Symbolic Regression by Exhaustive Search

Reducing the Search Space Using Syntactical Constraints and Efficient Semantic Structure Deduplication.

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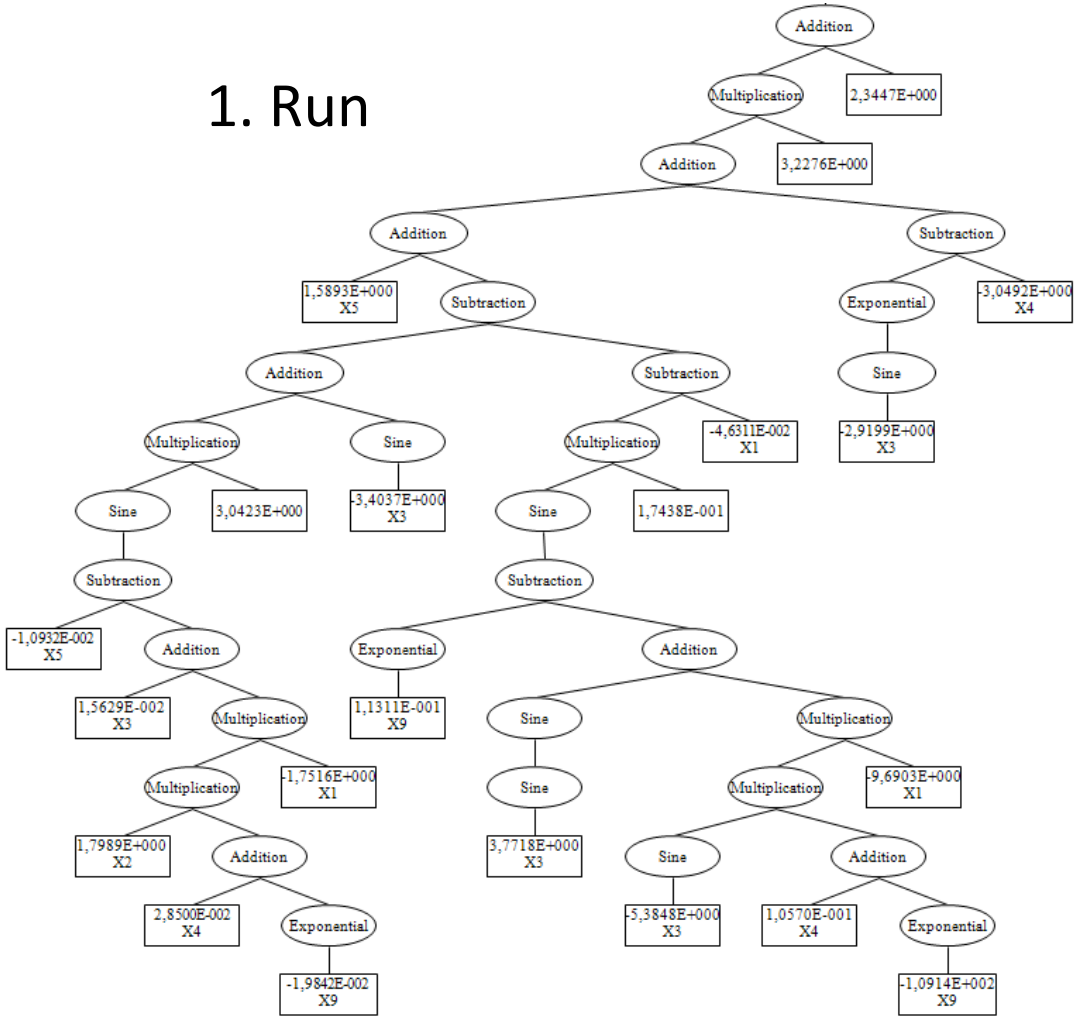
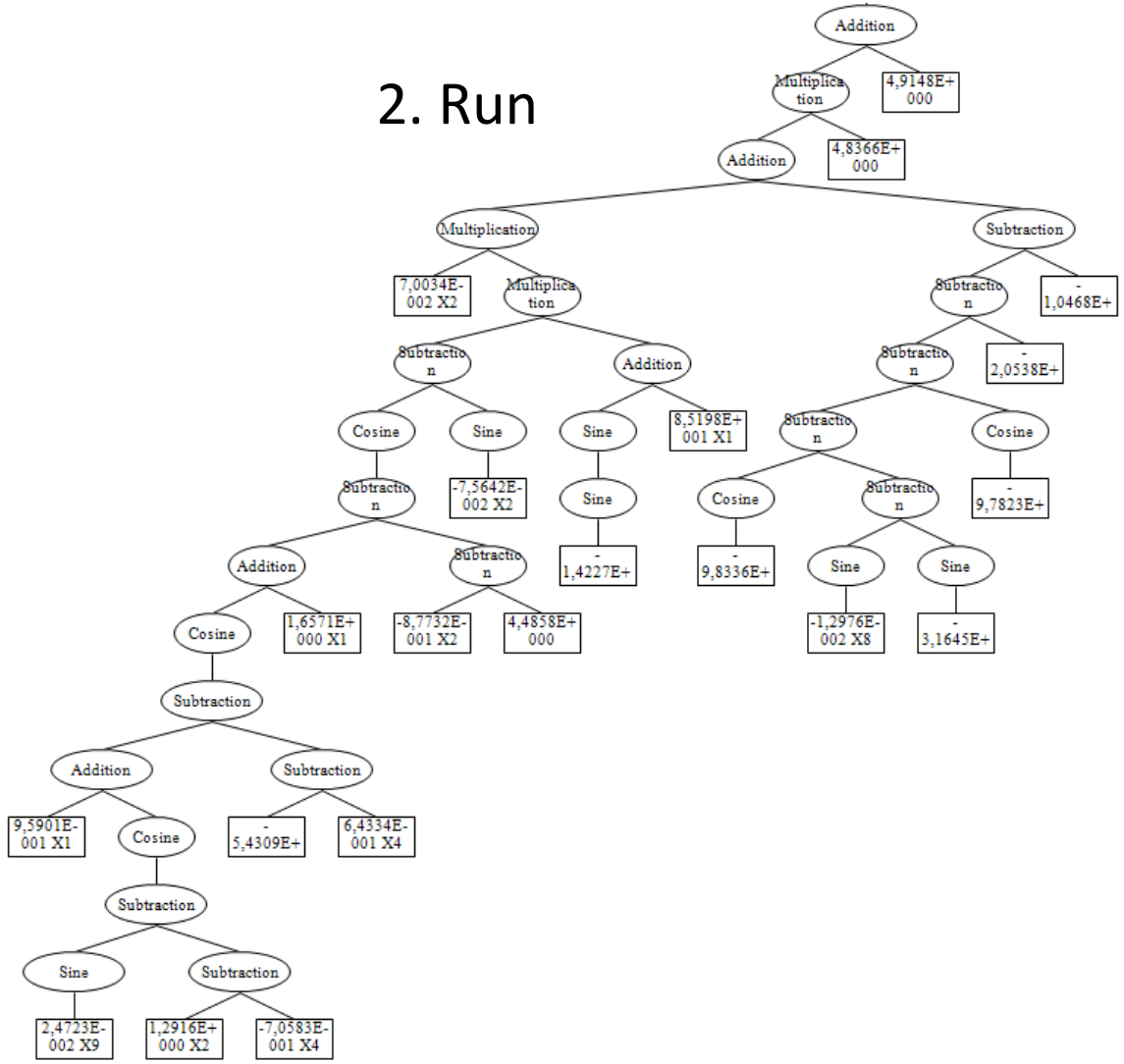
Motivation

