Differentiation of causal functions

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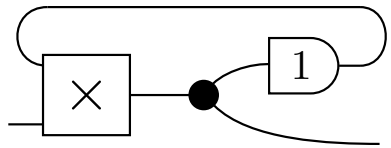
National Institute of Informatics
ERATO MMSD

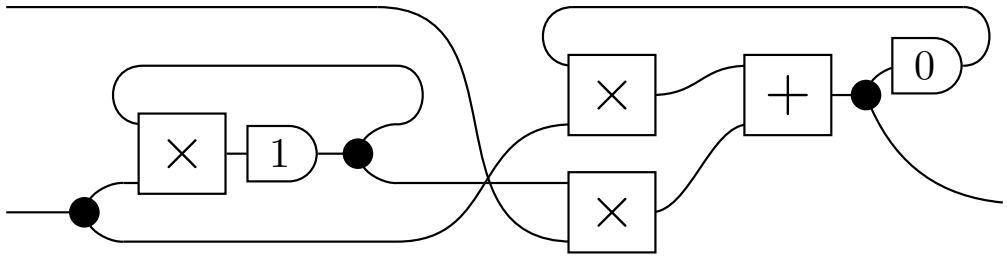
IU Logic Colloquium
March 21, 2019

Where we're heading

I would like to convince you the derivative of this function:



Is this:



How we get there

1. Causal functions
2. Computation sequences
   - Main ideas
   - Sanity check
3. Delayed trace
4. Neural networks
5. Cartesian differential categories
6. Recap and future directions

Causal functions on sequences

A^ω is the set of *A-valued infinite sequences*. The entries of $\sigma \in A^\omega$ are $[\sigma]_k = \sigma_k \in A$ for $k \in \mathbb{N}$, so $\sigma = (\sigma_0, \sigma_1, \ldots, \sigma_k, \ldots)$.

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Definition

A *causal* function $f : A^\omega \to B^\omega$ satisfies

$$\forall \sigma, \tau \in A^\omega, \forall k \in \mathbb{N}, [\sigma]_{0:k} = [\tau]_{0:k} \to [f(\sigma)]_{0:k} = [f(\tau)]_{0:k}$$

Intuitively, the first k outputs of f only depend on the first k inputs.

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$$[\mathtt{zip}(\sigma, \tau)]_k = \begin{cases} \sigma_{k/2} & \text{if } k \equiv 0 \pmod 2 \\ \tau_{(k-1)/2} & \text{if } k \equiv 1 \pmod 2 \end{cases}$$ is causal.

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5. $\mathtt{tl} : A^\omega \to A^\omega$ defined by $[\mathtt{tl}(\sigma)]_k = \sigma_{k+1}$ is **not causal**, since output k is input $k + 1$.

Background

Causal functions appear all over computer science:

1. Mealy machines [Mealy, 1955 and Eilenberg, 1974]
2. Coalgebra [Rutten, 2006]
3. Synchronous digital circuits [Leiserson and Saxe, 1986]
4. Signal flow graphs [Bonchi, Sobociński and Zanasi, 2014 and Milius, 2010]
5. Recurrent neural networks [Rumelhart, 1986 and Hochreiter and Schmidhuber, 1997]

(If you have examples from mathematics where this class of functions is important, let me know!)

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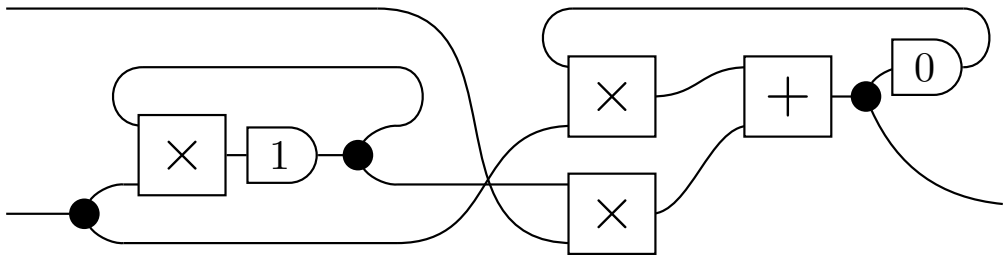
Thus one way to specify a causal function is to specify a state in a Mealy machine. This is the basis of the *syntactic (GSOS) method* in stream differential equations. [Hansen, Kupke and Rutten, 2017]

Digital circuit / signal flow graph approach

Circuit diagram treatments of causal functions are more explicit about how state is stored, how it is updated, and how outputs are produced. For example:



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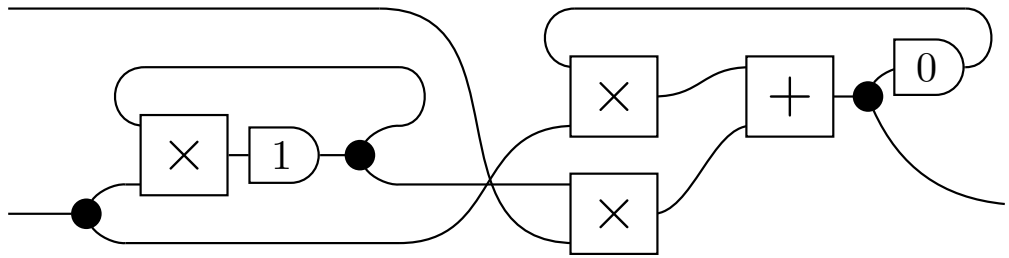

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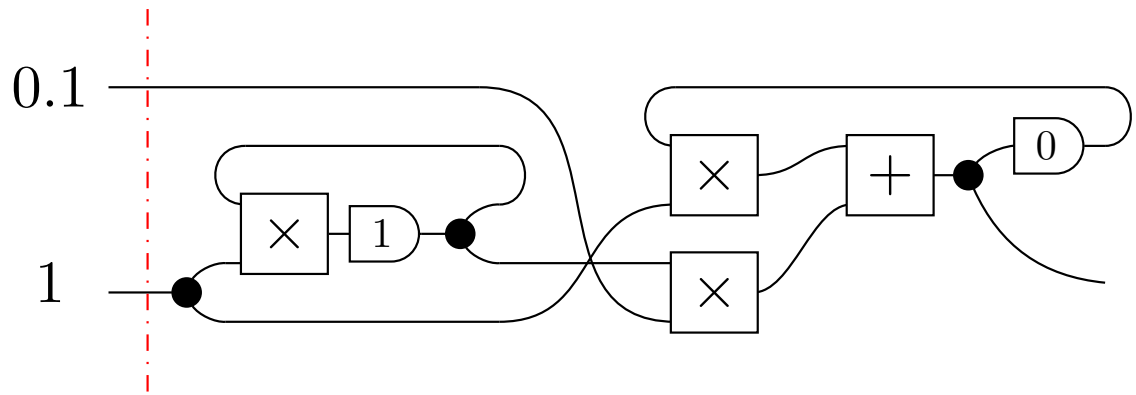

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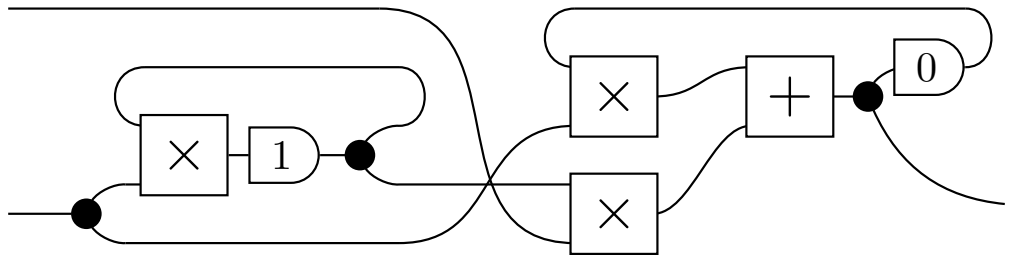

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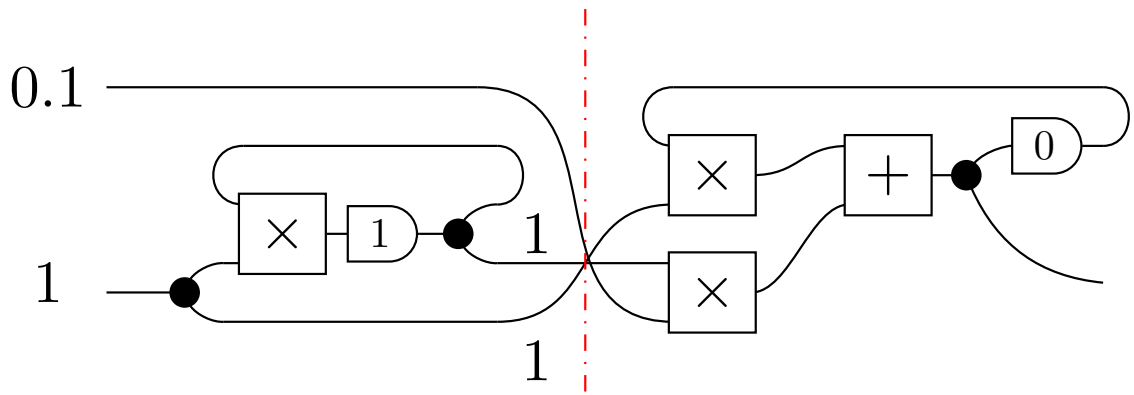

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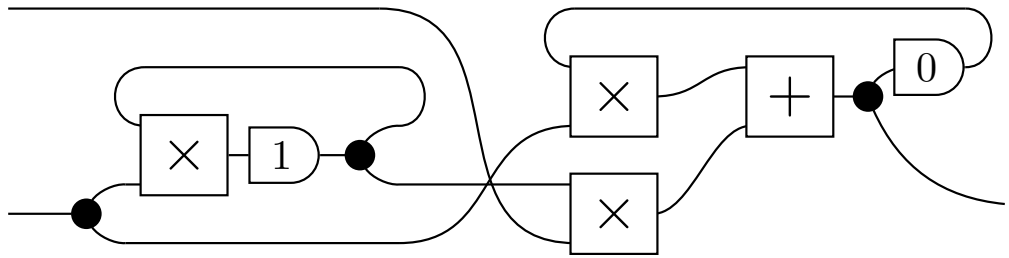

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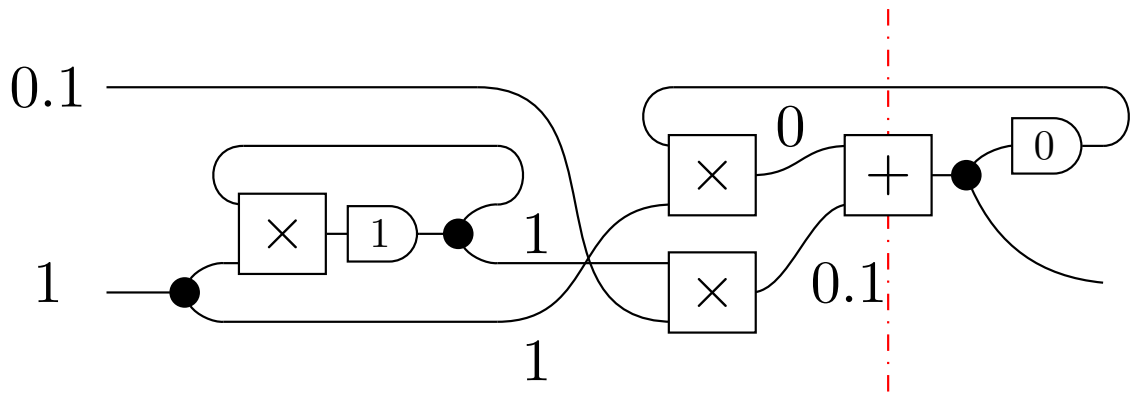

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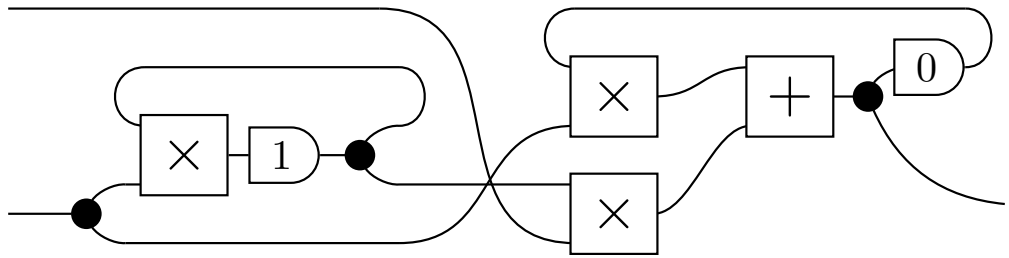

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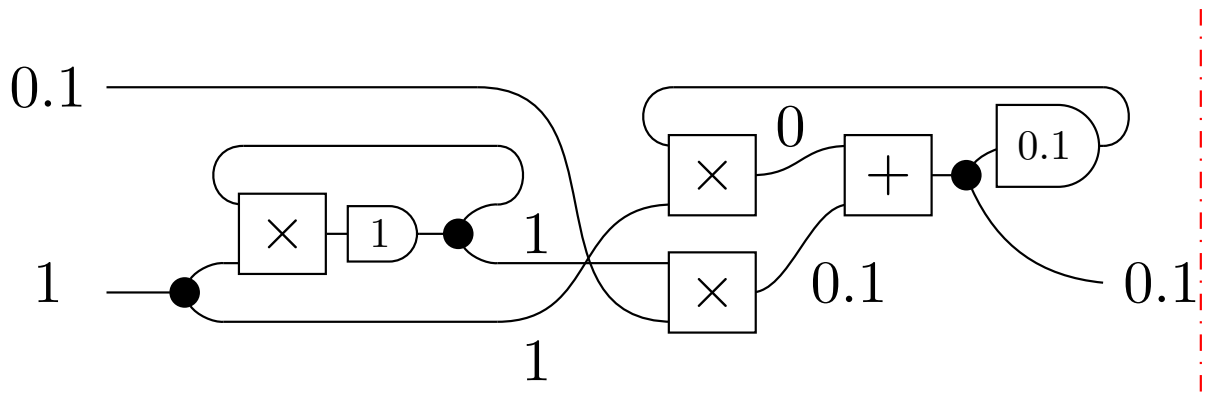


Recurrent neural networks

RNNs are special instances of the circuit diagram approach with the requirement that the functions involved are *differentiable*.

