# Introduction to Schema Theory

*A survey lecture of pessimistic & exact schema theory*

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# Outline of Discussion

Part I: Overview of Schema Theory ←

Part II: Pessimistic Schema Theory

Part III: Exact Schema Theory

Part IV: Conclusions

# What is a Theory?

- Set of analytical tools to help answer questions
- Particular domain in which to ask questions

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**What do theories *do*?**

- Predict
- Explain

# What are Schemata?

- Can view Schemata in many ways
  - Templates specifying groups (sets) of ”similar” chromosomes
  - Partitions of genome space
  - Descriptions of hyperplanes through genome space
  - Sets of search points sharing some ”syntactic feature”

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  - Templates specifying groups (sets) of "similar" chromosomes
  - Partitions of genome space
  - Descriptions of hyperplanes through genome space
  - Sets of search points sharing some "syntactic feature"
- Example for binary representation:

"*" $\Leftrightarrow$ "Don't care"

| Schema | Members |
|---|---|
| 1**0 | 1000 |
| | 1010 |
| | 1100 |
| | 1110 |

# What is Schema Theory?

- Describes how schemata are *expected* to propagate from one generation to the next
- More specifically:
  - Divides the space into subspaces
  - Quantifies these subspaces
  - Explains how & why individuals move between subspaces

# What are Schema Theorems?

- *Specific* analytical models
- Usually reflect particular representational choices
- May provide only a lower bound schemata growth
- May provide tight bounds on schemata growth

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**Explanation**

# Advantages of Schema Theory

- Appeals to our intuition of how problems may be solved (i.e., building blocks)
- Can be formulated in a concise way, such that specific instantiations for particular EAs can be ”plugged in” to main theorems
- With exact models, we can get correct predictions of expectation, as well as bounds on the probability of those expectations

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  - Operates under the assumption that knowing what schemata are doing helps us understand how & why the GA is working (it doesn't always)
- Applicability is low. Why?
  - Large effort to produce very specific models
  - Most EAs modeled under ST are simple EAs, not used in practice

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- Attempts to give insight
  - About *how* GAs work
  - Describes how the expected number of schemata will *at least* grow in the next generation
- Generally assumes
  - Binary, fixed-length representation
  - Bit flip mutation, 1-point crossover
  - Proportional selection

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$$E[\,\#\text{ strs} \in \text{schema @ gen } t+1] \geq (\#\text{ strs} \in \text{schema @ } t)\cdot$$
$$(\text{rel. value of schema})\cdot$$
$$(\text{prob } \sim\text{destroyed})$$

# Notation

- Individual are fixed-length binary strings, $v \in \{0,1\}^l$
- Schema are fixed length ternary strings, $s \in \{0,1,*\}^l$
- Schema define a set of individual strings. $v \in s$ iff $\forall i \in \{0 \ldots l\}, v_i = s_i \vee s_i = *$
- Population at time $t$ is a set of binary strings, $P_t = \{v^{(1)}, v^{(2)}, \ldots, v^{(n)}\}$, $v^{(i)} \in \{0,1\}^l$
- Match is no. of strings in $P_t$ also in schema $s$. $m(s,t) = \|\{v \in P_t, v \in s\}\|$

# Notation (continued)

- Mean fitness of strings in schema $s$ also in $P_t$, $f(s,t)$
- Mean fitness of the population, $\overline{f}(t)$
- Probability of mutation, $p_m$
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$$E[m(s,t+1)] \geq m(s,t)\frac{f(s,t)}{f(t)}Pr[\text{surv mut}]Pr[\text{surv xover}]$$

# Measures of Schema

- **Order** of schema is the # of fixed positions, $o(s) = \|\{\forall i \in \{1 \ldots l\}, s_i \neq *\}\|$
- **Defining length** is the longest distance between two fixed positions,

$$\delta(s) = \max\left(|i - j|,\ \forall i, j \in \{1 \ldots l\}, s_i \neq * \wedge s_j \neq *\right)$$

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**Example:**

$s =$ `* 0 * 1 1 * * 1 *`

$o(s) = 4$

$\delta(s) = 6$

# Surviving Mutation

- Probability no mutation at a given position occurs is $1 - p_m$
- All mutations are independent
- We only care about the fixed positions
- So probability schema survives disruption is $(1 - p_m)^{o(s)}$

# Surviving Crossover

- A crossover event which does not divide the defined positions in the schema is harmless
- The probability the crossover breaks the schema is $\frac{\delta(s)}{l-1}$
- Thus the probability to survive crossover is $1 - p_c \frac{\delta(s)}{l-1}$

# The Traditional Schema Theorem

$$E[m(s,t+1)] \geq m(s,t)\frac{f(s,t)}{f(t)}(1-p_m)^{o(s)}\left(1-p_c\frac{\delta(s)}{l-1}\right)$$

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But we can do better, since this ignores the possibility that you select a breeding partner from the same schema...

$$m(s,t)\frac{f(s,t)}{f(t)}(1-p_m)^{o(s)}\left(\left(1-p_c\frac{\delta(s)}{l-1}\right)\left(1-\frac{m(s,t)f(s,t)}{n\cdot f(t)}\right)\right)$$

