String diagrams for layered structures

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Outline

Monoidal categories and string diagrams as models of compositional systems

Layers of abstraction

Case study: diagrammatic electrical circuit theory

Case study: retrosynthetic analysis

Layered props

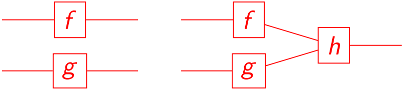
Layered props - semantically

Monoidal categories and string diagrams

Definition

A *monoidal category* is a triple $(\mathcal{C}, \otimes, I)$, where $\mathcal{C}$ is a category, $\otimes : \mathcal{C} \times \mathcal{C} \to \mathcal{C}$ is a functor and I is an object of $\mathcal{C}$, such that the appropriate associativity and unitality conditions hold.

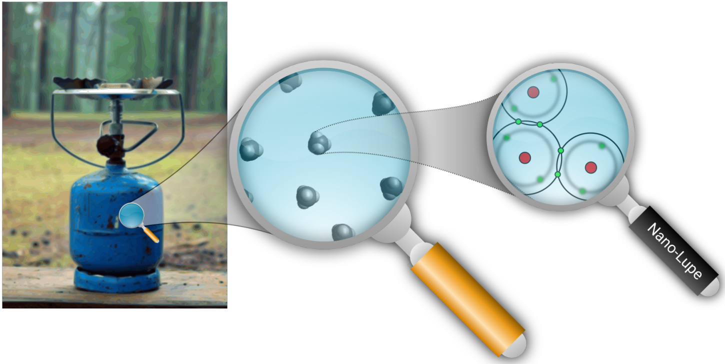
Objects of $\mathcal{C}$ are represented by *wires*, morphisms by *boxes*, the unit I by the empty diagram, the monoidal product $\otimes$ by juxtaposition, and composition in $\mathcal{C}$ by joining the wires.



Applications of string diagrams

- Quantum computing: ZX-calculus (Coecke, Duncan and many others), dagger-compact categories (Heunen, Vicary)
- Electrical circuit theory (and linear algebra): Bonchi, Piedeleu, Sobociński, Zanasi, Boisseau
- Logic: game semantics (Melliès), Peirce's existential graphs (Haydon, Sobociński), semantics of linear logic (Acclavio)
- Computer science: computability theory (Pavlovic), rewrite theory (Bonchi, Gadducci, Kissinger, Sobociński, Zanasi), dataflow programming (Román)

Layers of abstraction



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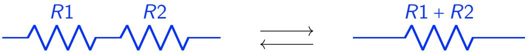
Electrical circuits

- View electrical circuit diagrams as a free prop (= strict symmetric monoidal category with the natural numbers as objects) *ECirc*

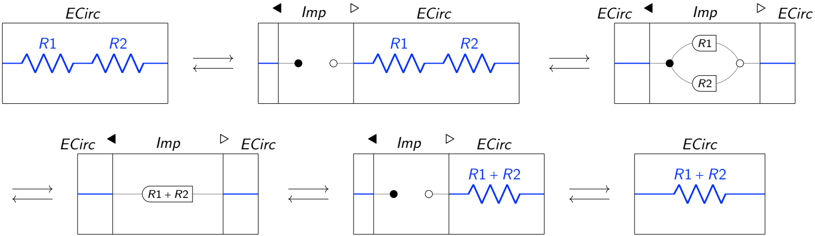
- Functorially interpret the electrical circuit diagrams in *graphical affine algebra GAA*
- This captures the behaviour of electrical components!

