From Small-Step to Big-Step, Abstractly

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HO Mathematical Operational Semantics Project

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

.. and rolling

Project in Nutshell

- ▶ Motto: Make operational semantics more mathematical
- Main Idea: Given operational specification (set of O/S rules), devise methods/properties of the language
- ► Main Tool: Category theory



- ► Methods: Abstract logical relations, Abstract Howe's method
- Properties: Compositionality, safety, adequacy
- ► Side-effect: categorical methods → functional implementation (Haskell, Agda, Coq)

Our Hobbyhorse: (Extended) Combinatory Logic

►
$$I (= \lambda p. p)$$
 $K (= \lambda p. \lambda q. p)$ $S (= \lambda p. \lambda q. \lambda r. (p \cdot r) \cdot (q \cdot r))$

 \triangleright plus S', S" and K' for partially reduced terms

Small-step semantics (cf. lazy λ -calculus[†]):

$$K \xrightarrow{p} K'(p)$$
 $K'(p) \xrightarrow{q} p$ $S''(p,q) \xrightarrow{r} (p \cdot r) \cdot (q \cdot r)$...
$$\frac{p \to p'}{p \cdot q \to p' \cdot q} \qquad \frac{p \xrightarrow{q} p'}{p \cdot q \to p'}$$

Example:

$$\frac{K \xrightarrow{S} K'(S)}{K \cdot S \to K'(S)} \xrightarrow{K'(S) \xrightarrow{I} S} S \text{ so } (K \cdot S) \cdot I \to^{\star} S$$

[†] Abramsky, "The lazy λ-calculus", 1990.

Big-Step Semantics

- Notion of value: $v, w := I \mid K \mid S \mid K'(t) \mid S'(t) \mid S''(s, t)$
- ▶ Evaluation relation: $\Downarrow \subseteq Terms \times Values$
- Big-step rules:

Equivalence Theorem:
$$t \Downarrow v \iff t \rightarrow^* v \land v$$
 is a value

? How to prove it abstractly?

How to prove

```
t \Downarrow v \iff t \rightarrow^* v \land v \text{ is a value}
```

abstractly?

Abstract Higher-Order GSOS

A Bit of Category Theory

From the programming perspective:

- (Endo-)functor is a type constructor, e.g. $FX = X \times X$
- Natural transformation $\alpha: F \to G$ is a polymorphic function $\alpha_X \colon FX \to GX$, e.g. $swap \colon X \times X \to X \times X$
- ▶ Algebra is a map $a: FX \to X$, e.g. the free algebra of Σ-terms $\iota: \Sigma(\Sigma^*X) \to \Sigma^*X$ over variables X, and $\mu\Sigma := \Sigma^*\emptyset$
- ▶ Monad is such a functor T that morphisms $(f: X \to TY)_{X,Y \in \mathcal{C}}$ form a category, e.g. for $T = \mathcal{P}$ we obtain the category of relations

Dinaturality

Given two functors F, $G: \mathbb{C}^{op} \times \mathbb{C} \to D$,

$$\alpha = (\alpha_{X,Y} \colon F(X,Y) \to G(X,Y))_{X,Y \in \mathcal{C}}$$
 is a dinatural transformation if

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

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

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

commutes for any $f: X \to Y$

Example: evaluation transformation ev: $C^X \times X \rightarrow C$

Higher-Order Abstract GSOS

A higher-order GSOS law in category ${\mathcal C}$ consists of

- ▶ Signature functor Σ : $\mathcal{C} \to \mathcal{C}$
- ▶ Behaviour functor $B: \mathcal{C}^{op} \times \mathcal{C} \rightarrow \mathcal{C}$
- ► 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

For combinatory logic:

- ▶ C category of sets
- $\Sigma X = \coprod_{f \in Ops} X^{arity(f)}, Ops = \{S, S', S'', K, K', I, \cdot \}$
- \triangleright $B(X, Y) = Y^X + Y$
- \triangleright ρ is induced by rules of operational semantics