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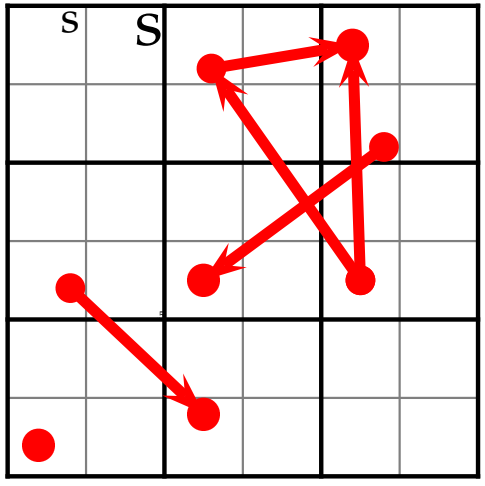
More generally, we can replace the selection method...

$$n\cdot p(s,t)(1-p_m)^{o(s)}\left(\left(1-p_c\frac{\delta(s)}{l-1}\right)(1-p(s,t))\right)$$

Where $p(s,t)$ is the probability of selecting schema $s$ at generation $t$. For proportional selection $p(s,t)=\frac{m(s,t)}{n}\cdot\frac{f(s,t)}{f(t)}$.

# What does this tell us?




- Helps explain how $m(s,t)$ is affected by GA operators
- Helps predict how $m(s,t)$ varies from one generation to the next
- Provides only a *lower bound*

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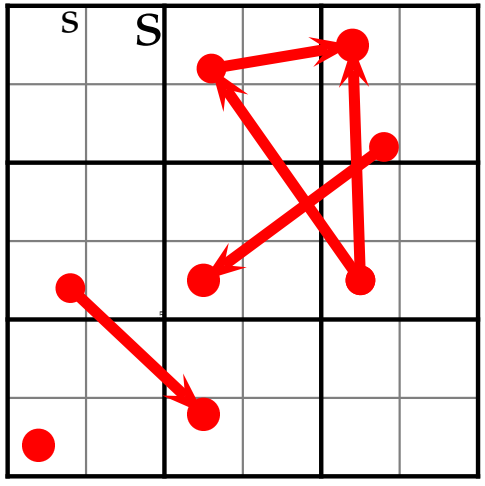


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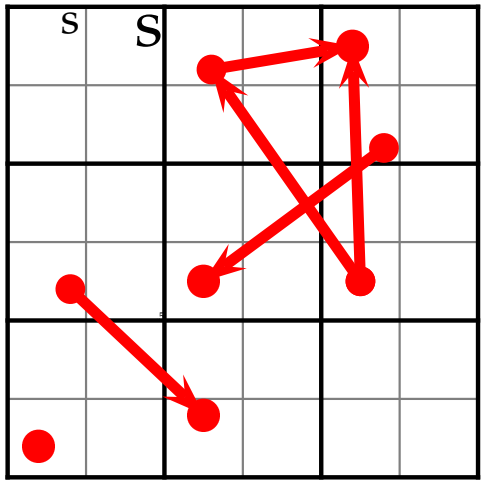


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  - No. indiv in schema
  - Avg fitness of schema
  - Avg fitness of pop
  - Disruption of ops
  - etc.

# Genetic Programming Schemata

- We can express schemata as a list of ordered pairs

  $0 * 1 * * 1\ 1 \Leftrightarrow [(0,1),(1,3),(11,6)]$

- Supposing $v \in \{a,b,c,d\}^l$,

  $a * b\ c * a\ d \Leftrightarrow [(a,1),(bc,3),(ad,6)]$

- Traditional ST specifies the complete string, so position is important.
- But we could match partial strings...
- And we could match strings independent of position...

# GP Schemata (continued)

- No. of individuals matching $s$ in $P_t$ is $m(s,t)$
- No. of substrings matching $s$ in $P_t$ is $\iota(s,t)$ *(instantiations)*

**Example Population:**

a b a a c

a c c a b

c c c c b

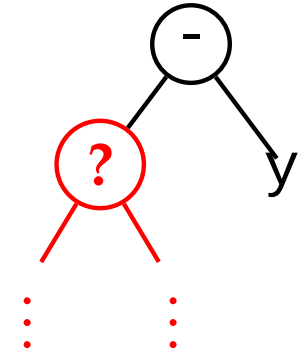
a b c a b

$$m([ab],t) = 3, \quad \iota([ab],t) = 4$$

$$m([a,b],t) = 4, \quad \iota([a,b],t) = 12$$

# Rosca's Rooted Tree Schemata

- Syntactically:
  - Every schema is a contiguous tree fragment
  - Every schema includes the root node of the tree
  - Use '#' character rather than '*' for *don't care* symbol
- Semantically:
  - A schema defines a set of programs
  - $s =$ ( - # y ) defines the set of programs:



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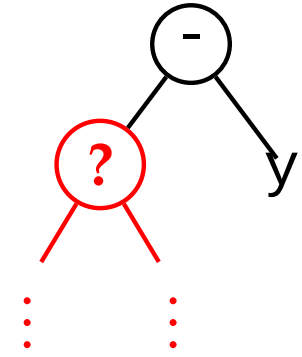

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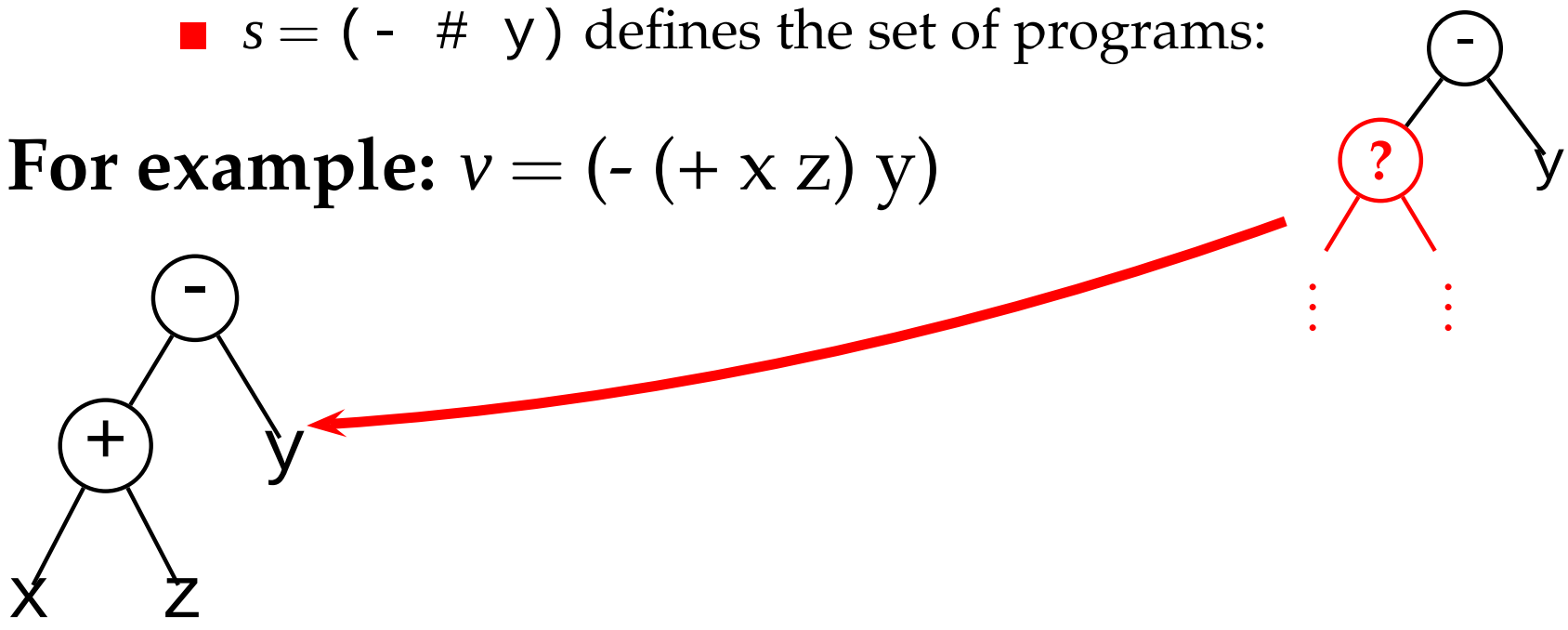

# Rosca's Schemata Notation/Measures

- Size of program $v$ matching schema $s$ is $N(v)$
- The fitness of program $v$ is $f(v)$
- The order of schema is number of defining symbols it contains, $O(v)$
- The population at time $t$ is the multiset $P(t)$
- All programs in $P(t)$ which are also members of the schema $s$ is denoted $s \cap P(t)$
- The probability (per child) that mutation is applied is $p'_m$

# Rosca's Schema Theorem

$$E[m(s,t+1)] \geq$$
$$m(s,t)\frac{f(s,t)}{f(t)}\left[1-(p'_m+p_c)\sum_{v\in s\cap P(t)}\frac{O(s)}{N(v)}\frac{f(v)}{\sum_{v\in s\cap P(t)}f(v)}\right]$$

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- Divide space into subspaces containing programs of different sizes and shapes
- Estimate fragility of schema instances
- Use wt'd sum & prob of seln. to est. prob. of disrupting schema