1. Run



2. Run



Previous Work

- Trent McConaghy. "FFX: Fast, Scalable, Deterministic Symbolic Regression Technology." *GPTP IX*. 2011

- Tony Worm and Kenneth Chiu. "Prioritized Grammar Enumeration: Symbolic Regression by Dynamic Programming." *Proceedings of the 15th GECCO*. 2013.

- Michael Korns. "A baseline symbolic regression algorithm." *GPTP X*. 2013

- Gabriel Kronberger et al. „Cluster Analysis of a Symbolic Regression Search Space.“ *GPTP XVI*.

- Discussions at GPTP XVII

General Idea

1. Separate structure and coefficients

$$f(x,y) = 2y + 3x + 4x(5x + 6y)$$

$$f(x,y) = c_1 y + c_2 x + c_3 x(c_4 x + c_5 y)$$

cf. Korns, Michael. "A baseline symbolic regression algorithm." GPTP X. 2013.

cf. Worm, Tony, and Kenneth Chiu. "Prioritized grammar enumeration: symbolic regression by dynamic programming." *Proceedings of the 15th GECCO*. 2013.

Kommenda, Michael, et al. "Effects of constant optimization by nonlinear least squares minimization in symbolic regression." *Proceedings of the 15th GECCO*. 2013.

General Idea

1. Separate structure and coefficients

2. Restrict the search space

$$f(x,y) = c_1 y + c_2 x + \underline{c_3 x(c_4 x + c_5 y)}$$

$$f(x,y) = c_1 y + c_2 x + \underline{c_3 x^2 + c_4 xy}$$

General Idea

1. Separate structure and coefficients

2. Restrict the search space

$$f(x,y) = \sin\left(\mathrm{e}^{\mathrm{e}^{yx}x}\cos\left(\mathrm{e}^{-29}x\right)\right)^{\log(\sin(4x))}$$

General Idea

1. Separate structure and coefficients

2. Restrict the search space

3. Generate all solutions

$$f(x,y) = c_1 x + c_2 x$$

$$f(x,y) = c_1 x + c_2 x^2$$

$$f(x,y) = c_1 x + c_2 x^3$$

$$f(x,y) = c_1 x + c_2 y$$

$$\vdots$$

General Idea

1. Separate structure and coefficients
2. Restrict the search space
3. Generate all solutions
4. Identify semantic duplicates

$$f(x,y) = c_1 y + c_2 x + c_3 x^2 + c_4 xy$$

$$f(x,y) = c_1 x + c_2 x^2 + c_3 y + c_4 xy$$

Search Space

$$G(Expr):$$

$$Expr = c_0 \ + \ c_1 \ Term_1 \ + \ c_2 \ Term_2 \ + \ ...$$

$$Term_i = Factor_0 \ Factor_1 ...$$

$$Factor_i \in \{var, \frac{1}{Expr}, \log(arg), \exp(arg), \sin(arg), \sqrt{arg}, \sqrt[3]{arg}\}$$