Electrical circuits

We wish to derive the rule for the sequential composition of resistors:

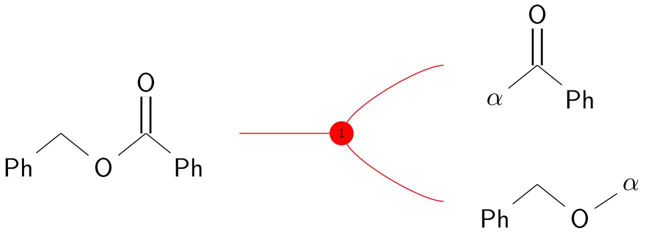


Electrical circuits

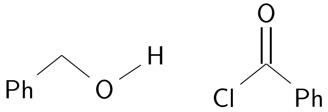


Retrosynthetic analysis

- Start with a target compound
- Formally decompose the target compound into smaller (formal!) "molecules" (called *synthons*):



- Search for chemically equivalent molecules which actually exist or are theoretically possible (called *synthetic equivalents*):



- Repeat until actually existing compounds are reached

Layered props

Definition

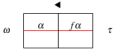
A *layered signature* is a functor $\Omega : P \to \mathbf{StrMon}$ from a poset P which does not send non-isomorphic objects to isomorphic objects.

Definition

A *layered prop* generated by Ω is a 2-category whose 0-cells are lists $(\omega_1, a_1; \ldots; \omega_n, a_n)$ of pairs (ω, a), where $\omega \in P$ and $a \in \Omega(\omega)$,and whose 1-cells are generated by the procedure below:

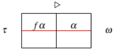
Layered props: 1-cells

$$\frac{\omega \le \tau \quad \alpha \in \Omega(\omega) \quad \Omega(\omega \le \tau) = f}{\blacktriangleleft}$$



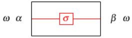
$: (\omega, \alpha \mid \tau, f\alpha)$

$$\frac{\omega \le \tau \quad \alpha \in \Omega(\omega) \quad \Omega(\omega \le \tau) = f}{\triangleright}$$



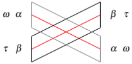
$: (\tau, f\alpha \mid \omega, \alpha)$

$$\alpha, \beta \in \Omega(\omega) \quad \sigma : \alpha \to \beta$$



$: (\omega, \alpha \mid \omega, \beta)$

$$\alpha \in \Omega(\omega) \quad \beta \in \Omega(\tau)$$



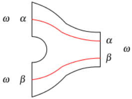
$: (\omega, \alpha; \tau, \beta \mid \tau, \beta; \omega, \alpha)$

$: (\varepsilon \mid \varepsilon)$

$: (\varepsilon \mid \omega, I_\omega)$

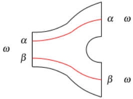
$: (\omega, I_\omega \mid \varepsilon)$

$$\alpha, \beta \in \Omega(\omega)$$



$: (\omega, \alpha; \omega, \beta \mid \omega, \alpha \otimes_\omega \beta)$

$$\alpha, \beta \in \Omega(\omega)$$



$: (\omega, \alpha \otimes_\omega \beta \mid \omega, \alpha; \omega, \beta)$

$$\frac{x : (t \mid s) \quad y : (s \mid u)}{x;y : (t, u)} \qquad \frac{x : (t \mid s) \quad y : (u \mid w)}{x \otimes y : (t;u \mid s;w)}$$

Layered props: 2-cells

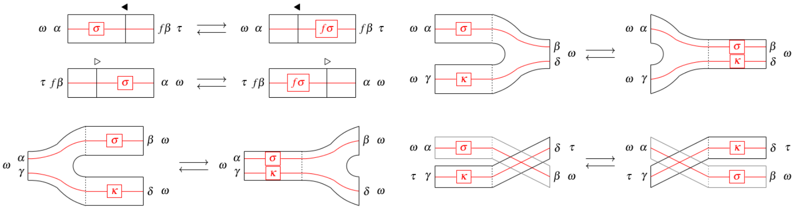


Figure 2: 2-cells of a layered prop expressing functoriality of refinement, coarsening, pants and copants.