# Poli-Langdon Schemata

- Fixed size and shape
- Set of functions is denoted, $\mathcal{F}$
- Set of terminals is denoted, $\mathcal{T}$
- The "=" symbol is "don't care" for a *single* function or terminal
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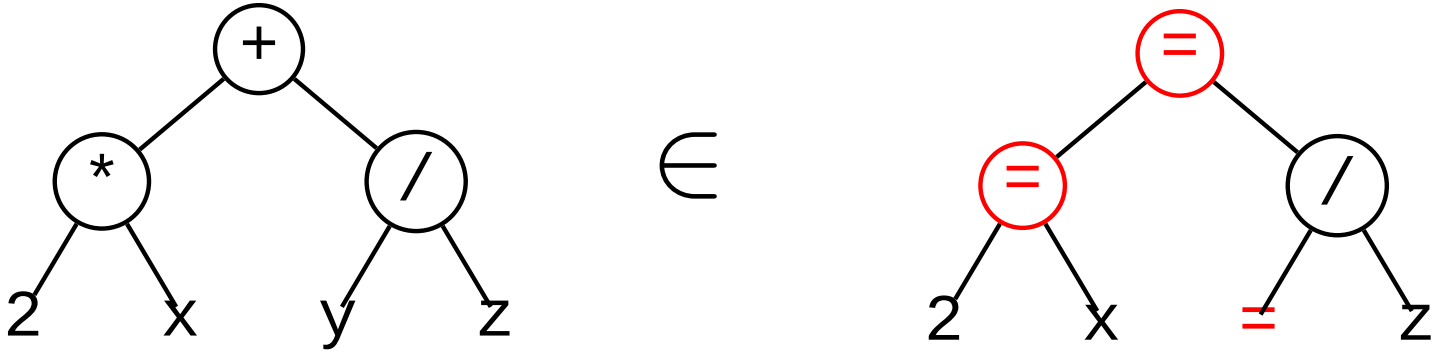
**For example:** $\mathcal{F} \in \{+,-,*,/\}, \mathcal{T} \in \{1,\ldots,9,x,y,z\}$



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- The order is the number of non-= symbols of the schema, $O(s)$
- The length is the total number of nodes in the schema, $N(s)$
- The defining length is the number of links in the minimum tree fragment including all non-= symbols in a schema, $L(s)$

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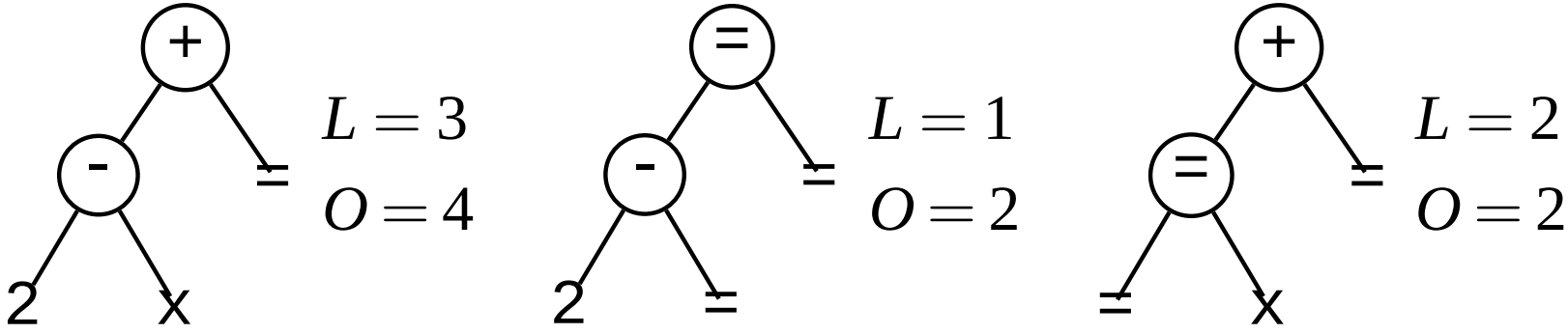

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- The zeroth order schema with the same structure as schema $s$ is G(s)
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- The prob. of selecting the $s$ from population at time $t$ is $p(s,t)$

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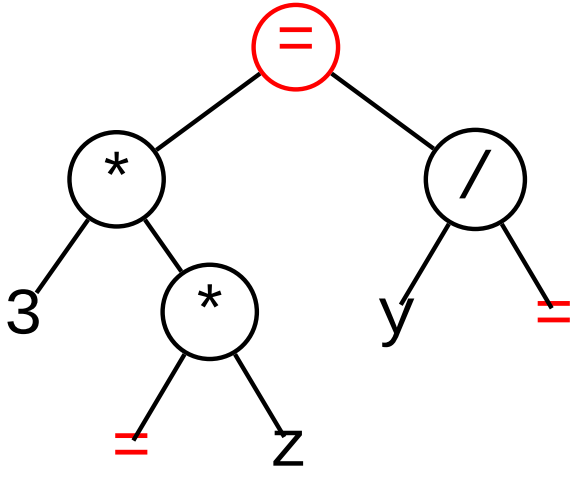


