Recurrent Neural Networks: A Categorical Perspective

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10 September 2019

Outline

Motivations (general to specific)

- Re-examining the foundations of machine/deep learning

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- Understanding recurrent neural networks and their training
- Striking up collaboration

Machine learning, as a field

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  - Experimental results can be better tied to theory

Examples of confusion

A recent answer on the data science StackExchange: "gradient descent . . . relies on local information only. . . .

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Some common ideas about LSTMs: "Remembering information for long periods of time is practically their default behavior!" (Chris Olah's introduction)

This makes training difficult. It is common practice to create an "unrolled" version of the network; this finite approximation of the RNN is then trained. (Tensorflow documentation)

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This talk: mostly on the treatment of state and the techniques we use (!)

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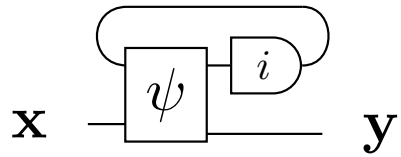

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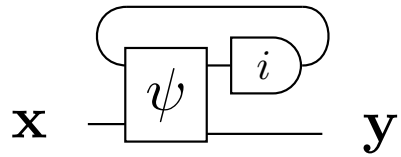

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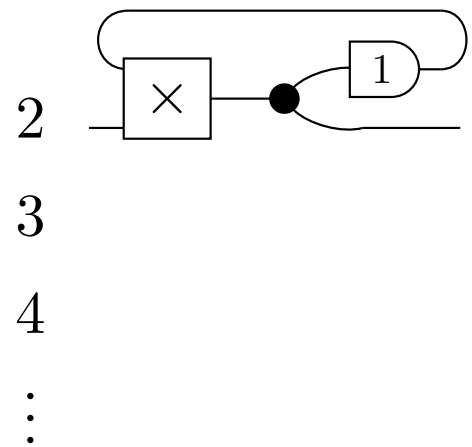

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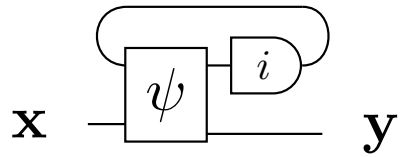

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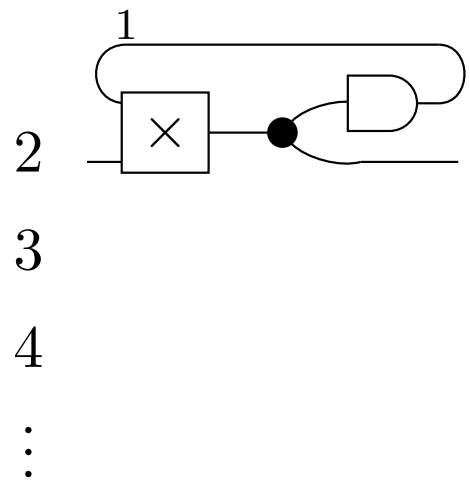

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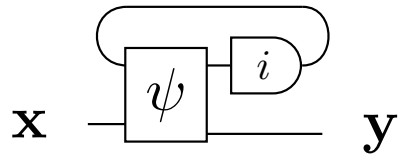

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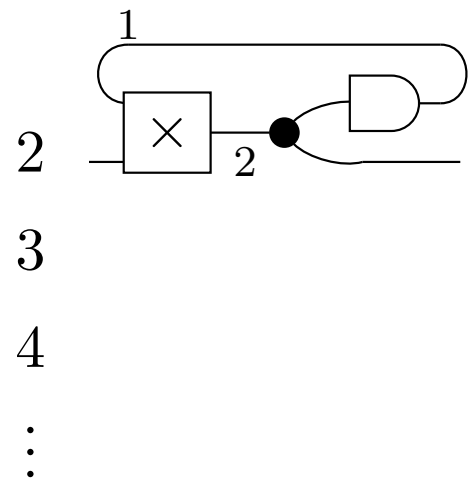

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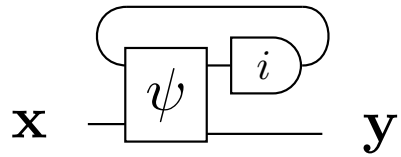

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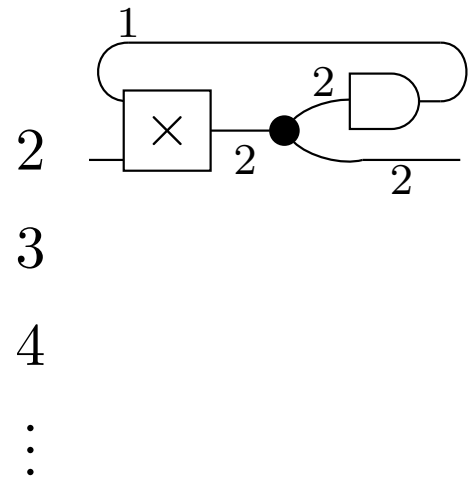

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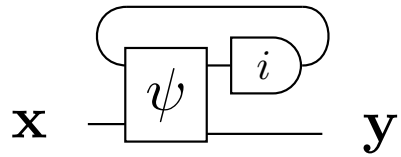

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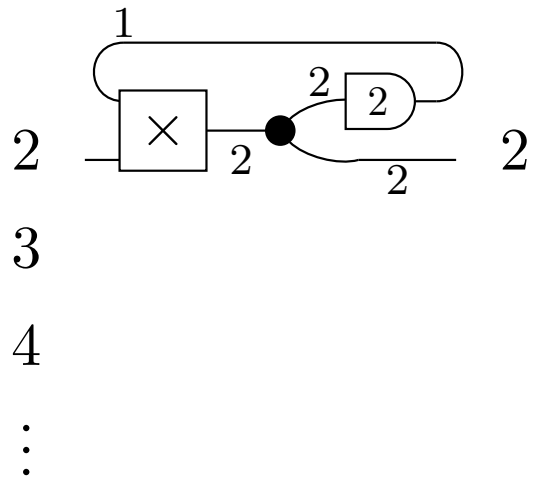

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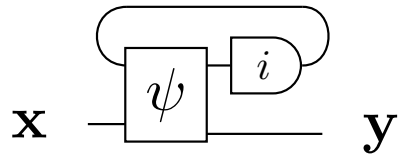

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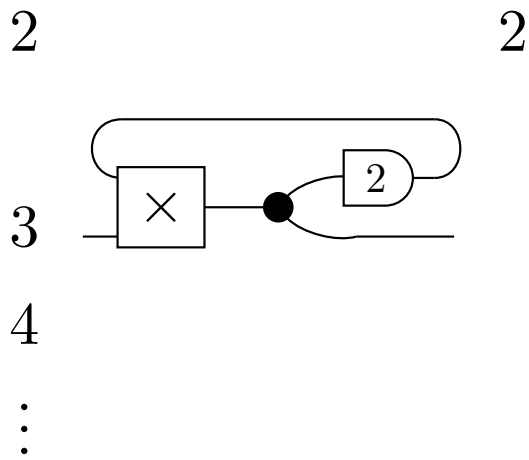

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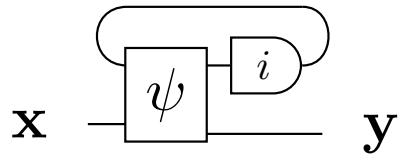

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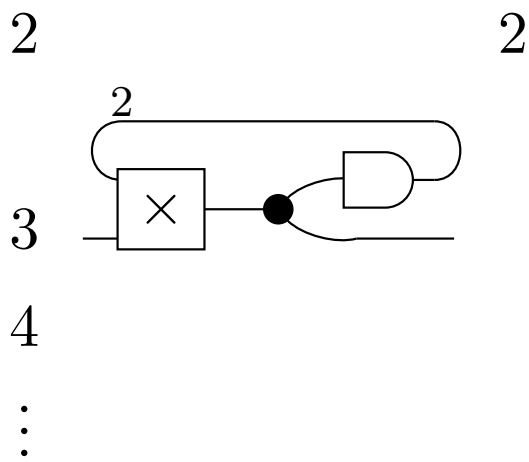

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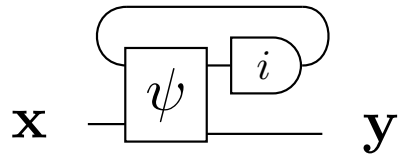

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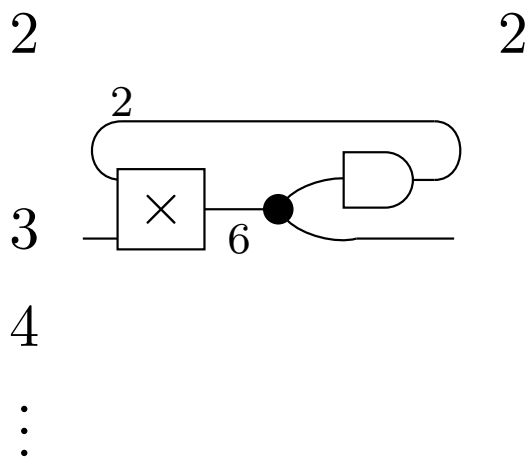

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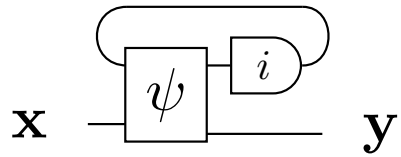

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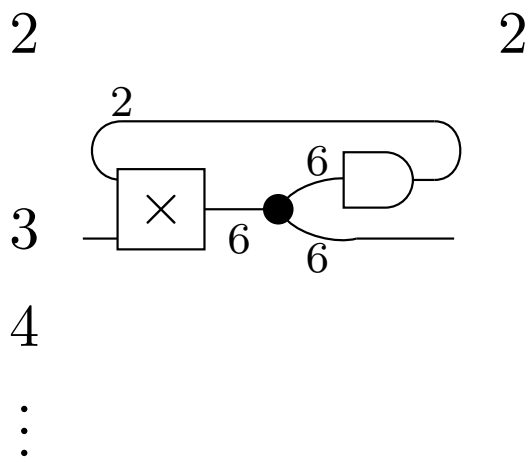

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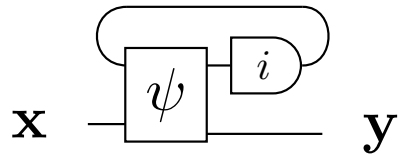

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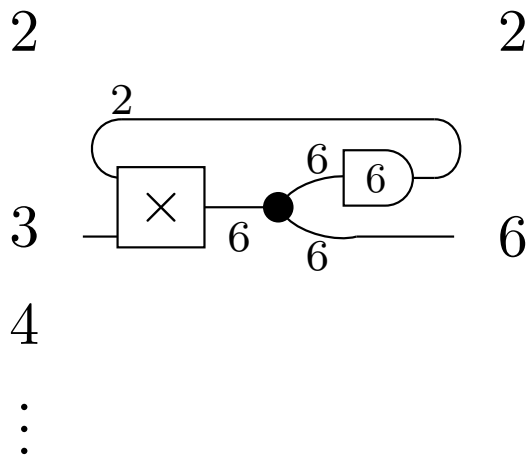

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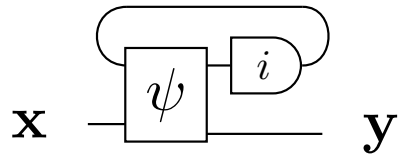

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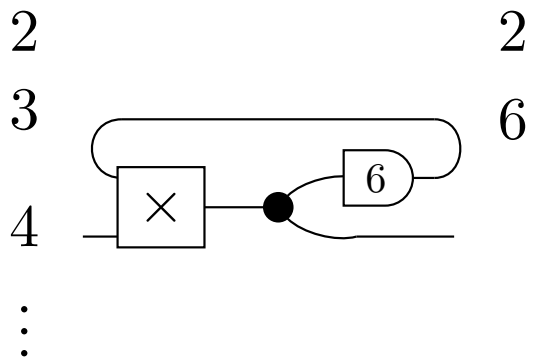

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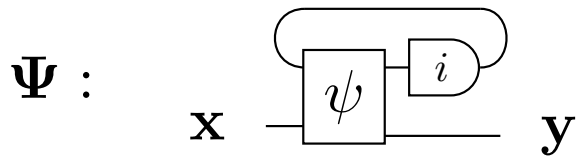

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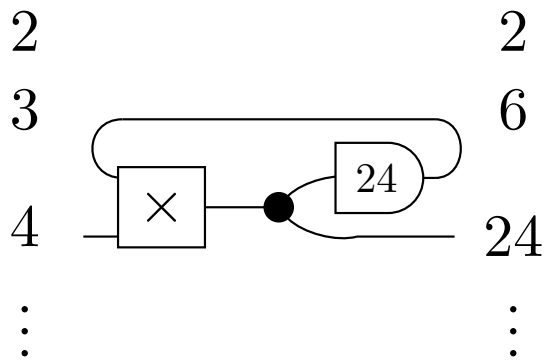
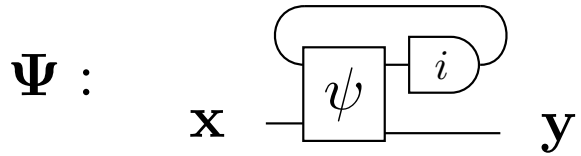
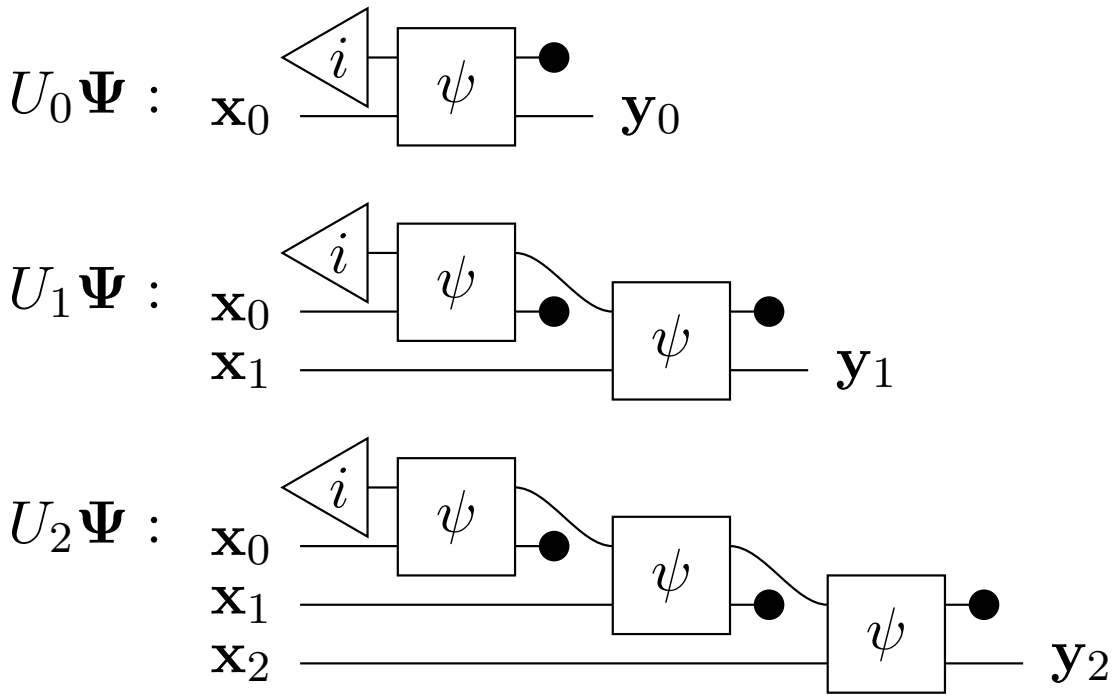


Unrolling semantics

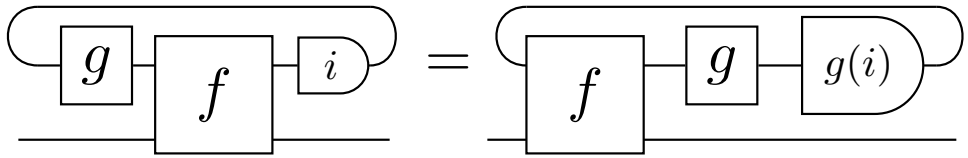


A common semantics of RNNs uses the *unrollings* of the network:



A (desired) consequence of these semantics

From the unrolling semantics, we can infer that these two RNNs should be equal:

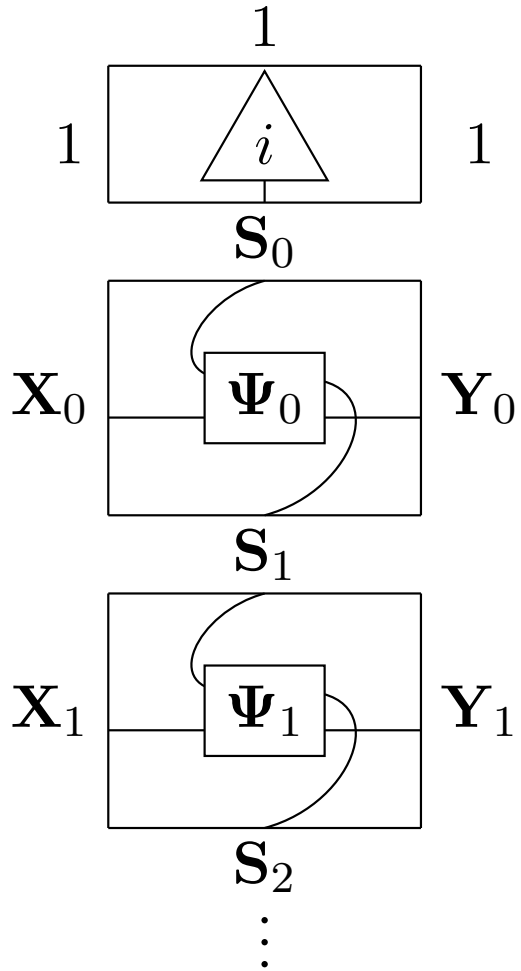


Outline

Stateful **computations**

Let $(\mathbb{C}, \times, 1)$ be a strict Cartesian category, whose morphisms we think of as stateless functions. A stateful sequence computation looks like this:

$$\mathbf{\Psi}_i \in \mathbb{C}(\mathbf{S}_i \times \mathbf{X}_i, \mathbf{S}_{i+1} \times \mathbf{Y}_i)$$



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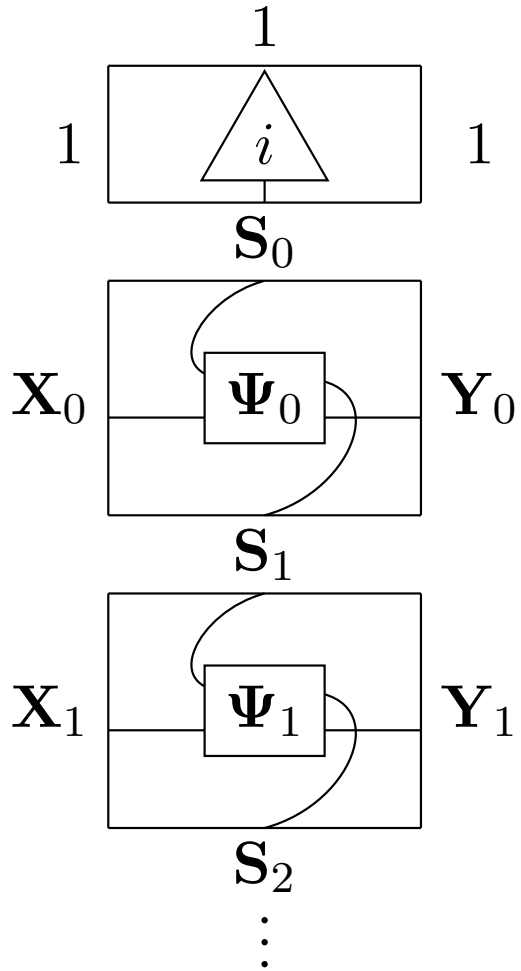
This is a sequence of 2-cells in a double category based on $\mathbb{C}$, with a restriction on the first 2-cell.



