# Introduction to Higher-Order Mathematical Operational Semantics

Sergey Goncharov

# In(tro)duction to Higher-Order Mathematical Operational Semantics

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# **HO Mathematical Operational Semantics Project**

- Goncharov, Milius, Schröder, Tsampas, and Urbat, "Towards a Higher-Order Mathematical Operational Semantics", POPL 2023
- Urbat, Tsampas, Goncharov, Milius, and Schröder, "Weak Similarity in Higher-Order Mathematical Operational Semantics", LICS 2023
- Goncharov, Santamaria, Schröder, Tsampas, and Urbat, "Logical Predicates in Higher-Order Mathematical Operational Semantics", FoSSaCS 2024
- Goncharov, Milius, Tsampas, and Urbat, "Bialgebraic Reasoning on Higher-Order Program Equivalence", LICS 2024
- Goncharov, Tsampas, and Urbat, "Abstract Operational Methods for Call-by-Push-Value", POPL 2025

.. and rolling

# Context: Applied Category Theory

- ► Somewhat like
  https://en.wikipedia.org/wiki/Applied\_category\_theory
- More specifically: using category theory as an organization device
- Yet more specially: proving classes of statements at once

## **Example:** Coalgebraic Modal Logic

- ▶ Parameters: functor F (for transitions), predicate liftings  $\heartsuit: 2^X \to 2^{FX}$  (for modalities), axioms
- ► **Results:** soundness, completeness, Hennessy–Milner property, complexity bounds, etc.

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Our **Grand Objective**: develop a similar approach to operational semantics

# Semantics: Operational v.s. Denotational

Operational Semantics (how programs behave?)

$$s(s(0)) + s(s(0)) \rightarrow s(s(0) + s(s(0)))$$
  
  $\rightarrow s(s(0 + s(s(0)))) \rightarrow s(s(s(s(0))))$ 

Denotational Semantics (what programs denote?)

$$[s(s(0)) + s(s(0))] = [s(s(0))] + [s(s(0))] = 2 + 2 = 4$$

## Semantics in Use

#### **Denotational:**

© Compositional by design:

$$[\![p]\!] = [\![q]\!] \Rightarrow [\![C[p]\!]] = [\![C[q]\!]]$$

for any program context C

- Mathematically rigorous and precise
- Ease to define: from hard to impossible

#### Operational:

- © Lightweight and easy to define even for complex languages
- Nonuniform and fraggile
- Hard to reason about (because of lack of compositionality)

Overall: not (sufficiently) mathematical

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Turi and Plotkin's abstraction of GSOS rule format<sup>1</sup>:

- ightharpoonup Signature endo-functor  $\Sigma$
- ► Behaviour endo-functor B
- ▶ GSOS law natural transformation  $\rho_X$ :  $\Sigma(X \times BX) \to B(\Sigma^*X)$

#### **Example (Process Algebra):**

- ▶  $\Sigma = \{ \text{ par } /2, \emptyset /0 \} \cup \{ a. (-)/1 \mid a \in A \}$
- $\triangleright$   $BX = \mathcal{P}(A \times X)$
- GSOS law encodes rules like:

$$\frac{p \xrightarrow{a} p'}{p \text{ par } q \xrightarrow{a} p' \text{ par } q}$$

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$$\triangleright$$
  $BX = \mathcal{P}(A \times X)$ 

GSOS law encodes rules like:

behaviour from B

operation from 
$$\Sigma$$
 
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## First-Orded GSOS

Theory of first-order GSOS takes  $\Sigma$ , B,  $\rho$  as input parameters, and produces

- $\bigcirc$  operational semantics  $\gamma \colon \Sigma^* \emptyset \to B(\Sigma^* \emptyset)$  (operational model)
- $\bigcirc$  notion of program equivalence  $\sim \subseteq \Sigma^*\emptyset \times \Sigma^*\emptyset$  (strong bisimilarity)
- $\bigcirc$  generic compositionality:  $p \sim q \Rightarrow C[p] \sim C[q]$  for any context

#### But

- $\odot$  ~ is too fine-grained for programming languages
- $\bigcirc$  first-order  $\subsetneq$  higher-order  $\rightsquigarrow$  no  $\lambda$ -calculus