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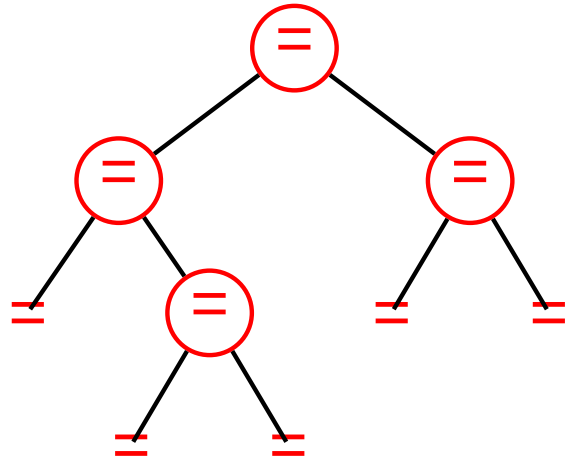
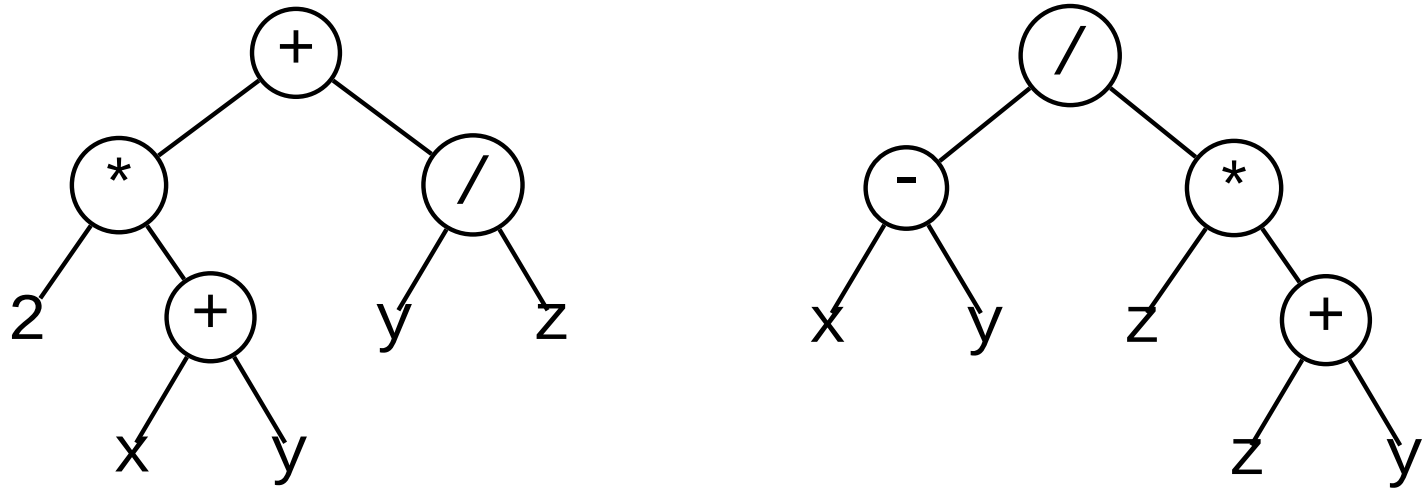


# GP One-Point Crossover

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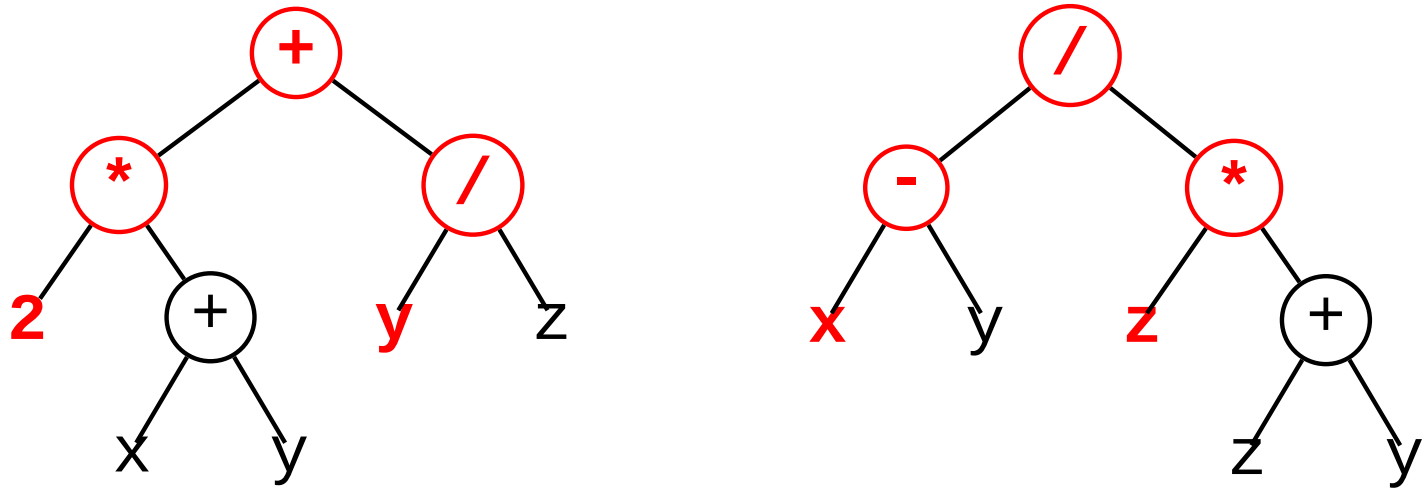