Representing Rules

For C = Set, $\Sigma X = \coprod_{f \in Ops} X^{arity(f)}$, $B(X, Y) = Y^X + Y$, HO-GSOS precisely correspond to sets of rules of the form[†]:

$$\frac{(x_j \to y_j)_{j \in W} \quad (x_i \xrightarrow{z} y_i^z)_{i \in \overline{W}, z \in \{x_1, \dots, x_n\}}}{f(x_1, \dots, x_n) \to t}$$

or

$$\frac{(x_j \to y_j)_{j \in W} \quad (x_i \xrightarrow{z} y_i^z)_{i \in \overline{W}, z \in \{x, x_1, \dots, x_n\}}}{f(x_1, \dots, x_n) \xrightarrow{x} t}$$

$$(W \subseteq \{1,\ldots,n\}, \overline{W} = \{1,\ldots,n\} \setminus W)$$

Proof Idea: Yoneda-style argument



Generally, HO-GSOS vastly abstract this situation

[†] Goncharov, Milius, Schröder, Tsampas, and Urbat, "Towards a Higher-Order Mathematical Operational Semantics", 2023.

Combinatory Logic as HO-GSOS

For example,

$$\begin{array}{c|cccc} p \rightarrow p' & & p \stackrel{q}{\rightarrow} p' \\ \hline p \cdot q \rightarrow p' \cdot q & & \hline p \cdot q \rightarrow p' \end{array}$$

correspond to

$$\rho((\begin{array}{c} p \end{array}, \begin{array}{c} p' \end{array}) \cdot (\begin{array}{c} q \end{array}, _)) = \begin{array}{c} p' \cdot q \\ \\ \rho((\begin{array}{c} p \end{array}, \begin{array}{c} f \end{array}) \cdot (\begin{array}{c} q \end{array}, _)) = \begin{array}{c} f(q) \end{array}$$

$$\left(\rho_{X,Y} \colon \Sigma(\begin{array}{c} X \end{array} \times (\begin{array}{c} Y \end{array} + \begin{array}{c} Y^X \end{array})) \rightarrow \begin{array}{c} \Sigma^*(X + Y) \end{array} + (\Sigma^*(X + Y))^X \right)$$

Operational Model

- ▶ Operational model γ : $\mu\Sigma \to B(\mu\Sigma, \mu\Sigma)$ abstracts derivability of one-step transitions $p \to p', p \xrightarrow{t} p'$
- ► It is a unique solution to

$$\begin{array}{ccc} \Sigma(\mu\Sigma) & \xrightarrow{t} & \mu\Sigma \\ & \Sigma\langle \mathrm{id},\gamma\rangle & & & \downarrow\gamma \\ & \Sigma(\mu\Sigma \times B(\mu\Sigma,\mu\Sigma)) & \xrightarrow{\rho} & B(\mu\Sigma,\Sigma^{\star}(\mu\Sigma+\mu\Sigma)) & \xrightarrow{B(\mathrm{id},\nabla^{\sharp})} & B(\mu\Sigma,\mu\Sigma) \end{array}$$

- ► Alternatively: $\gamma = B(id, \nabla^{\sharp}) \cdot \rho \cdot \Sigma \langle id, \gamma \rangle \cdot \iota^{-1}$ (structural recursion)
- ► For combinatory logic: $\gamma(p) = p'$ iff $p \to p'$ and $\gamma(p) = f$ iff $\forall x. p \xrightarrow{x} f(x)$

Separation

Strict and Lazy Arguments

Rule

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

really means two rules

$$\frac{p \to p' \qquad q \to q'}{p \cdot q \to p' \cdot q} \qquad \frac{p \to p' \qquad (q \xrightarrow{r} q_r)_r}{p \cdot q \to p' \cdot q}$$



We cannot allow such ambivalence in big-step semantics:

$$\frac{s \Downarrow K'(r) \quad r \Downarrow v}{s \cdot t \Downarrow v} \quad \text{behaves differently than} \quad \frac{s \Downarrow K'(r) \quad t \Downarrow w \quad r \Downarrow v}{s \cdot t \Downarrow v}$$

Separating example: $K'(I) \cdot \Omega$ (where $\Omega = (S \cdot I \cdot I) \cdot (S \cdot I \cdot I)$)

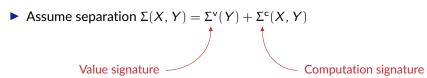
Solution: binary $\Sigma: \mathcal{C} \times \mathcal{C} \to \mathcal{C}$, for strict and lazy arguments

Separation

In $t \!\!\!\! \downarrow v \iff t \to^\star v \land v$ is a value we need to define multistep semantics \to^\star and values

Solution:

Involve ω -continuous monad T, i.e such monad that morphisms $X \to T(Y+X)$ can be iterated. Examples TX = X+1, $TX = \mathcal{P}X$, TX = D(X+1), D = monad of probability distributions