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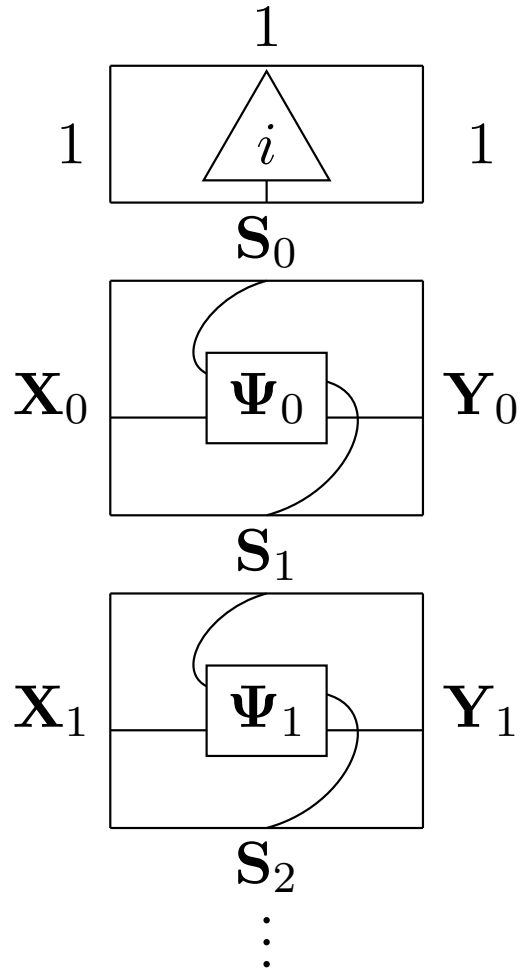
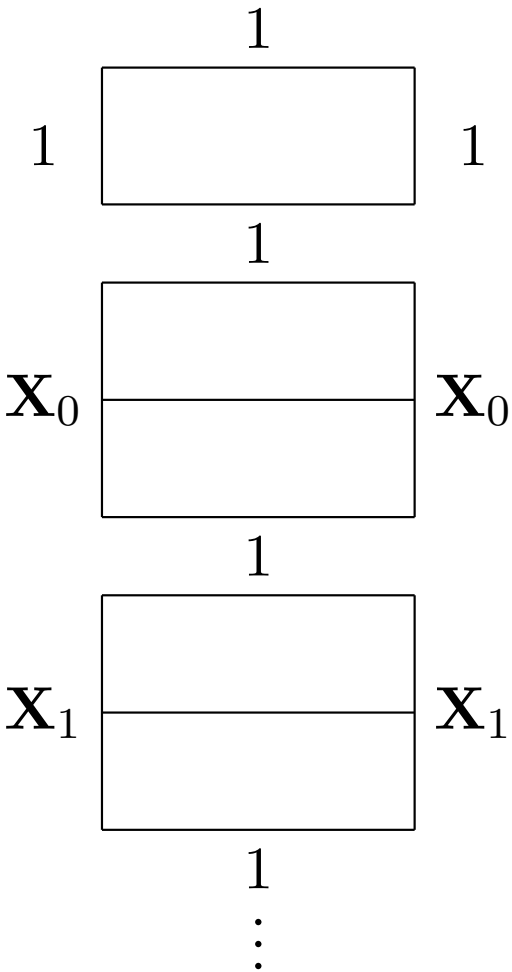
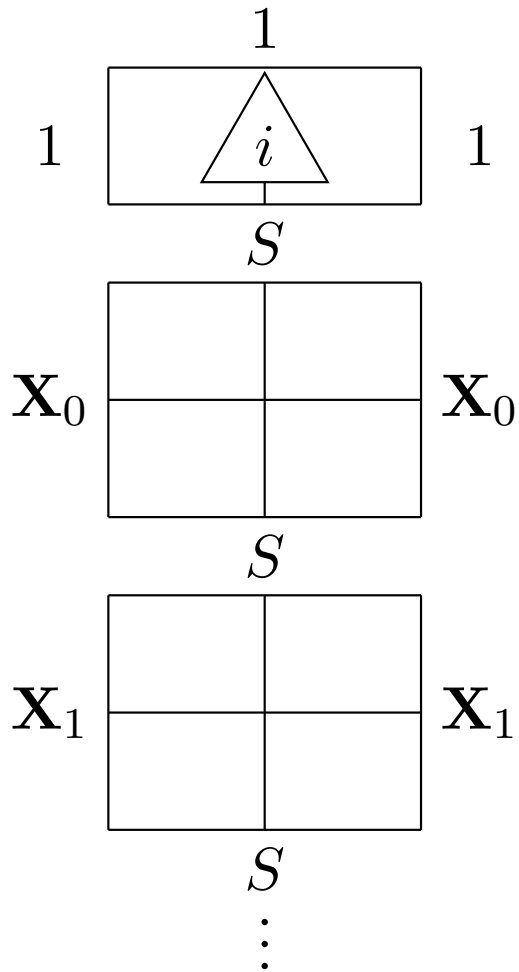


At time i, the computation executes function $\mathbf{\Psi}_i$, which takes a *value* of type $\mathbf{X}_i$ from the environment and a *state* of type $\mathbf{S}_i$ prepared by the previous step and returns a value of type $\mathbf{Y}_i$ and a state of type $\mathbf{S}_{i+1}$.

Stateful **functions**

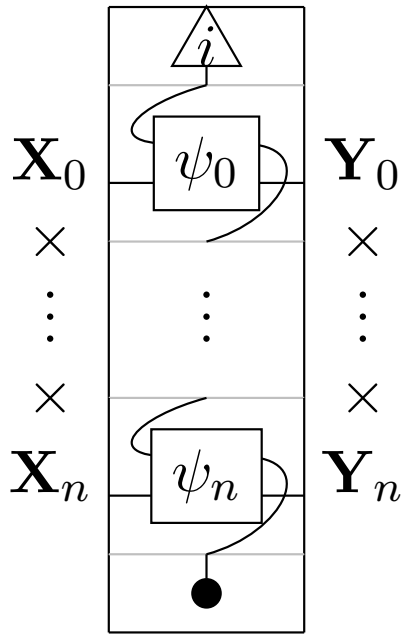
Two computation sequences might have different state spaces and still compute the same function. For example:





Stateful **functions**

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



Definition

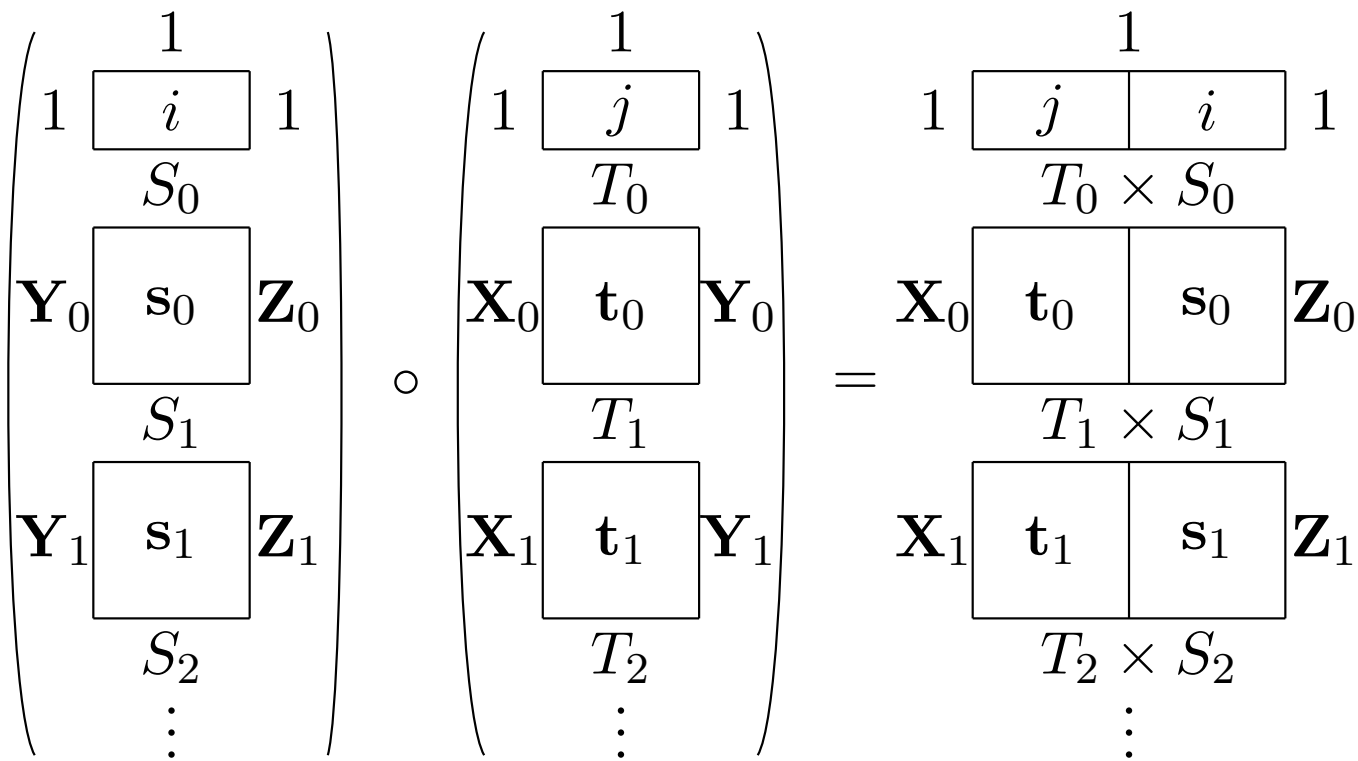
Two computation sequences are *extensionally equivalent* means they have the same nth truncation for all $n \in \mathbb{N}$. A *stateful (sequence) function* is an extensional equivalence class of computation sequences.

Stateful **functions**

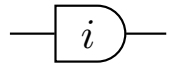
Definition

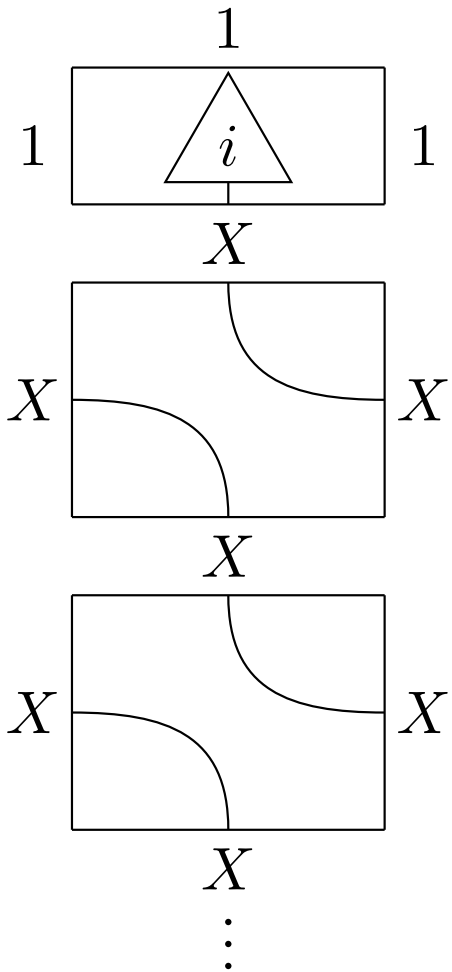
If $\mathbb{C}$ is a strict Cartesian category, then its *stateful sequence extension* is a category $\mathrm{St}(\mathbb{C})$ where

- objects are infinite sequences of objects in $\mathbb{C}$ and
- morphisms are stateful functions $\mathbf{\Psi} : \mathbf{X} \to \mathbf{Y}$.



Example computation sequences

Here is  as a computation sequence:



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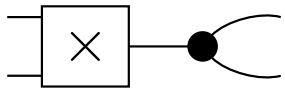
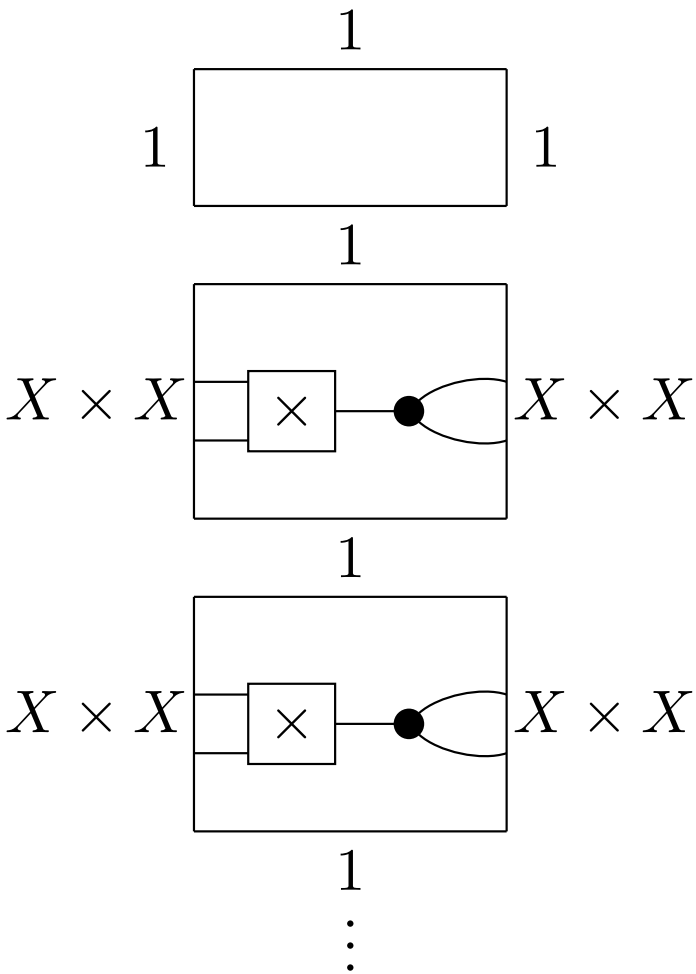
Here is  as a computation sequence:



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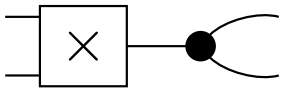
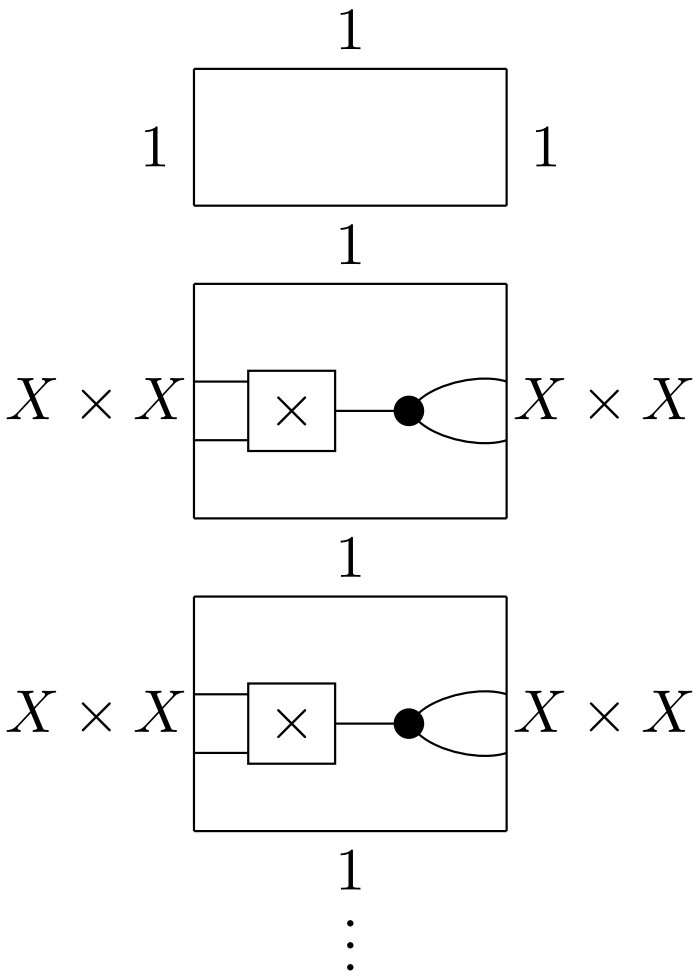
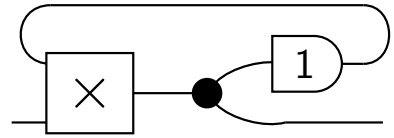
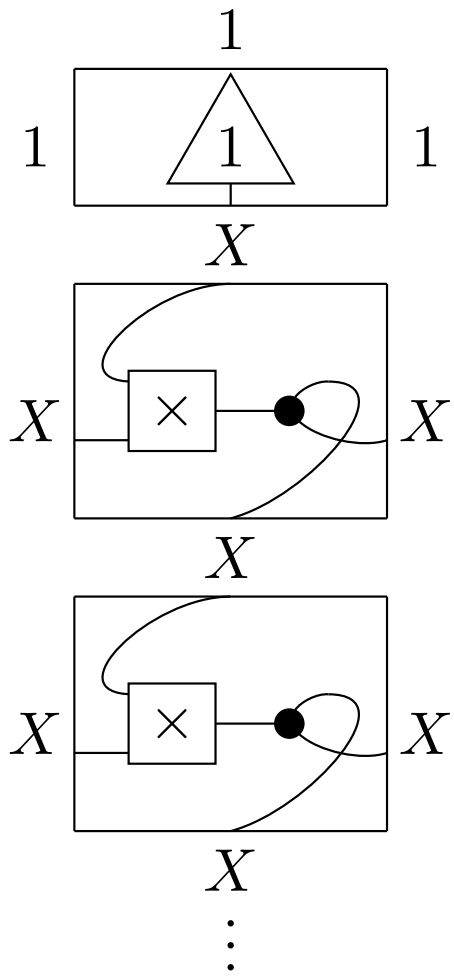
Here is  as a computation sequence:



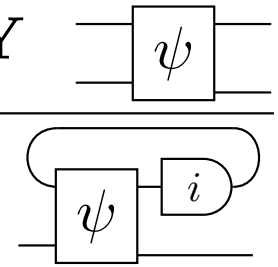
Here is  as a computation sequence:



Delayed trace

This loop-with-register is a like a trace (Joyal+ '96)—we call it a *delayed trace*. It satisfies several properties of an ordinary trace:

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



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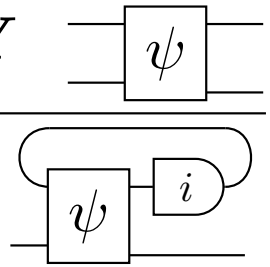
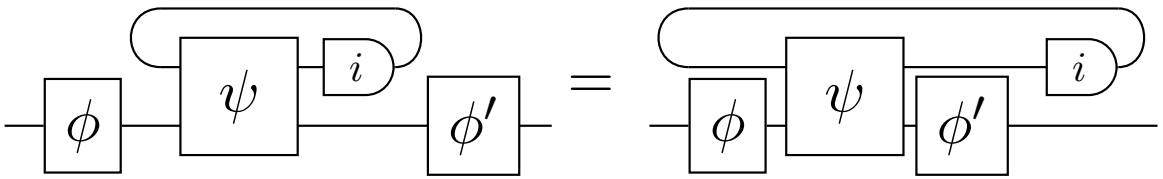


S/T naturality:



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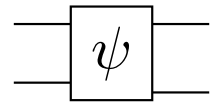
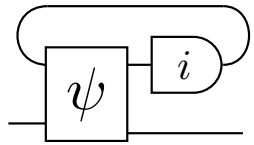


$$dtr_i^{\mathbf{S}}(\psi) : \mathbf{X} \to \mathbf{Y}$$



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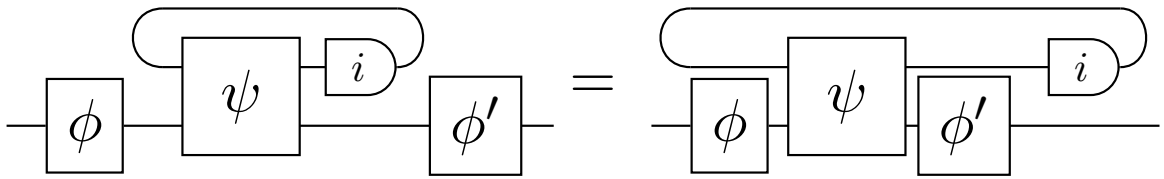
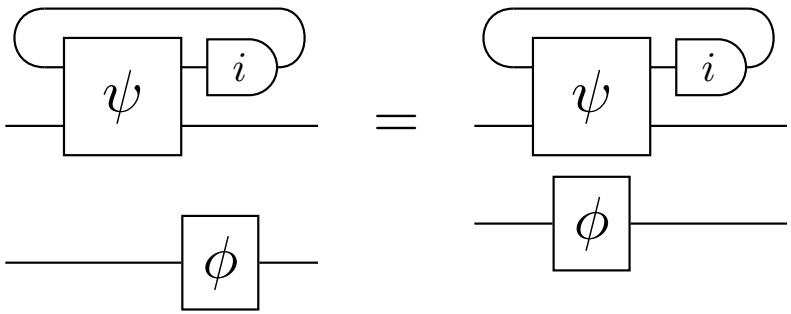


Superposition:



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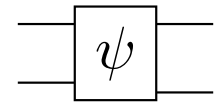
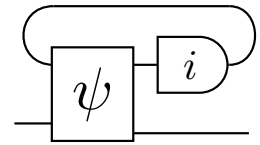
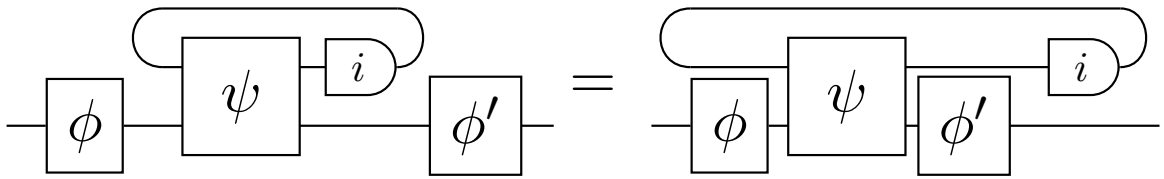
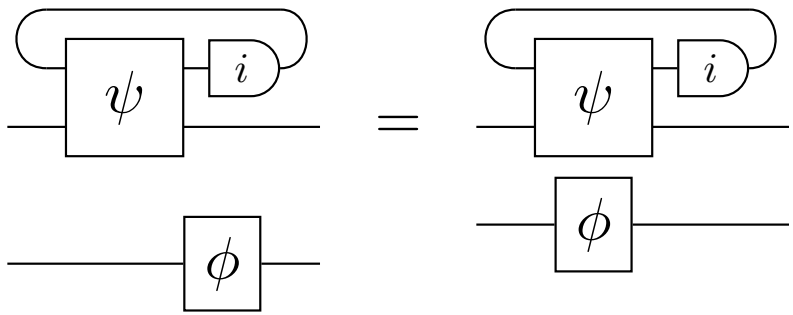




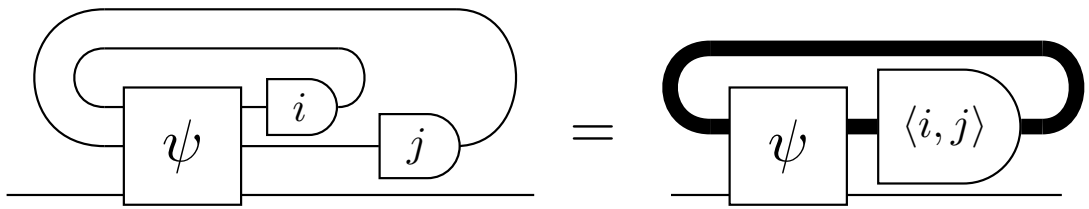
S/T naturality:



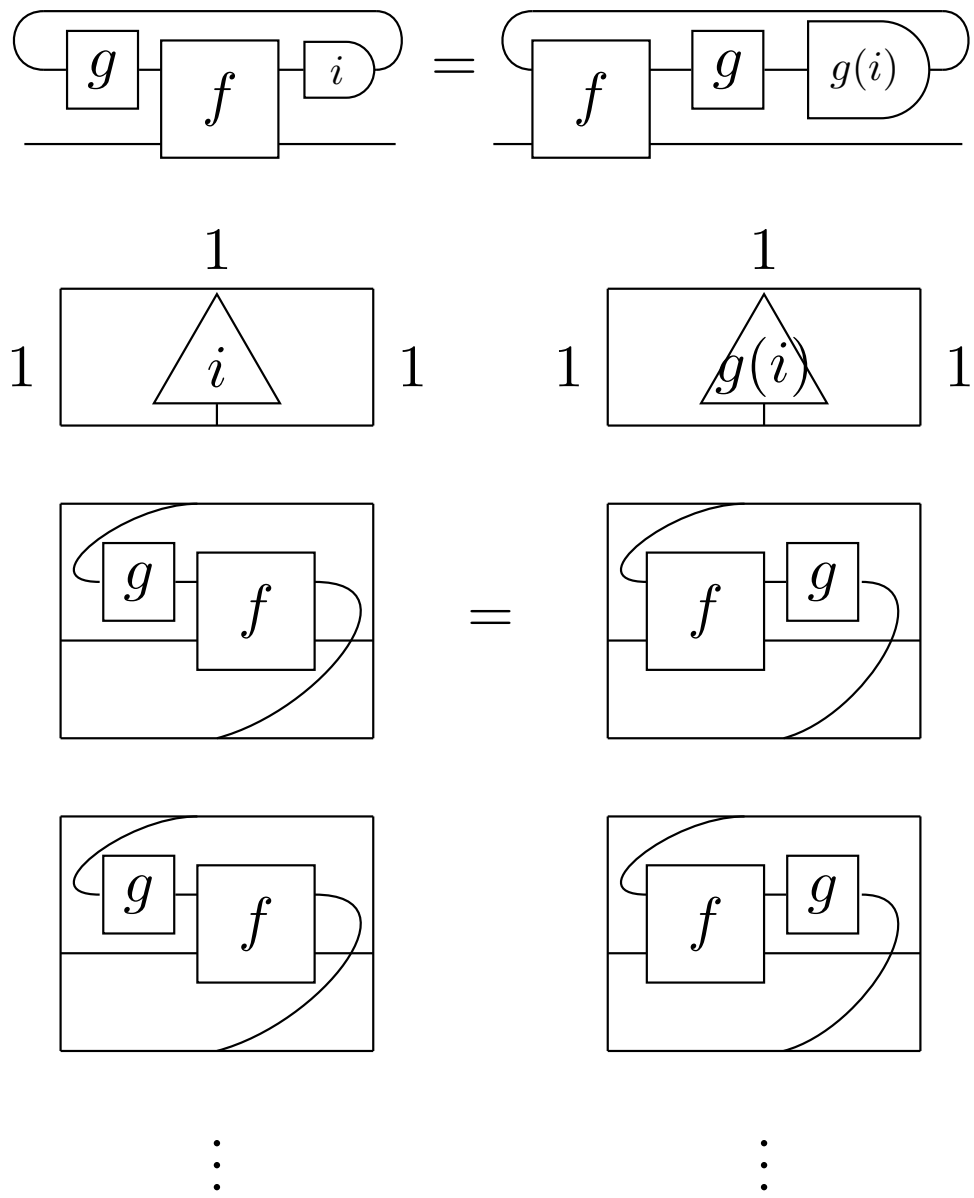
Superposition:



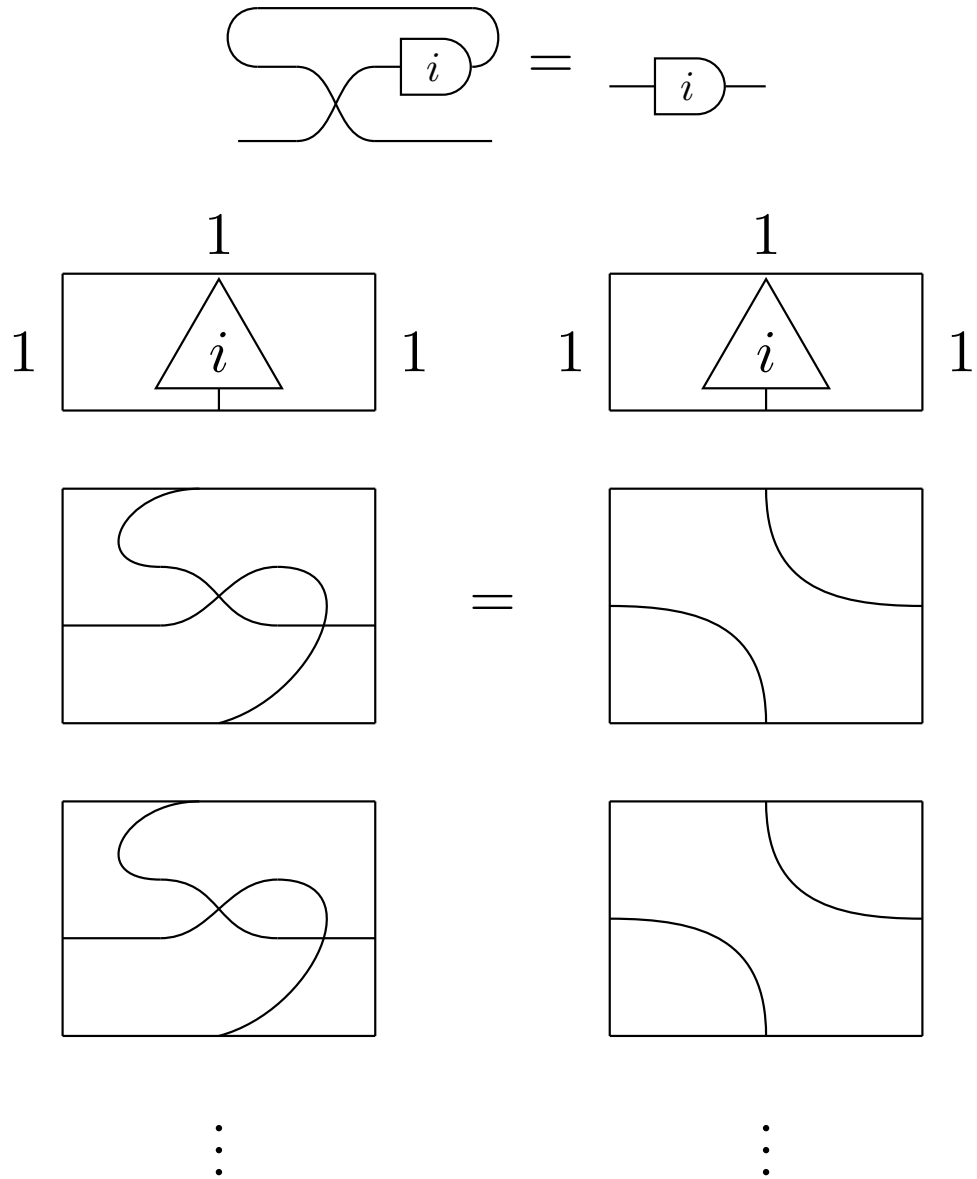
Vanishing $\times$:



~~Dinaturality~~ → retiming



~~Yanking~~ → delay

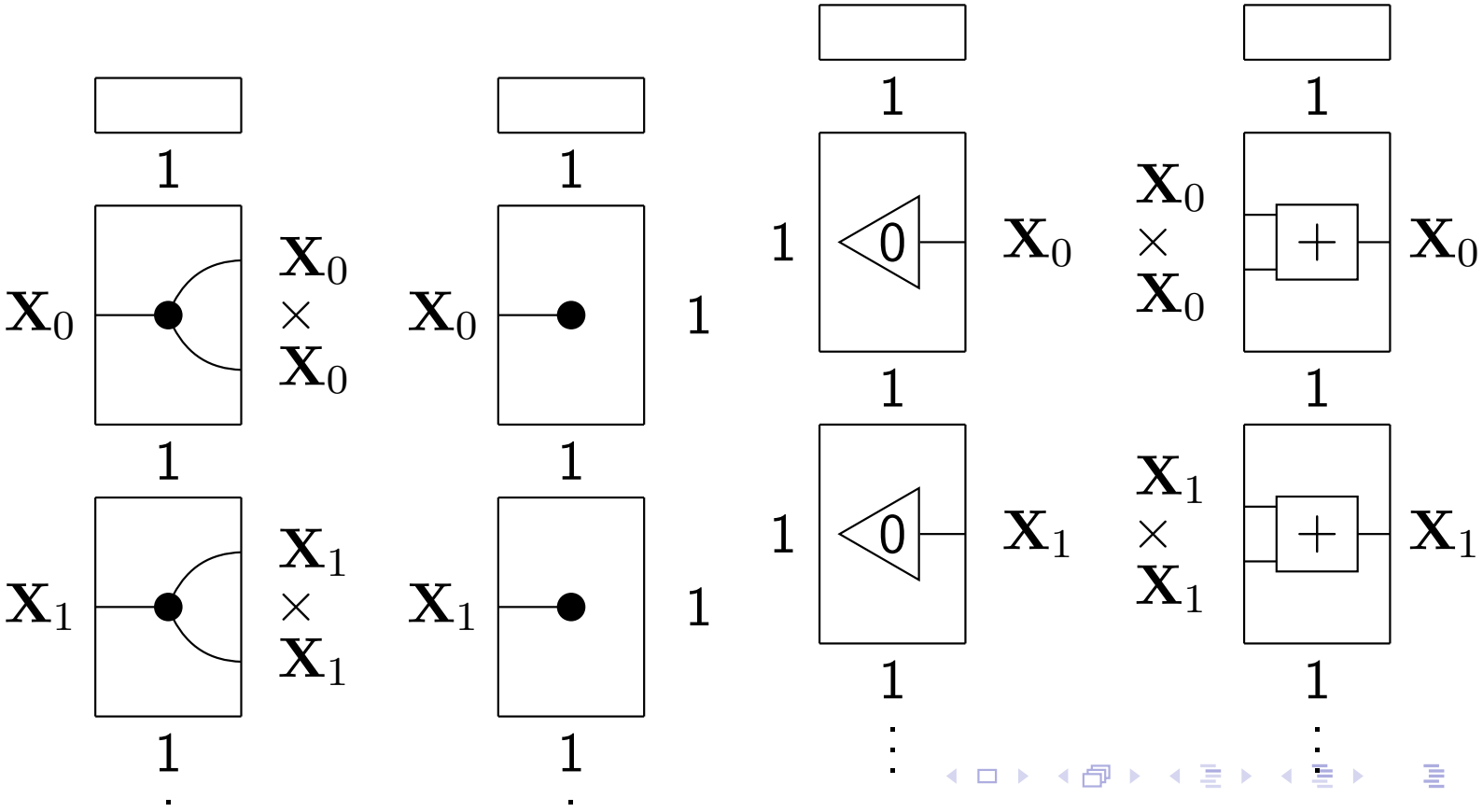


$\mathrm{St}(-)$ preserves a lot of structure

Theorem

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

The first two are easy:



Sanity checks

Proposition: $\mathbb{C}$ embeds in $\mathrm{St}(\mathbb{C})$

There is a finite-product preserving functor $H : \mathbb{C} \to \mathrm{St}(\mathbb{C})$. It takes A to $(A, A, A, \ldots)$ and f to the stateless sequence executing f at each step.

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Proposition: Normal forms for $\mathrm{St}(\mathbb{C})$

Every $\Psi \in \mathrm{St}(\mathbb{C})(\mathbf{A}, \mathbf{B})$ can be written as $\Psi = dtr_i^{\mathbf{S}}(\psi)$ where ψ has a stateless representative and $i : 1 \to S$.

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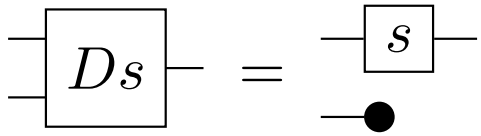
Adding state to computations is common:

1. Bicategorically—Katis, Sabadini, & Walters '97
2. Digital circuits—Ghica & Jung, '16
3. Signal flow graphs—Bonchi, Sobociński, & Zanasi, '14

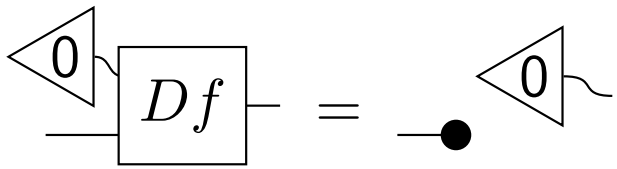
Outline

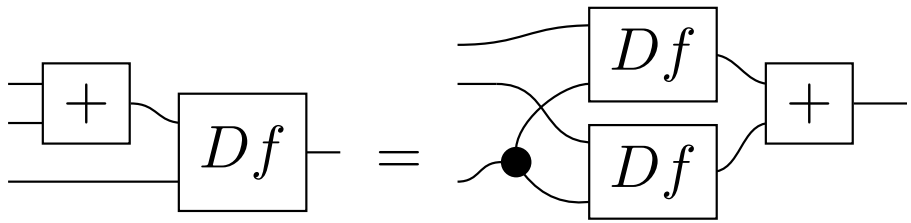
Cartesian differential categories [Blute, Cockett, Seely '09]

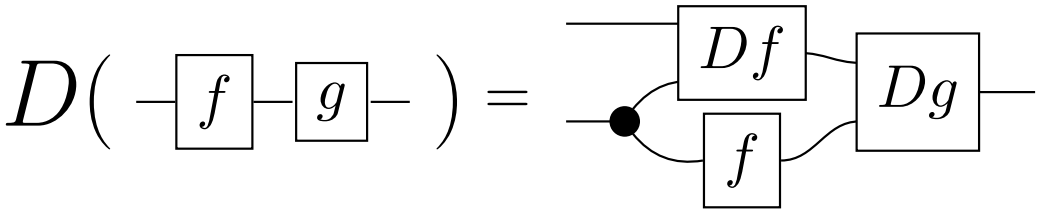
A *Cartesian differential category* has a differential operation on morphisms sending $f : X \to Y$ to $Df : X \times X \to Y$, satisfying seven axioms:

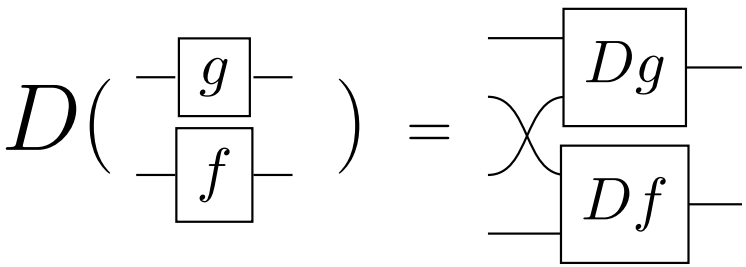
CD1. 

for $s \in \{\mathrm{id}_X, \sigma_{X,Y}, !_X, \Delta_X, 0_X, +_X\}$.