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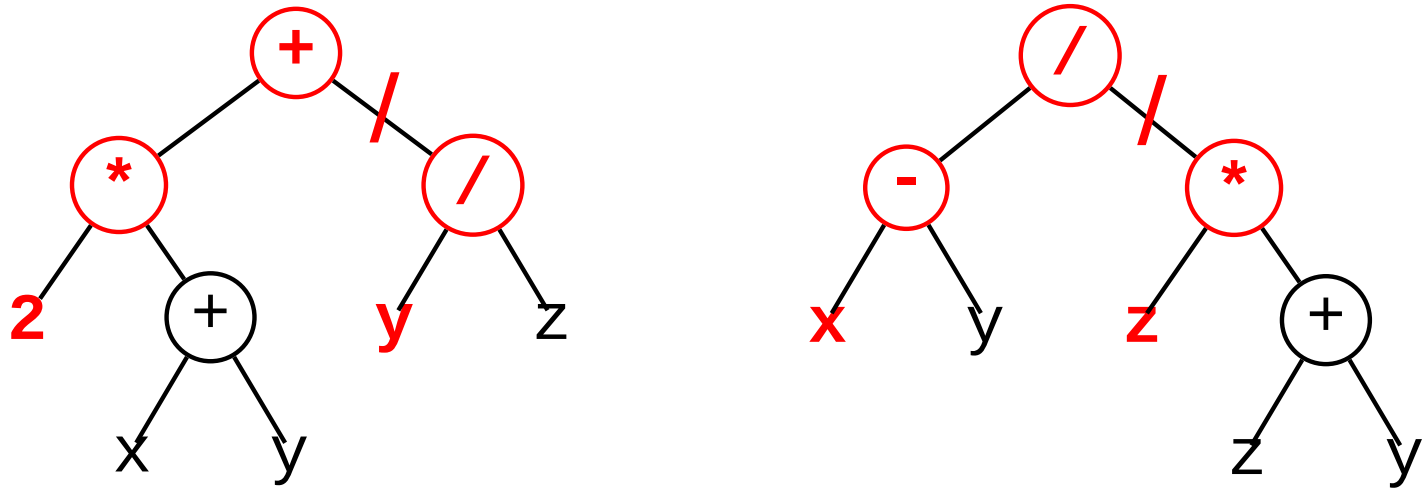


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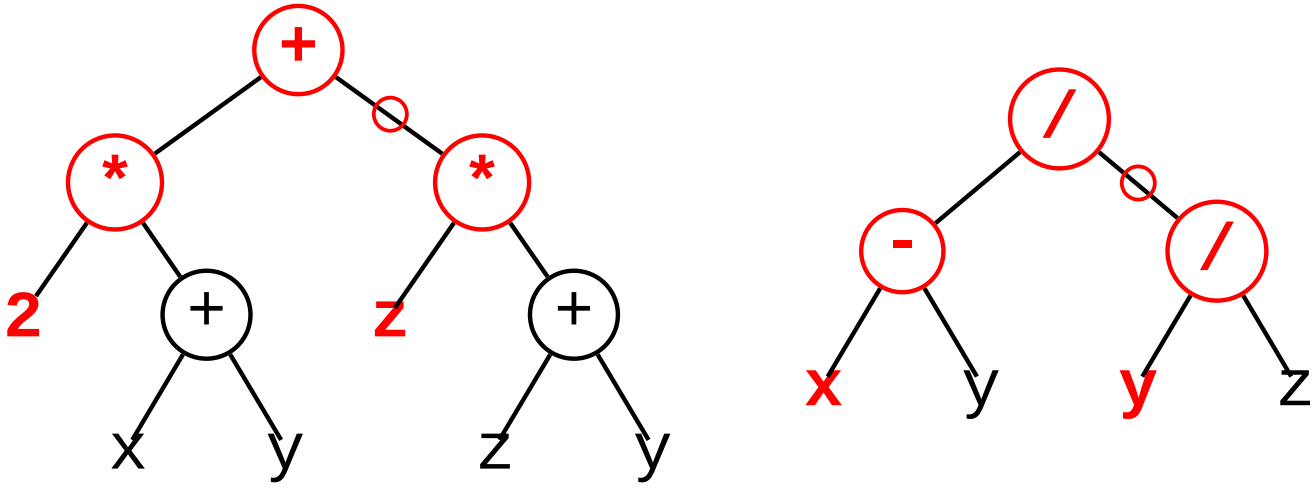


- Align the two parents
- Identify the region which is struct. common
- Choose a x-over pt from within that region
- Perform subtree crossover at that point

# Poli-Langdon Theorem (pess, 1-pt x-over)

$$E[m(s,t+1)] \geq n \cdot \underbrace{p(s,t)}_{\text{selection}} \underbrace{(1-p_m)^{O(s)}}_{\text{mutation}}$$

$$\left\{1 - p_c \left[p_{diff}(t)(1 - p(G(s),t) + \frac{L(s)}{N(s)}(p(G(s),t) - p(s,t))\right]\right\}$$

- Pessimistic ST for 1-pt crossover using any selection

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**"Exact" in what sense?**

Because it is possible to predict with a known certainty whether $m(s,t+1)$ will be above a certain threshold, the expectation operator can be removed from the theorem.