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#### But

# **Higher-Order Abstract GSOS**

# (Call-by-Name, Extended) Combinatory Logic

- $\blacktriangleright$   $I (=\lambda p. p)$
- $\blacktriangleright$   $K (= \lambda p. \lambda q. p)$
- $\triangleright$  S (= $\lambda p.\lambda q.\lambda r.(p \cdot r) \cdot (q \cdot r)$ )
- ightharpoonup plus S', S'' and K' for partially reduced terms

$$I \xrightarrow{p} p \qquad K \xrightarrow{p} K'(p) \qquad K'(p) \xrightarrow{q} p \qquad S \xrightarrow{p} S'(p)$$

$$S'(p) \xrightarrow{q} S''(p,q) \qquad S''(p,q) \xrightarrow{r} (p \cdot r) \cdot (q \cdot r)$$

$$\frac{p \to p'}{p \cdot q \to p' \cdot q} \qquad \frac{p \xrightarrow{q} p'}{p \cdot q \to p'}$$

**Example:** 
$$S \cdot p \cdot q \cdot r \rightarrow S'(p) \cdot q \cdot r \rightarrow S''(p,q) \cdot r \rightarrow (p \cdot r) \cdot (q \cdot r)$$

This is very similar to original GSOS, but it is not

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## **Higher-Order Abstract GSOS**

A higher-order GSOS law consists of

- Signature Σ
- ► Mixed variance (!) behaviour functor B
- ► Family of maps  $\rho_{X,Y}$ :  $\Sigma(X \times B(X,Y)) \to B(X,\Sigma^*(X+Y))$  natural in Y and dinatural in X

**Example:** For combinatory logic:  $B(X, Y) = Y^X + Y$ ,  $\rho$  is induced by rules of operational semantics

- Most (but not all!) of Turi and Plotkin's theory caries over
- $\bigcirc$  In particular: strong applicative bisimilarity  $\sim$  is implied and is a congruence

# Strong Applicative Bisimilarity

Strong applicative bisimilarity is the largest symmetric relation ~
 on programs, such that

1. 
$$p \rightarrow p' \wedge p \sim q \implies \exists q'. q \rightarrow q' \wedge p' \sim q'$$

2. 
$$p \xrightarrow{t} p' \wedge p \sim q \Rightarrow \exists q'. q \xrightarrow{t} q' \wedge p' \sim q'$$

- ▶ Key expected property congruence:  $p \sim q$  implies  $C[p] \sim C[q]$
- Then it is sound method for proving contextual equivalence of p and q (for every C, C[p] and C[q] are "behaviorally equivalent")

# Strong Applicative Bisimilarity: Examples

#### **Bisimilar Terms:**

- $\qquad \qquad \bullet \quad \Omega_0 = (\mathit{SII})(\mathit{SII}), \, \Omega_1 = (\mathit{I}(\mathit{SII}))(\mathit{I}(\mathit{SII})), \, \Omega_2 = (\mathit{II}(\mathit{SII}))(\mathit{I}(\mathit{SII})), \, \text{etc.}$
- ► Then  $\Omega_0 = (SII)(SII) \rightarrow (S'(I)I)(SII) \rightarrow (S''(I,I))(SII) \rightarrow \Omega_1$
- ▶ Analogously,  $\Omega_n \to^* \Omega_{n+1}$
- ▶ Proof that  $\Omega_n \sim \Omega_{n+1}$ :
  - Arr  $\mathcal{R} = \{(P, Q) \mid \Omega_0 \to^* P, \Omega_0 \to^* Q\}$  is bisimulation,
  - ▶ hence  $(\Omega_n, \Omega_m) \in \mathcal{R} \subseteq \sim$

### **Non-Bisimilar Terms**: Generally, for $P \rightarrow Q$ , $P \not\sim Q$

E.g. 
$$K'(I)I \rightarrow I$$
, but  $I \rightarrow$ 

## **Proving Congruence**

- Structural induction won't do: given  $p \sim q$ ,  $S'(p) \sim S'(q)$  would require  $S''(q, t) \sim S''(p, t)$
- Proving that

$$\widehat{\sim} = \{ (C[p], C[q]) \mid p \sim q \}$$

is bisimulation won't do, for  $S''(s, t)p \rightarrow (sp)(tp)$ 

- Proving that  $\{(C[\overline{p}], C[\overline{q}]) \mid p_i \sim q_i\}$  is bisimulation won't do:  $p_1p_2 \sim q_1q_2$  may require  $p' \sim q'$  where  $p_1 \xrightarrow{p_2} p'$  and  $q_1 \xrightarrow{q_2} q'$
- $\bigcirc$  Worked approach: bisimulation up-to congruence  $\iff$   $\widehat{\sim}^*$  is a bisimulation. Hence  $\widehat{\sim} \subseteq \widehat{\sim}^* \subseteq \widehat{\sim}$