$$arg = c_0 + c_1 var \ var ... + c_2 var \ var ... + ...$$

Search Space

$$G(Expr):$$

$$Expr = c_0 \ + \ c_1 \ Term_1 \ + \ c_2 \ Term_2 \ + \ ...$$

$$Term_i = Factor_0 \ Factor_1 ...$$

$$Factor_i \in \{var, \frac{1}{Expr}, \log(arg), \exp(arg), \sin(arg), \sqrt{arg}, \sqrt[3]{arg}\}$$

$$arg = c_0 + c_1 var \ var ... + c_2 var \ var ... + ...$$

Example: $c_0 + c_1 xxy + c_2 xx$

$$c_0 + c_1 xxy + c_2 \log(c_3 + c_4 xy + x)$$

$$c_0 + c_1 x \frac{1}{c_2 + \sin(c_3 + c_4 x + c_5 y)}$$

Search Space

Prevent:

$$x(x+y)$$

$$\sin(\sin(x))$$

$$\frac{1}{\frac{1}{x}}$$

$$\frac{1}{x+y}\ \frac{1}{x}$$

$$\sqrt{x}\ \sqrt{x}$$

$$\exp(x+x)$$

$$\vdots$$

Search Space

```
G(Expr):

Expr -> "const" "*" Term "+" Expr |
        "const" "*" Term "+" "const"

Term -> RecurringFactors "*" Term | RecurringFactors |
        OneTimeFactors


RecurringFactors -> VarFactor | LogFactor |
                    ExpFactor | SinFactor


VarFactor  -> <variable>

LogFactor  -> "log" "(" SimpleExpr ")"

ExpFactor  -> "exp" "(" "const" "*" SimpleTerm ")"

SinFactor  -> "sin" "(" SimpleExpr ")"


OneTimeFactors -> <every combination of InvFactor,
                   SqrtFactor and CbrtFactor>
```

```
InvFactor  -> "1/" "(" InvExpr ")"

SqrtFactor -> "sqrt" "(" SimpleExpr ")"

CbrtFactor -> "cbrt" "(" SimpleExpr ")"


SimpleExpr -> "const" "*" SimpleTerm "+" SimpleExpr |

              "const" "*" SimpleTerm "+" "const"

SimpleTerm -> VarFactor "*" SimpleTerm | VarFactor


InvExpr -> "const" "*" InvTerm "+" InvExpr |

           "const" "*" InvTerm "+" "const"

InvTerm -> RecurringFactors "*" InvTerm  |

           <every combination of RecurringFactors,
            SqrtFactor and CbrtFactor>
```

Identifying Semantic Duplicates

$$c_0 + c_1 yx = c_0 + c_1 xy$$

$$c_0 + c_1 x + c_2 x = c_0 + c_3 x$$

$$c_0 + c_1 \mathrm{e}^{c_2 x} \mathrm{e}^{c_3 x} = c_0 + c_1 \mathrm{e}^{c_3 x}$$

