpler version of (14).

#### Controlled-U gates

Generalizing, **controlled-U** gates are captured by the **generic** combinator:

 $C: (A \rightarrow B) \rightarrow (2 + A \rightarrow 2 + B)$   $C (U) = id \oplus U$ where  $2 \xrightarrow{id} 2$ , whereby fredkin = C swap  $xor_{-} = C \neg$   $toffoli = C (C \neg)$ 

and so on. Moreover,  $C_{-}$  is a **functor**:

$$C \ id = id \tag{16}$$
$$C \ (M \cdot N) = (C \ M) \cdot (C \ N) \tag{17}$$

#### Unitary gates

The isomorphisms (reversible functions) we have seen so far are special cases of so-called **unitary** matrices.

A  $\mathbb{C}$ -valued matrix U is unitary iff  $U \cdot U^* = U^* \cdot U = id$ , where  $U^*$  is the **conjugate** transpose of U.

**Isomorphisms** admit further decompositions in terms of such matrices, for instance "the sqrt of not"

 $\neg = (\sqrt{\neg}) \cdot (\sqrt{\neg})$ 

where

$$\sqrt{\neg} = \frac{1}{2} \left( \top + i \left( id - \gamma \right) \right) = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$$

Thus one gets into the wonderful world of **actual** quantum gates in which classical logic operations are no longer primitive.

Suppose we want to apply the Hadamard gate

$$2 \stackrel{H}{\longleftarrow} 2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$$

*n* times to qubit q — a kind of **for**-loop: **for** H n q

Expanding — and ignoring the quantum essence of H for the moment:

for  $H \ 0 \ q = q$ for  $H \ (n+1) \ q = H$  (for  $H \ n \ q$ )

From the type of for  $H: \mathbb{N}_0 \to 2 \to 2$ , or the isomorphic  $\mathbb{N}_0 \times 2 \to 2$ , we see that for H cannot be reversible.

But type  $N_0 \times 2 \rightarrow N_0 \times 2$  would have room to accommodate one such reversible computation.

So we go for the uncurried version, paired with fst as before — the **constant complement** trick again — abbreviated to f:

$$f(0,q) = (0,q) f(n+1,q) = (n+1, H (snd (f (n,q))))$$

Because H is not a function, we have to go **pointfree** (in LA) to have the right definition:

 $f \cdot (\underline{0} \otimes id) = \underline{0} \otimes id$  $f \cdot (succ \otimes id) = (succ \cdot fst) \lor (H \cdot snd \cdot f)$ 

Putting the two lines together using **coproducts** and converse, we get the **recursive** matrix,

 $f = [\underline{0} \otimes id|(succ \cdot fst) \circ (H \cdot snd \cdot f)] \cdot (([\underline{0}|succ] \otimes id) \cdot \beta)^{\circ}$ 

cf. diagram



where  $\beta$  is the obvious isomorphism.

To test this quantum program in MATLab we fix an approximation to  $N_0$ , for instance we restrict to *n*-bit numbers in  $\{0...2^n - 1\}$ , taking  $\beta = id$  valid at matrix level into account:



Then we iterate over  $f = \underbrace{[\underline{0} \otimes id|(succ \cdot fst) \circ (H \cdot snd \cdot f)] \cdot ([\underline{0}|succ] \otimes id)^{\circ}}_{F f}$ 

starting with  $f_0 = 2^n \times 2 \stackrel{\perp}{\longleftarrow} 2^n \times 2$  holding zeros only.

References

#### MatLab checking

In  $2^n$  iterations we reach the fixpoint:

```
>> f4=[ (kron(z,id)) kr(s*fst(4,2),H*snd(4,2)*f3) ]*out
```

f4	=							
	1.0000	0	0	0	0	0	0	0
	0	1.0000	0	0	0	0	0	0
	0	0	0.7071	0.7071	0	0	0	0
	0	0	0.7071	-0.7071	0	0	0	0
	0	0	0	0	1.0000	0	0	0
	0	0	0	0	0	1.0000	0	0
	0	0	0	0	0	0	0.7071	0.7071
	0	0	0	0	0	0	0.7071	-0.7071

Note the type  $f_4: 2^n \times 2 \to 2^n \times 2$ .

Since it is a real valued, symmetric matrix, it is **unitary**.

References

#### MatLab checking

Suppose we want to check the outcome of for  $H \ 3 (|0\rangle - |1\rangle)$ .

We obtain this by running 
$$f_4 \cdot (\underline{3} \vee \begin{bmatrix} \underline{1} \\ -1 \end{bmatrix}) = f_4 \cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \vee \begin{bmatrix} \underline{1} \\ -1 \end{bmatrix}$$
, cf.

This corresponds to the pair  $(3, |0\rangle + \frac{|1\rangle}{\sqrt{2}})$ , as expected.

References

#### Phase-shift gates

The for-loop above gets more interesting when we replace the Hadamard gate by the so-called **phase shift gate** defined by

$$R_{\phi} = (\sigma \ \phi) \ ^{\forall} \ id = \begin{bmatrix} 1 & 0 \\ 0 & e^{i \ \phi} \end{bmatrix}$$

where

$$\sigma \phi = [1 \ e^{i \phi}].$$

Recalling  $e^{i\phi} = \cos\phi + i\sin\phi$ the fixpoint of



for the same types is given in the next slide.



#### Iterating a phase-shift gate



Complex matrix  $f_4$  is unitary.

Note the effect of the constant complement (*fst*  $\neg$  \_) shifting the corresponding iteration of gate  $R_{\frac{\pi}{c}}$  along the diagonal.

#### Summary

Very experimental still.

Previous work on stochastic folds in LA (Murta and Oliveira, 2015) showed that we can have **quantitative** algebras of programming

Would like to investigate the AoP of  ${\color{black} \textbf{unitary}}$  (recursive) matrices now

Towards **correct by construction** quantum programs, who knows...

Need to investigate Ralph Hinze's "Adjoint folds" not in CCCs but rather in MCCs

Also studying previous WG2.1 work in the field (Mu and Bird, 2001)

Acknowledgement

References

#### Acknowledgement

The idea of a *"linear algebra of programming"*, which underlies this talk, was first put forward by Amílcar Sernadas (1952–2017), the key idea being



"to adopt linear algebra as the lingua franca of **software verification**" (SQIG-Group, 2011).

I thank Amílcar for his friendship and good advice, and his research group for this and so many other inspirations.

Prelude

Quantum gates

Quantum folds?

Acknowledgement

References

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Prelude

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