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- Proving that  $\{(C[\overline{p}], C[\overline{q}]) \mid p_i \sim q_i\}$  is bisimulation won't do:  $p_1p_2 \sim q_1q_2$  may require  $p' \sim q'$  where  $p_1 \stackrel{p_2}{\longrightarrow} p'$  and  $q_1 \stackrel{q_2}{\longrightarrow} q'$
- Worked approach: bisimulation up-to congruence  $\iff \hat{\sim}^*$  is a bisimulation. Hence  $\hat{\sim} \subseteq \hat{\sim}^* \subseteq \sim$

Key insight of HO-MOS: This generalizes to: regular categories, mono-preserving B and "finitary"  $\Sigma$ 

## Lambda-Calculus

Standard rules

$$\frac{s \to s'}{s \ t \to s' \ t} \qquad \qquad \frac{(\lambda x. \, s) \ t \to s[t/x]}{(\lambda x. \, s) \ t \to s[t/x]}$$

▶ We take:  $C = Set^{\mathbb{F}}$  ( $\mathbb{F}$  – category of finite cardinals)

$$\Sigma: \mathsf{C} \to \mathsf{C} \qquad \qquad \Sigma X = V + \delta X + X \times X$$
 
$$B: \mathsf{C}^{\mathsf{op}} \times \mathsf{C} \to \mathsf{C} \qquad B(X,Y) = \langle\!\langle X,Y \rangle\!\rangle \times (Y + Y^X + 1)$$

$$V(n) = \{n\}$$
 (variables),  $(\delta X)(n) = X(n+1)$ ,  $\langle\!\langle X, Y \rangle\!\rangle(n) = C(X^n, Y)$ 

 $\triangleright$   $(\Sigma^*\emptyset)(n) \cong \lambda$ -terms over *n* free variables<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>Fiore, Plotkin, and Turi, "Abstract Syntax and Variable Binding".

## Lambda-Calculus

Standard rules

"substitution" behavior

"reduction" behavior

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$$\overline{(\lambda x.\,s)\,\,t\to s[t/x]}$$

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$$\Sigma: C \to C$$
 
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# **Further Advances**

## First-Orded GSOS [Recall]

Theory of first-order GSOS takes  $\Sigma$ , B,  $\rho$  as input parameters, and produces

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- $\bigcirc$  generic compositionality:  $p \sim q \Rightarrow C[p] \sim C[q]$  for any context

#### But

- $> \sim$  is too fine-grained for programming languages  $\leftarrow$

 $\forall$  first-order  $\subseteq$  higher-order  $\rightsquigarrow$  no  $\lambda$ -calculus

# Weak Bisimilarity

# Weak Applicative (Bi)similarity

- ▶ Weak transitions: let  $\Rightarrow$  be  $\rightarrow^*$ ,  $\stackrel{t}{\Rightarrow}$  be  $(\Rightarrow \cdot \stackrel{t}{\rightarrow})$
- ► Weak applicative similarity largest such ≤ that
  - 1.  $t \to t'$  implies  $s \Rightarrow s'$  and  $t' \lesssim s'$  for some s'
  - 2.  $t \stackrel{r}{\rightarrow} t'$  implies  $s \stackrel{r}{\Rightarrow} s'$  and  $t' \lesssim s'$  for some s'
- ▶ Weak applicative bisimilarity  $\approx$  =  $\lesssim$   $\cap$   $\gtrsim$

**Example:**  $f \lesssim S \cdot (K \cdot I) \cdot f$  (analogue of  $f \lesssim \lambda x. fx$ ), but

$$S \cdot (K \cdot I) \cdot \Omega \lesssim \Omega$$
, because

$$S \cdot (K \cdot I) \cdot \Omega \xrightarrow{t} (K \cdot I \cdot t)(\Omega \cdot t)$$
 but  $\Omega \to \Omega \to \dots$ 

**Key Property:** pre-congruence of ≤

Proof Idea: Bisimulation up-to Howe's closure (Howe's method)

## Howe's Method

For a relation  $\mathcal{R} \subseteq \Sigma^*\emptyset \times \Sigma^*\emptyset$ , Howe's closure  $\mathcal{R}^H$  is generated by

$$\frac{t_1 \, \mathcal{R}^H \, t_1' \quad \dots \quad t_n \, \mathcal{R}^H \, t_n' \quad f(t_1', \dots, t_n') \, \mathcal{R} \, s}{f(t_1, \dots, t_n) \, \mathcal{R}^H \, s}$$