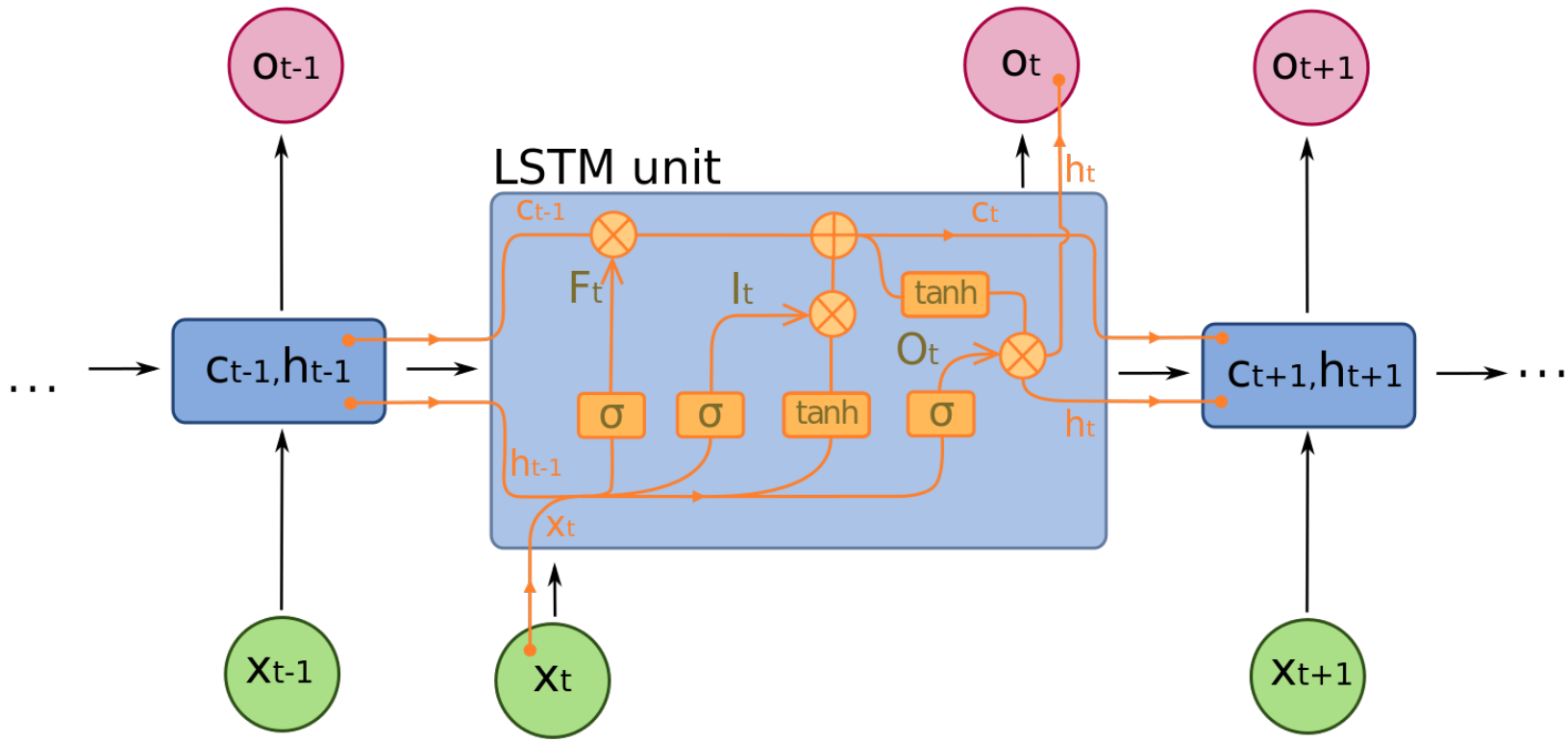


Figure: François Deloche - Own work, CC BY-SA 4.0, wikimedia

Finite approximations approach

Another perspective on causal functions is to treat them as a limit of functions on finite lists. This is based on the following observation:

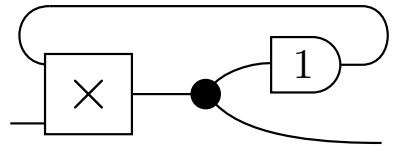
Theorem

The following are equivalent:

1. *a causal function* $f : A^\omega \to B^\omega$,
2. *an infinite sequence of functions* $u_k : A^{k+1} \to B$, *and*
3. *an infinite sequence of functions* $t_k : A^{k+1} \to B^{k+1}$ *satisfying* $[t_{k+1}(\vec{a})]_{0:k} = t_k([\vec{a}]_{0:k})$ *for all* $\vec{a} \in A^{k+2}$.

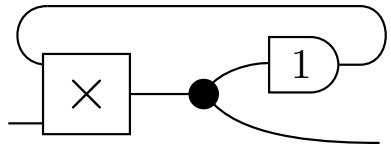
Proof Idea. u_k gives the $k+1^{\text{st}}$ entry in the sequence produced by f, and t_k provides the first $k+1$ entries.

What causal function is represented by this circuit?



Where we're heading, update I

I would like to convince you the derivative of the running product:



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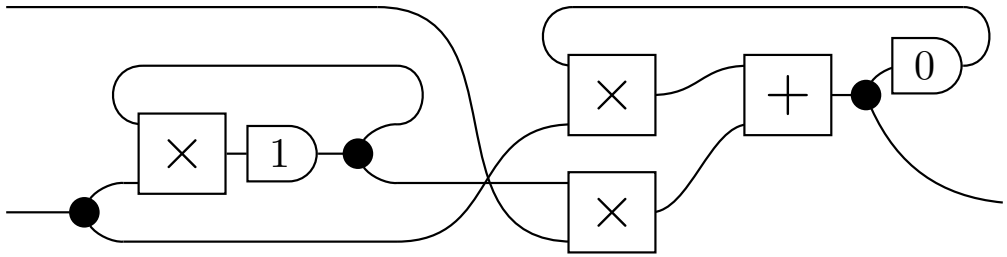

Outline

Main ideas

We start from a (strictified Cartesian) category $\mathbb{C}$ whose morphisms represent simple computations. Our goal is to define an extended category whose morphisms are causal functions.

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There are three steps:

1. describe a single step of the computation, including a mechanism for sending and receiving state
2. chain single steps together to get a computation sequence
3. quotient these computation sequences by their observable behaviour.

Step 1: Single computation steps

We separate inputs and outputs of a $\mathbb{C}$-morphism into two classes: *values*, exchanged with the environment, and *states*, exchanged with next/previous steps of the computation.

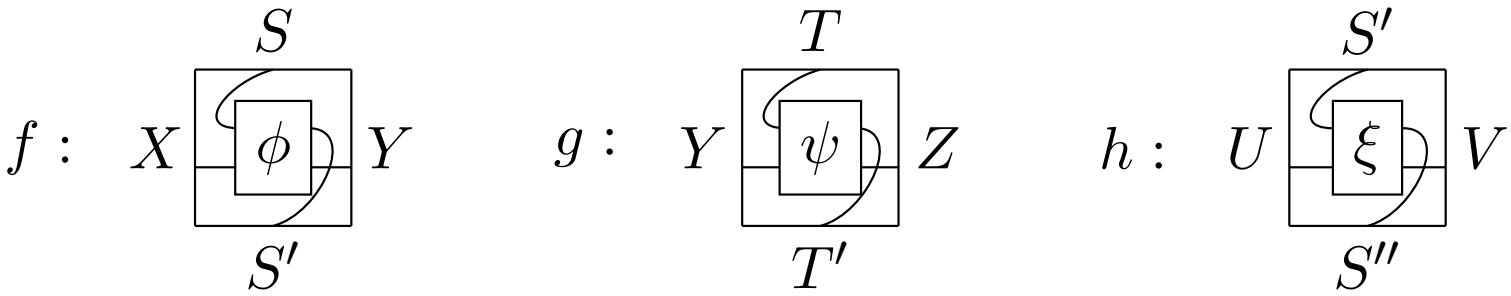
Definition

A *computation step* $f : X \xrightarrow[S']{S} Y$ is four objects and a morphism:

1. S — the input state received from the previous step
2. X — the input value received from the environment
3. S' — the output state sent to the next step
4. Y — the output value sent to the environment
5. $\phi : S \times X \to S' \times Y$ — the $\mathbb{C}$-morphism doing the computation

Step 1: Single computation steps

We can draw a single step like so:



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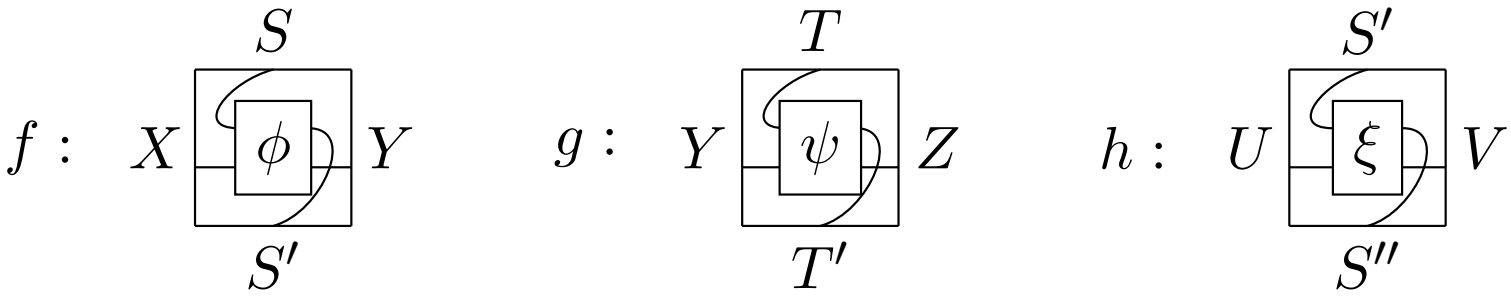
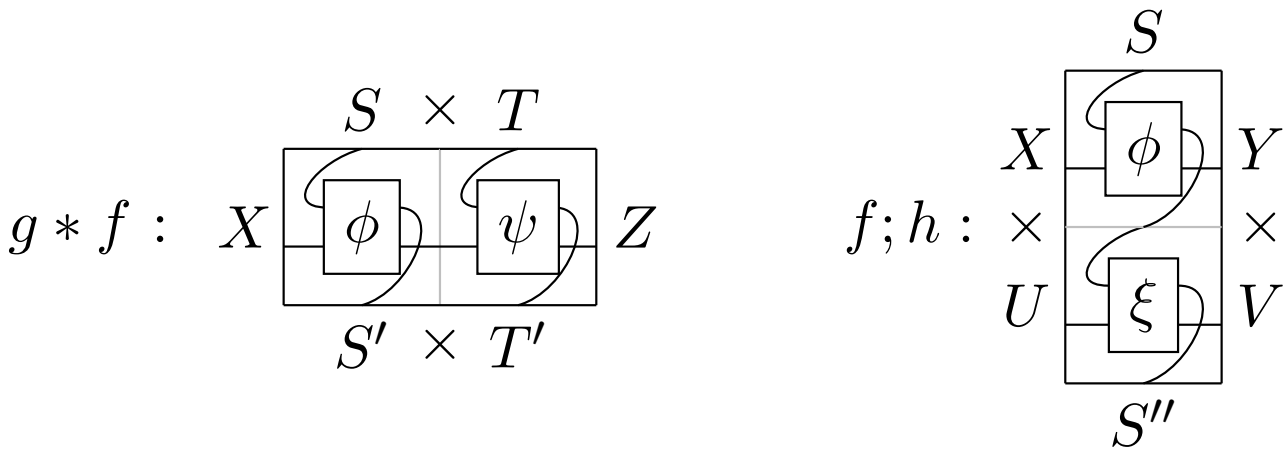


Computation steps can be composed in two different ways:



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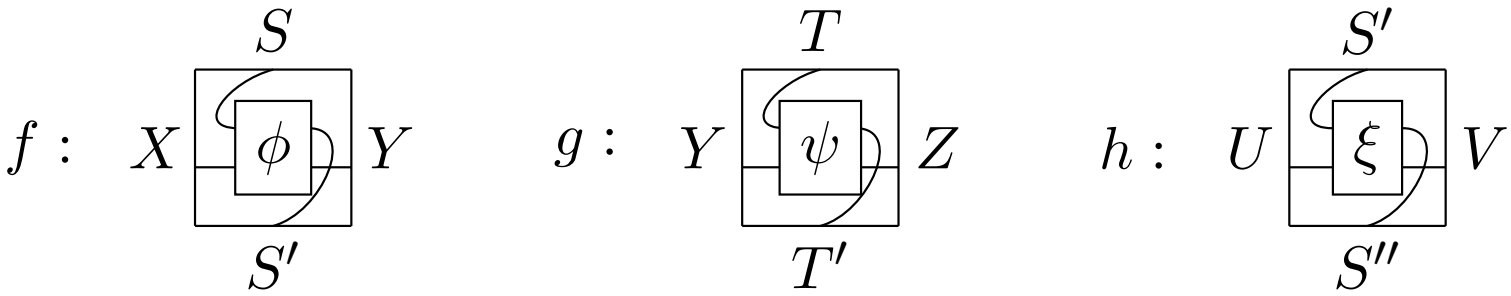

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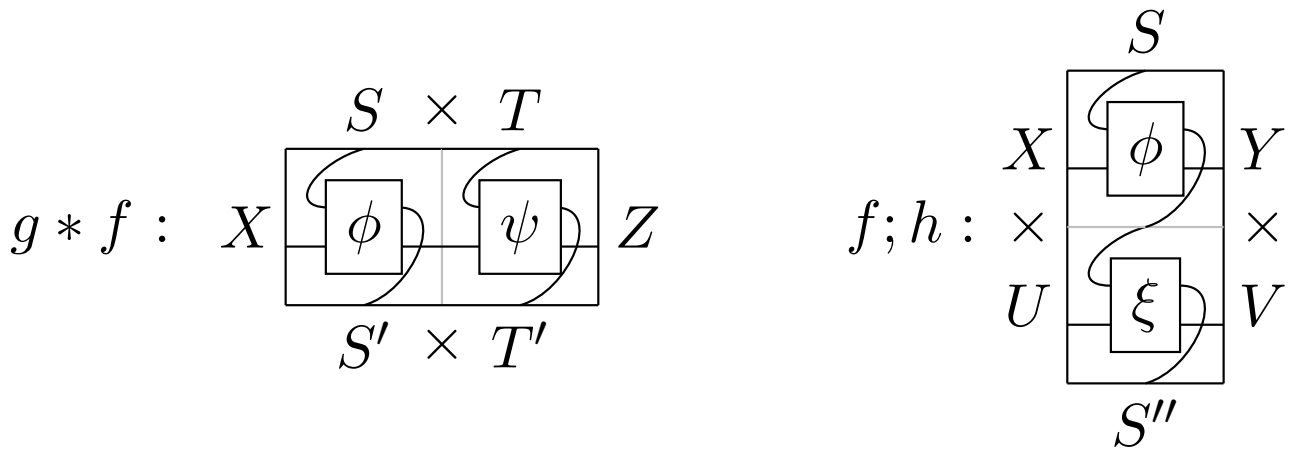


psst . . . double category

Step 2: Computation sequences

Next, we chain together infinitely many of these computation steps to compute a sequence of outputs.