$$c_0 + c_1 \exp(x) + c_2 \exp(x) \neq c_0 + c_3 \exp(x)$$

$$c_0 + c_1 \sin(x) + c_2 \sin(x) \neq c_0 + c_3 \sin(x)$$

Identifying Semantic Duplicates

$$c_0 + c_1 yx = c_0 + c_1 xy$$

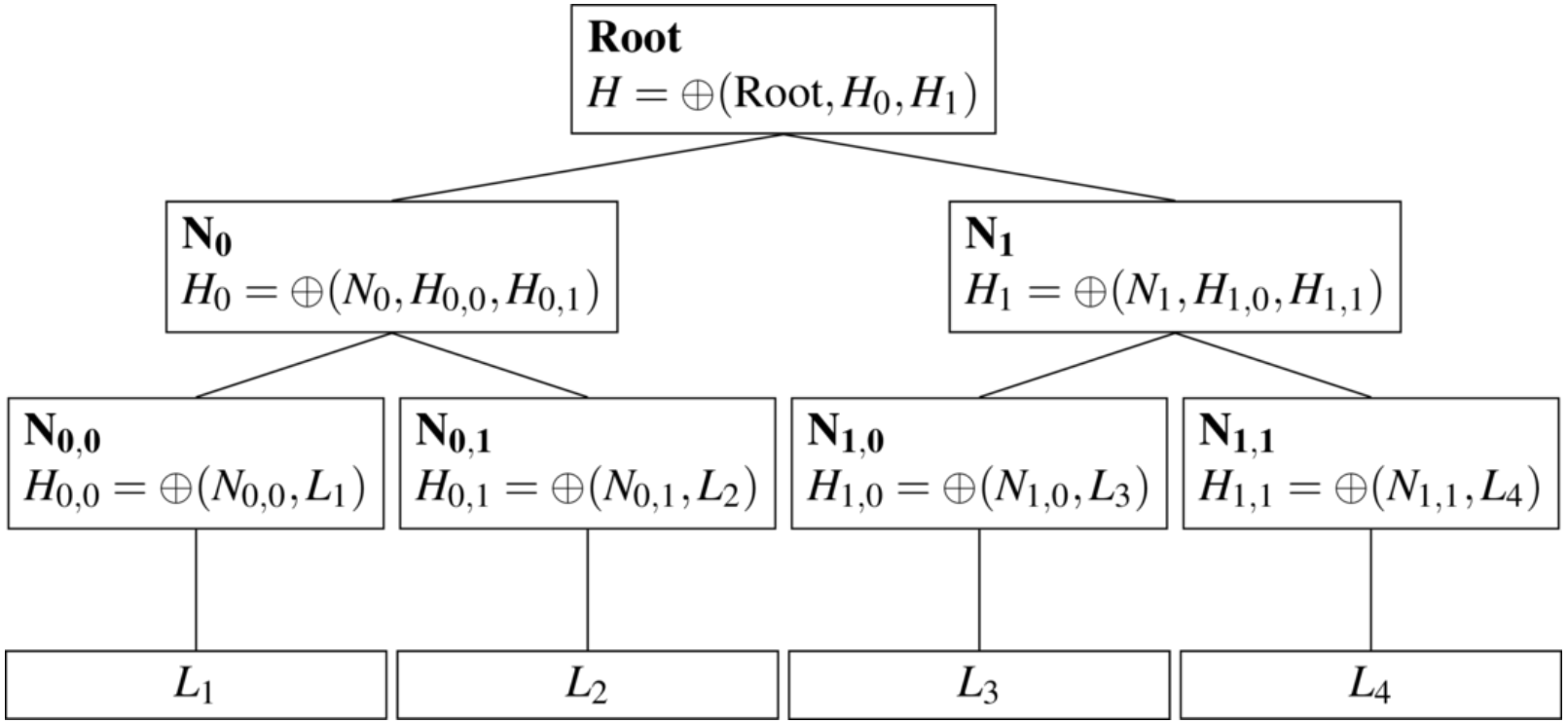
$$c_0 + c_1 x + c_2 x = c_0 + c_3 x$$

$$c_0 + c_1 \mathrm{e}^{c_2 x} \mathrm{e}^{c_3 x} = c_0 + c_1 \mathrm{e}^{c_3 x}$$

$$c_0 + c_1 \exp(c_2 + c_3 x) + c_4 \exp(c_5 + c_6 x) \neq c_0 + c_7 \exp(c_8 + c_9 x)$$

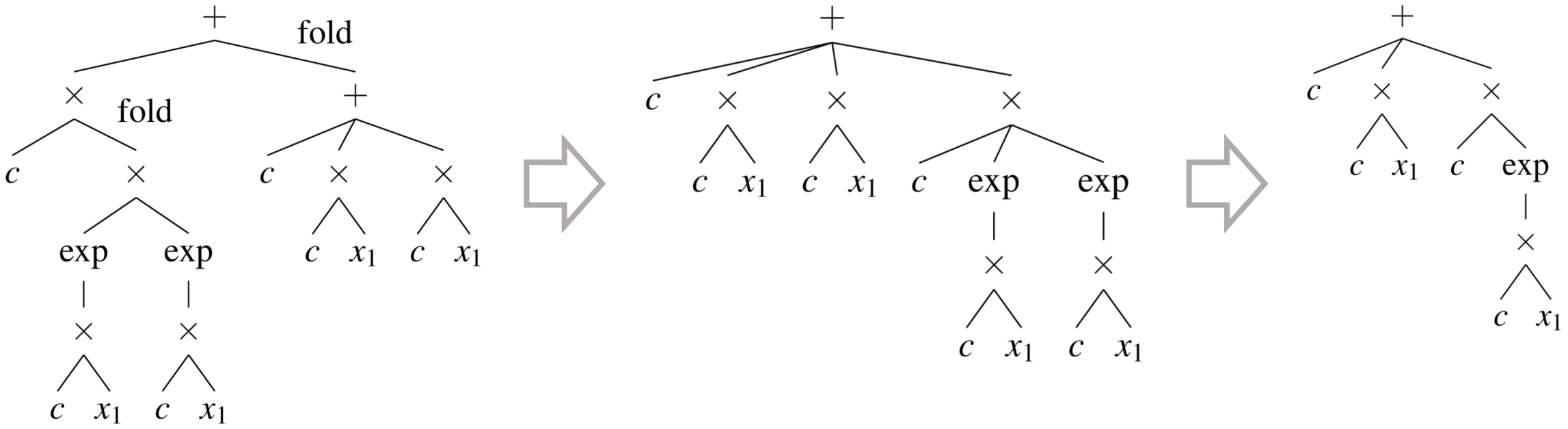
$$c_0 + c_1 \sin(c_2 + c_3 x) + c_4 \sin(c_5 + c_6 x) \neq c_0 + c_7 \sin(c_8 + c_9 x)$$