# Transmission Probability

- Want to know $\alpha(s,t)$:
  - The probability that at generation $t$, individuals produced via genetic operators (including selection & cloning) will be in schema $s$.
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- But assuming we knew it, if parents are selected independently...

# Transmission Probability

- Want to know $\alpha(s,t)$:
  - The probability that at generation $t$, individuals produced via genetic operators (including selection & cloning) will be in schema $s$.
  - $\alpha(s,t) = Pr[s \text{ survives}] + Pr[s \text{ constructed}]$
- $\alpha(s,t)$ can be quite difficult to elcit
- But assuming we knew it, if parents are selected independently...

**Then $m(s,t)$ is binomially distributed!**

$$\therefore \quad Pr[m(s,t+1)] = \binom{n}{k} \alpha(s,t)^k \left(1-\alpha(s,t)\right)^{n-k}$$

# Distribution of $m(s,t+1)$

- Now we can compute expectation and variance exactly:
  - $E[m(s,t+1)] = n \cdot \alpha(s,t)$
  - $Var[m(s,t+1)] = n \cdot \alpha(s,t)\ (1-\alpha(s,t))$
- Now we can compute a probabilistic ST:
  - Using Chebyshev's inequality & some algebra
  - $Pr\left[m(s,t+1) > n\alpha(s,t) - k\sqrt{n\alpha(s,t)(1-\alpha(s,t))}\right] \geq 1 - \frac{1}{k^2}$

    for any given constant $k$
  - Now have a relationship between the bounding condition and accuracy of the prediction

# Stephens & Waelbroeck's ST

- Exact ST for GAs with fixed-length binary representations
- One-point crossover (no mutation)

$$\alpha(s,t) = (1-p_c)p(s,t) + \frac{p_c}{l-1}\sum_{i=1}^{l-1} p\left(L(s,i),t\right)\ p\left(R(s,i),t\right)$$

where:

$L(s,i)$ replaces right $(i+1)\ldots l$ positions with "*"

$R(s,i)$ replaces left $1\ldots i$ positions with "*"

# Fixed Size/Shape GP ST

- All programs have same size and shape
- One-point GP crossover

$$\alpha(s,t) = (1-p_c)p(s,t) + \frac{p_c}{N(s)} \sum_{i=1}^{N(s)-1} p\left(l(s,i),t\right)\ p\left(u(s,i),t\right)$$

where:

$N(s)$ is number of nodes in schema $s$

$l(s,i)$ repl all nodes above x-over pt $i$ with "=" nodes

$u(s,i)$ repl all nodes below x-over pt $i$ with "=" nodes

# Hyperschemata

- Set of functions is denoted, $\mathcal{F}$
- Set of terminals is denoted, $\mathcal{T}$
- The "=" symbol is "don't care" for a *single* function or terminal
- The "#" symbol is "don't care" for any *valid subtree*
- Schema $s$ is a rooted tree composed of:
  - Internal nodes from $\mathcal{F} \cup \{=\}$
  - Leaf nodes from $\mathcal{T} \cup \{=, \#\}$