① This is crucially weaker than saying that  $\mathbb{R}^H$  is closure of  $\mathbb{R}$  under contexts and transitivity

**Key property:**  $\approx^H$  is a bisimulation

- $\implies$   $\hat{\approx} \subseteq \approx^H \subseteq \approx$
- $\rightarrow$   $\approx$  is congruence

**Analogously:** ≤ is pre-congruence

# Howe's Method Abstractly

► Together with  $\gamma \colon \Sigma^{\star} \emptyset \to B(\Sigma^{\star} \emptyset, \Sigma^{\star} \emptyset)$  for strong transitions "→", we require new parameter

$$\widetilde{\gamma} \colon \Sigma^{\star} \emptyset \to B(\Sigma^{\star} \emptyset, \Sigma^{\star} \emptyset)$$

for weak transitions "⇒"

▶ We need liftings to the category of relations:

.. and some other assumptions

**Result:**  $\lesssim$  (i.e. largest relation R, such that  $R \leqslant (\gamma \times \widetilde{\gamma})^{-1}[\overline{B}(\Delta, R)]$ ) is a congruence (i.e.  $\overline{\Sigma}(\lesssim) \leqslant (\iota \times \iota)^{-1}[\lesssim]$ )

# **Step-Indexing Logical Relations**

## Step-Indexing, Concretely

The step-indexed logical relation  $\mathcal{L}$  for combinatory logic is the inductively defined family  $(\mathcal{L}^{\alpha} \subseteq \Sigma^{\star}\emptyset \times \Sigma^{\star}\emptyset)_{\alpha \leqslant \omega}$ :

$$\mathcal{L}^0 = \top, \qquad \mathcal{L}^{n+1} = \mathcal{L}^n \cap \mathcal{E}(\mathcal{L}^n) \cap \mathcal{V}(\mathcal{L}^n, \mathcal{L}^n), \qquad \mathcal{L}^\omega = \bigcap_{n < \omega} \mathcal{L}^n$$

where  $\mathcal{E}$  and  $\mathcal{V}$  are relation transformers:

$$\mathcal{E}(R) = \{(t,s) \mid \text{if } t \to t' \text{ then } \exists s'. \, s \Rightarrow s' \land R(t',s')\}$$

$$\mathcal{V}(Q,R) = \{(t,s) \mid \text{for all } r_1, r_2, \ Q(r_1,r_2),$$

$$\text{if } t \xrightarrow{r_1} t' \text{ then } \exists s'. \, s \xrightarrow{r_2} s' \land R(t',s')\}$$

As a slogan: "related programs applied to related arguments produce related results"

# **Step-Indexing: Properties**

- $\mathcal{L}^{\omega}$  is a fixpoint  $\mathcal{L}^{\omega} = \mathcal{L}^{\omega} \cap \mathcal{E}(\mathcal{L}^{\omega}) \cap \mathcal{V}(\mathcal{L}^{\omega}, \mathcal{L}^{\omega})$
- ► In first-order case we would reduce to the familiar fixpoint theory and Kleene/Knaster-Tarski theorems, but because of higher-order, we generally do not (!)
- ightharpoonup Every  $\mathcal{L}^{\alpha}$  is a congruence
- $\triangleright \mathcal{L}^{\omega}$  is sound for contextual preorder

**Bottom Line:** Step-indexing is another sound method for proving contextual equivalence

# Step-Indexing, Abstractly

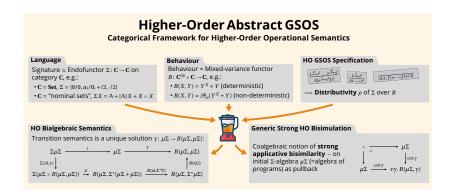
Under similar (but weaker) assumptions, as for weak applicative bisimilarity,

- 1. There is an abstract (ordinal-indexed) logical relation  $(\mathcal{L}^{\alpha})_{\alpha}$
- 2. The limit  $\mathcal{L}^{\nu} = \bigcap_{\alpha} \mathcal{L}^{\alpha}$  exists
- 3. Every  $\mathcal{L}^{\alpha}$  is a congruence
- 4.  $\mathcal{L}^{\nu}$  is sound for contextual equivalence