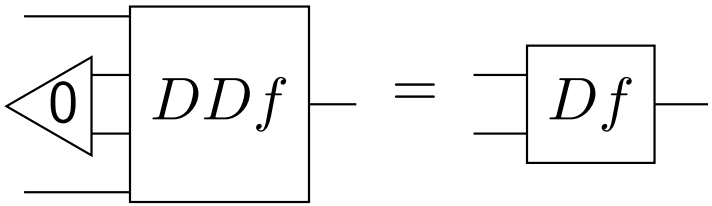
CD2. 

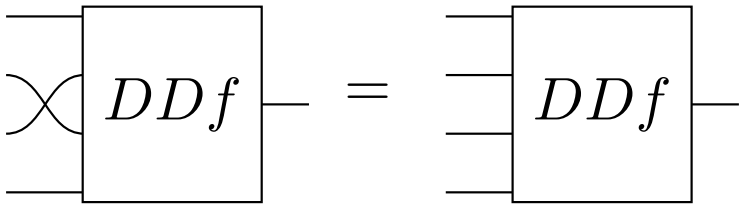
CD3. 

CD4. 

CD5. 

Cartesian differential category axioms, continued

CD6. 

CD7. 

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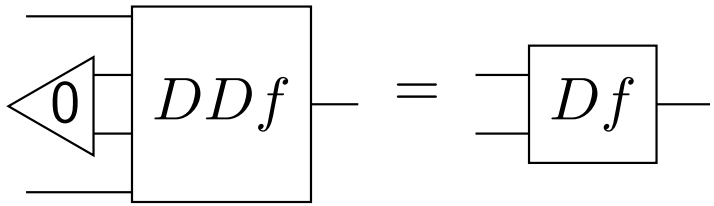
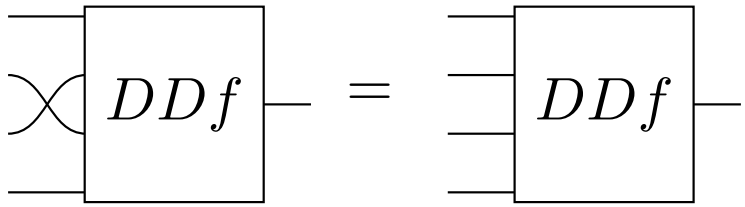
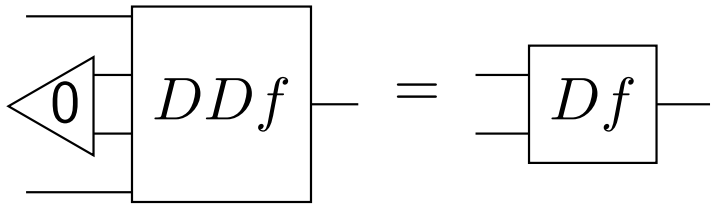
CD6. 

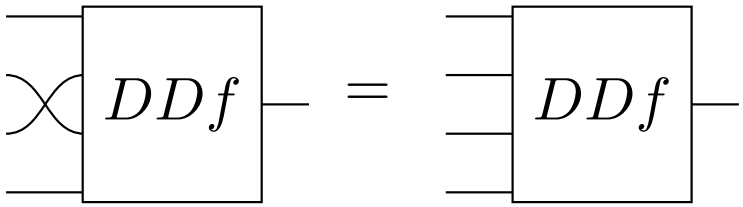
CD7. 

Example

Objects of the category $\mathbf{Euc}_\infty$ are $\mathbb{R}^n$ for $n \in \mathbb{N}$, maps are smooth maps between them. $\mathbf{Euc}_\infty$ is a Cartesian differential category with the (curried) Jacobian sending $f : \mathbb{R}^n \to \mathbb{R}^m$ to $Df : (\Delta x, x) \mapsto Jf|_x \times \Delta x$.

Cartesian differential category axioms, continued

CD6. 

CD7. 

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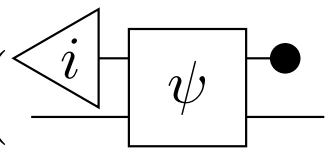
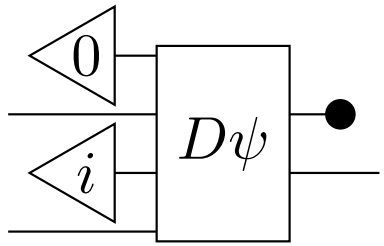
What's the right rule for delayed trace?

Differentiating the unrollings of a simple RNN

$D($ 

$) =$ 

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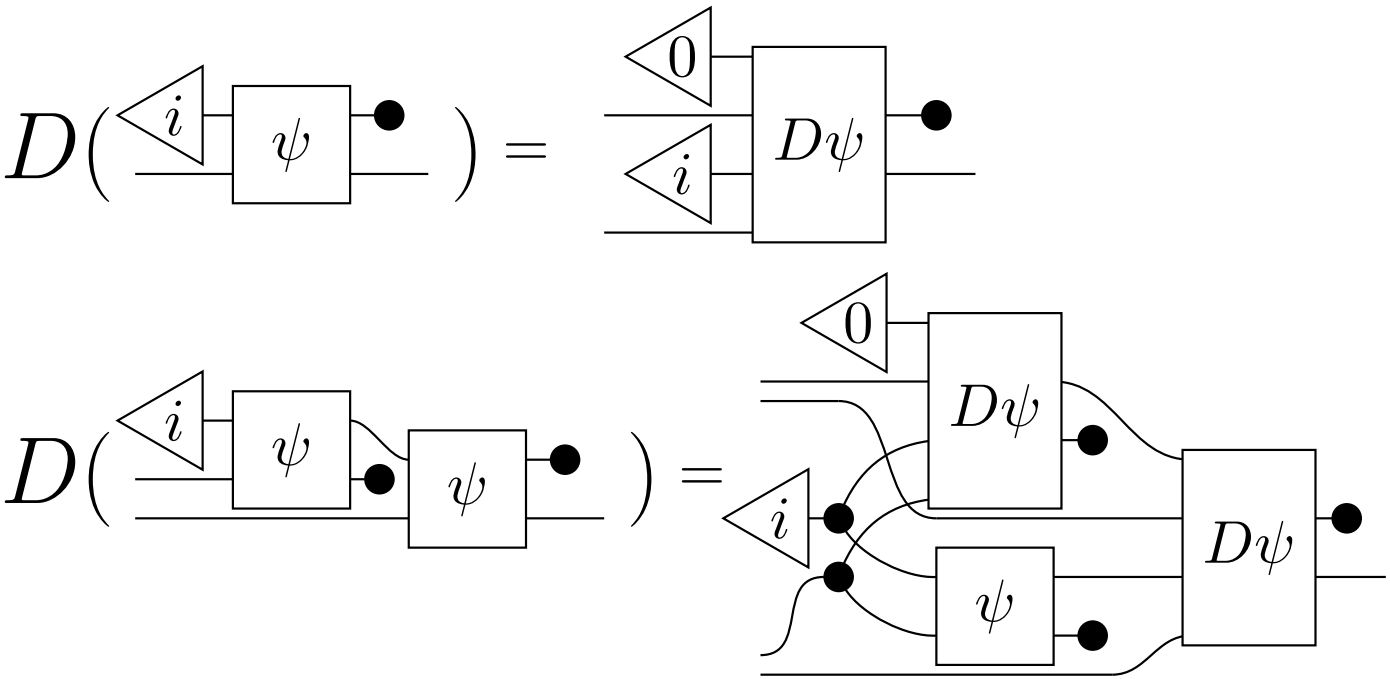

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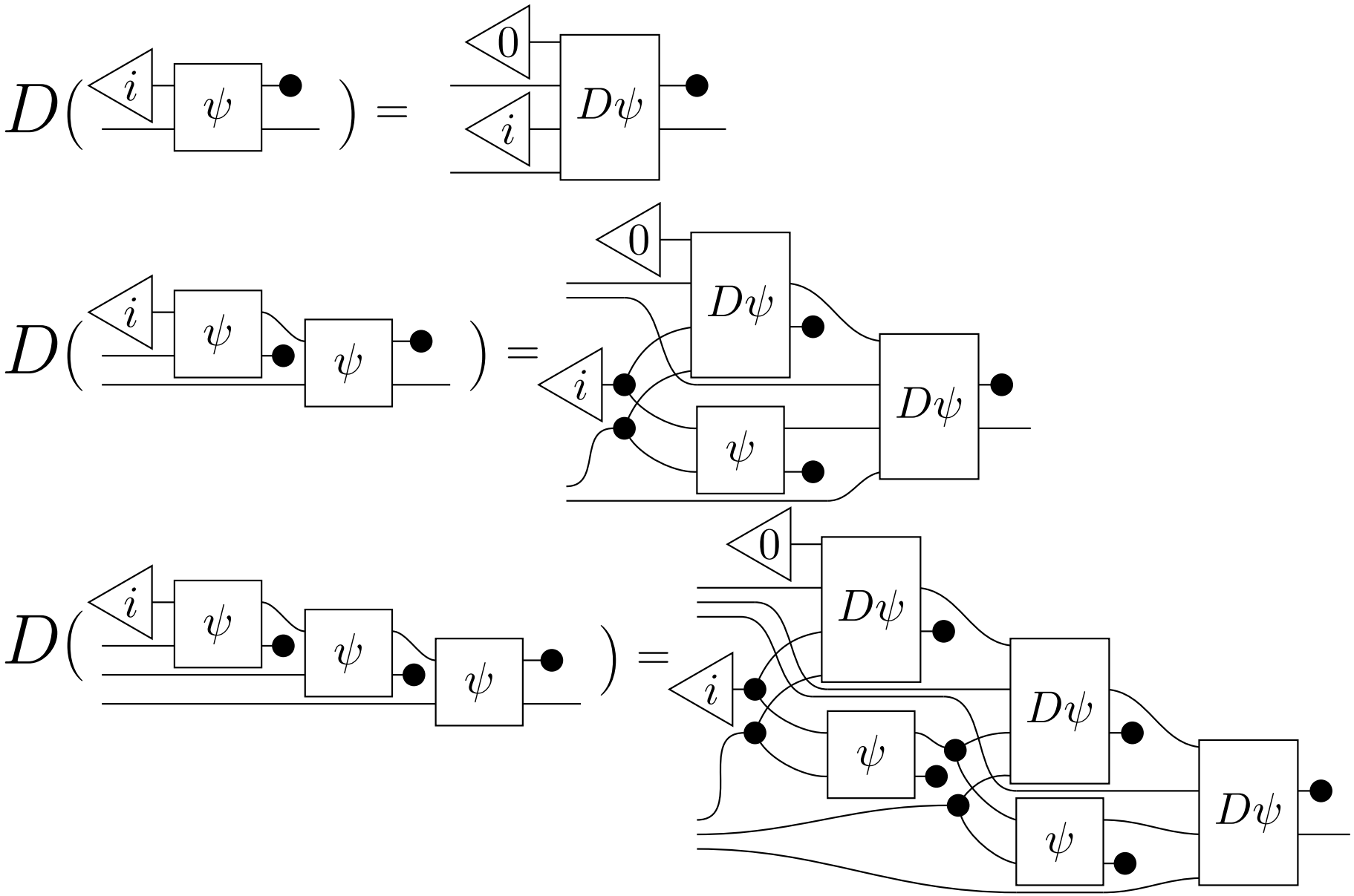
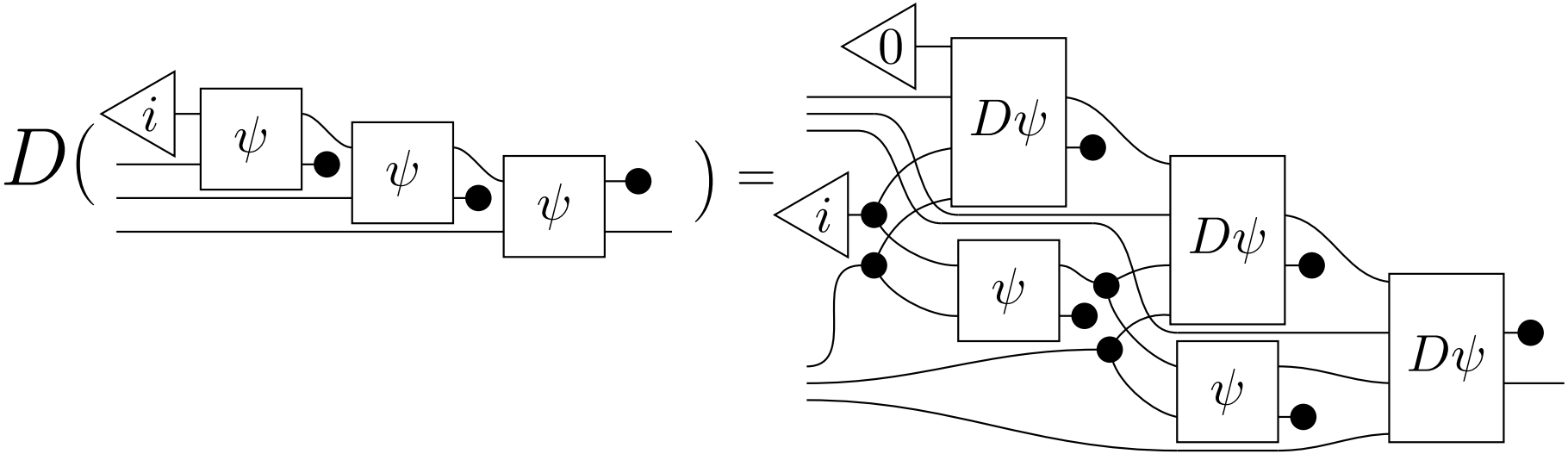
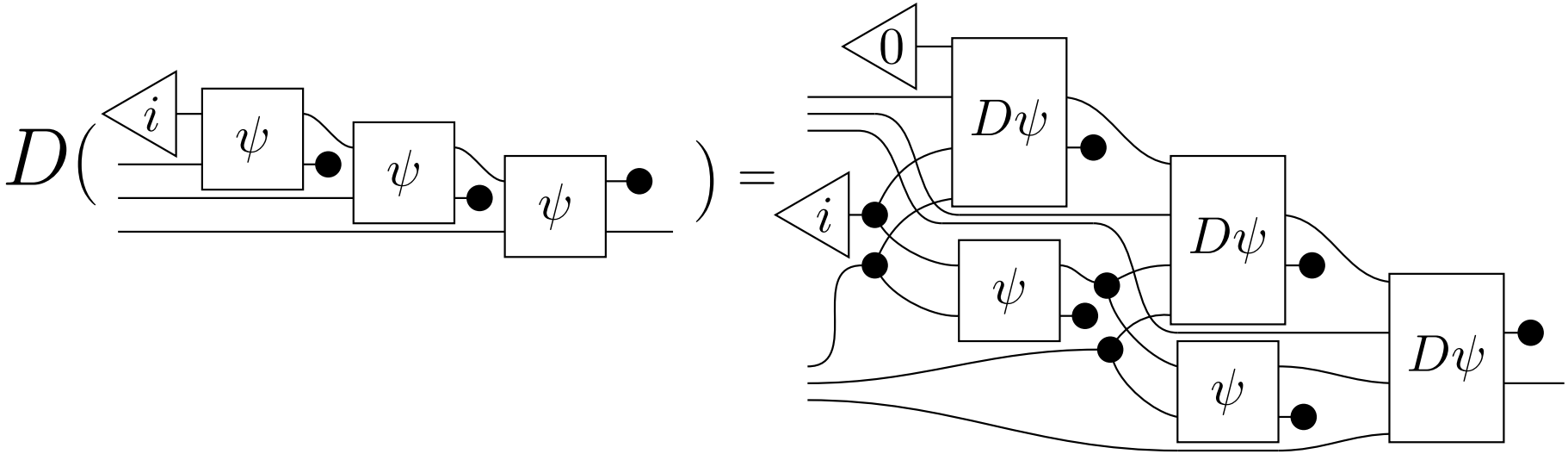




This suggests a hypothesis:



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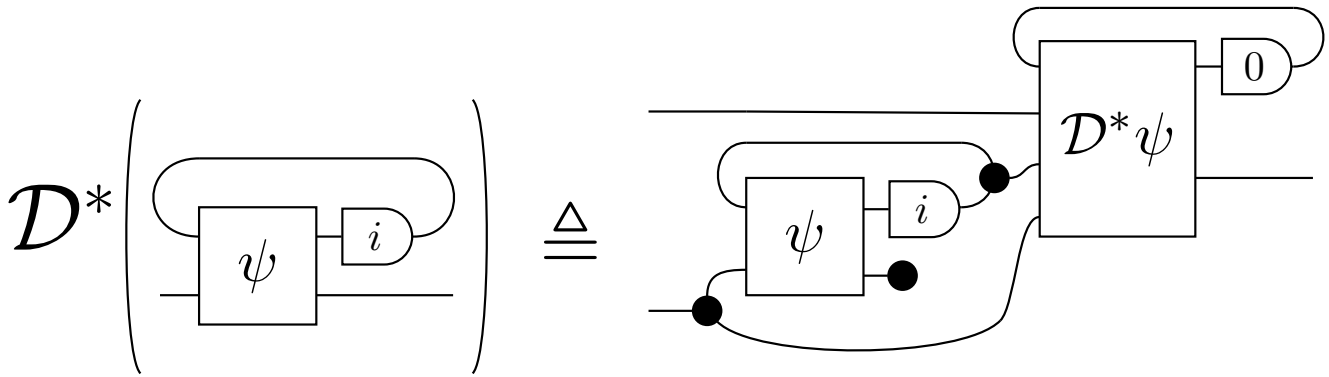
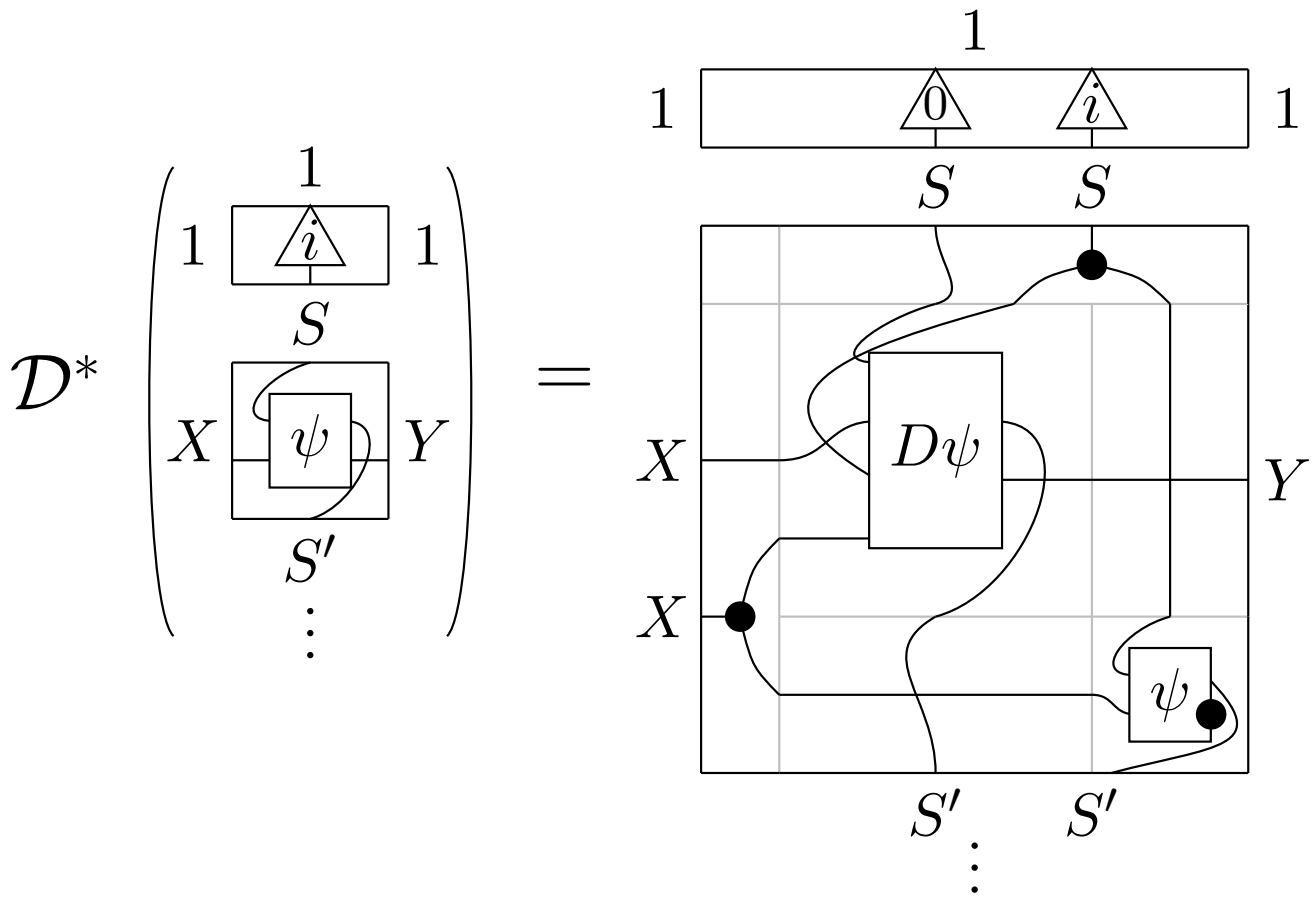


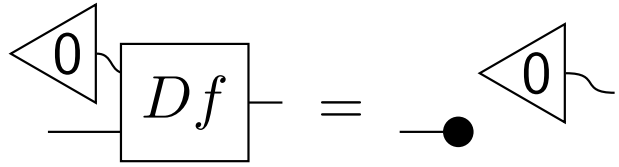
Differentiation for stateful functions

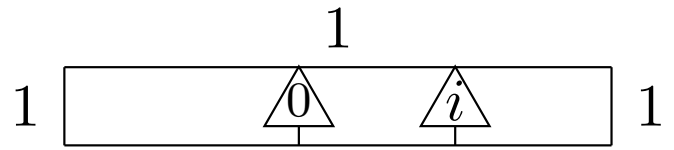
Let $\mathbb{C}$ be Cartesian differential with differential operator D. The following is a Cartesian differential operator on $\mathrm{St}(\mathbb{C})$:

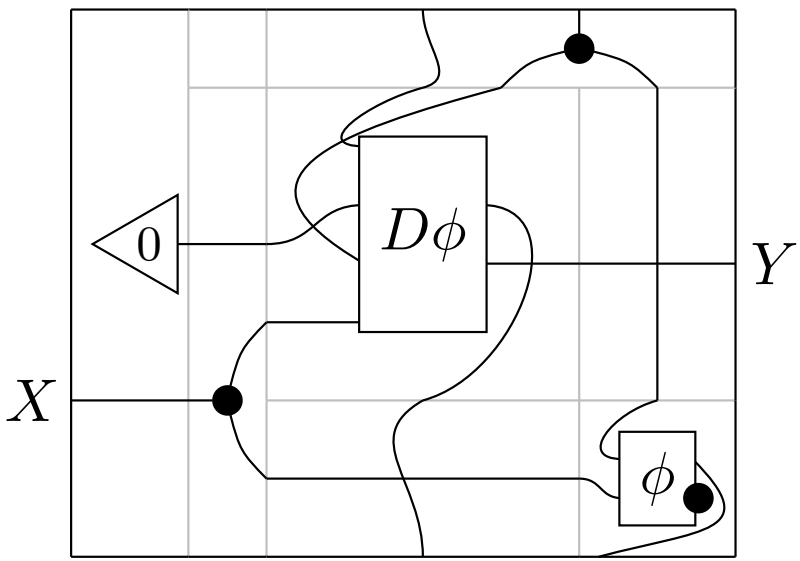


$\mathcal{D}^*$ is a Cartesian differential operator

Proof idea. For CD2:







$\vdots$

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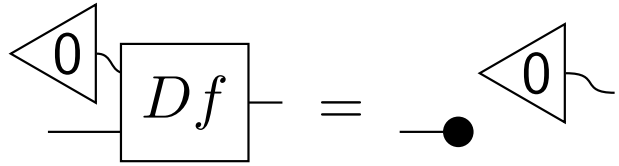

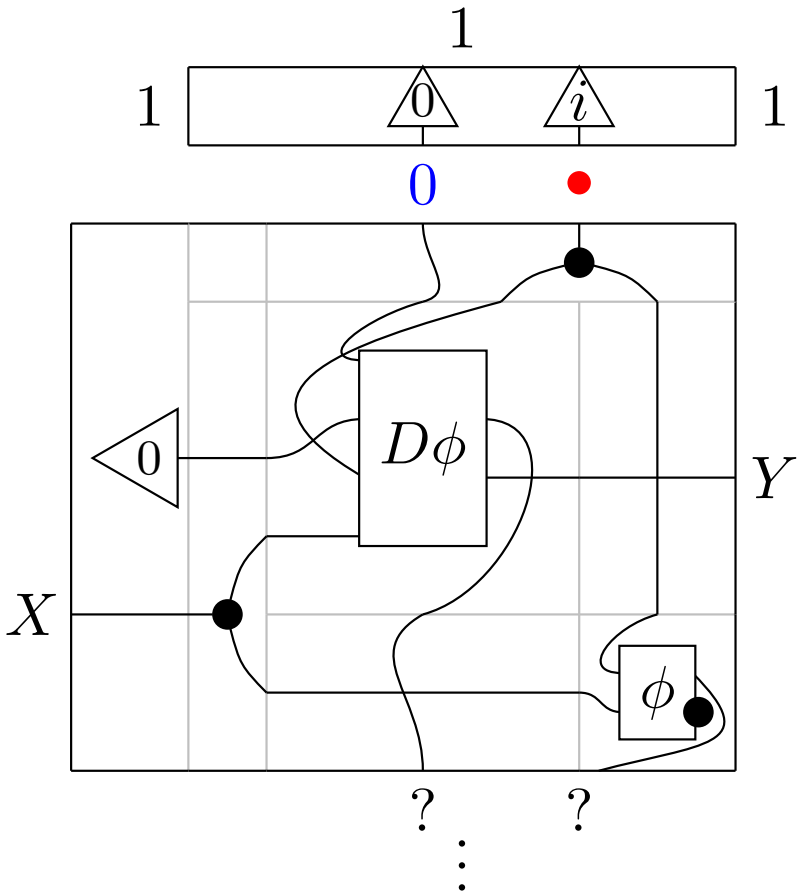

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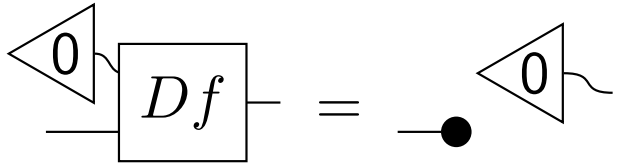
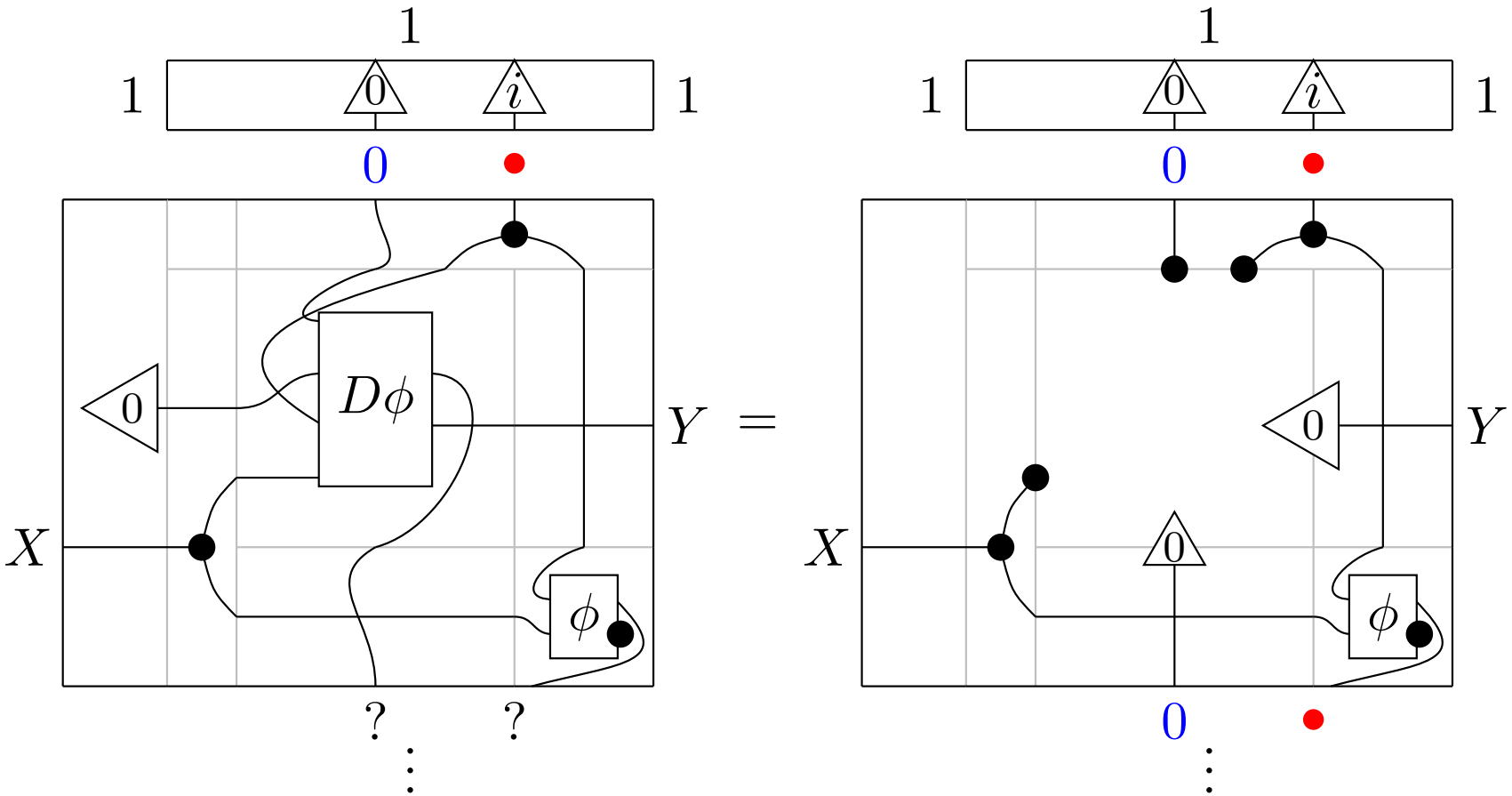
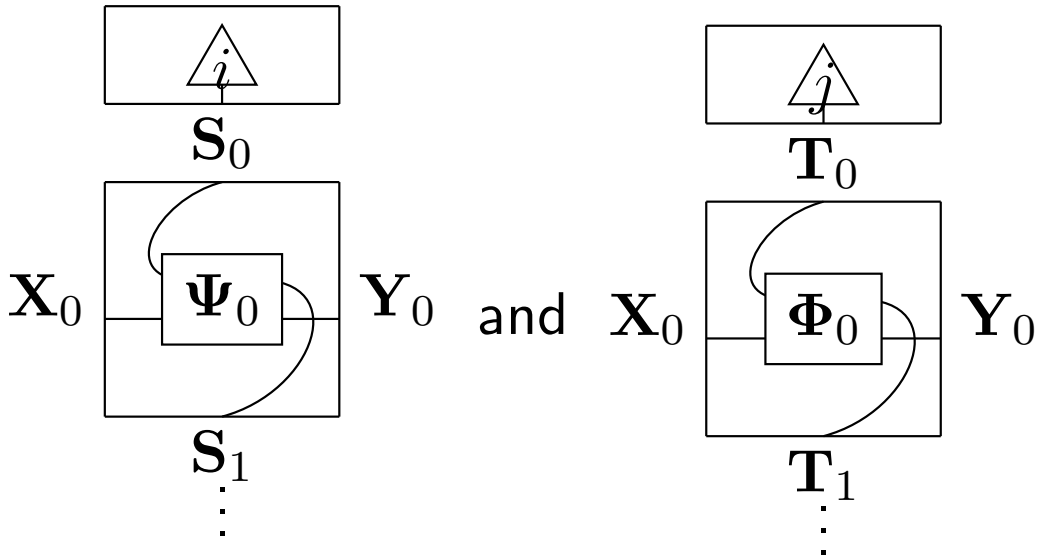


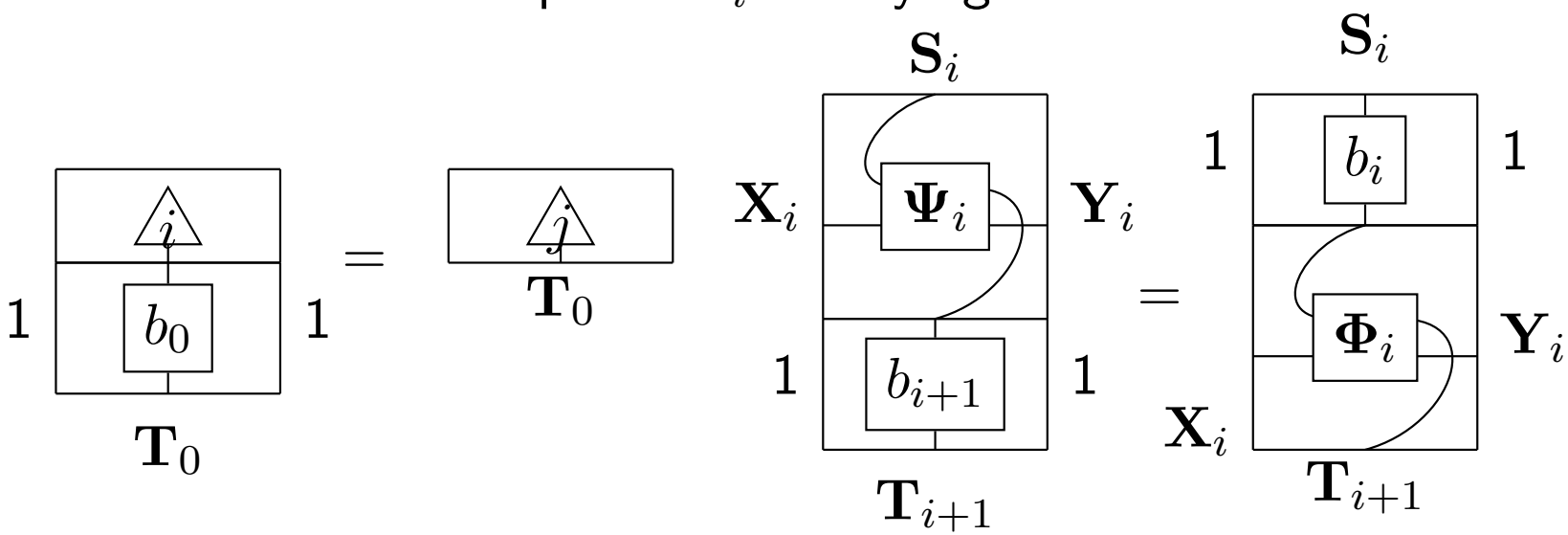


The (illustrated) shim lemma

In order to show the extensional equivalence of

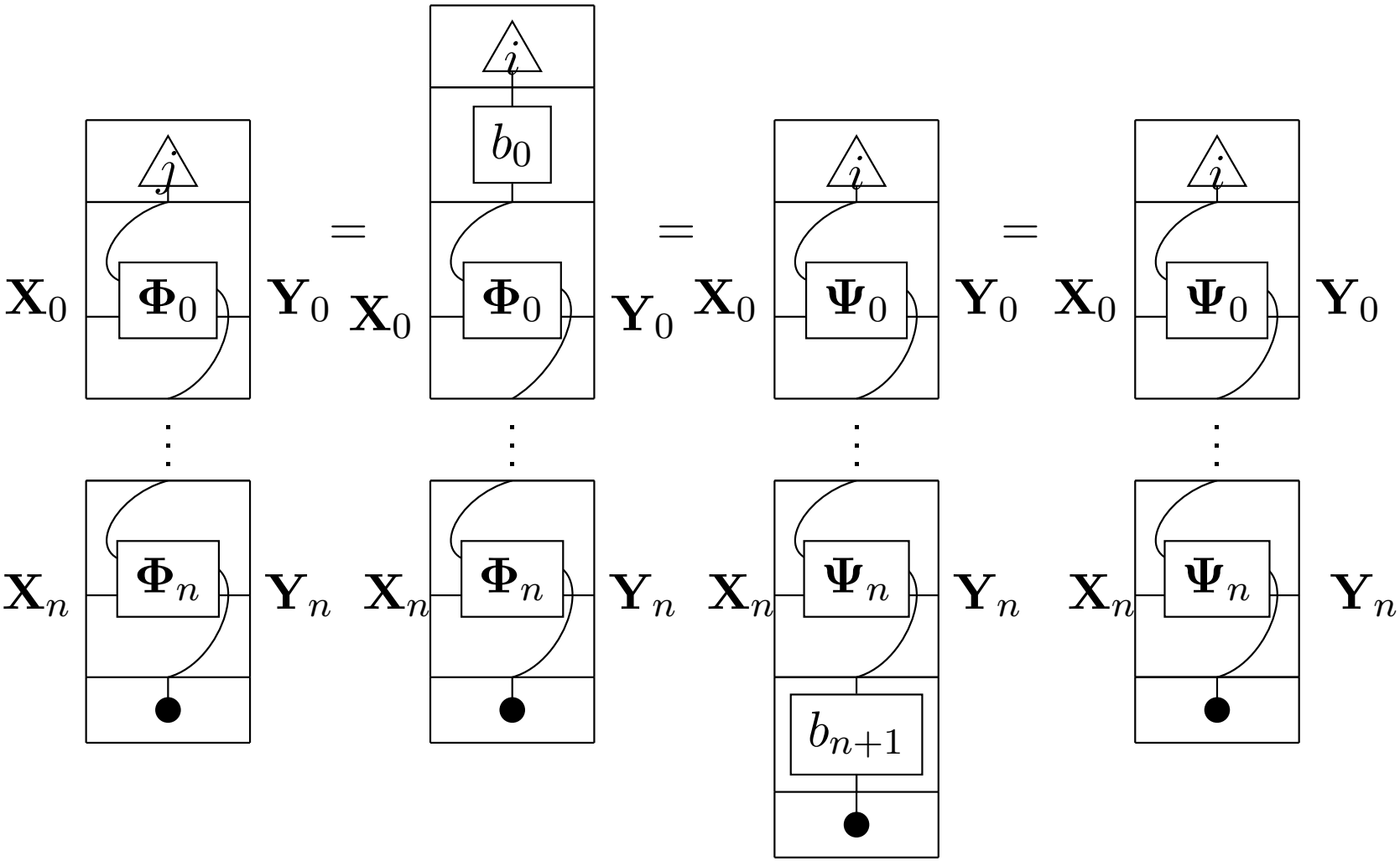


it suffices to find a sequence b_i satisfying:



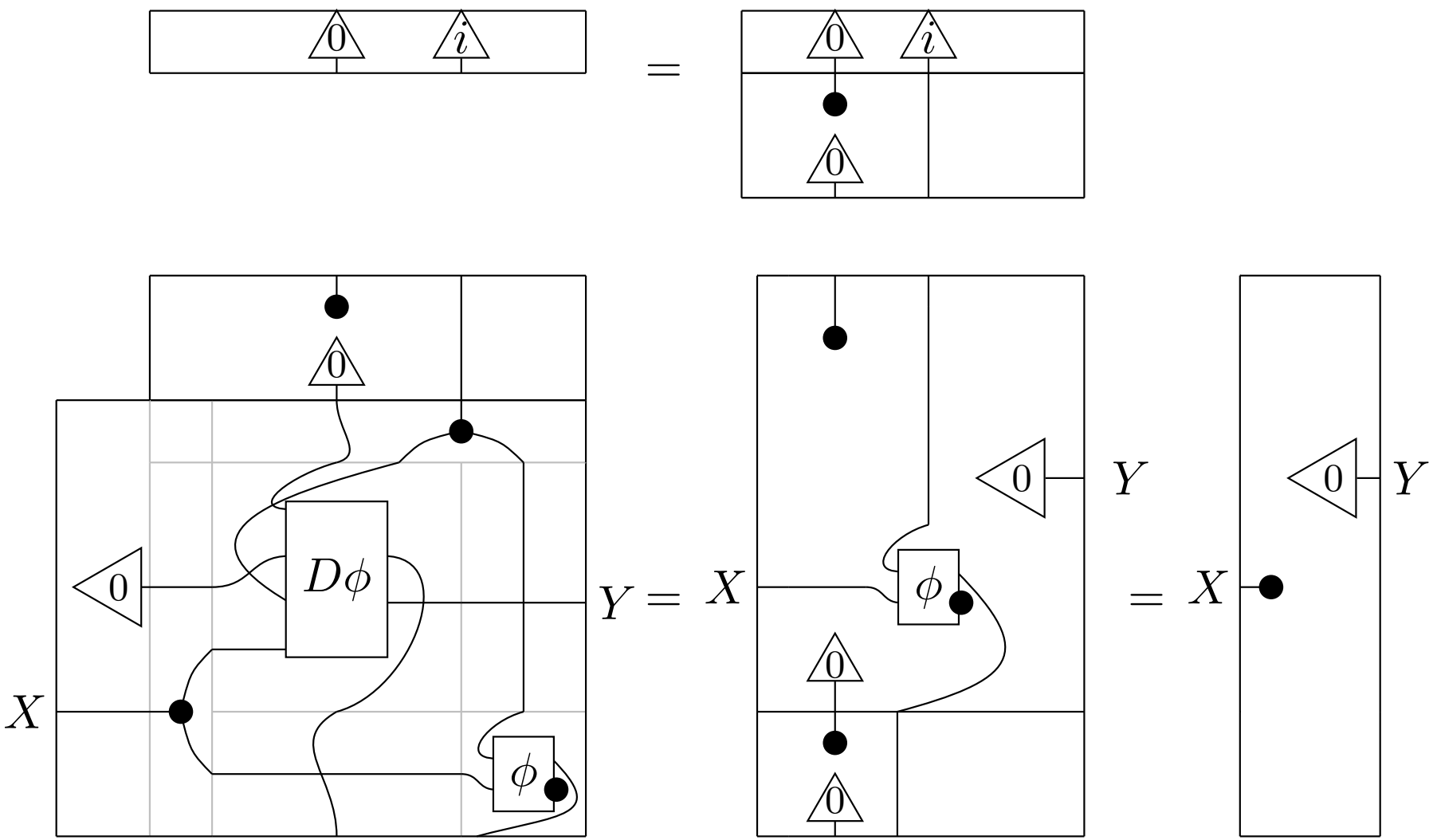
Proof of shim lemma

For all $n \in \omega$,



$\mathcal{D}^*$ is a Cartesian differential operator

Proof. For CD2:



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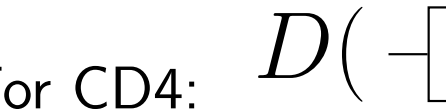
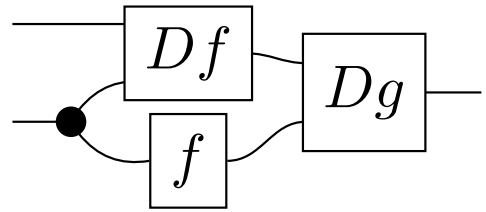
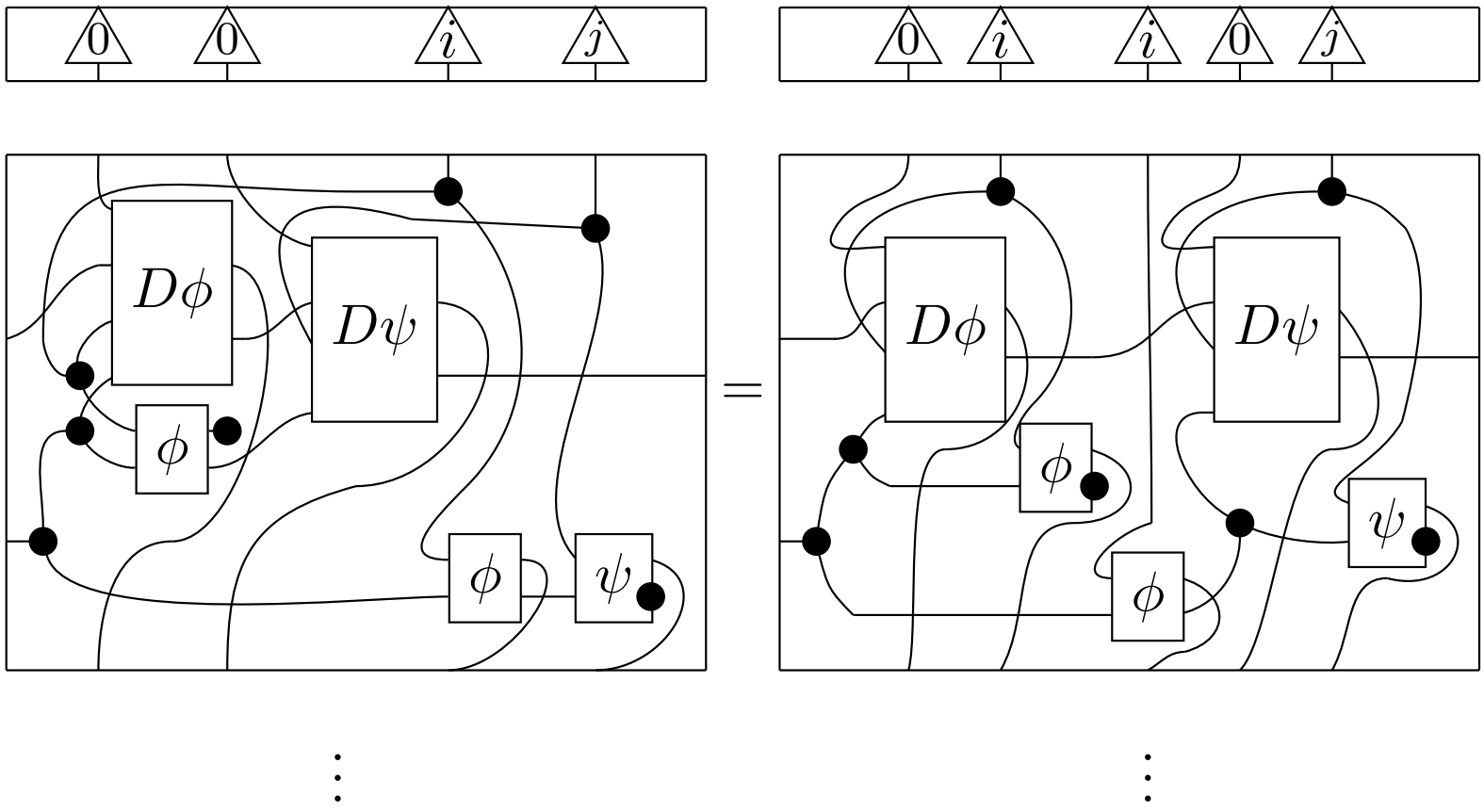
Proof idea. For CD4: $D($  $) =$ 



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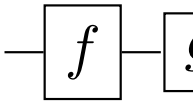
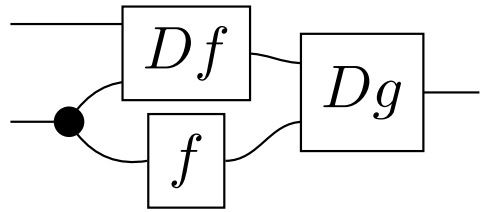
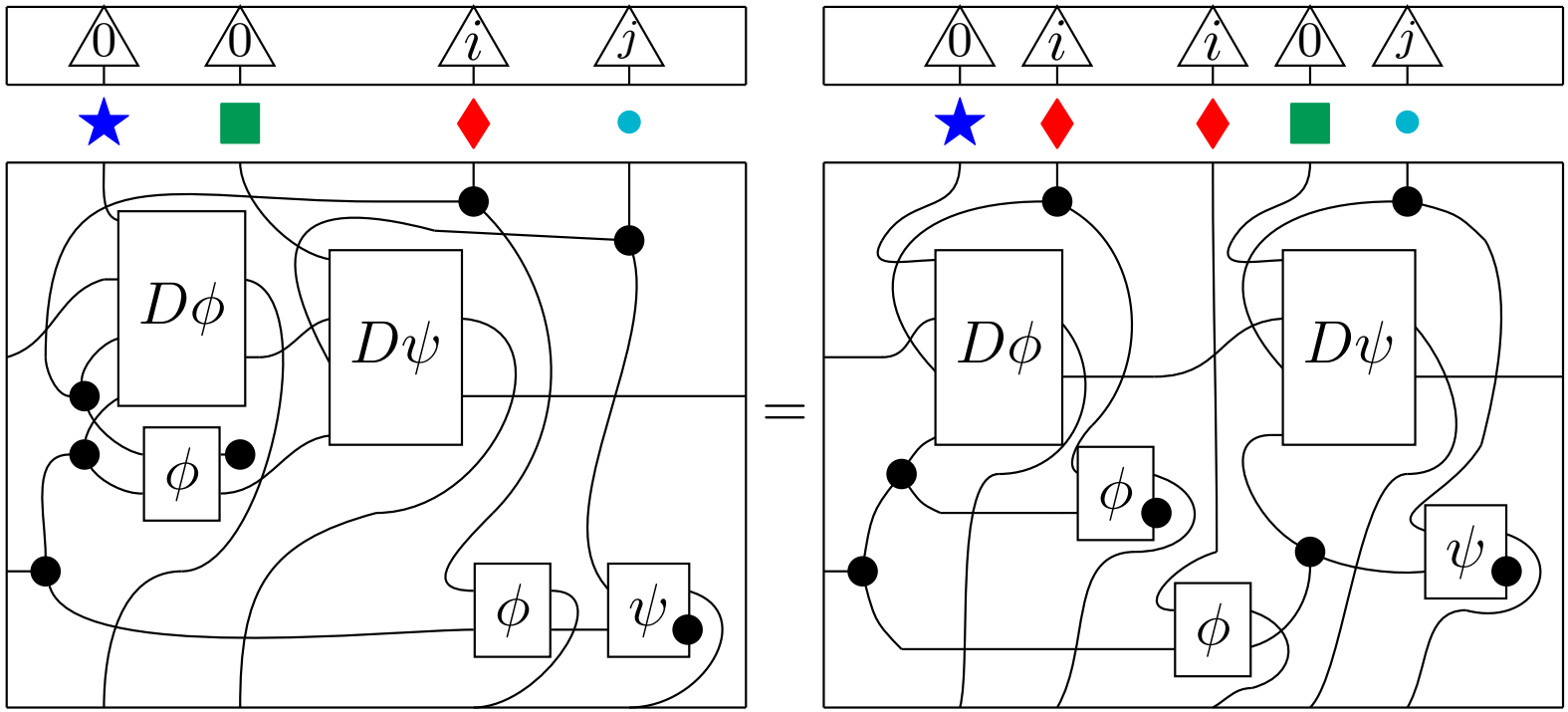
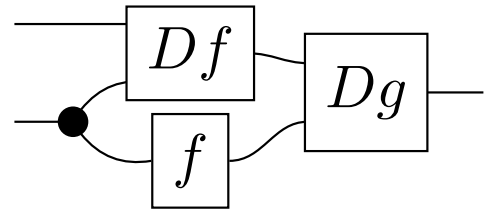
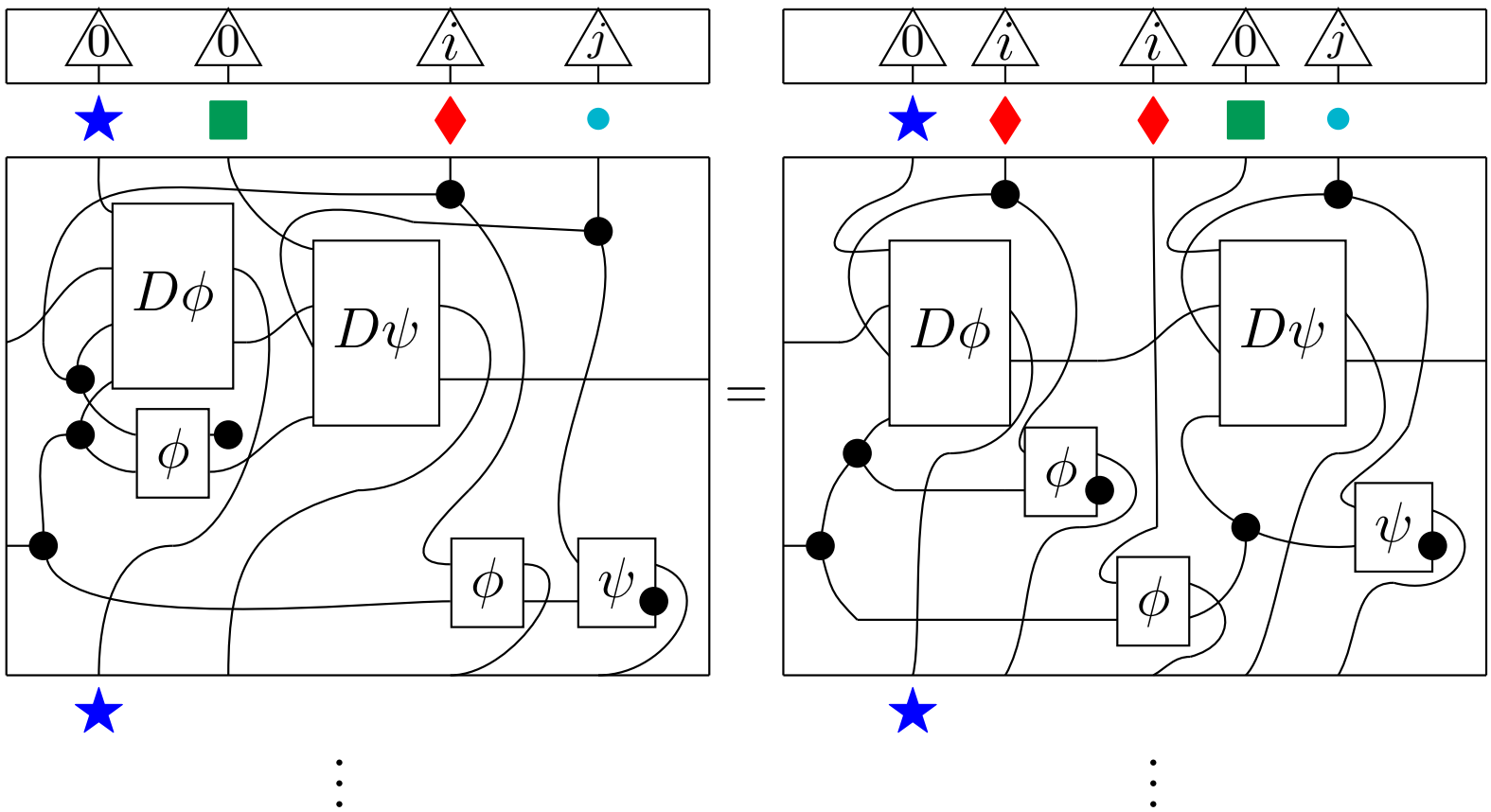
Proof idea. For CD4: $D($  $) =$ 