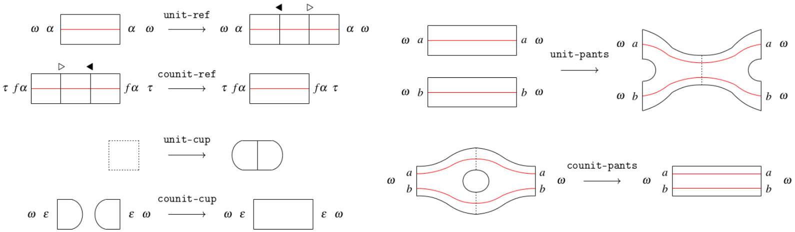


Figure 3: 2-cells of a layered prop that exhibit pants-copants and refinement-coarsening as two adjoint pairs.

Layered props: 2-cells

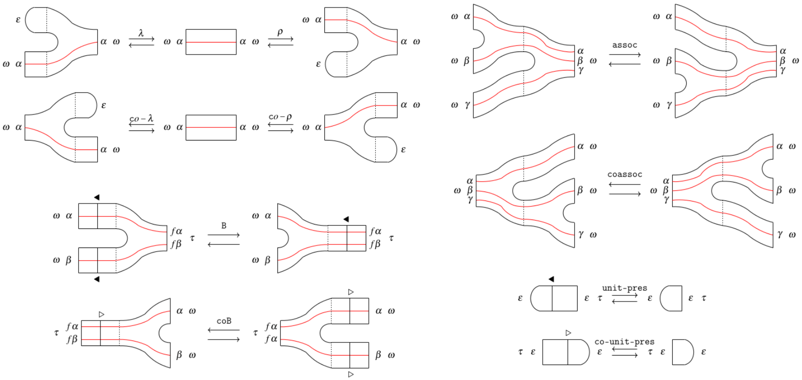


Figure 4: 2-cells of a layered prop that are motivated by monoidal categories and functors.

Layered props - semantically

Definition

An *ordered monoid* is a tuple $(M, \cdot, 1, \leq)$ such that $(M, \cdot, 1)$ is a monoid, and $\leq$ is a partial order on M such that $x \leq y$ and $z \leq w$ imply $xz \leq yw$.

Definition

Let P be a poset. The *free ordered monoid* generated by P has the free monoid P^* as its monoid structure, and the relation $\leq$ on P^* is generated by

- $\varepsilon \leq \varepsilon$,
- for $x, y \in P$, we have $x \leq y$ in P^* if and only if $x \leq y$ in P,
- for $n, m \geq 2$, we have $x_1 \cdots x_n \leq y_1 \cdots y_m$ if and only if $n = m$ and for each $i = 1, \ldots, n$ we have $x_i \leq y_i$.

The free *symmetric* ordered monoid generated by P additionally has for all $x, y \in P$ the inequality $xy \leq yx$.

Layered props - semantically

Definition

Let P be a poset. Let us denote by $\mathcal{L}(P)$ the free symmetric ordered monoid generated by P, to which for all $x \in P$, we freely add morphisms $xx \to x$ and $\varepsilon \to x$.

Proposition

Any layered signature $\Omega : P \to \mathbf{StrMon}$ uniquely extends to a monoidal functor $\Omega : \mathcal{L}(P) \to \mathbf{StrMon}$ which maps the morphisms $xx \to x$ to $\otimes : \Omega(x) \times \Omega(x) \to \Omega(x)$ and $\varepsilon \to x$ to the unique monoidal functor $\mathbf{1} \to \Omega(x)$.

Layered props - semantically

$\Omega : \mathcal{L}(P) \to \mathbf{StrMon}$ gives rise to two 2-categories, both having pairs $(\omega, a \in \Omega(\omega))$ as objects.A morphism $(F, f) : (\omega, a) \to (\tau, b)$ is given by one of the following:

- $F : \omega \to \tau$ and $f : \Omega(F)(a) \to b$, denote: $Gr(\Omega)$
- $F : \omega \to \tau$ and $f : b \to \Omega(F)(a)$, denote: $Gr^{\leftarrow}(\Omega)$.