Semantic Expression Hashing



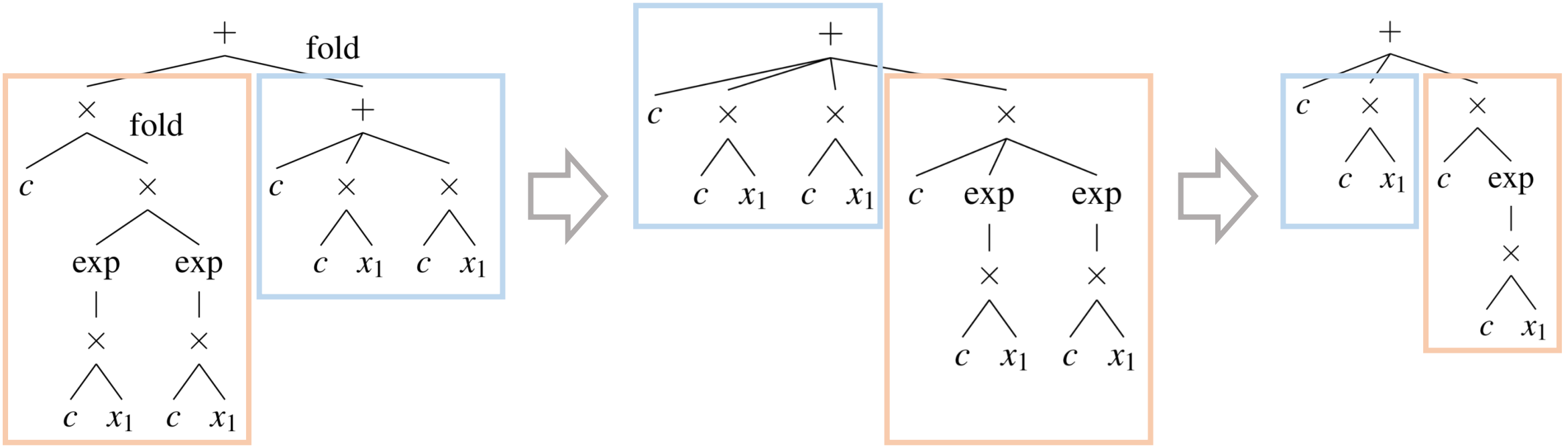
cf. Merkle, Ralph C. "A digital signature based on a conventional encryption function." *Conference on the theory and application of cryptographic techniques*. Springer, Berlin, Heidelberg, 1987.

Semantic Expression Hashing



original folded reduced

Semantic Expression Hashing



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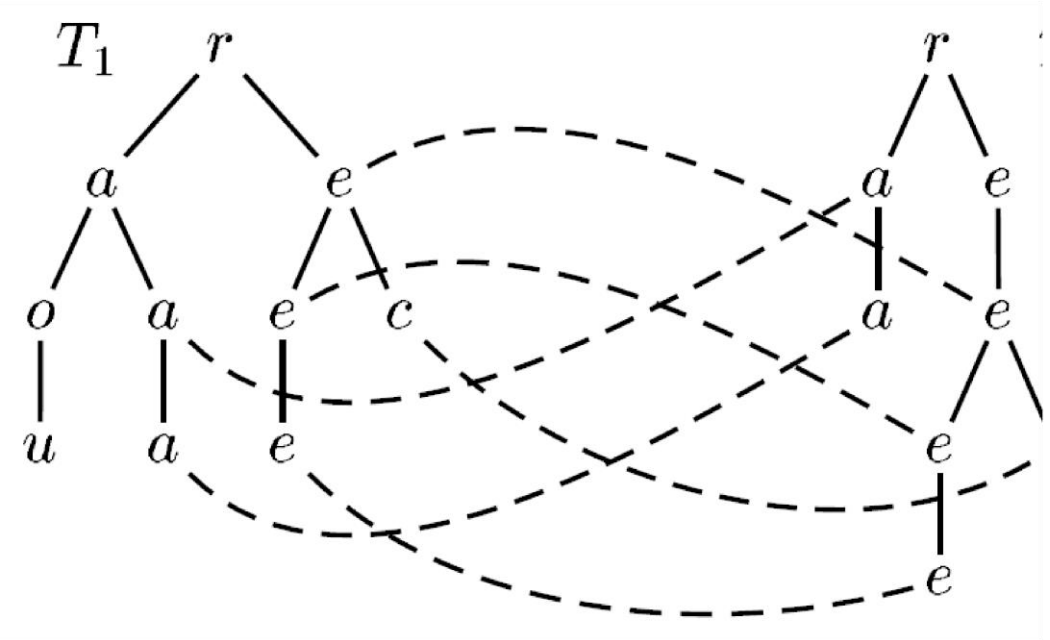
Semantic Expression Hashing vs. Bottom-Up Tree Distance



cf. Valiente, Gabriel. "An Efficient Bottom-Up Distance between Trees." *Proceedings of the 8th International Symposium of String Processing and Information Retrieval*. 2001