Separated Abstract HO-GSOS

Given $D: \mathcal{C}^{op} \times \mathcal{C} \to \mathcal{C}$, $\Sigma_v: \mathcal{C} \to \mathcal{C}$, $\Sigma_c: \mathcal{C} \times \mathcal{C} \to \mathcal{C}$ and a monad T, separated abstract HO-GSOS consists of

$$\begin{split} \rho_X^{\mathsf{v}} \colon \Sigma_{\mathsf{v}} X &\to D(X, \Sigma^{\star} X) \\ \rho_{X,Y}^{\mathsf{c}} \colon \Sigma_{\mathsf{c}} (X \times (TD(X,Y) + TY), X) &\to T\Sigma^{\star} (X + Y) \end{split}$$

dinatural in X and natural in Y, and a distributive law

$$\chi_{X,Y} \colon \Sigma_{c}(TX,Y) \to T\Sigma_{c}(X,Y)$$

Abstract HO-GSOS can be recovered:

$$ho = \eta \cdot D(id, \Sigma^* inl) \cdot \rho^v + \rho^c$$

Separated Abstract HO-GSOS: Properties

- Combinatory logic is separated (and so many others)
- ▶ Operational model β: $\mu\Sigma \to TD(\mu\Sigma, \mu\Sigma)$ gets separated to

$$\gamma^v \colon \Sigma_v \mu \Sigma \to \mathit{TD}(\mu \Sigma, \mu \Sigma) \qquad \gamma^c \colon \Sigma_c(\mu \Sigma, \mu \Sigma) \to \mathit{T} \mu \Sigma$$

(Slogan: Values behave as values, computions as computations)

► We can define multi-step semantics $β: μΣ → T(Σ^νμΣ)$ as least fixpoint: Klesili lifting $β^\sharp: TμΣ → TD(μΣ, μ$

$$\beta = [\eta, \beta^{\sharp} \cdot \gamma^{c}] \cdot \iota^{-1}$$
 Klesili lifting $\beta^{\sharp} \colon \mathcal{T}\mu\Sigma \to \mathcal{T}\mathcal{D}(\mu\Sigma, \mu\Sigma)$

Monad can be used for modelling other effects, e.g. add erratic choice with $p+q \rightarrow p$, $p+q \rightarrow q$, and $T=\mathcal{P}$

Abstract Big-Step SOS

Abstract Big-Step SOS

Abstract big-step SOS is a natural transformation

$$\xi: \Sigma_{c}(\Sigma_{v} X, X) \to T(\Sigma^{*}X)$$

Assuming that T = Id, this captures two kinds of rules:

$$\frac{p_1 \Downarrow g_1(\begin{array}{ccc} p_1^1, \dots, p_n \end{pmatrix} \Downarrow g(p_1, \dots, p_n)}{f(p_1, \dots, p_k, \dots, p_n) \Downarrow v} (g \in \Sigma_v) \\
\frac{p_1 \Downarrow g_1(\begin{array}{ccc} p_1^1, \dots, p_{n_1}^1 \end{pmatrix} \dots p_k \Downarrow g_k(\begin{array}{ccc} p_1^k, \dots, p_{n_k}^k \end{pmatrix} & t \Downarrow v \\
\hline f(p_1, \dots, p_k, \dots, p_n) \Downarrow v & (f \in \Sigma_c, g_i \in \Sigma_v)$$

where precisely k first arguments are strict

Abstract Big-Step SOS: Properties

 Big-step operational model is defined as least solution of simple recursive equation

$$\zeta = [\eta, \zeta^{\sharp} \cdot T\mu \cdot \xi^{\sharp} \cdot \chi \cdot \Sigma_{c}(\zeta, id)] \cdot \iota^{-1}$$

This is neither structural, nor tail recursion, and so it must, e.g.

$$\frac{s \Downarrow S''(r,q) \quad (r \cdot t)(q \cdot t) \Downarrow v}{s \cdot t \Downarrow v}$$

► There is simple translation:

Separated Abstract HO-GSOS \Rightarrow Abstract Big-Step SOS

(This is how big-step semantics of combinatory logic is obtained)

Separation isn't Enough

Consider separated semantics

$$\frac{1}{g(p) \xrightarrow{q} f(q)} \qquad \frac{1}{\Omega \to \Omega} \qquad \frac{p \to p'}{f(p) \to g(p')} \qquad \frac{p \xrightarrow{p} p'}{f(p) \to p'}$$