Definition

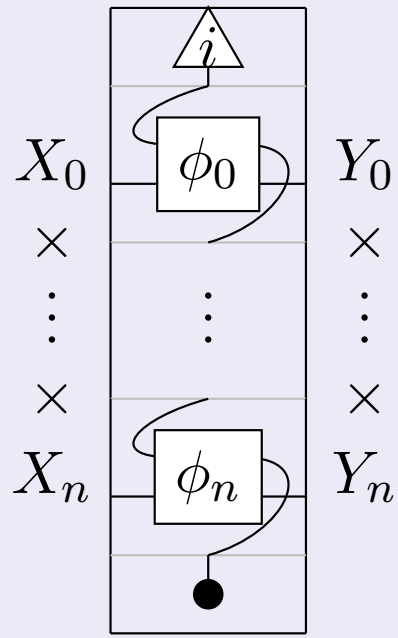
A *computation sequence* $\mathbf{f} = (i, [f_k])$ is an infinite sequence of computation steps $f_k : X_k \xrightarrow[S_{k+1}]{S_k} Y_k$, and an initial state $i : 1 \xrightarrow[S_0]{1} 1$. We say $\mathbf{f}$ takes sequences of type $[X_k] = (X_0, X_1, \ldots)$ to sequences of type $[Y_k] = (Y_0, Y_1, \ldots)$.

Note that f_k and f_{k+1} are vertically composable, as are i and f_0.

Step 3: Comparing computation sequences

Definition

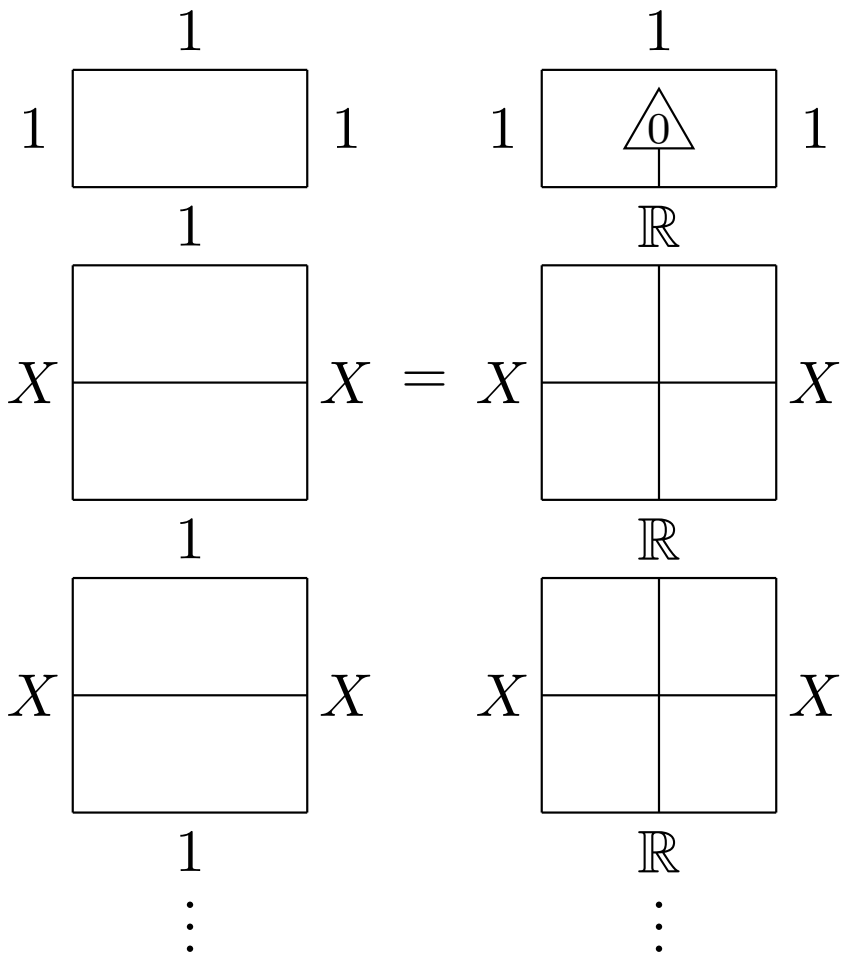
The n*th truncation* of a computation sequence is the morphism of the vertical composite of the first $n+1$ steps:



Definition

Two computation sequences $\mathbf{f}, \mathbf{g} : [X_k] \to [Y_k]$ are *extensionally equivalent* means they have the same nth truncation for all $n \in \mathbb{N}$.

Step 3: Extensionally equivalent identity computations



Step 3: Comparing computation sequences

Definition

A *stateful (sequence) function* is an extensional equivalence class of computation sequences.

Definition

If $\mathbb{C}$ is a (strict) Cartesian category, then its *stateful extension* is a category $\mathrm{St}(\mathbb{C})$ where

- objects are $[X_k]$, i.e. infinite sequences of objects in $\mathbb{C}$ and
- morphisms are stateful functions $\mathbf{f} : [X_k] \to [Y_k]$.

Sanity check

Theorem

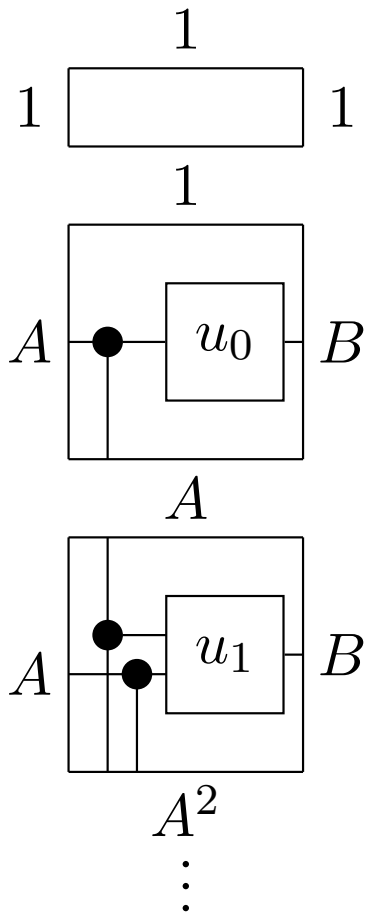
The homset $\mathrm{St}(\mathit{Set})([A],[B])$ *is in 1-1 correspondence with the set of causal functions from* A^ω *to* B^ω*.*

Sanity check

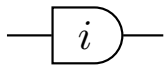
Theorem

The homset $\mathrm{St}(Set)([A],[B])$ *is in 1-1 correspondence with the set of causal functions from* A^ω *to* B^ω*.*

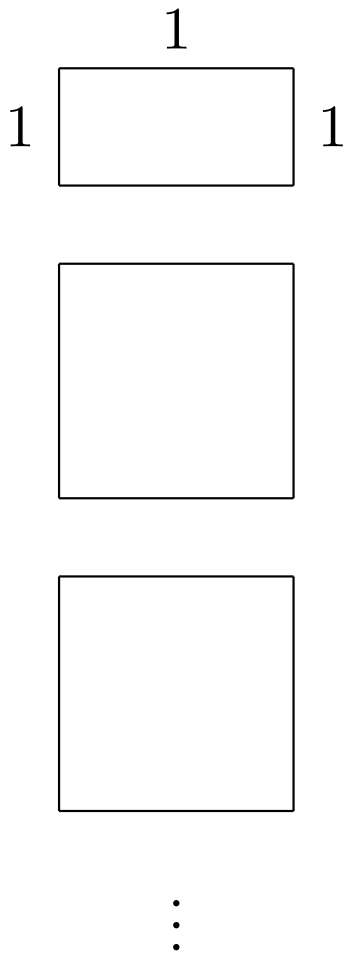
Idea. A causal $f : A^\omega \to B^\omega$ determines a unique sequence of functions $u_k : A^{k+1} \to B$. Form a computation sequence as follows:



Quiz

How would you implement 

as a computation sequence?



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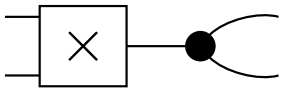
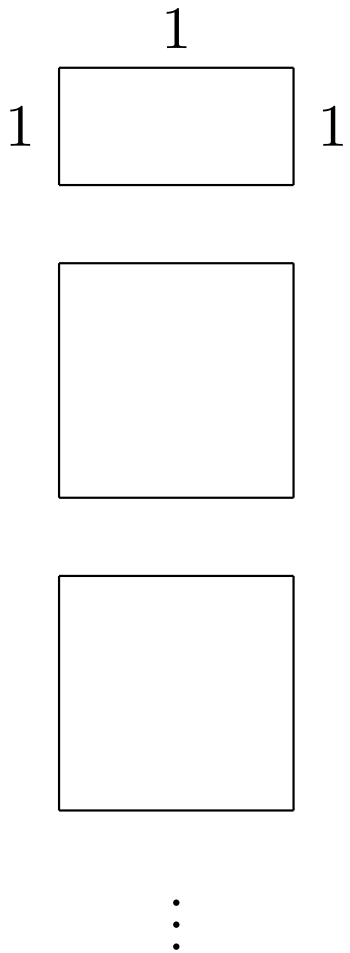
How would you implement  as a computation sequence?



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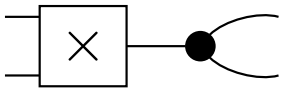
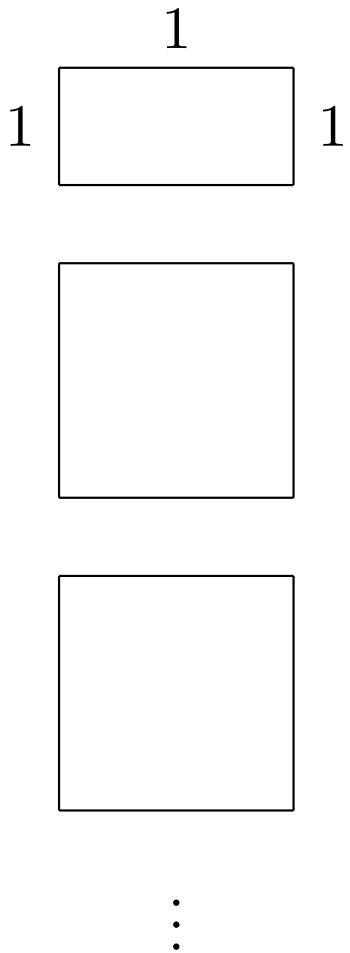
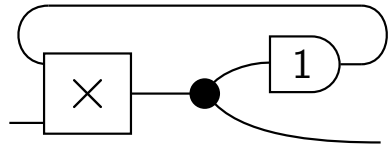
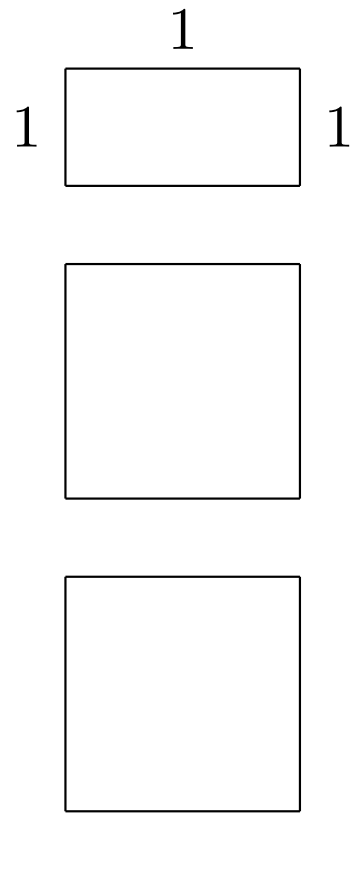
How would you implement  as a computation sequence?



How would you implement  as a computation sequence?

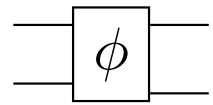


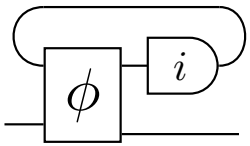
Outline

Delayed trace

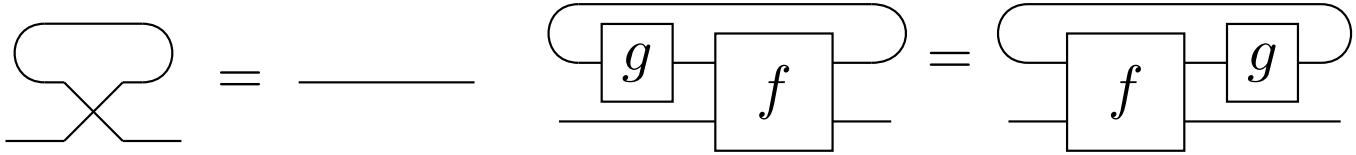
This loop-with-delay-gate is a trace-like operation.