$\mathcal{D}^*$ is a Cartesian differential operator

Proof idea. For CD4: $D(\ -[f]-[g]-\ ) =$ 



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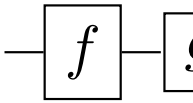
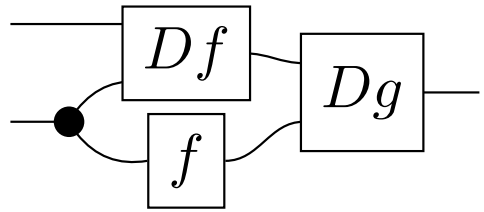
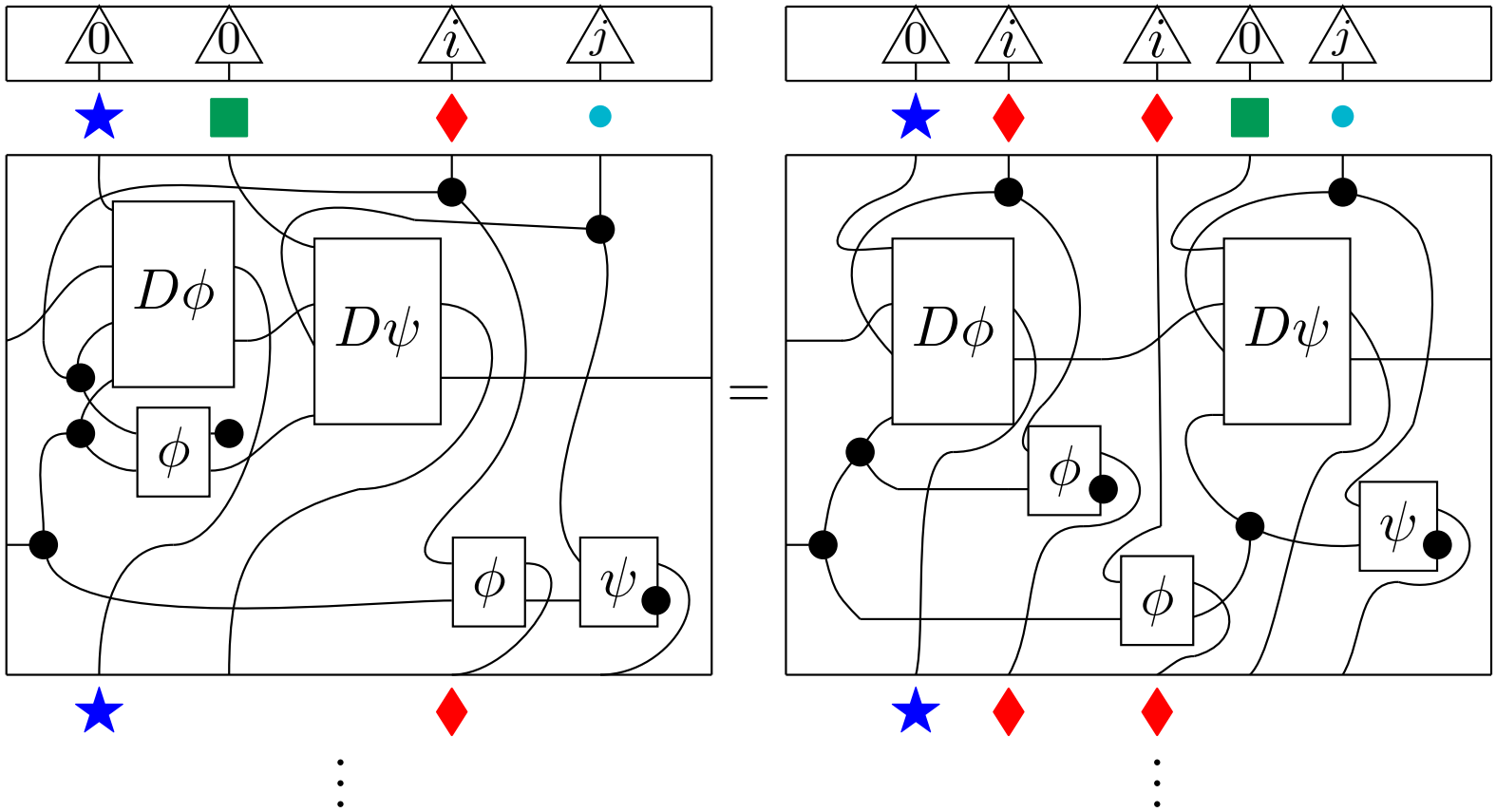
Proof idea. For CD4: $D($  $) =$ 



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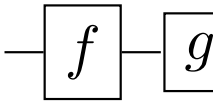
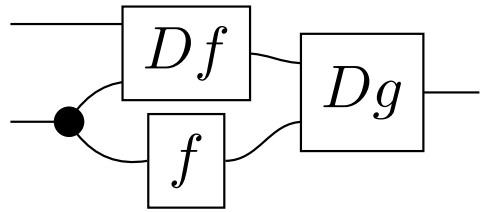
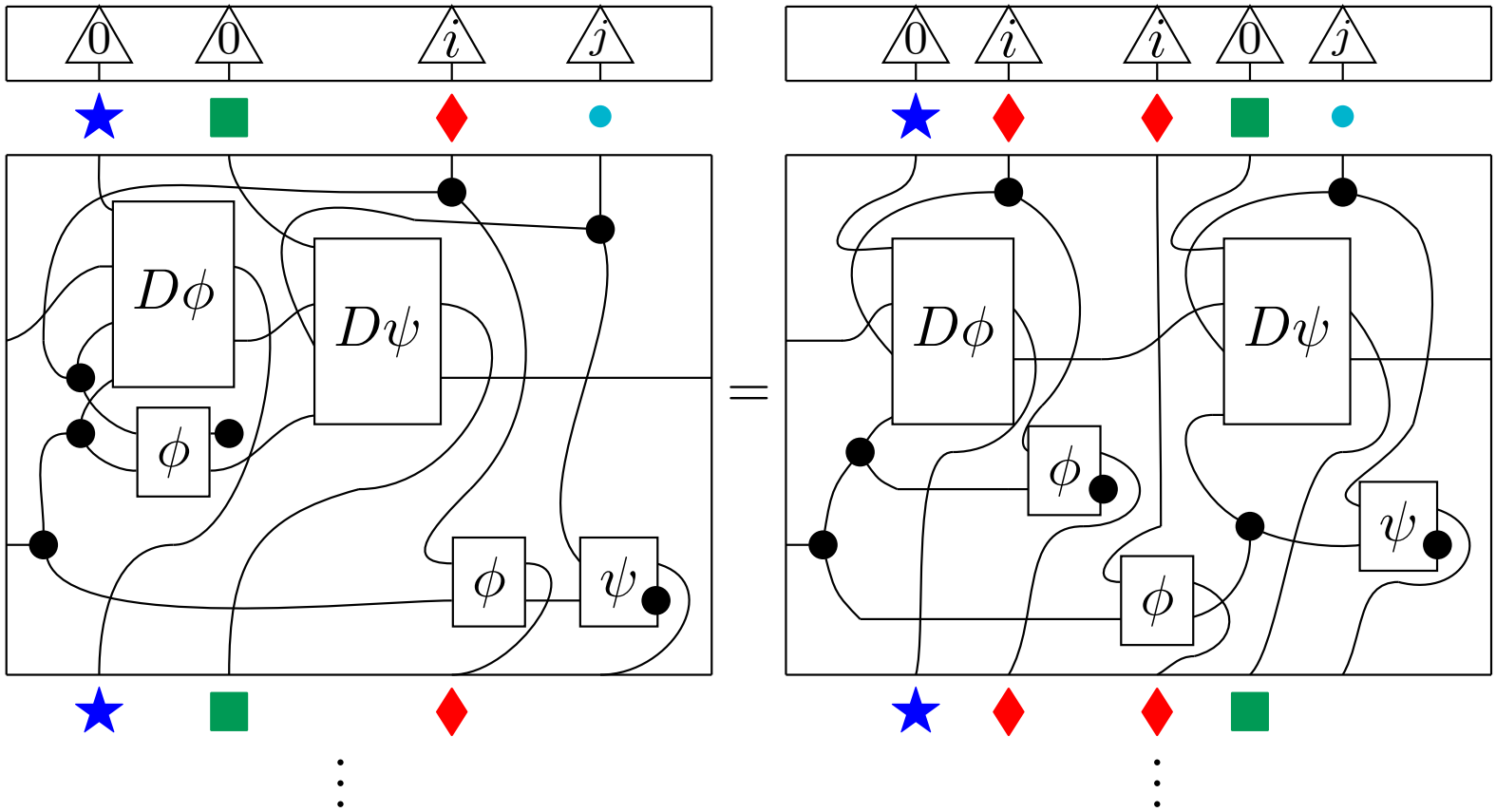
Proof idea. For CD4: $D($  $) =$ 



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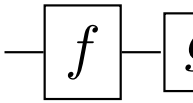
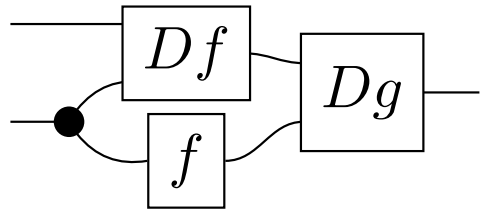
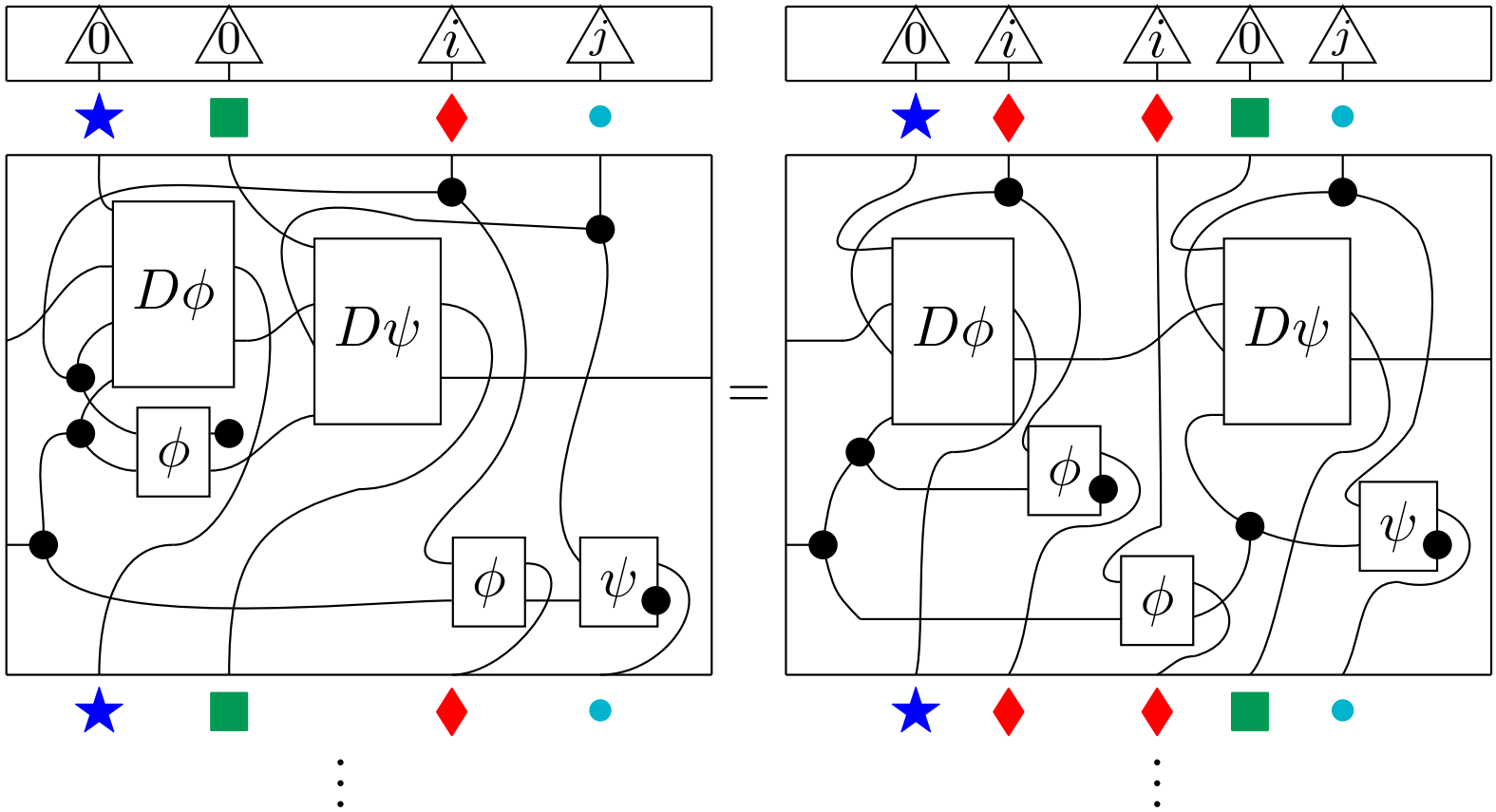
Proof idea. For CD4: $D($  $) =$ 



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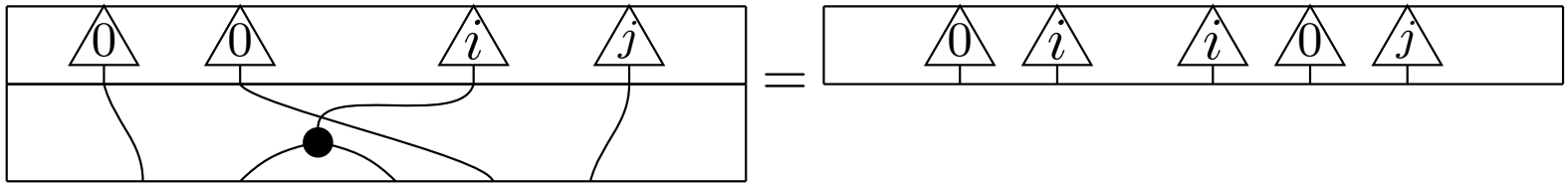
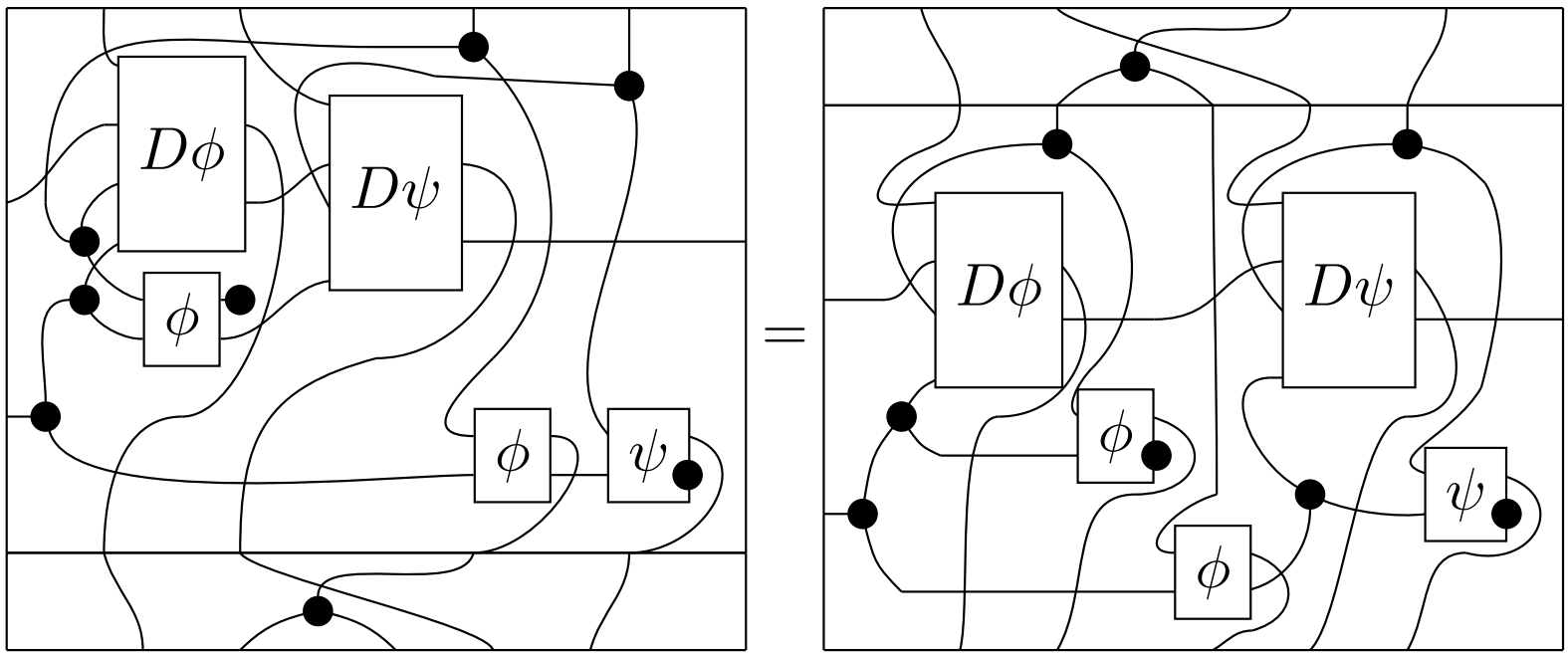
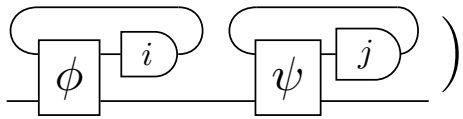




Stateful chain rule

$\mathcal{D}^*($ 

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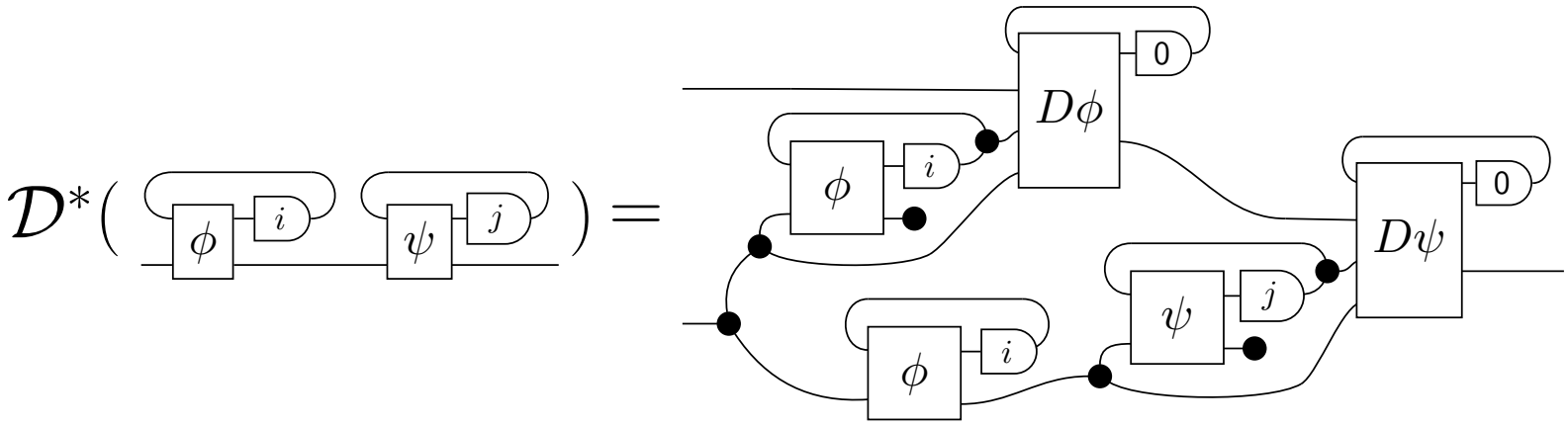

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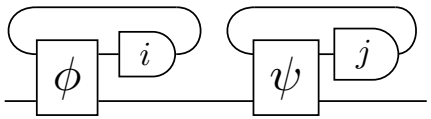
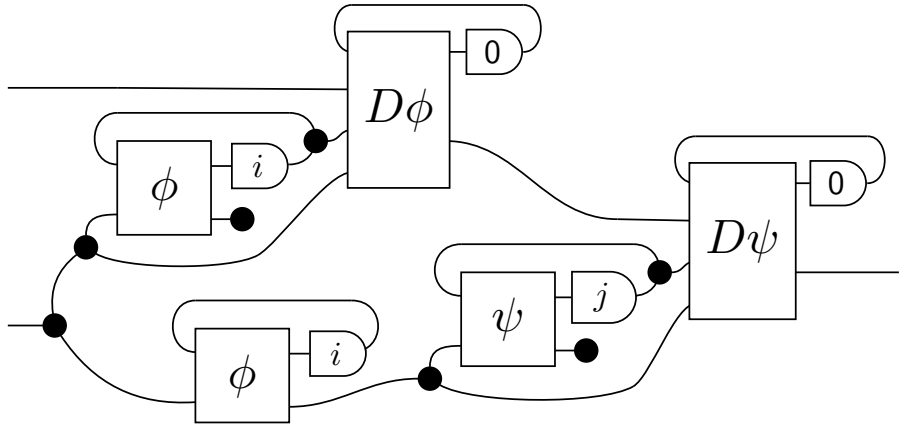
$\mathcal{D}^*($ 