► Only sensible big-step semantics is

$$\frac{p \Downarrow g(q) \qquad g(q) \Downarrow v}{f(p) \Downarrow v}$$

However $t \Downarrow v \iff t \to^* v \land v$ is a value fails (!): $f(f(g(\Omega))) \to g(g(\Omega))$, but $f(f(g(\Omega))) \Downarrow g(\Omega)$

Strong Separation

Strong separation condition (omitted) abstracts the following: if a rule has at least one premise of the form $x_k \to x'_k$ then the conclusion of the rule must be

$$f(x_1,\ldots,x_n,y_1,\ldots,y_m) \rightarrow f(x_1',\ldots,x_n',y_1,\ldots,y_m)$$

where either $x_i \to x_i'$ occurs in the premise, or else, the premise contains a labeled transition for x_i , in which case $x_i' = x_i$.

Example:

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

Non-Example:

$$\frac{p \to p'}{f(p) \to g(p')}$$

Main Result

Theorem: if (ρ^v, ρ^c, χ) is strongly separated, and abstract big-step SOS law (ξ, χ) is generated by it, then multi-step semantics and big-step operrational model agree:

$$\beta = \zeta$$

Example: Call-by-Value

Call-by-value combinatory logic: combinators as before, plus

$$\frac{t \to t'}{t \cdot s \to t' \cdot s} \ (a) \qquad \frac{t \stackrel{r}{\to} t' \quad s \to s'}{t \cdot s \to t \cdot s'} \ (b) \qquad \frac{t \stackrel{s}{\to} t' \quad s \stackrel{r}{\to} s'}{t \cdot s \to t'} \ (c)$$

But no rule

$$\frac{t \to t' \quad s \to s'}{t \cdot s \to t' \cdot s'}$$

Hence, no strong separation. Solution: replace (b)-(c) with

$$\frac{s \xrightarrow{r} s'}{s \cdot t \to s \cdot t} \qquad \frac{s \to s'}{t \cdot s \to t \cdot s'}$$

$$\frac{t \xrightarrow{r} t'}{s \cdot t \to s \cdot t} \qquad \frac{t \to t'}{t \cdot s \to t' \cdot s} \qquad \frac{t \xrightarrow{s} t'}{t \cdot s \to t'}$$

This produces "pretty-big-step semantics"†

[†] Charguéraud, "Pretty-Big-Step Semantics", 2013.

Languages with Binders

► Small-step rules:

$$\frac{p \to p'}{(\lambda x. p)q \to p[q/x]} \ (\beta) \qquad \frac{p \to p'}{pq \to p'q} \ (app)$$

▶ Big-step rules:

$$\overline{\lambda x. p \Downarrow \lambda x. p}$$

$$\frac{p \! \Downarrow \! \lambda x. \, p' \quad p'[q/x] \! \Downarrow v}{pq \! \Downarrow v}$$

We need to decompose (β) to

$$\frac{p[q/x] = p'}{\lambda x. p \xrightarrow{q} p'}$$

$$\frac{p \stackrel{q}{\rightarrow} p'}{pq \rightarrow p'}$$

Space of substitution actions

So, p[q/x] = p' becomes new kind of transitions (!)

Solution: Upgrade ρ^{v} to $\rho^{\mathsf{v}}_{X,Y} \colon \Sigma_{\mathsf{v}}(X \times (X - Y)) \to D(X, \Sigma^{\star}(X + Y))$ use a presheave category as \mathbb{C} , for modeling languages with binders[†]

[†] Fiore, Plotkin, and Turi, "Abstract Syntax and Variable Binding", 1999.

Conclusions

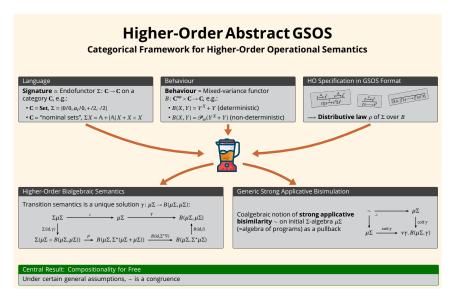
- Abstract notions of small-step/big-step semantics
- ▶ A general and abstract $t \Downarrow v \iff t \rightarrow^* v \land v$ is a value
- Functional implementation (in Haskell)

Further Work:

- Implementing proofs in proof assistant (WIP Meta-Semantics Agda Library†)
- Cost semantics, probabilistic semantics (by varying T)
- Stateful semantics
- Other uses of (strong) separation (compositionality of observational equivalences?)

https://github.com/sergey-goncharov/agda-meta-semantics

Thank You for Your Attention!