$$\frac{\phi : S \times X \to S \times Y}{dtr_i^S(\phi) : X \to Y}$$

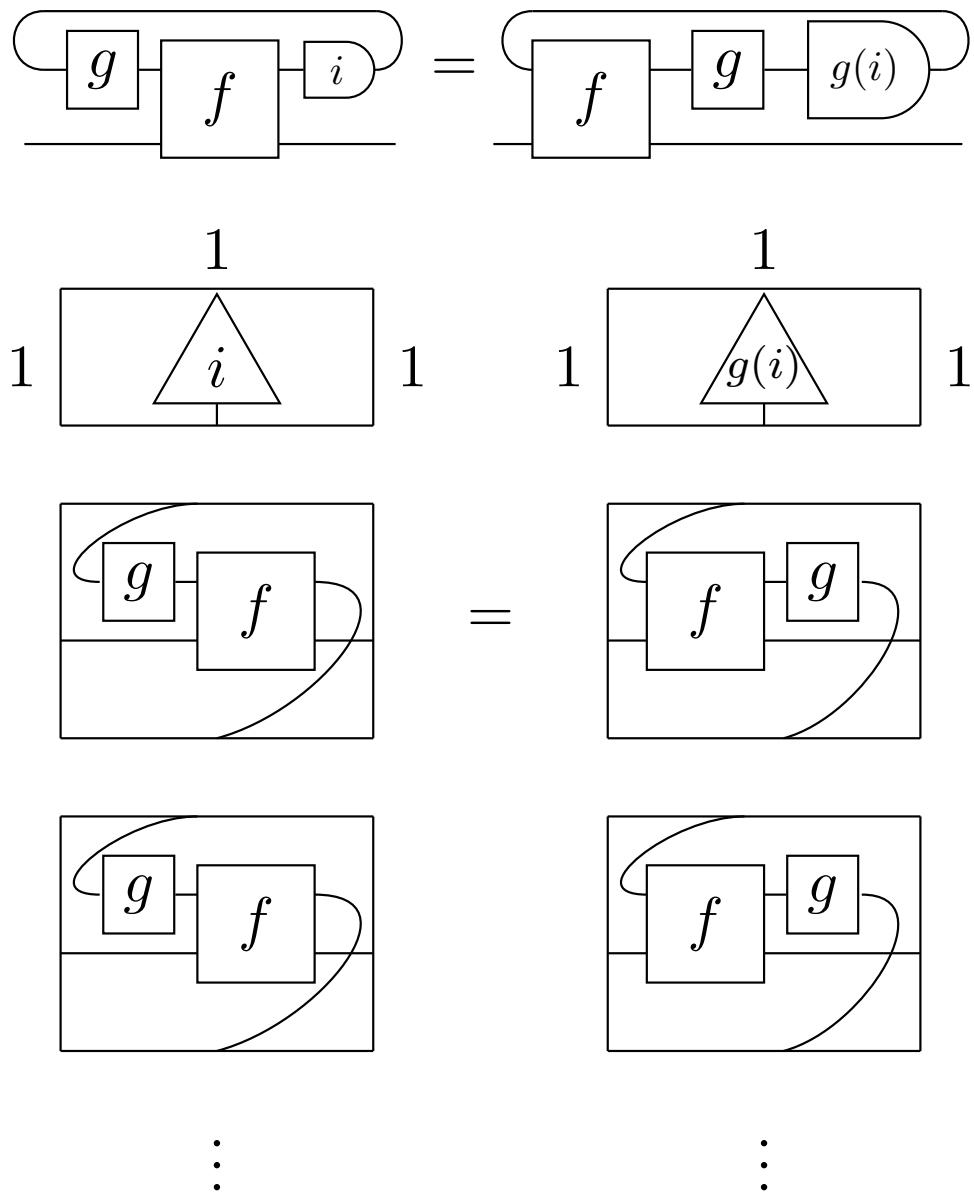




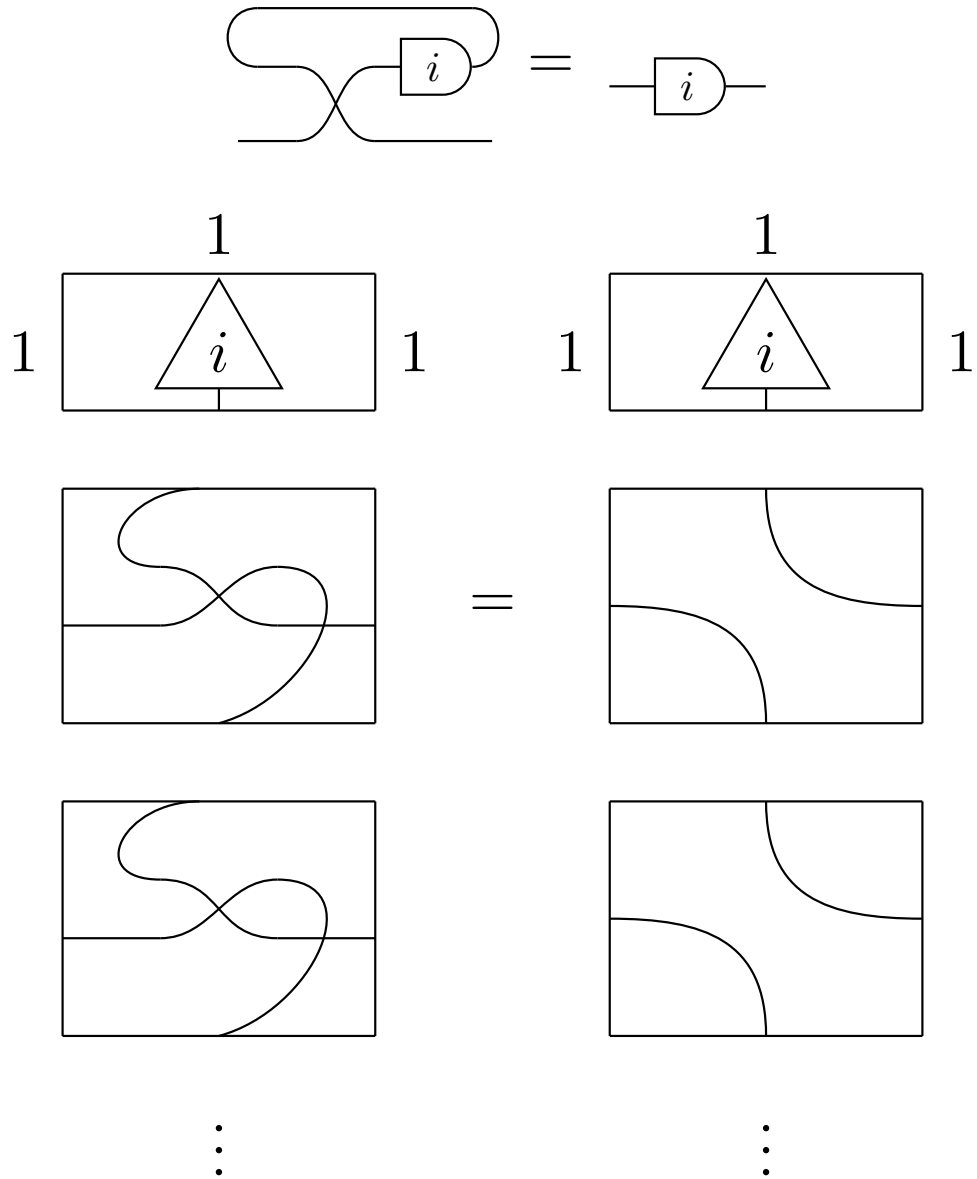
It satisfies **most** of the the trace axioms [Joyal, Street, Verity, 1996] but misses two: yanking and dinaturality. For monoidal trace, those are



~~Dinaturality~~ → retiming



~~Yanking~~ → delay



Advantages of delayed trace

Often, people formalizing circuits in category theory use these steps:

1. add registers to the category,
2. add trace to the category,
3. restrict to a subcategory such that all traces are taken on positions guarded by a register.

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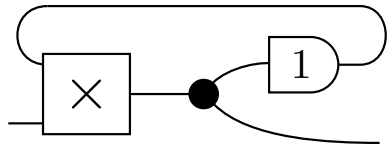
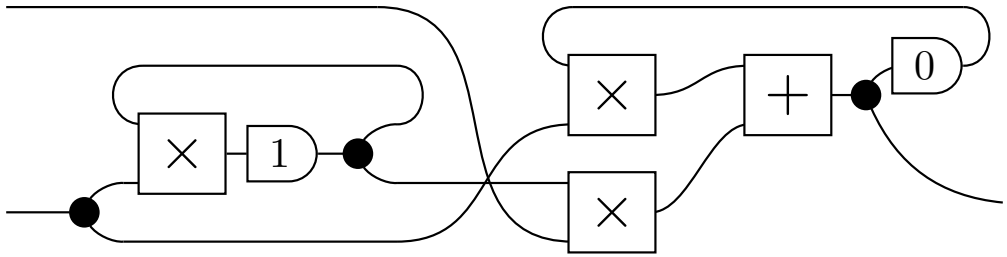
We are also interested in looking at delayed traces abstractly...

Where we're heading, update II

I would like to convince you the derivative of the running product:



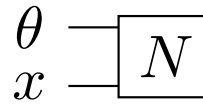
Is this:



Now we know how to represent these circuits as computation sequences.

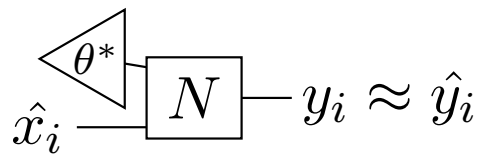
Outline

(Feedforward) neural networks

A *neural network* looks like 

. We assume its input and output spaces are real Euclidean spaces $\mathbb{R}^n$.

Training a neural network (with data $\hat{x}_i, \hat{y}_i$) means finding θ^* so that:



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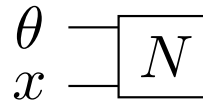
A *neural network* looks like 

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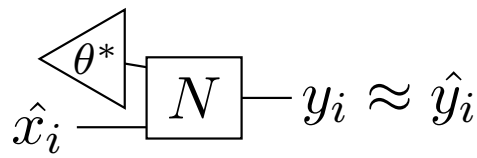

Gradient-based training algorithms are based on the insight that $\frac{\partial N}{\partial \theta}$ is a good approximation for the change in y that results from a small change in θ. This allows us to make smart updates to θ^*.

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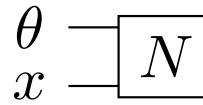
A *neural network* looks like 

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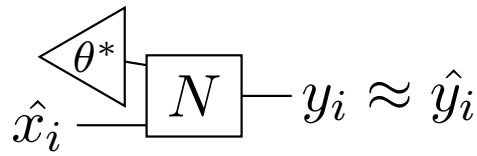
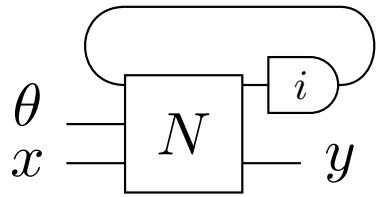


Gradient-based training algorithms are based on the insight that $\frac{\partial N}{\partial \theta}$ is a good approximation for the change in y that results from a small change in θ. This allows us to make smart updates to θ^*.

Various algorithms can be used to compute these partial derivatives, including *backpropagation* [Rumelhart, 1986].

(Feedback/recurrent) neural networks

Recurrent neural networks (RNNs) are designed to process sequences of inputs using some internal state:



It's less clear what the derivatives of these functions are.

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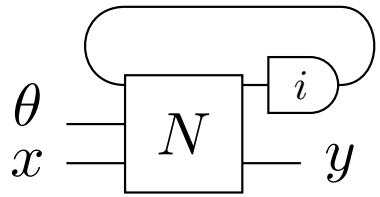
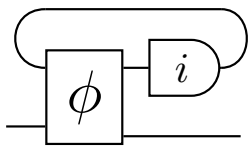


It's less clear what the derivatives of these functions are.

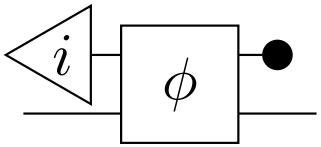
The most common training method for RNNs relies on a gradient-finding algorithm called *backpropagation through time*.

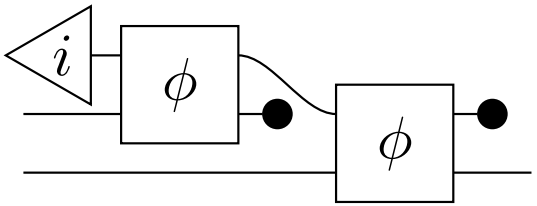
Backpropagation through time

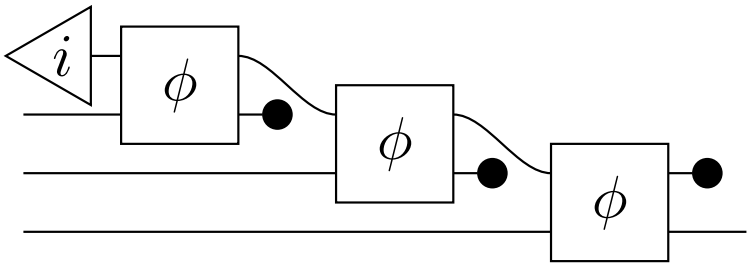
First, we *unroll* the network:

$\Phi =$ 

$\Rightarrow$

$u_0 =$ 

$u_1 =$ 

$u_2 =$ 

$\vdots$

Then, whenever the derivative of Φ is needed at an input of length $k+1$, the derivative of u_k is supplied instead.

Does BPTT make sense, or is it just a hack?

Does BPTT make sense, or is it just a hack?

"Making sense" means having the usual properties of derivatives:

1. a sum rule,
2. a chain rule,
3. being linear when evaluated at any base point,
4. symmetry of mixed partial derivatives,

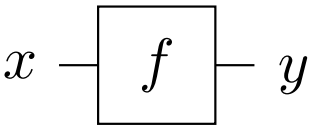
⋮

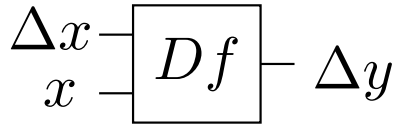
Outline

Derivatives, diagrammatically

The derivative of x — f — y is $\begin{matrix}\Delta x \\ x\end{matrix}$ — Df — Δy, which gives the best linear approximation to f at a base point x.