Iterating the Search Space

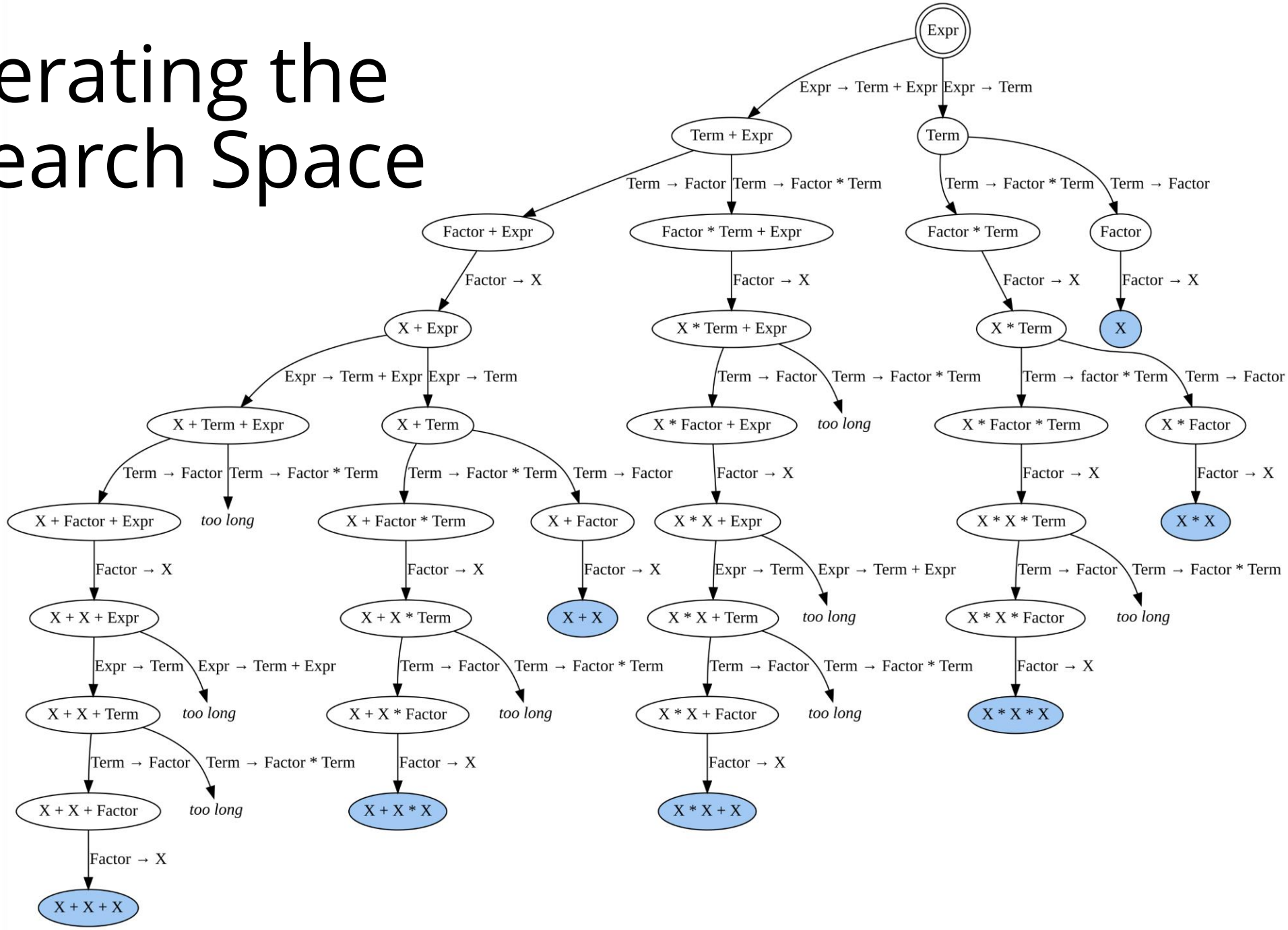
```
1    openPhrases = { StartSymbol }
2    seenHashes = { }
3    while openPhrases not empty
4         openPhrase = fetch from openPhrases
5         expandedSymbol = leftmost nonterminal symbol in openPhrase
6         foreach prod in expandedSymbol's productions
7              newPhrase = derive from openPhrase with prod
8              if hash(newPhrase) not in seenHashes
9                   if newPhrase is sentence
10                       add hash(newPhrase) to seenHashes
11                       optimize coefficients in newPhrase
12                       evaluate newPhrase
13                  else
14                       push newPhrase to openPhrases
```