Separated Abstract HO-GSOS and Abstract BSSOS in Haskell

Free Functors, and Signatures

```
data Free s x = Res x | Cont (s (Free s x))
type Initial s = Free s Void

newtype Mrg s x = Mrg (s x x)
sigOp = Cont . Mrg

data SepSig' sv sc x y = SigV (sv y) | SigC (sc x y)
type SepSig sv sc = Mrg (SepSig' sv sc)
```

Values, Computations, Behaviours

```
type InitialV sv sc = sv (Initial (SepSig sv sc))
type InitialC sv sc = sc (Initial (SepSig sv sc))
(Initial (SepSig sv sc))

data SepBeh d x y = BehV (d x y) | BehC y
```

SepHOGSOS Type Class

```
class (MixFunctor d, Functor sv, Bifunctor sc) =>
    SepHOGSOS sv sc d where

rhoV :: sv x -> d x (Free (SepSig sv sc) x)

rhoC :: sc (x, SepBeh d x y) x
    -> Free (SepSig sv sc) (Either x y)
```

Operational Model

```
gammaV :: InitialV sv sc ->
1
        d (Initial (SepSig sv sc)) (Initial (SepSig sv sc))
2
     gammaV t = mvmap id join $ rhoV t
3
4
     gammaC :: Proxy d ->
5
        InitialC sv sc -> Initial (SepSig sv sc)
6
     gammaC (p :: Proxy d) t =
7
      (rhoC @_ @_ @d $ first (id &&& gamma) t) >>= nabla
8
         where
9
           nabla = either id id
10
           gamma (Cont (Mrg (SigV v))) = BehV $ gammaV v
11
           gamma (Cont (Mrg (SigC c))) = BehC $ gammaC p c
12
```

Multi-Step Semantics

XCL Signature

```
data XCLV x
     = S
     | K
3
   | S' x
  | K' x
     | S'' x x
8
   data XCLC x y
     = Comp x y
10
```

XCL as SepHOGSOS

```
instance SepHOGSOS XCLV XCLC (->) where
     rhoV S = sigOp . SigV . S' . Res
2
     rhoV K = sigOp . SigV . K' . Res
3
     rhoV I = Res
4
     rhoV (S' t) = sigOp . SigV . S'' (Res t) . Res
5
     rhoV(K't) = const(Res t)
6
     rhoV (S'' t s) = \r -> sigOp $ SigC $ Comp
7
         (sigOp $ SigC $ Comp (Res t) (Res r))
8
         (sigOp $ SigC $ Comp (Res s) (Res r))
9
10
     rhoC (Comp (_, BehC s) r) =
11
         sigOp (SigC $ Comp (Res $ Right s) (Res $ Left r))
     rhoC (Comp (_, BehV f) r) = Res (Right $ f r)
13
```

BSSOS Type Class

```
class (Functor sv, Bifunctor sc) => BSSOS d sv sc where
    xi :: sc (sv x) x \rightarrow Free (SepSig sv sc) x
2
3
    zeta' :: Initial (SepSig sv sc) -> InitialV sv sc
4
    zeta' (Cont (Mrg (SigV v))) = v
5
    zeta' (Cont (Mrg (SigC c))) = zeta' @d $ join $ xi @d
6
        $ first (zeta' @d) c
7
    zeta :: InitialC sv sc -> InitialV sv sc
8
    zeta = zeta' @d . sigOp . SigC
9
```

From SepHOGSOS to BSSOS

```
instance (SepHOGSOS sv sc d) => BSSOS d sv sc where
xi :: sc (sv x) x -> Free (SepSig sv sc) x
xi t = rhoCV (bimap ((sigOp . SigV &&&
mx_second @d join . rhoV)
fmap return
return t)
>>= nabla
where nabla = either id id
```

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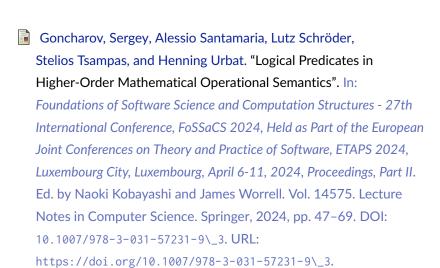
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