Derivatives, diagrammatically

The derivative of 

is 

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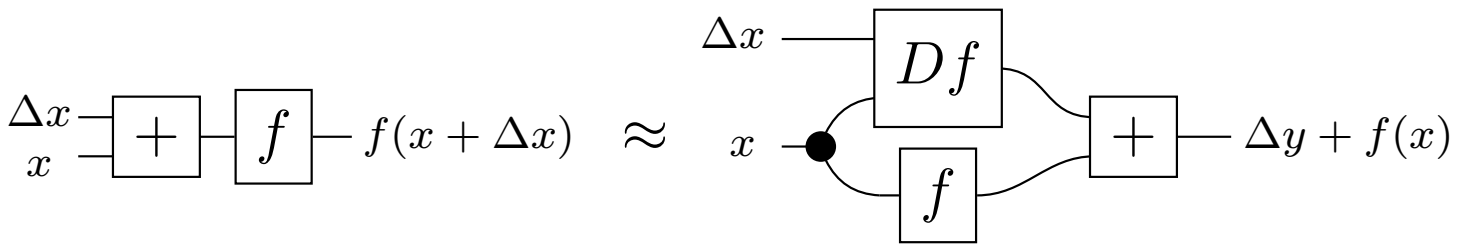

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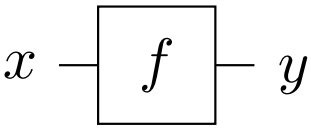
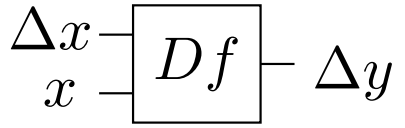
Derivatives, diagrammatically

The derivative of 

is 

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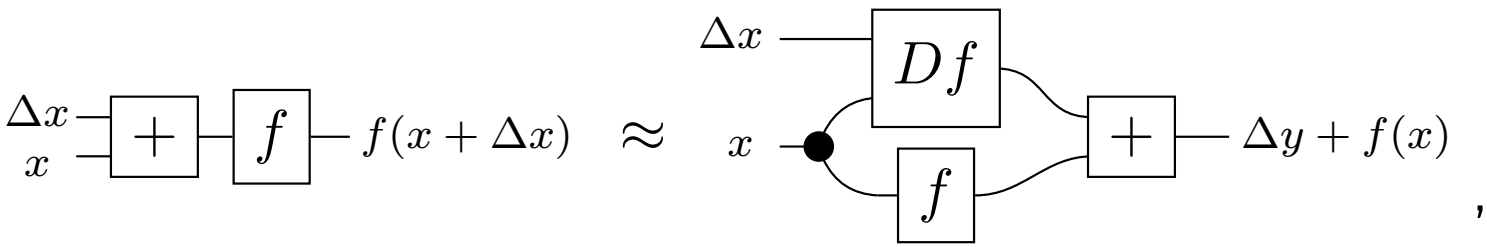

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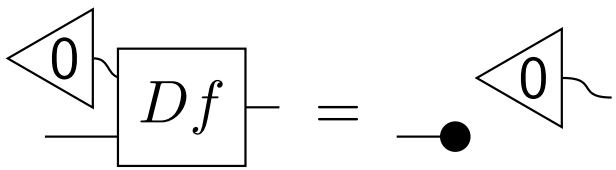
(CD2) 

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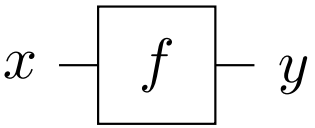
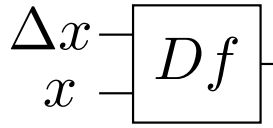
Derivatives, diagrammatically

The derivative of 

is 

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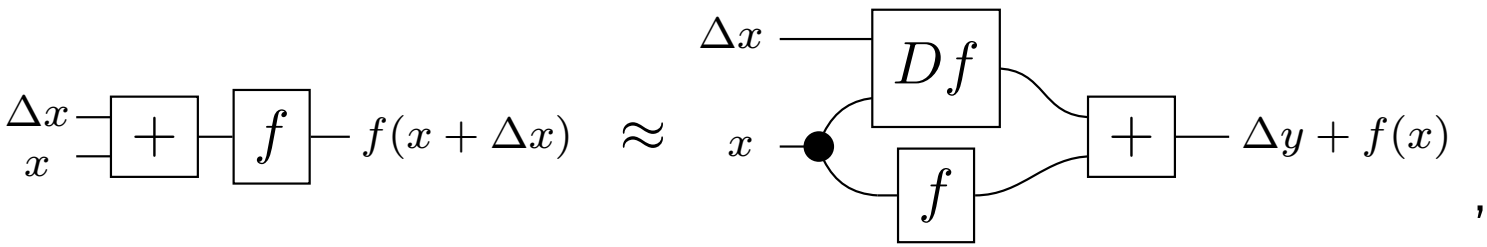

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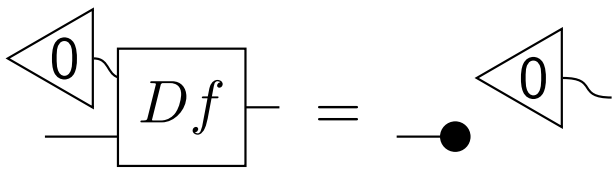
(CD2) 

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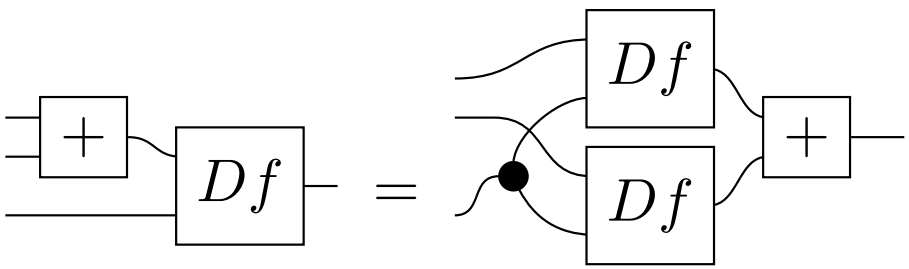
(CD3) 

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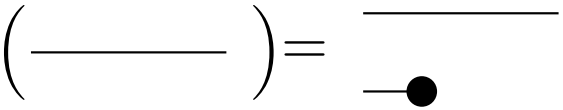
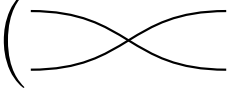
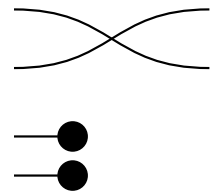
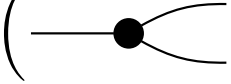
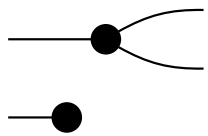
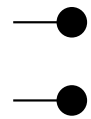
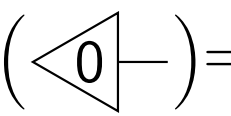
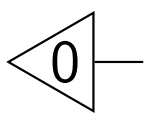
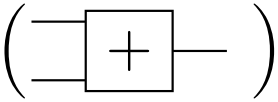
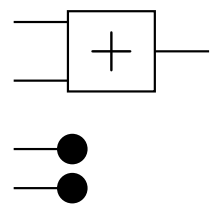
Derivatives of basic functions

The derivatives of some basic functions include:

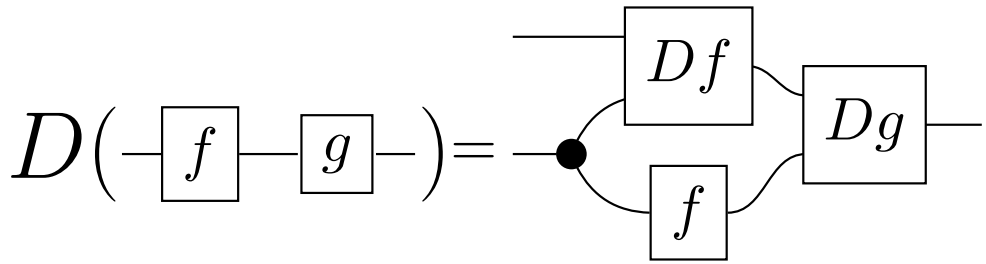
(CD1) $D($  $)=$ $D($  $)=$ 

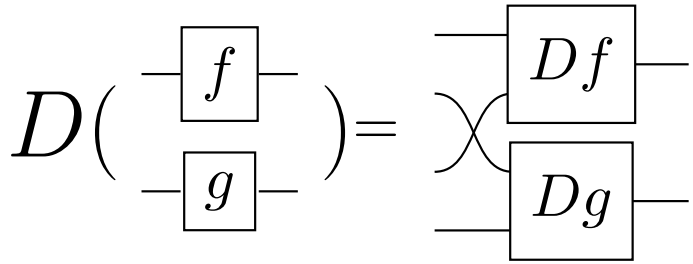
$D($  $)=$  $D($ $)=$ 

$D($  $)=$  $D($  $)=$ 

Properties of derivatives, diagrammatically

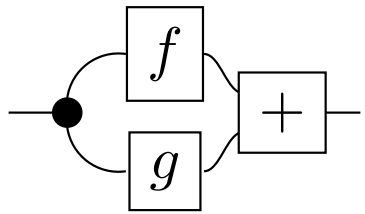
We can also express the chain rule and "parallel rule":

(CD4) 

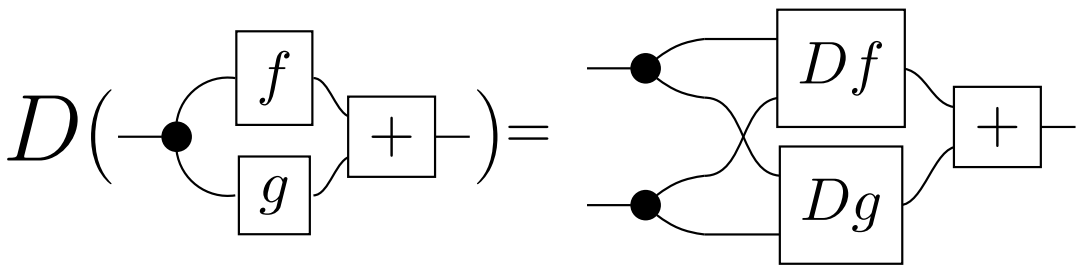
(CD5) 

Sum rule, diagrammatically

The sum rule is a consequence of the axioms we have seen so far. Here's a diagram for the sum of two functions:



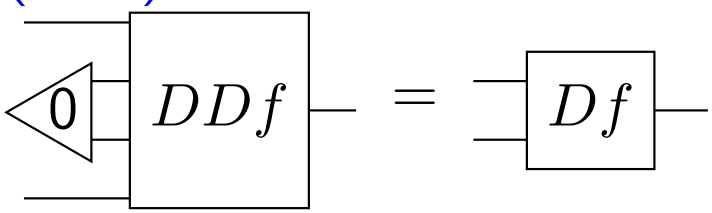
The rules we've seen allows us to compute:



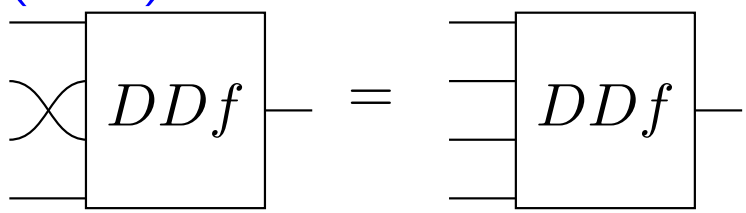
Properties of higher-order derivatives

It's also possible to express properties of higher order derivatives, but it's not worth the time to explain them in much detail.

(CD6)



(CD7)



Cartesian differential categories [Blute, Cockett, Seely '09]

A *Cartesian differential category* is a

- Cartesian category
- with left additive structure (providing 0 and $+$)
- an operation sending $f : X \to Y$ to $Df : X \times X \to Y$
- which satisfies CD1-7.

This is a categorical representation of the major algebraic properties of derivatives.

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This is a categorical representation of the major algebraic properties of derivatives.

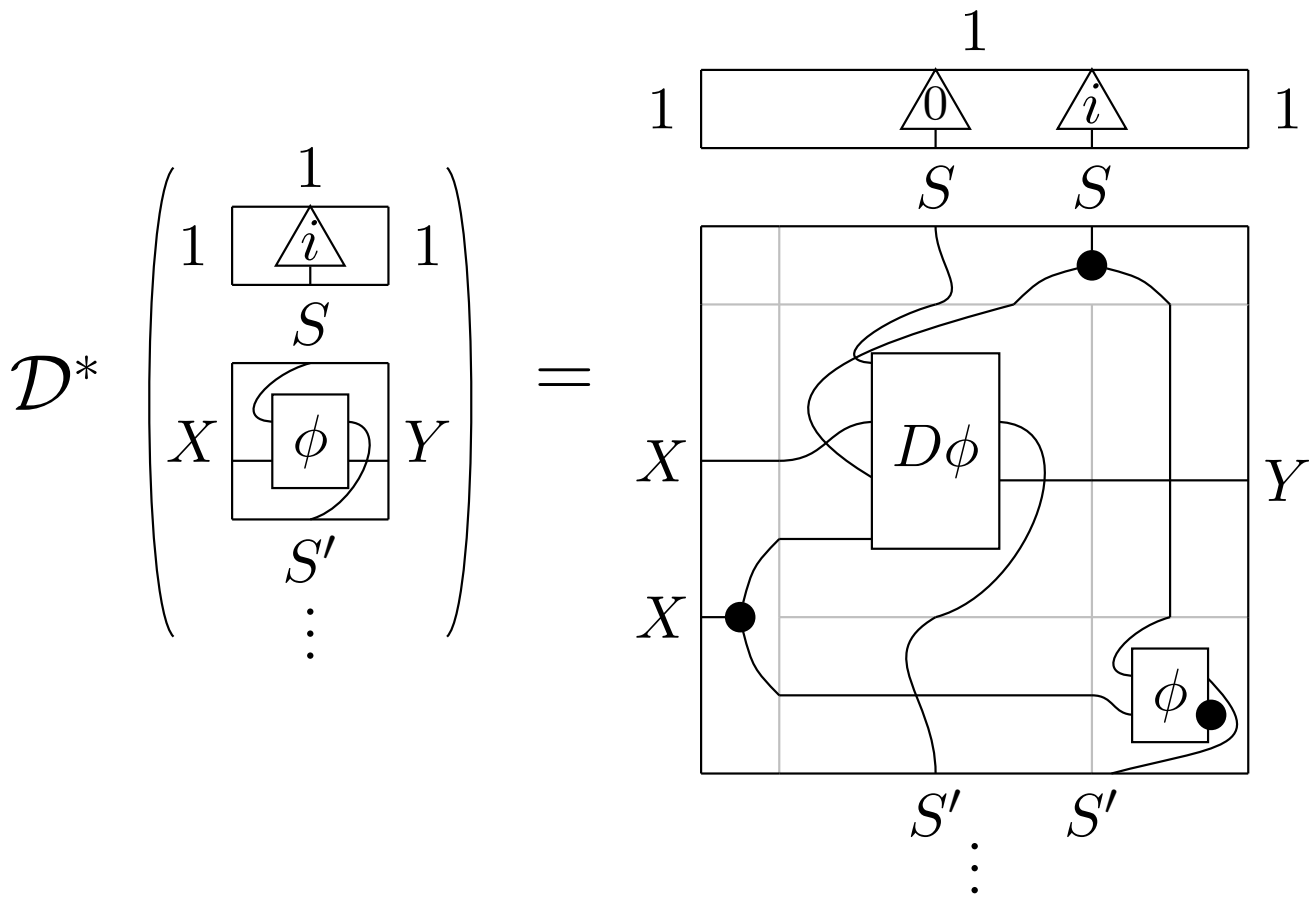
The canonical example of a Cartesian differential category is $\mathbf{Euc}_\infty$, where objects are $\mathbb{R}^n$ for all $n \in \mathbb{N}$ and morphisms are smooth functions.