derive phrases

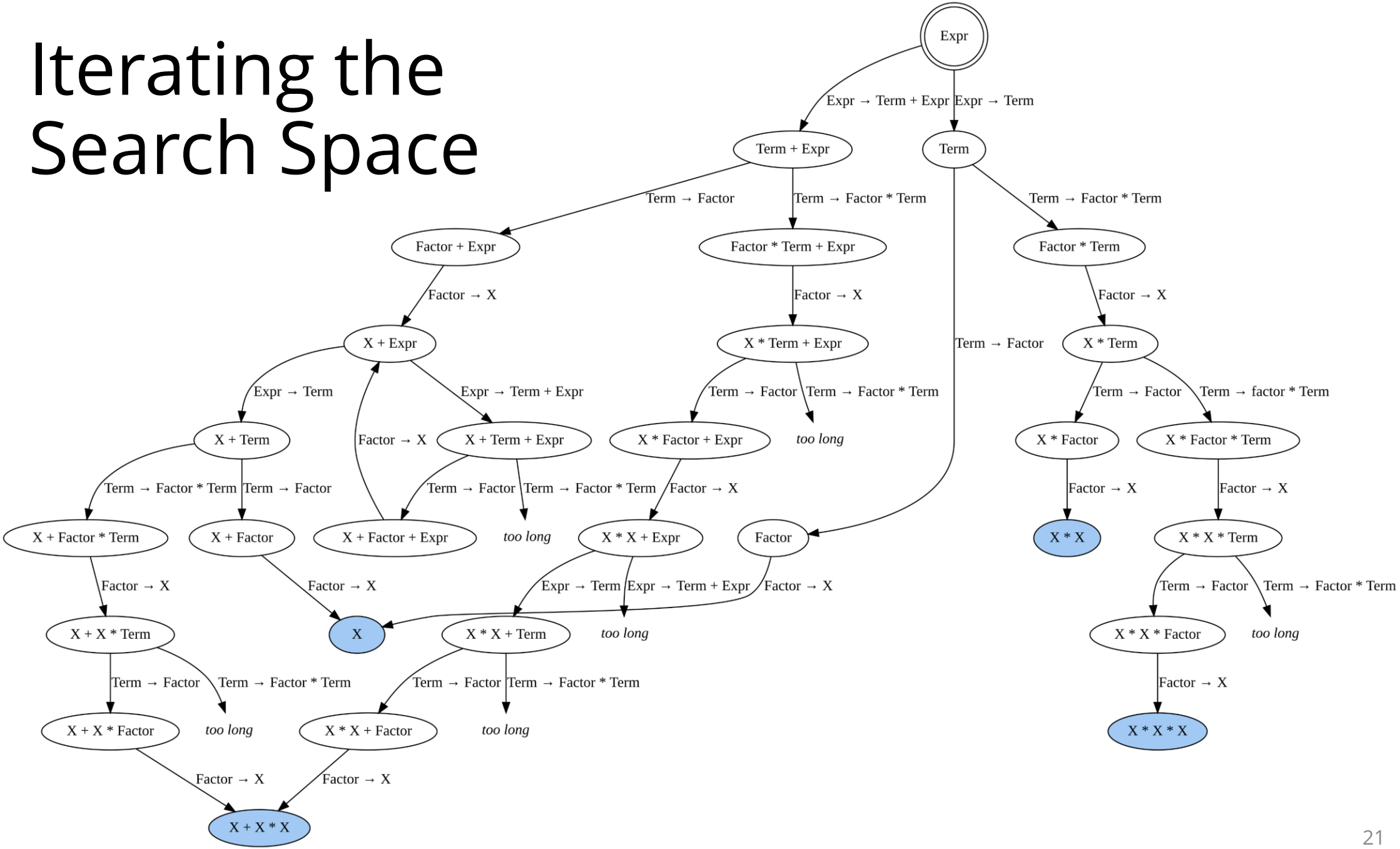
check for duplicates

evaluate previously unseen sentence

Iterating the Search Space



Iterating the Search Space



Guiding the Search

```
1   openPhrases = priority queue({ StartSymbol })
2   seenHashes = { }
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14                  prio = priority(newPhrase)
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derive phrases

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guide the search

Guiding the Search

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13              else
                    prio = priority(newPhrase)
                    push newPhrase with prio to openPhrases
```

derive phrases

check for duplicates

evaluate previously unseen sentence

guide the search

unfinished solution!

Steering the search

$$c_1 \log(c_2 x + c_3) \quad + \quad c_4 x x \quad + \quad Expr$$

Steering the search

$$\overbrace{c_1 \log(c_2 x + c_3)}^{finishedTerm_1} + \overbrace{c_4 x x}^{finishedTerm_2} + \underbrace{Expr}_{\text{Treat as coefficient}}$$

Steering the search

$$\overset{finishedTerm_1}{c_1 \log(c_2 x + c_3)} \quad + \quad \overset{finishedTerm_2}{c_4 x x} \quad + \quad \underbrace{Expr}_{\text{Treat as coefficient}}$$

$$finishedTerm_1 \quad + \quad finishedTerm_2 \quad + \quad \underbrace{c_5\, Term}_{\text{Can only improve quality}}$$

A Simple Heuristic

Length vs. Accuracy

$$priority(p) = -\underbrace{\frac{\text{len}(p)}{length_{\max}}}_{\in[0,1]} - w\,\text{NMSE}(p)$$

Experiment Results

Nguyen Problems

		Training NMSE	Test NMSE	Exact?
1	$x^3 + x^2 + x$	1.e-22	2.e-22	✓
2	$x^4 + x^3 + x^2 + x$	6.e-25	2.e-24	✓
3	$x^5 + x^4 + x^3 + x^2 + x$	4.e-22	7.e-22	✓
4	$x^6 + x^5 + x^4 + x^3 + x^2 + x$	1.e-13	7.e-12	
5	$\sin(x^2)\cos(x) - 1$	1.e-14	7.e-14	✓
6	$\sin(x) + \sin(x + x^2)$	9.e-13	1.e-07	
7	$\log(x + 1) + \log(x^2 + 1)$	9.e-14	1.e-12	✓
8	$\sqrt{x}$	5.e-18	1.e-17	✓
9	$\sin(x) + \sin(y^2)$	3.e-14	3.e-13	✓
10	$2\sin(x)\cos(y)$	4.e-18	6.e-18	✓
11	x^y	1.e-05	4.e-02	
12	$x^4 - x^3 + 0.5\,y^2 - y$	2.e-17	1.e-16	✓