## **Conclusions**

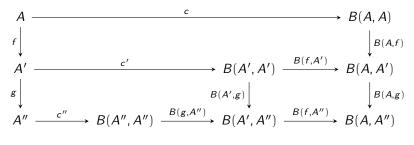
- We broke the barrier between (co-)algebraic methods and higher-order semantics
- ? A lot to be done:
  - Call-by-value
  - Big-step semantics (and equivalence thereof)
  - Other behavioral equivalence (e.g. trace equivalence)
  - ▶ Metric, probabilistic, quantialic, fibrational generalizations
  - Modelling polymorphic languages
  - ► Modelling effectful languages
  - $\blacktriangleright$   $\mathcal{L}^{\nu}$  is included in applicative bisimilarity. When they are equal?

## Thank You for Your Attention!



# Bialgebras Form a Category

If  $f: A \to A'$  and  $g: A' \to A''$  are  $\rho$ -bialgebra morphisms then so is the composition  $g \cdot f$ , for the diagram



obviously commutes.

## Lambda-Calculus

Operational semantics rules

$$\frac{s \to s'}{s \ t \to s' \ t} \qquad \qquad \overline{(\lambda x.s) \ t \to s[t/x]}$$

 $ightharpoonup C = \mathsf{Set}^{\mathbb{F}}$ , where  $\mathbb{F}$  is the category of finite cardinals

$$\begin{split} \Sigma\colon\mathsf{C}\to\mathsf{C}, & \Sigma X=V+\delta X+X\times X,\\ B\colon\mathsf{C}^\mathsf{op}\times\mathsf{C}\to\mathsf{C}, & B(X,Y)=\langle\!\langle X,Y\rangle\!\rangle\times(Y+Y^X+1) \end{split}$$

where  $Y^X$  is exponent in  $\mathsf{Set}^\mathbb{F}$ , V is the presheaf of variables  $\mathsf{Set}^\mathbb{F}(n) = n$ ,  $(\delta X)(n) = X(n+1)$ ,  $\langle\!\langle X, Y \rangle\!\rangle(n) = \mathsf{Set}^\mathbb{F}(X^n, Y)$ 

- ▶  $\mu\Sigma$  is the presheaf  $\Lambda \in Set^{\mathbb{F}}$  of  $\lambda$ -terms over n free variables
- ► H/O GSOS law is pointed:

$$\rho_{X,Y} \colon \Sigma(jX \times B(jX,Y)) \to B(jX, \Sigma^{\star}(jX+Y))^{3}$$

<sup>&</sup>lt;sup>3</sup>Fiore, Plotkin, and Turi, "Abstract Syntax and Variable Binding".

# Dinaturality

A dinatural transformation from  $F: C^{op} \times C \to D$  to  $G: C^{op} \times C \to D$  is a family  $(\sigma_X: F(X,X) \to G(X,X))_{X \in C}$ , such that

$$F(Y,X) \xrightarrow{\sigma_X} G(X,X)$$

$$F(Y,X) \xrightarrow{G(X,F)} G(X,Y)$$

$$F(Y,Y) \xrightarrow{\sigma_Y} G(Y,Y)$$

for every  $f: X \to Y$ 

**Example:** apply:  $X^Y \times Y \to X$ 

# Proving the "η-Law"

Recall:

$$t \stackrel{r}{\Rightarrow} s = (\exists t'. t \Rightarrow t' \land t' \stackrel{r}{\Rightarrow} s) \lor (\exists t'. t \Rightarrow t' \land s = t' r)$$

$$\mathcal{L}^{n+1} = \mathcal{L}^n \cap \mathcal{E}(\mathcal{L}^n) \cap \mathcal{V}(\mathcal{L}^n, \mathcal{L}^n)$$

$$\mathcal{E}(\mathcal{L}^n) = \{(t, s) \mid \text{if } t \to t' \text{ then } \exists s'. s \Rightarrow s' \land \mathcal{L}^n(t', s')\}$$

$$\mathcal{V}(\mathcal{L}^n, \mathcal{L}^n) = \{(t, s) \mid \text{for all } r_1, r_2, \mathcal{L}^n(r_1, r_2),$$

$$\text{if } t \stackrel{r_1}{\Rightarrow} t' \text{ then } \exists s'. s \stackrel{r_2}{\Rightarrow} s' \land \mathcal{L}^n(t', s')\}$$

▶ Proof of  $\mathcal{L}^n(S \cdot (K \cdot I) \cdot f, f)$  by induction on n, in particular:

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