Key contribution: differential operator lifts

Theorem (Katsumata, S)

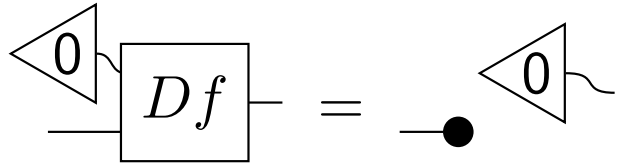
If $\mathbb{C}$ is a Cartesian differential category, so is $\mathrm{St}(\mathbb{C})$.

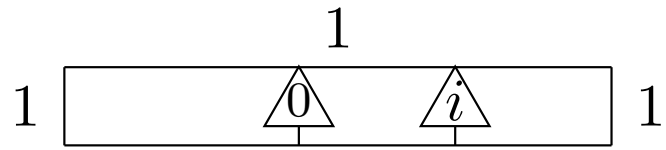
The Cartesian differential operator on $\mathrm{St}(\mathbb{C})$ is defined as follows:

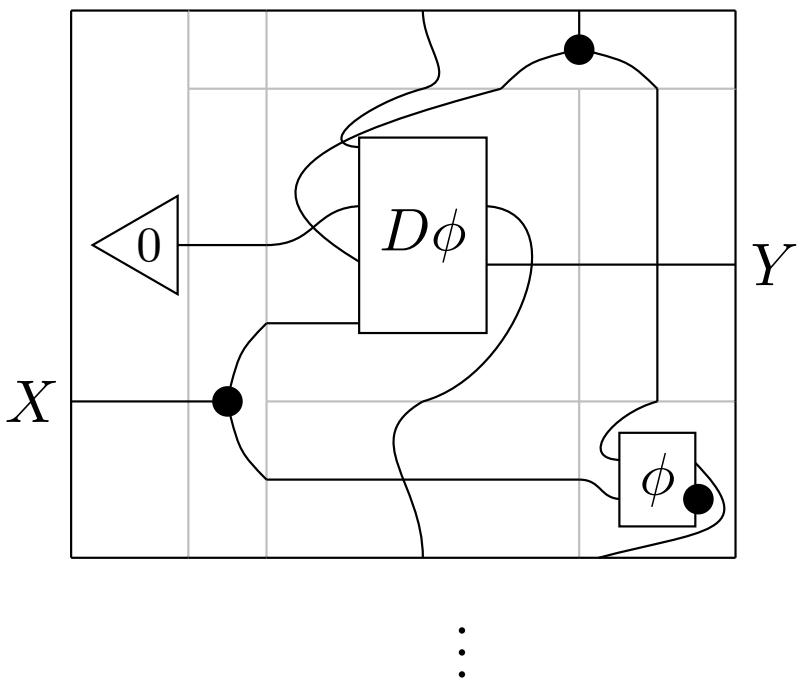


Key contribution: differential operator lifts

Proof idea. For CD2:







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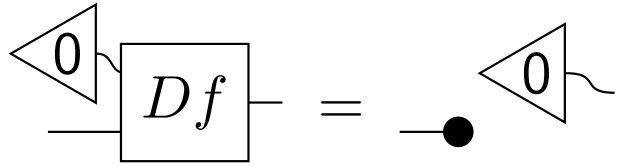

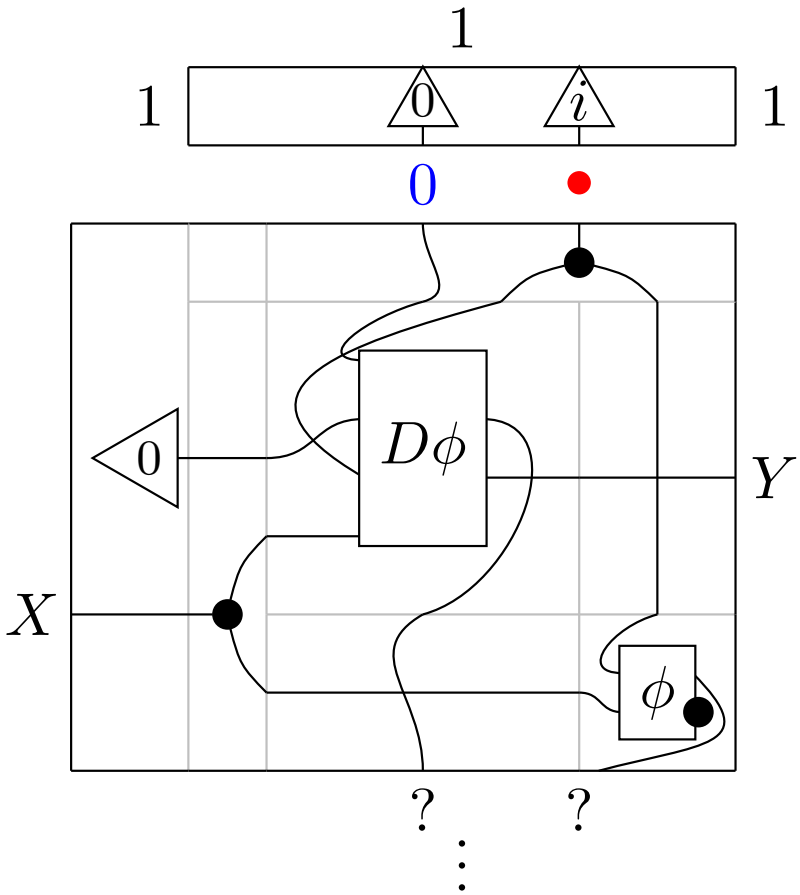

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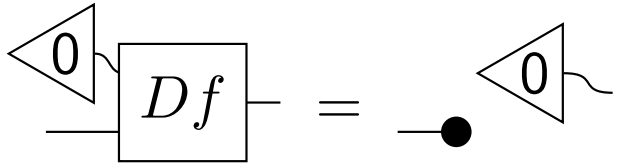
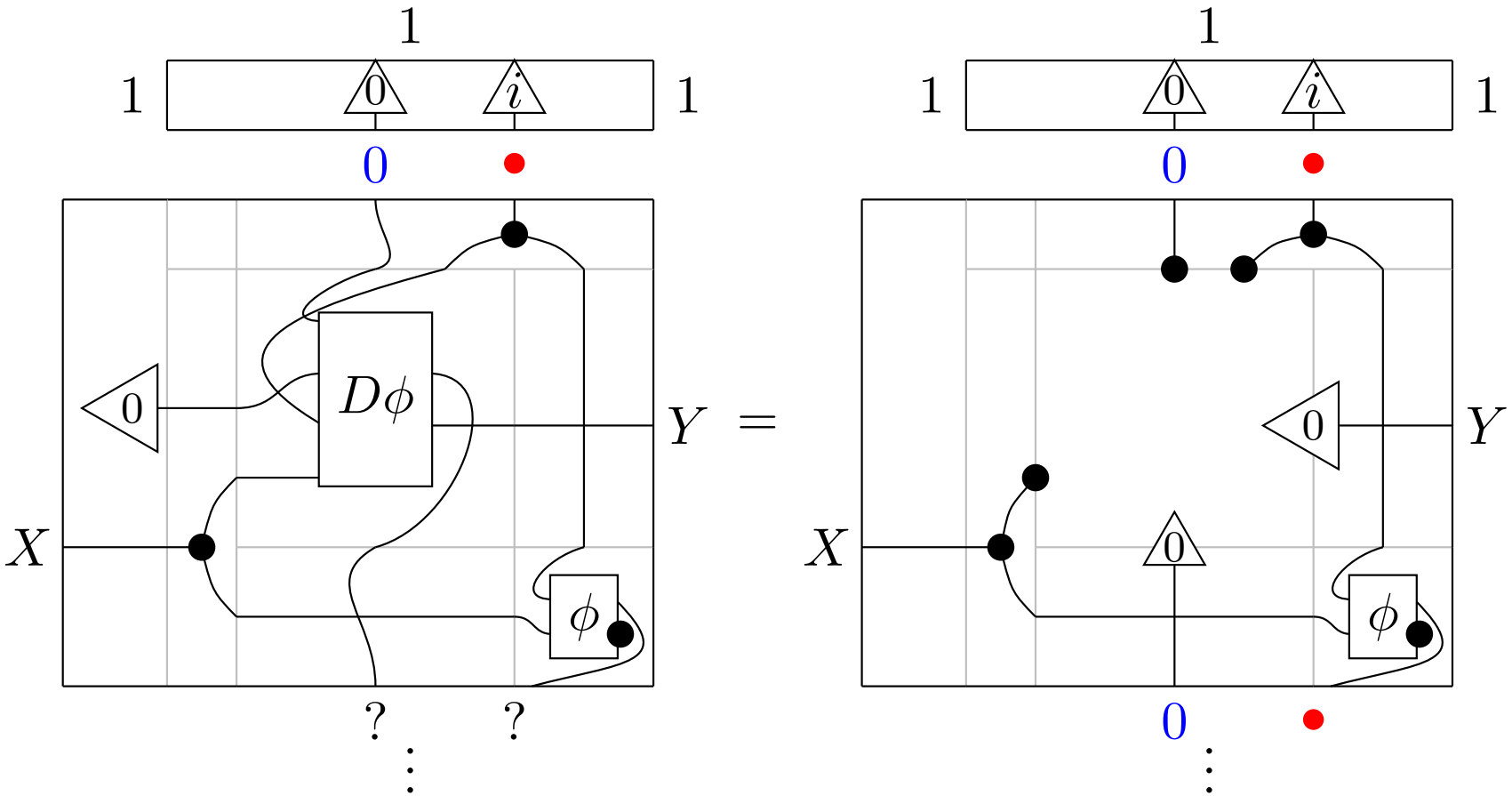
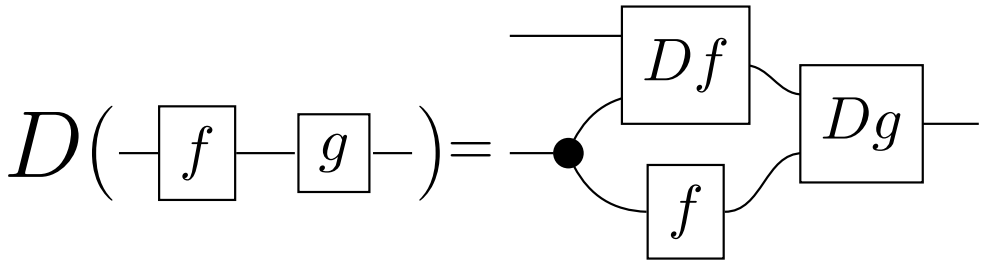
Proof idea. For CD2:

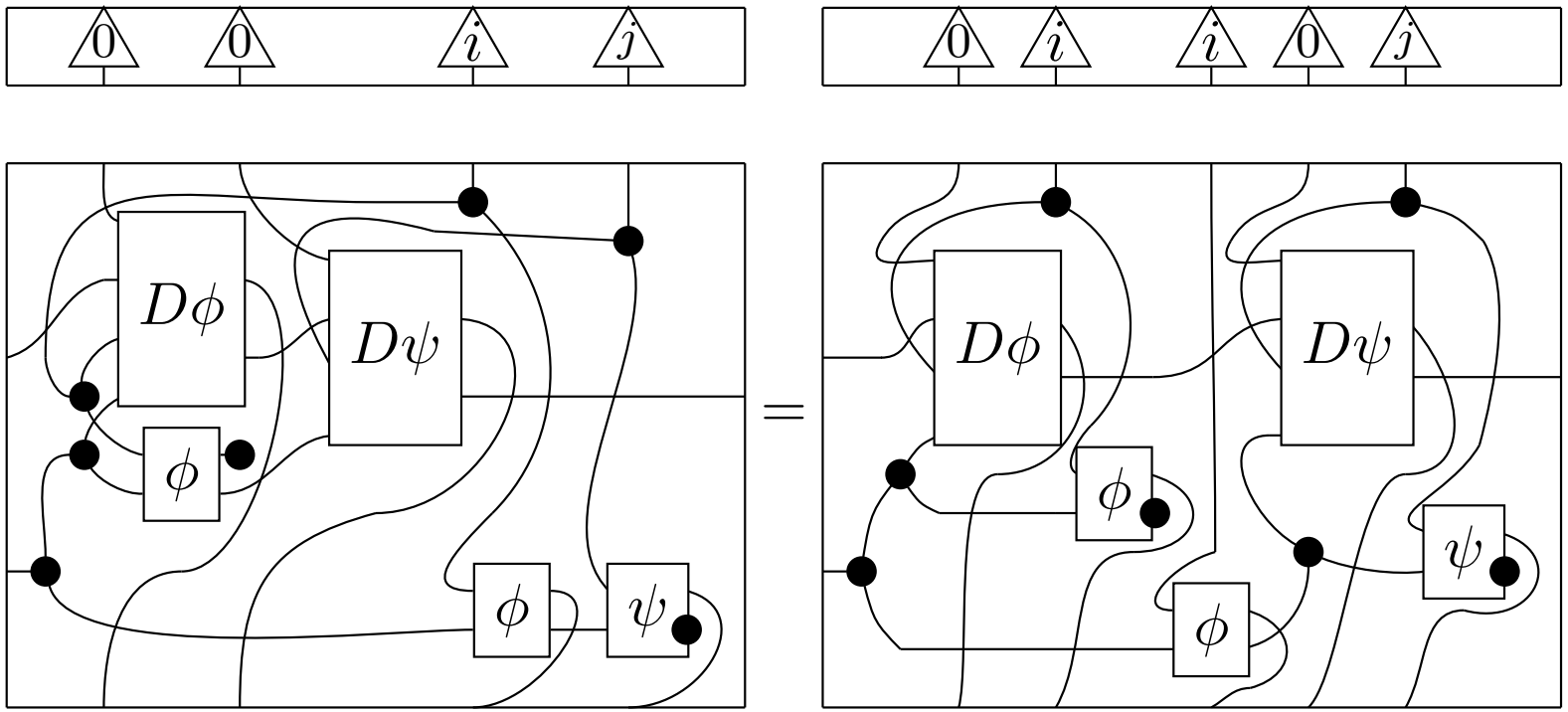




Key contribution: differential operator lifts

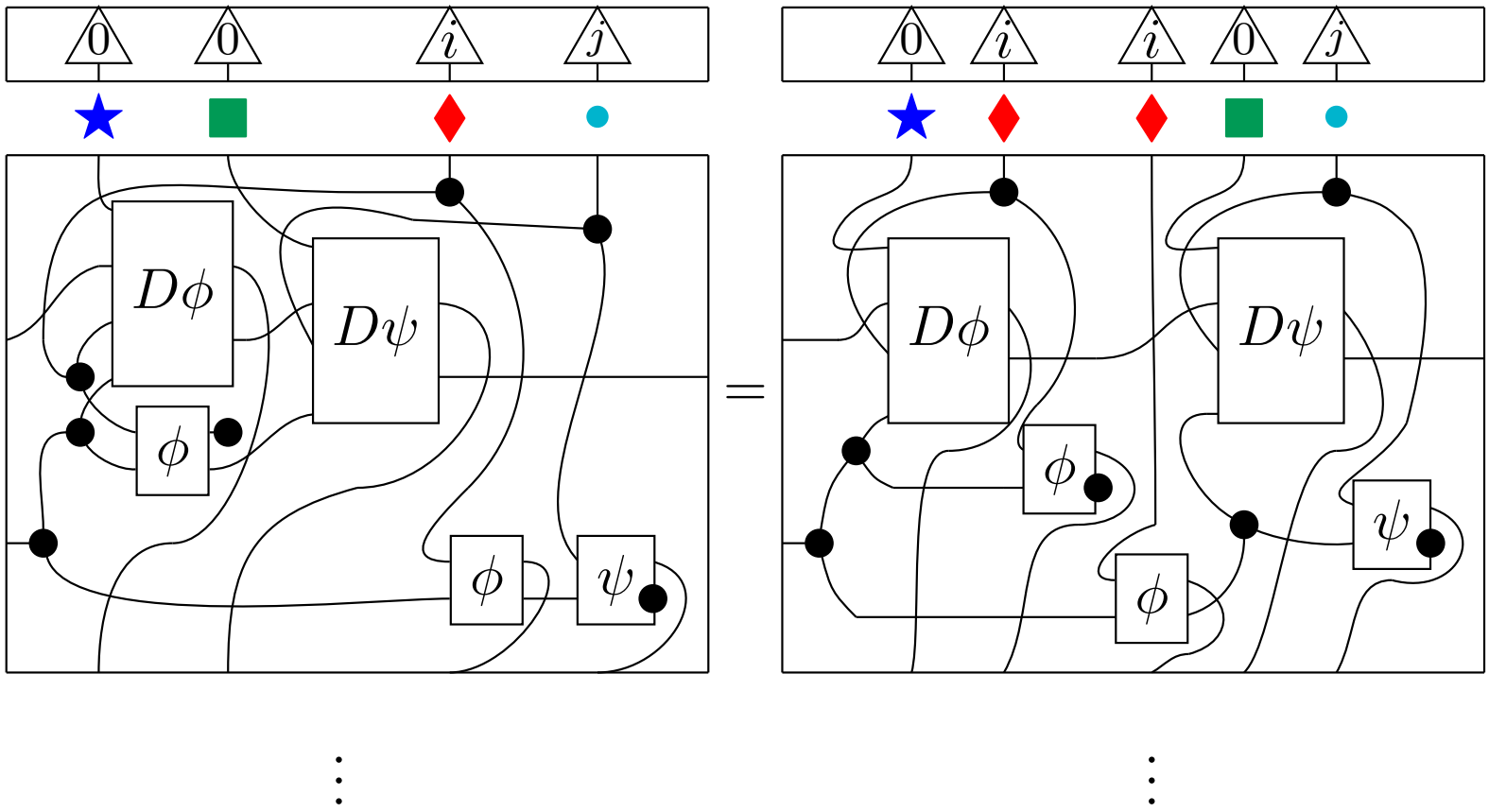
Proof idea. For CD4:





Key contribution: differential operator lifts

Proof idea. For CD4: $D(f \circ g) = Df \cdot f \circ Dg$



Key contribution: differential operator lifts

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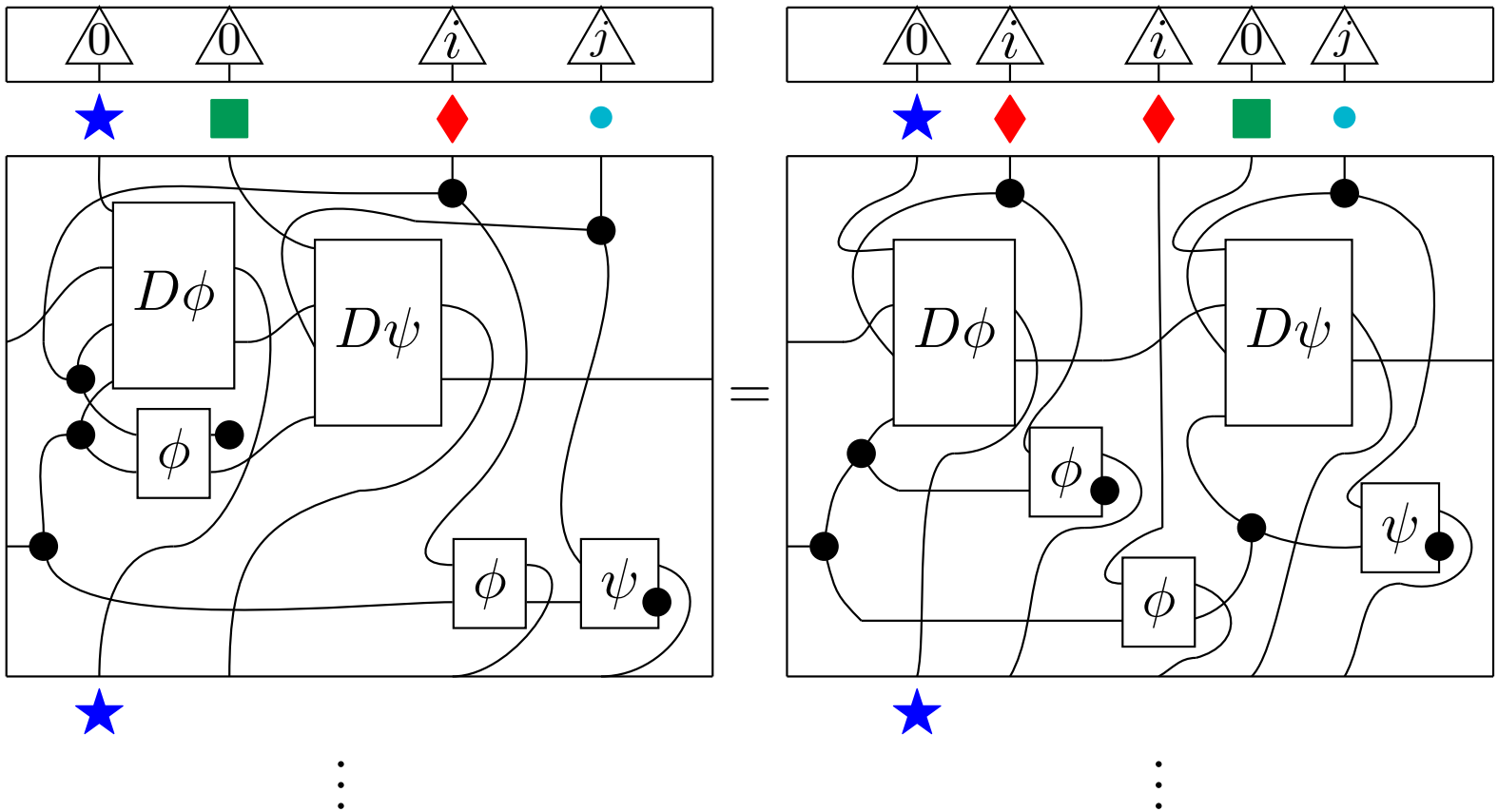
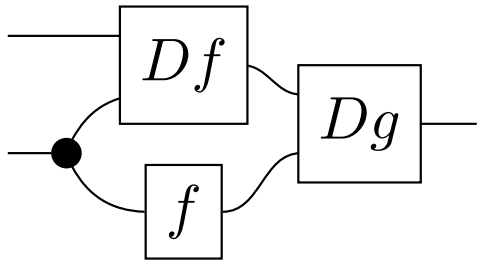
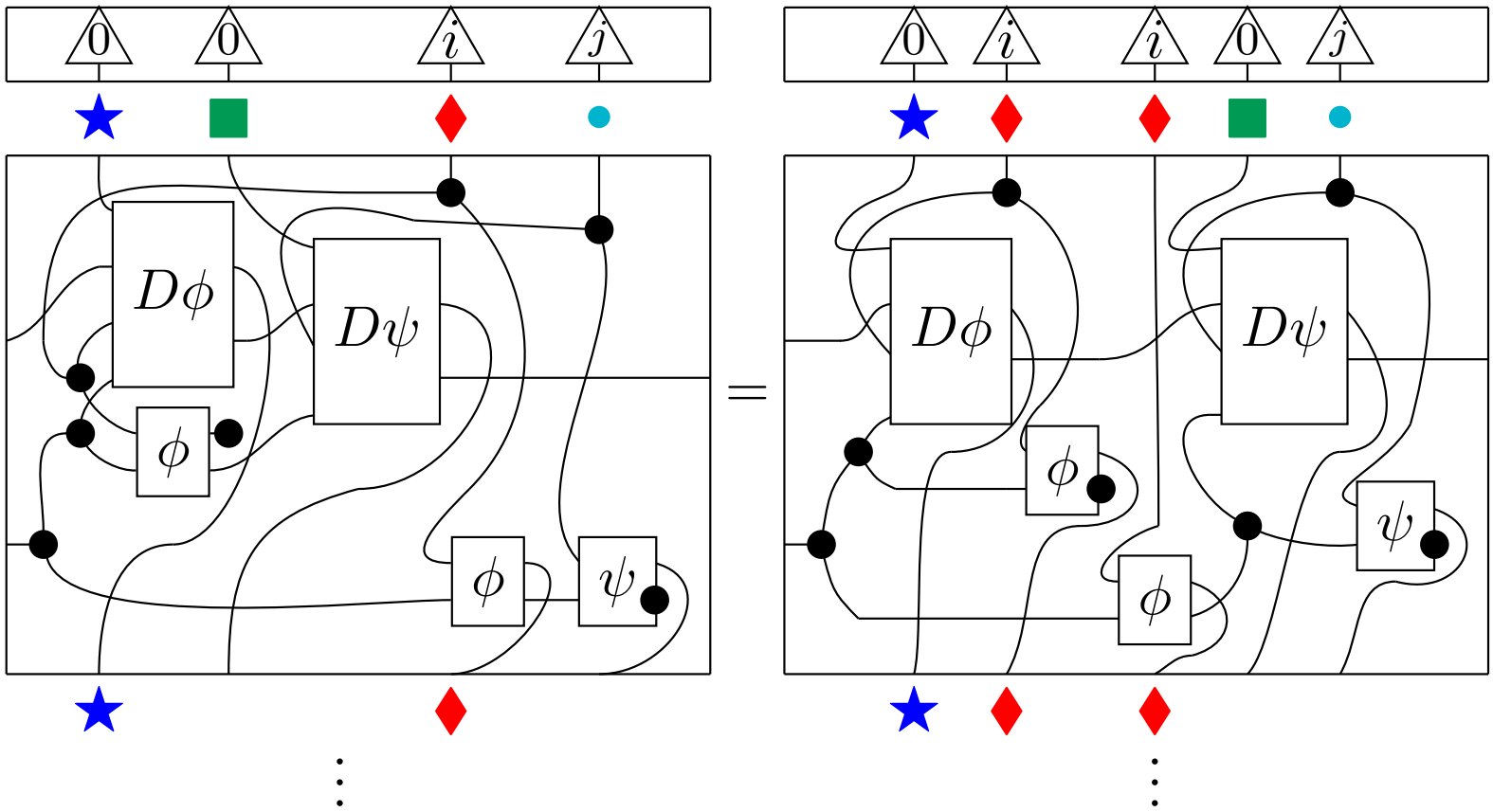