Experiment Results

Keijzer Problems

		Training NMSE	Test NMSE	Exact?
1,2,3	$0.3 \, x \sin(2 \pi x)$	7.E-13	2.E-12	✓
4	$x^3 \exp(-x) \cos(x) \sin(x) (\sin(x)^2 \cos(x) - 1)$	2.E-04	3.E-04	
5	$(30 \, x \, z) / ((x - 10) \, y^2)$	2.E-06	2.E-06	
6	Sum(1 / i) From 1 to x	9.E-13	8.E-09	
7	ln(x)	1.E-22	1.E-22	✓
8	sqrt(x)	1.E-17	1.E-17	✓
9	arcsinh(x) i.e. $\ln(x + \sqrt{x^2 + 1})$	4.E-14	1.E-05	
10	x ^ y	8.E-05	9.E-03	
11	$xy + \sin((x - 1)(y - 1))$	2.E-03	2.E-01	
12	$x^4 - x^3 + y^2 / 2 - y$	1.E-19	3.E-19	✓
13	$6 \sin(x) \cos(y)$	3.E-24	1.E-21	✓
14	$8 / (2 + x^2 + y^2)$	1.E-19	7.E+00	
15	$x^3/5 + y^3/2 - y - x$	3.E-20	3.E-20	✓

Experiment Results

Vladislavleva Problems

		Training NMSE	Test NMSE	Exact?
1	$\exp(-(x_1 - 1)^2) / (1.2 + (x_2 - 2.5)^2)$	2.E-03	4.E+00	
2	$\exp(-x)\, x^3 \cos(x) \sin(x) (\cos(x)\sin(x)^2 - 1)$	2.E-04	3.E-01	
3	$\exp(-x_1)\, x_1^3 \cos(x_1) \sin(x_1) (\cos(x_1)\sin(x_1)^2 - 1)(x_2 - 5)$	2.E-02	1.E-01	
4	$10 / (5 + \text{Sum}(x_i - 3)^2)$ for i in 1..5	1.E-01	3.E-01	
5	$30 ((x_1 - 1) * (x_3 - 1)) / (x_2^2 (x_1 - 10))$	3.E-03	1.E-02	
6	$6 \sin(x_1) \cos(x_2)$	3.E-20	2.E-18	✓
7	$(x_1 - 3)(x_2 - 3) + 2 \sin((x_1 - 4)(x_2 - 4))$	7.E-02	8.E-02	
8	$((x_1 - 3)^4 + (x_2 - 3)^3 - (x_2 - 3)) / ((x_2 - 2)^4 + 10)$	3.E-03	6.E-01	

Experiment Results

Other Benchmark Problems

	Training NMSE	Test NMSE	Exact?
Breiman - I	1.E-01	1.E-01	
Friedman - I	1.E-01	1.E-01	
Friedman – II	4.E-02	4.E-02	
Poly-10 $y = X_1 X_2 + X_3 X_4 + X_5 X_6 + X_1 X_7 X_9 + X_3 X_6 X_{10}$	3.E-17	4.E-17	✓
Spatial co-evolution $F(x,y) = 1/(1 + x^{-4}) + 1/(1 + y^{-4})$	6.E-04	5.E-03	

Limitations

Complex terms, many variables

Keijzer Problems		Training NMSE	Test NMSE
4	$x^3 \exp(-x) \cos(x) \sin(x) (\sin(x)^2 \cos(x) - 1)$	2.E-04	3.E-04
5	$(30 x z) / ((x - 10) y^2)$	2.E-06	2.E-06
Vladislavleva Problems			
1	$\exp(- (x_1 - 1)^2) / (1.2 + (x_2 - 2.5)^2)$	2.E-03	4.E+00
2	$\exp(-x) x^3 \cos(x) \sin(x) (\cos(x)\sin(x)^2 - 1)$	2.E-04	3.E-01

Limitations

Noise

	Training NMSE	Test NMSE
Breiman - I	1.E-01	1.E-01
Friedman - I	1.E-01	1.E-01
Friedman - II	4.E-02	4.E-02

Limitations

Noise

	Training NMSE	Test NMSE
Friedman - II	4.E-02	4.E-02

Ground Truth:

$\sqrt{X0*X0 + (x1 * x2 - 1 / (x1 * x3))^2} + N(0, 1)$.

Found:

-65.271025 +
exp(x3 * x3 * -0.32) * -48.14 +
exp(x1 * x2 * -2.66) * 118.35 +
342.59 x1 * x2 * exp(x2 * x1 * -1.14) +
-18.65 x3 +
5.28 x3 * x3 * x3 +
-0.21 x1 * x1 +
-0.23 x2 * x2 +
5.06 x5 +
0.22 x1 +
0.26 x2 +
9.95 x4

Limitations

Constants

Nguyen Problems			
6	$\sin(x) + \sin(x + x^2)$	9.e-13	1.e-07

Keijzer Problems		Training NMSE	Test NMSE
9	arcsinh(x) i.e. $\ln(x + \sqrt{x^2 + 1})$	4.E-14	1.E-05
11	$xy + \sin((x - 1)(y - 1))$	2.E-03	2.E-01

Limitations

Constants

Nguyen Problems

6	$\sin(x) + \sin(x + x^2)$	9.e-13	1.e-07

Found Model:

```
-0.021 +
-0.005 x*x*x*x +
 1.01 sin(0.02 + 0.98 x + 0.99 x*x) +
-0.15 x*x*x +
 1.01 x
```

Discussion

- Lack of heuristics for complex terms and many variables
- No mechanisms against overfitting
- No re-evaluation of solutions
- Nearly no bloat
- Less possibilities for parallelism
- Determinism

Discussion

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Thank you!

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