We have two locally full and faithful functors into pointed profunctors:

$$Gr(\Omega)^{co} \hookrightarrow \mathbf{Prof}_*$$
$$Gr^{\leftarrow}(\Omega)^{op} \hookrightarrow \mathbf{Prof}_*$$

Theorem

A layered prop generated by a layered signature Ω is 2-equivalent to the subcategory of $\mathbf{Prof}_*$ generated by the union of the images of the above embeddings.

Profunctors

Define the bicategory of *profunctors* **Prof** as:

- the 0-cells are (small) categories,
- the 1-cells, denoted by $\mathcal{C} \nrightarrow \mathcal{D}$, are functors

$$\mathcal{C}^{op} \times \mathcal{D} \to \mathbf{Set},$$

- the $2-\mathit{cells}$ are natural transformations $\alpha : F \Rightarrow G$,
- the composition

$$c_{\mathcal{A},\mathcal{B},\mathcal{C}} : \mathbf{Prof}(\mathcal{A},\mathcal{B}) \times \mathbf{Prof}(\mathcal{B},\mathcal{C}) \to \mathbf{Prof}(\mathcal{A},\mathcal{C})$$

takes profunctors $F : \mathcal{A} \nrightarrow \mathcal{B}$ and $G : \mathcal{B} \nrightarrow \mathcal{C}$ to the coend $G \circ F = \int^{B} F(-,B) \times G(B,=)$. Explicitly, we define

$$(G \circ F)(A,C) \coloneqq \int^{B \in \mathcal{B}} F(A,B) \times G(B,C).$$

Profunctors

There are two embeddings:

$$\begin{aligned} \mathfrak{p}^- &: \mathbf{Cat}^{co} \to \mathbf{Prof} \\ F : \mathcal{C} \to \mathcal{D} &\mapsto \mathcal{D}(F-, =) \\ \eta : F \to G &\mapsto - \circ \eta_C \end{aligned}$$

$$\begin{aligned} \mathfrak{p}_- &: \mathbf{Cat}^{op} \to \mathbf{Prof} \\ F : \mathcal{C} \to \mathcal{D} &\mapsto \mathcal{D}(=, F-) \\ \eta : F \to G &\mapsto \eta_C \circ - \end{aligned}$$

Both are locally fully faithful, and $\mathfrak{p}^F$ is the left adjoint to $\mathfrak{p}_F$.

Pointed profunctors

Define the bicategory of *pointed profunctors* $\mathbf{Prof}_*$ as:

- the 0-cells are pairs $(\mathcal{C}, c)$ of a (small) category $\mathcal{C}$ and an object $c \in \mathcal{O}b(\mathcal{C})$,
- the 1-cells $(P, f) : (\mathcal{C}, c) \to (\mathcal{D}, d)$ consist of a profunctor $P : \mathcal{C} \nrightarrow \mathcal{D}$, that is, a functor

$$P : \mathcal{C}^{op} \times \mathcal{D} \to \mathbf{Set},$$

  together with an element $f \in P(c, d)$,
- the 2-cells $\alpha : (P, f) \to (Q, g)$ are natural transformations $\alpha : P \Rightarrow Q$ such that $\alpha_{c,d}(f) = g$,
- the composition of $(P, f) : (\mathcal{C}, c) \to (\mathcal{D}, d)$ and $(Q, g) : (\mathcal{D}, d) \to (\mathcal{E}, e)$ is given by $(Q \circ P, [f, g])$, where $\circ$ is the composition of profunctors and $[f, g]$ the equivalence class of the pair (f, g) in $(Q \circ P)(c, e)$.

Conclusion and future work

- Layered props are a promising framework for scientific modelling with several layers
- Model “synthetic equivalence” using the language of layered props
- Model sequential decision making in layers of neural networks
- Model counterfactual reasoning/processes as a separate layer
- Integrate inconsistent data into a single framework

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Thank you for your attention!