Key contribution: differential operator lifts

Proof idea. For CD4: $D\big(-\boxed{f}-\boxed{g}-\big)=$ 



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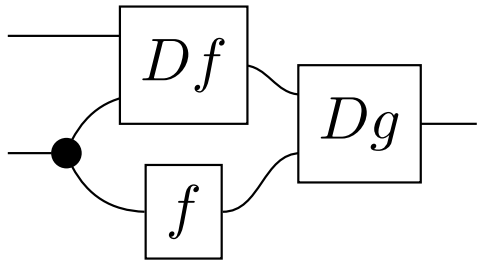
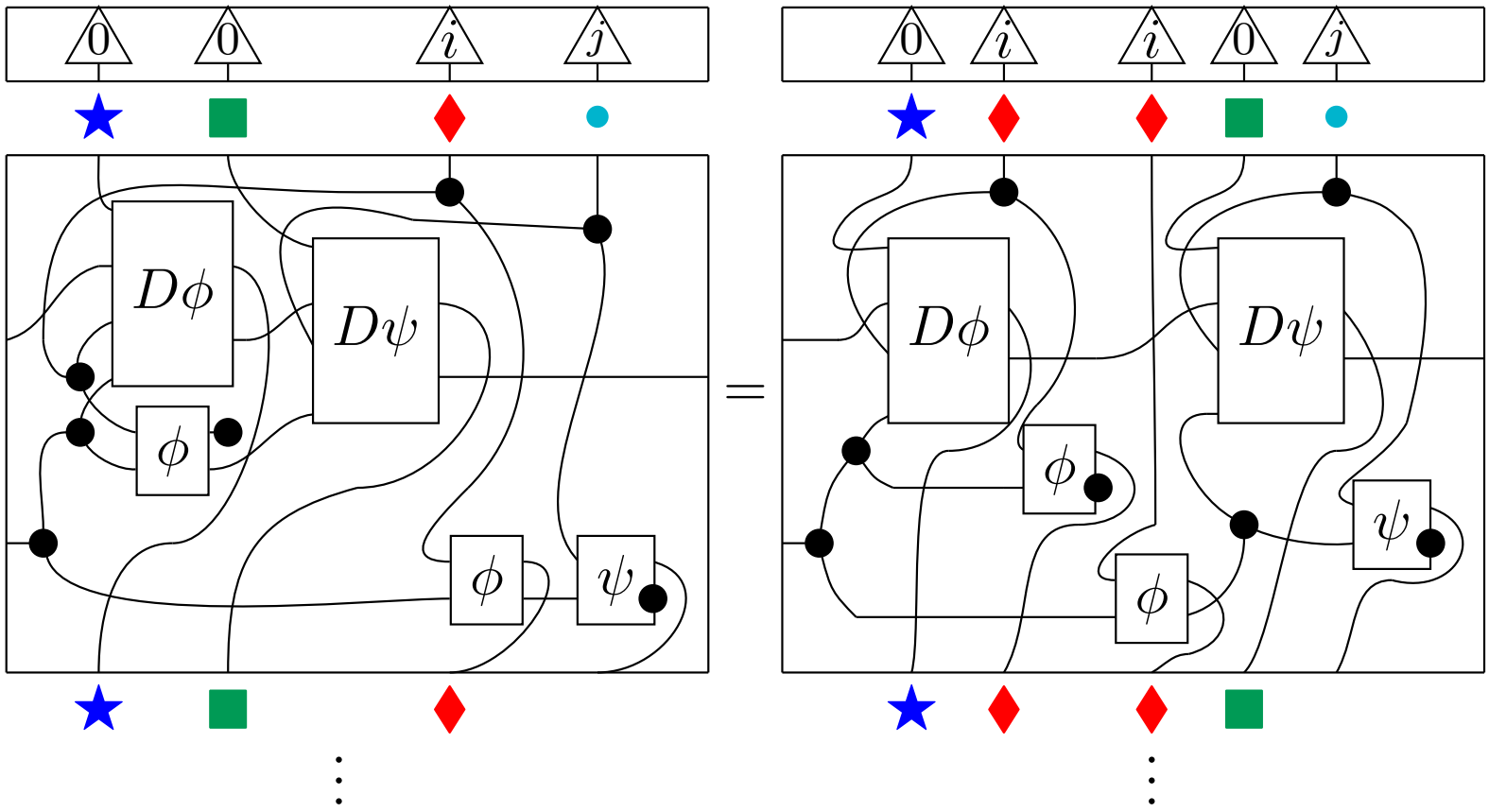
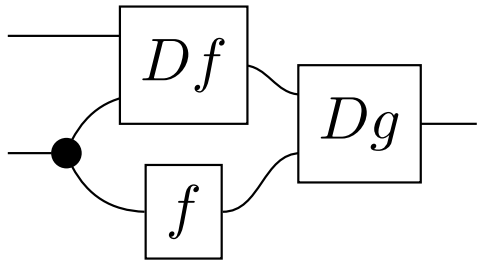
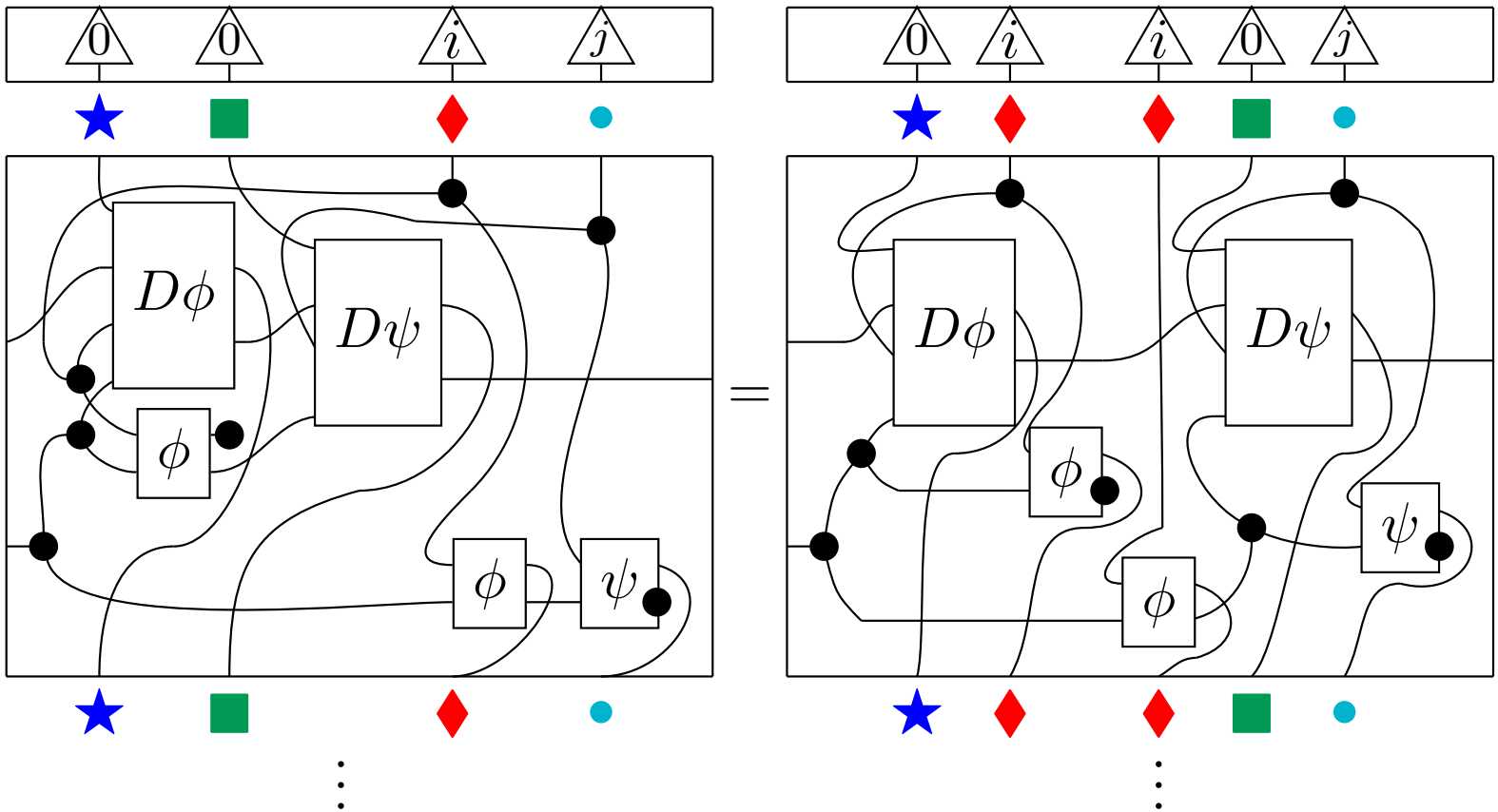
Proof idea. For CD4: $D\big(-\boxed{f}-\boxed{g}-\big)=$ 

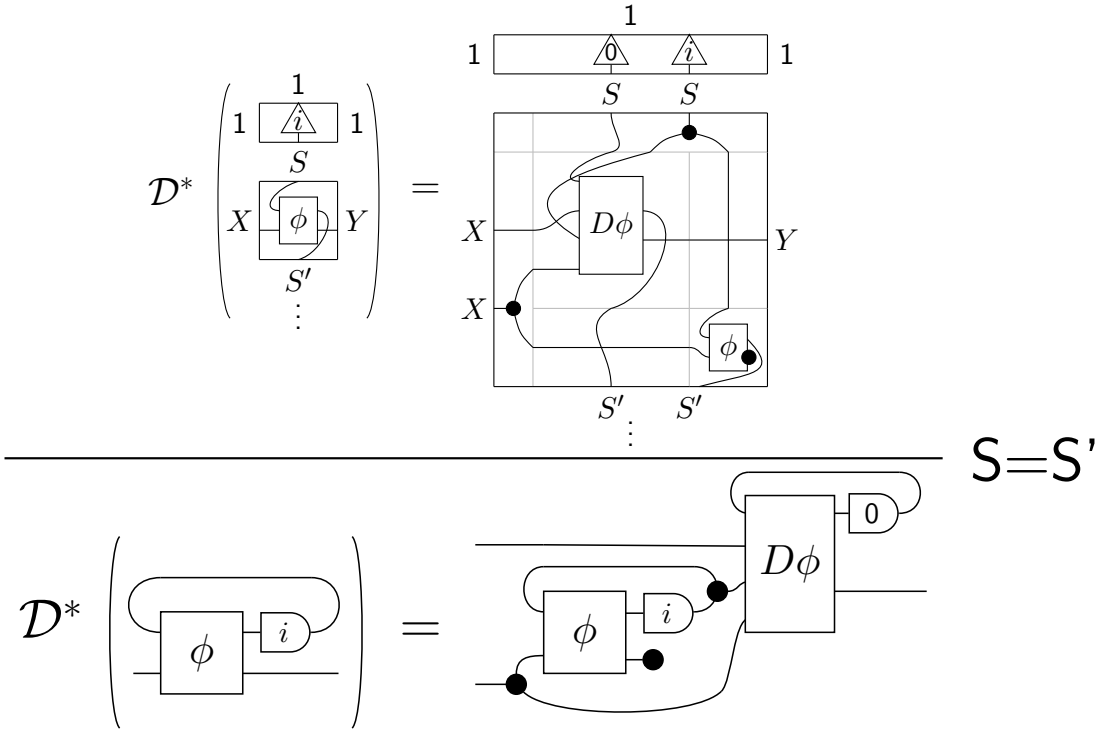


Key contribution: differential operator lifts

Proof idea. For CD4: $D\big(f\ g\big) =$ 



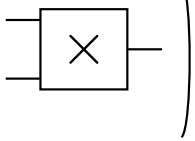
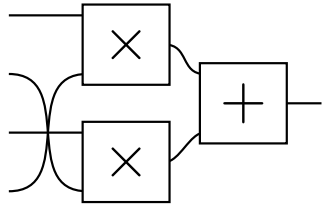
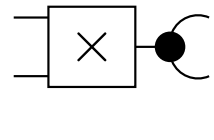
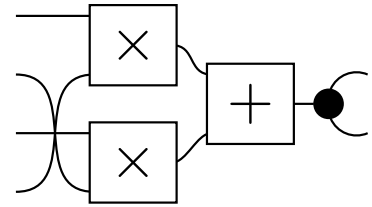
Differentiating circuits



Theorem ($\mathcal{D}^*$ matches BPTT)

The unrolling of $\mathcal{D}^*((i, [\phi]))$ is the component-wise application of D to the unrolling of $(i, [\phi])$.

Where we're heading, update III

$D\left($  $\right) =$  , so $D\left($  $\right) =$ 

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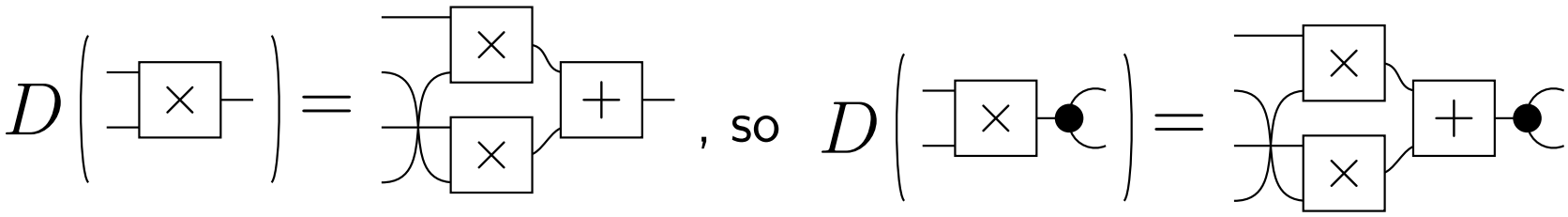
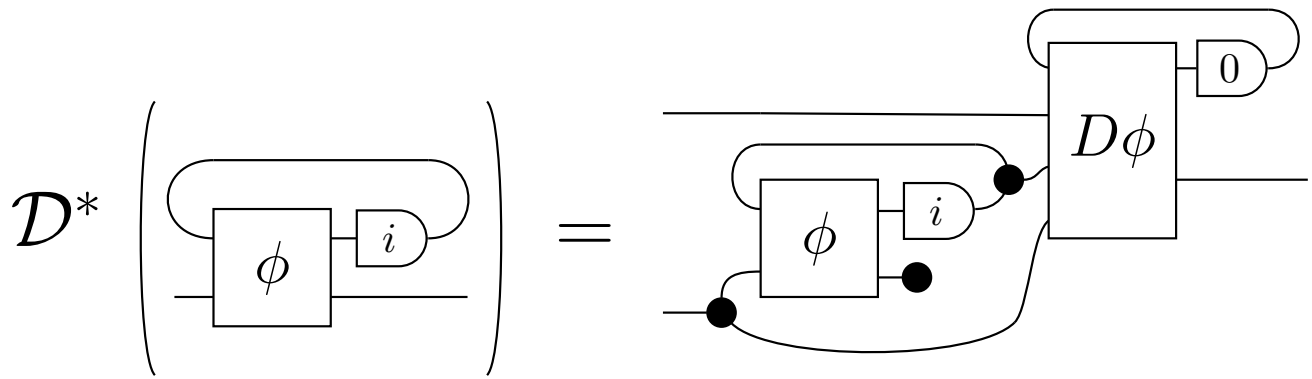
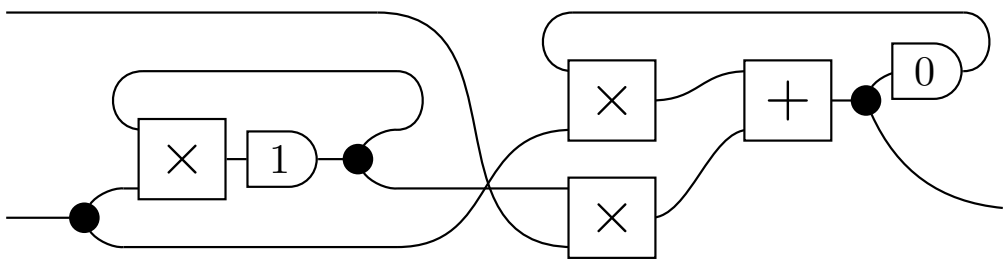


Then



becomes



Outline

Recap

We gave a mechanism for defining causal functions based on computation sequences. We organized these with a construction on Cartesian categories, $\mathrm{St}(-)$. These categories have a *delayed trace*.

We showed that if $\mathbb{C}$ is a Cartesian differential category, so is $\mathrm{St}(\mathbb{C})$. Taking $\mathbb{C} = \mathbf{Euc}_\infty$, we can find derivatives of recurrent neural networks. The differential operator on $\mathrm{St}(\mathbf{Euc}_\infty)$ matches the derivatives taken in backpropagation through time; the fact that it is a differential operator obtains many properties for BPTT.

Future questions (roughly mathematical to practical)

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2. $\mathcal{D}^*$ and derivatives in sequence spaces?
3. Bisimulations and extensional equality?
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11. Measuring complexity with string diagrams?
12. What happens when $\phi \in \{LSTM, GRU, \ldots\}$?
13. Implementation/plugin to neural net library?

Thanks!