$) =$ 

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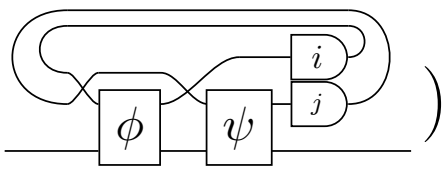
$\mathcal{D}^*($ 

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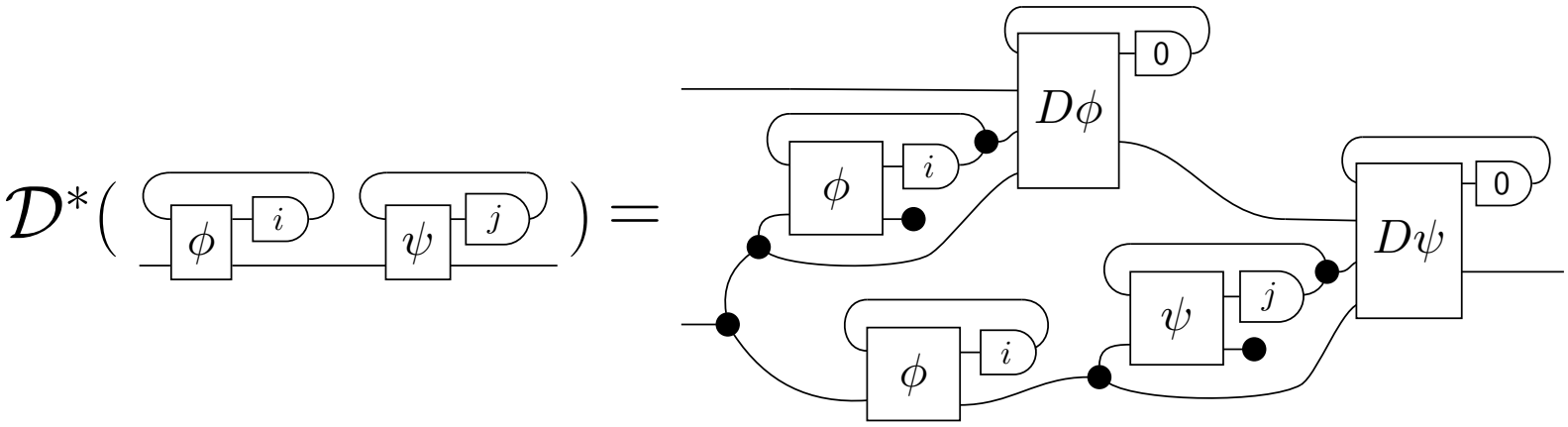

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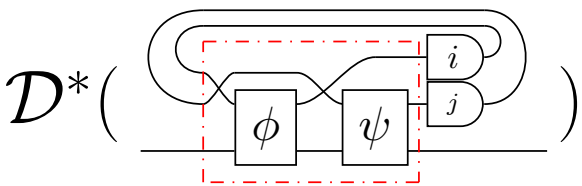

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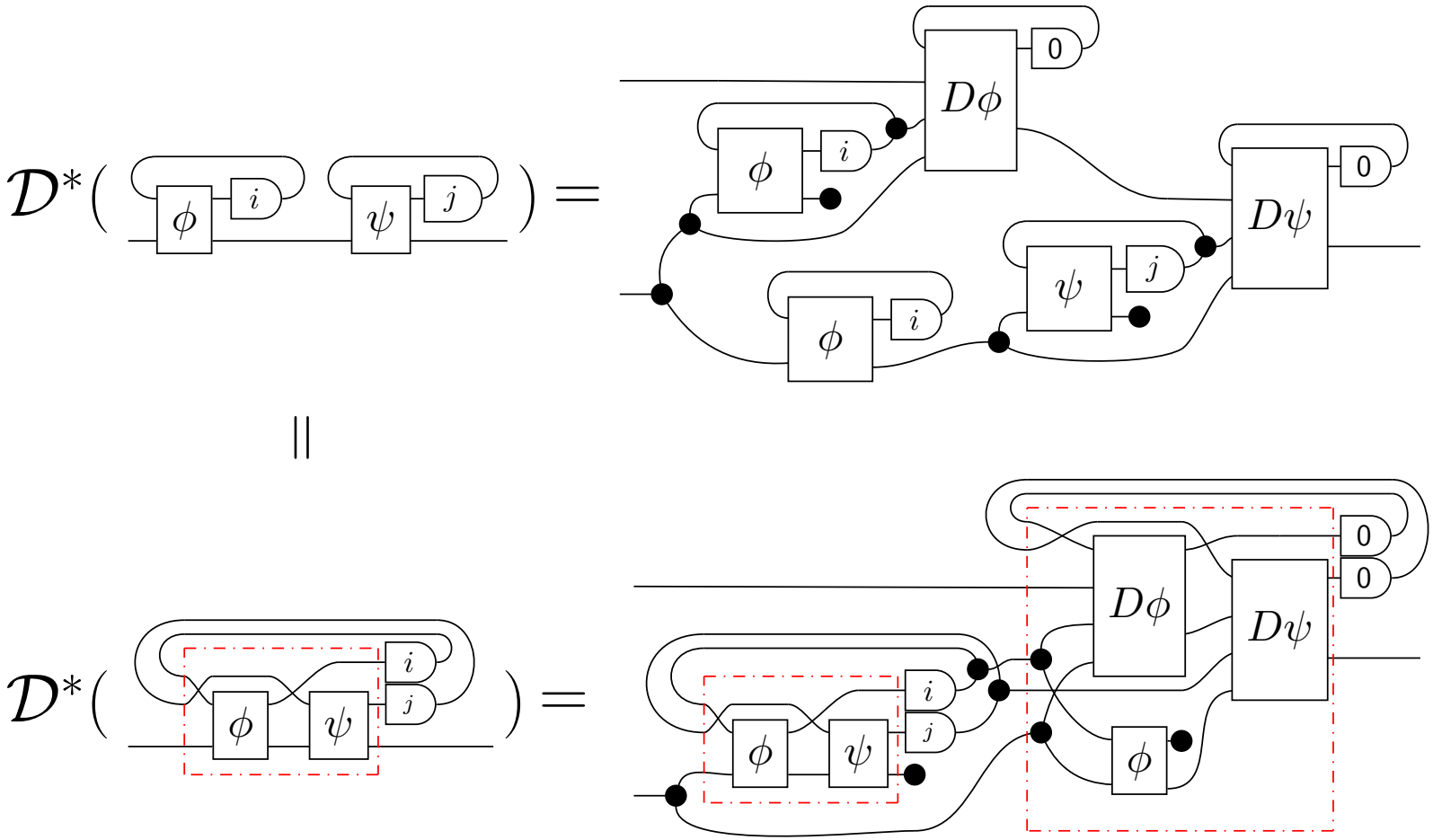

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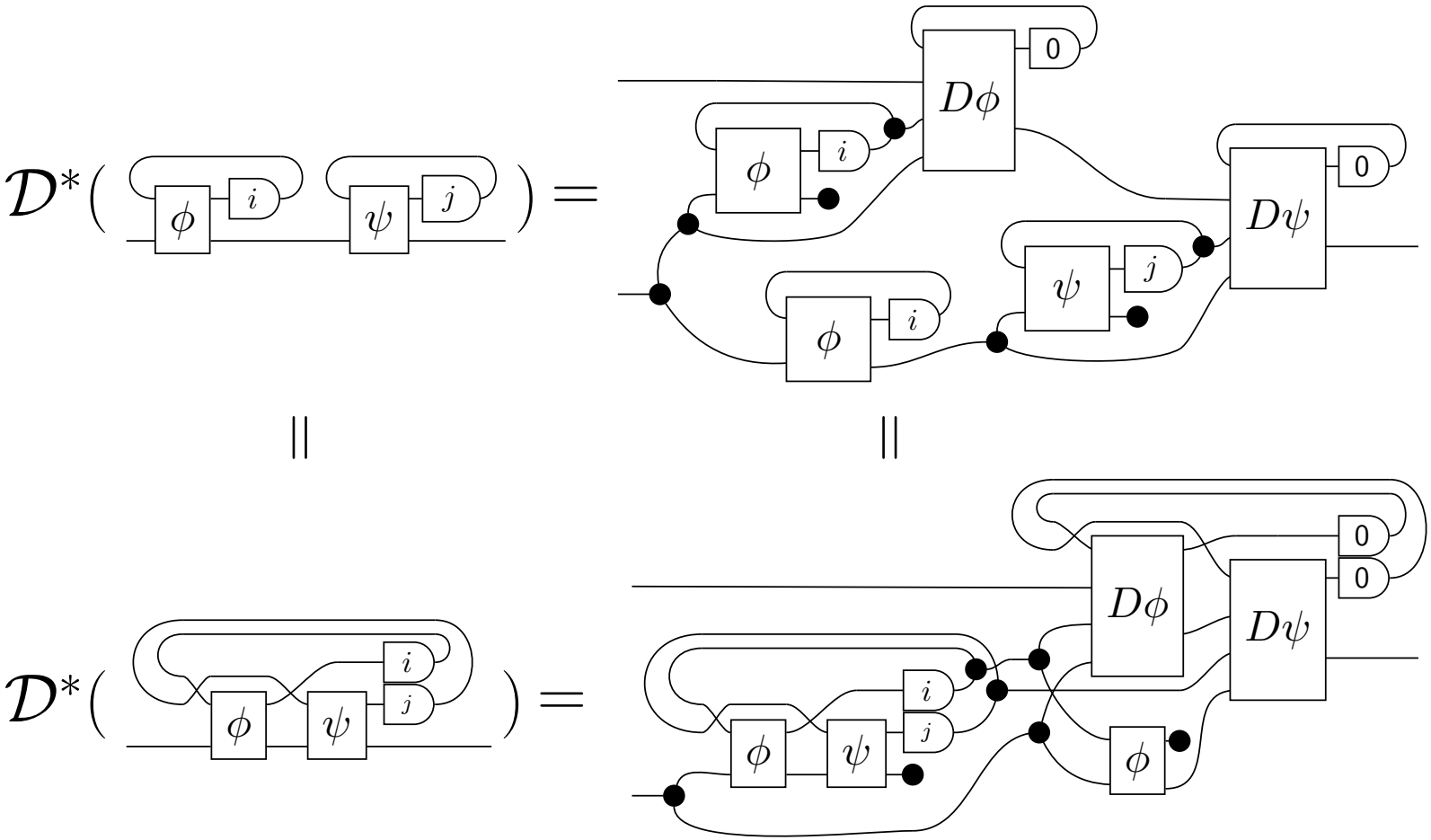

Outline

A recent observation

Since the paper was published, we noticed that $\mathrm{St}(\mathbb{C})$ is a full subcategory of the functor category $[\omega^{op}, \mathbb{C}]$, namely consisting of diagrams of the form:

$$X_0 \xleftarrow[\pi_0]{} X_0 \times X_1 \xleftarrow[\pi_0]{} X_0 \times X_1 \times X_2 \xleftarrow[\pi_0]{} \dots$$

Together with natural transformations ϕ

$$\begin{array}{ccccccc} X_0 & \xleftarrow[\pi_0]{} & X_0 \times X_1 & \xleftarrow[\pi_0]{} & X_0 \times X_1 \times X_2 & \xleftarrow[\pi_0]{} & \dots \\ \downarrow{\scriptstyle \phi_0} & & \downarrow{\scriptstyle \phi_1} & & \downarrow{\scriptstyle \phi_2} & & \\ Y_0 & \xleftarrow[\pi_0]{} & Y_0 \times Y_1 & \xleftarrow[\pi_0]{} & Y_0 \times Y_1 \times Y_2 & \xleftarrow[\pi_0]{} & \dots \end{array}$$

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Perhaps we can use this trick to find differential categories for more exotic network types (e.g. *recursive* neural networks)?

Future directions

Several obstacles prevent us from applying these ideas in practice right away:

1. Need non-smooth, partly differentiable, or partial functions
2. Need a transpose for computational efficiency

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Several obstacles prevent us from applying these ideas in practice right away:

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There are some questions related to the theory that we would like to understand better:

1. Can we add more advanced differential category structure (restriction, join, tangent, reverse, . . .)?
2. Categorical properties of $\mathrm{St}(-)$?
3. Bisimulations and extensional equality?
4. Basic results for delayed trace categories?
5. Other data shapes (trees, distributions, . . .)?

Summary

1. $\mathrm{St}(-)$ adds a delayed trace to a category.
2. $\mathrm{St}(-)$ preserves Cartesian differential category structure.
3. This notion of differentiation is connected to RNNs.
4. Cartesian differential categories are a useful tool for organizing unusual derivatives.
5. Machine learning needs compositional thinkers.

Thanks!

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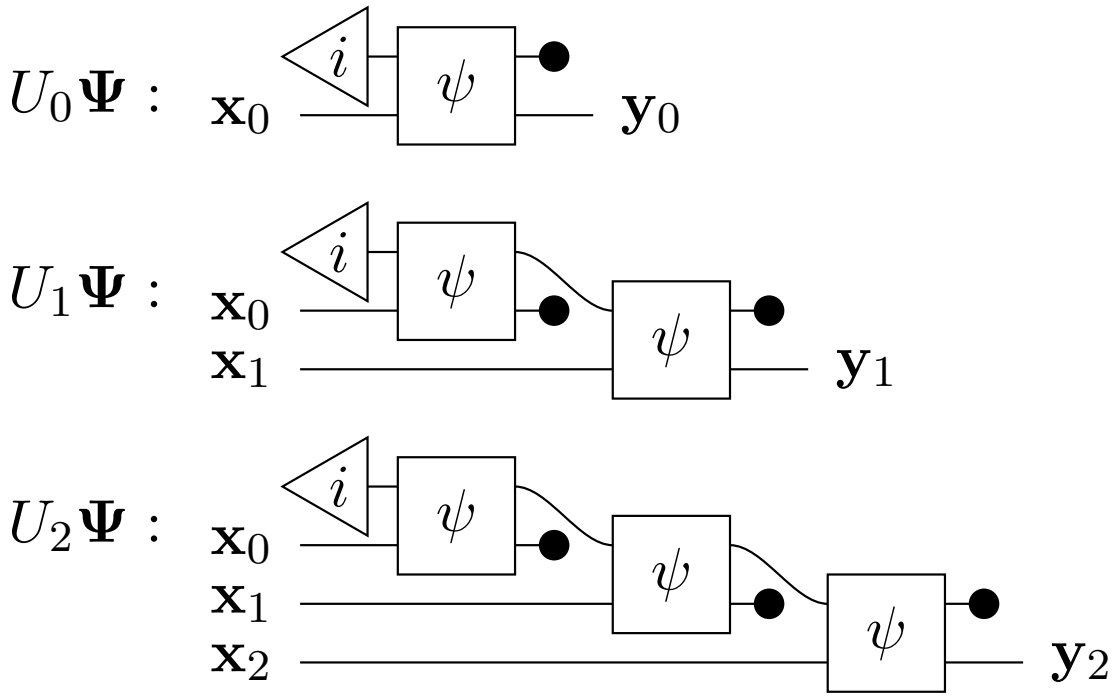
Unrollings and backpropagation through time (BPTT)

RNN training uses its *unrollings*:



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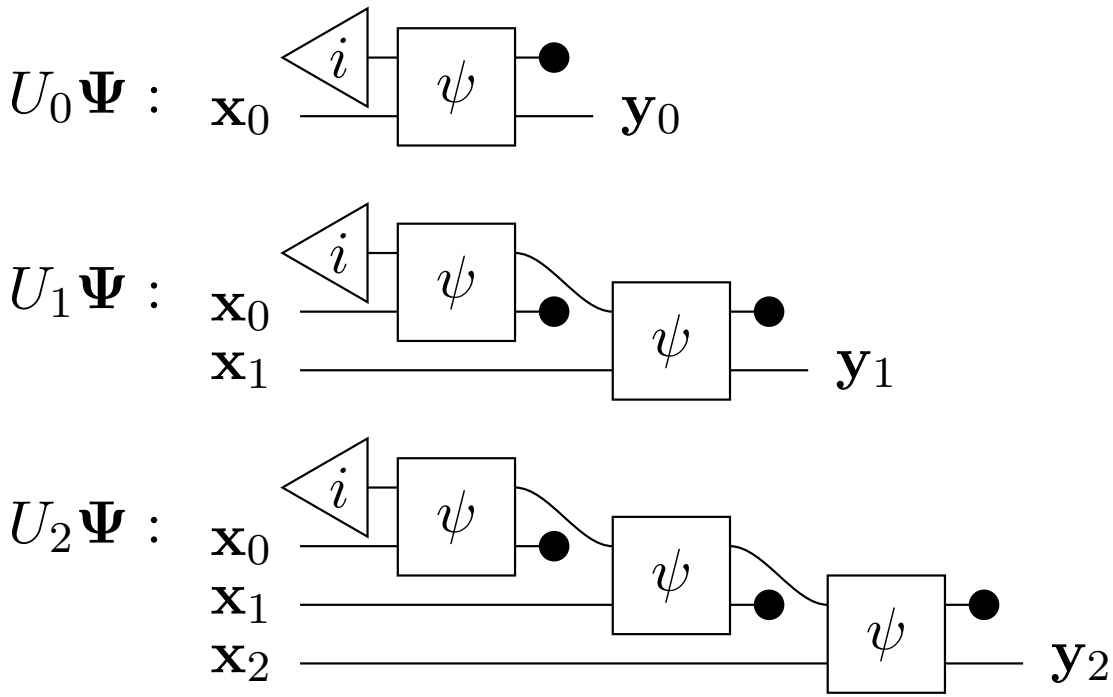

Backpropagation through time (BPTT, Werbos '90): Whenever the derivative of $\mathbf{\Psi}$ is needed at an input of length $k+1$, the derivative of $U_k\mathbf{\Psi}$ is used instead.

BPTT with category theory

BPTT generates good hints, but it leaves some questions:

1. $U_k(\mathbf{\Psi} \circ \mathbf{\Phi}) \neq U_k \mathbf{\Psi} \circ U_k \mathbf{\Phi}$. Did we lose the chain rule? What properties of derivatives hold for BPTT?

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Theorem: categorical BPTT

$DU_k(\Psi) = U_k(\mathcal{D}^*\Psi) \circ z_k$ for all $k \in \mathbb{N}$ and $\Psi \in \mathrm{St}(\mathbb{C})(\mathbf{A}, \mathbf{B})$.
($z_k : (\prod X_i) \times (\prod Y_i) \to \prod (X_i \times Y_i)$ is a zipping isomorphism.)

Upshot: All the properties of derivatives in Cartesian differential categories hold for backpropagation through time!