# Hyperschema Example

**For example:** $\mathcal{F} \in \{+,-,*,/\}, \mathcal{T} \in \{1,\ldots,9,x,y,z\}$

```
(+ (* 2 (+ x y)) (/ y z))
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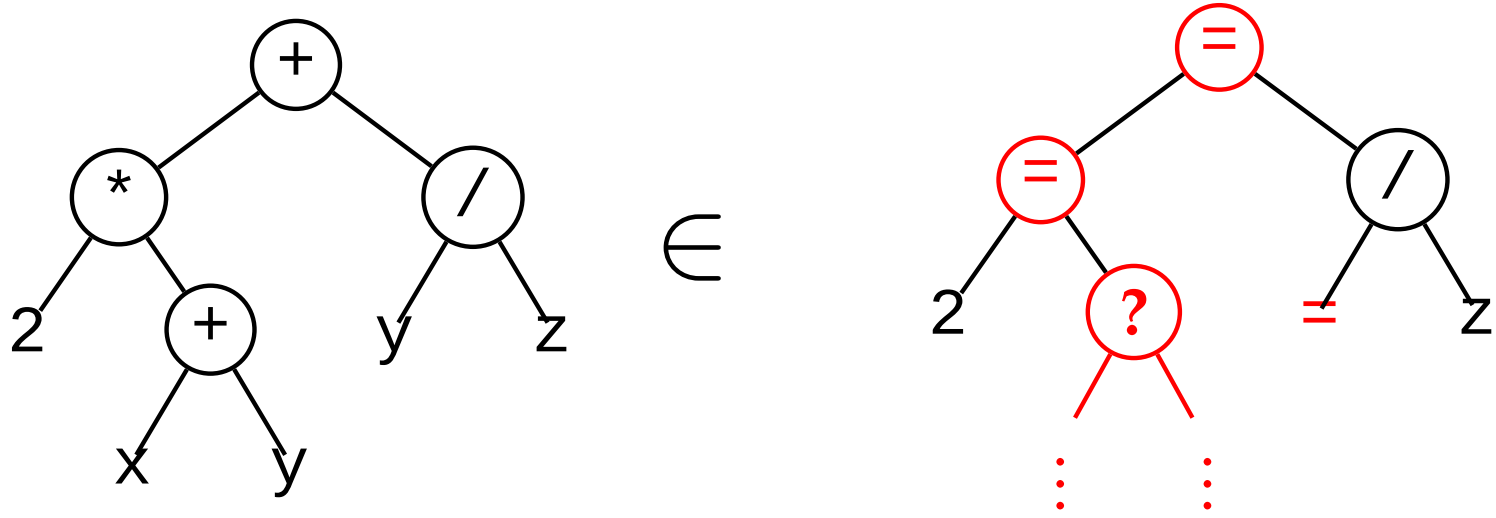

# Hyperschemata Notation/Measures

Let's now denote a member of $P_t$ as $v_i$

- No. nodes in tree fragment rep. common region b/w programs $v_1$ and $v_2$ is $NC(v_1, v_2)$
- Set of indices of crossover points in common region is $C(v_1, v_2)$
- Durak delta function, $\delta(x) = 1$ if x is true, and 0 otherwise
- $L(s, i)$ is hyperschema obtained by replacing all nodes on path between x-over pt. $i$ and root node with "=" nodes and all subtrees connected to those nodes with "#"
- $U(s, i)$ is hyperschema obtained by replacing all nodes below x-over pt. $i$ with "#" node

# Microscopic Exact GP ST

- Valid for populations of programs of any size and shape
- Generalization of Rosca's & P/L schemata (hence "hyper")
- One-point crossover, no mutation
- "Microscopic" since it must consider in detail each member of the population

$$\alpha(s,t) = (1-p_c)\,p(s,t) + p_c \sum_{v_1} \sum_{v_2} \frac{p(v_1,t)p(v_2,t)}{NC(v_1,v_2)} \sum_{i \in C(v_1,v_2)} \delta(v_1 \in L(s,i))\delta(v_2 \in U(s,i))$$

Where first two sums are over all individuals in the population.

# Advantages of Macroscopic ST

- Way of "course-graining" the right-hand side
  - Do not have to consider each individual in population
  - Mainly we are interested in *average properties*
- Becomes a proper generalization of all ST so-far described
  - Holland's ST
  - Stephens & Waelbroeck's ST
  - Poli-Langdon's fixed size & shape ST
  - Poli-Langdon's microscopic exact ST

# Macroscopic Exact GP ST

- $G_i$ represents all possible schemata of order 0 of the $i^{th}$ fixed size & shape.
- Enumerating all fixed size & shape order 0 schemata, $G_1, G_2, \ldots$, we cover the entire search space
- One-point crossover, no mutation

$$\alpha(s,t) = (1-p_c)\,p(s,t) +$$
$$p_c \sum_j \sum_k \frac{1}{NC(G_j,G_k)} \sum_{i \in C(G_j,G_k)} p\left(L(s,i) \cap G_j, t\right) p\left(R(s,i) \cap G_k, t\right)$$

# Other Macroscopic GP ST

- Homologous crossover
- Node-invariant subtree-crossing crossover
- ∴ Standard crossover
- Linear, length-only ST:
  - Homologous crossover
  - Headless chicken crossover
  - Subtree mutation crossover

# GP and the Building Block Hypothesis

- O'Reilly (1995) suggests crossover too destructive, so no BBH for GP
- Langdon & Poli (for 1-pt crossover) suggest otherwise:
  - $L(s.i) \cap G_j$ and $U(s.i) \cap G_k$ behave like GA BBs
  - GP really builds solutions via construction of lower order BBs
  - But GP BBs do not have to be above average fitness, short, or even of particularly low order

# Outline of Discussion

| | | |
|---|---|---|
| Part I: | Overview of Schema Theory | $\surd$ |
| Part II: | Pessimistic Schema Theory | $\surd$ |
| Part III: | Exact Schema Theory | $\surd$ |
| Part IV: | Conclusions | $\leftarrow$ |

# Traditional versus Exact Schema Theory

| **Traditional** | **Exact** |
|---|---|
| GA/Binary representation | Main focus has been in GP |
| Fixed length rep. | Variable length rep. |
| ”Pessimistic” inequality provides lower bound on expectation | Uses equality, so correctly predicts the expectation |
| | Can compute probability of expectation |

# Riccardo Poli's View of GP ST

- Compatibility with existing theory
  - GP Schema Theory is a superset of GA Schema Theory

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- Framework for est. specialized theorems
  - There is no "correct" schema theorem, it depends on the context of the question
    Must find the right level of granularity
  - Different operators lead to different ST
- Valid and useful tool for researchers
  - The meaning of GP building blocks is clearer
  - Exact GP ST can help (and has helped) guide designers to create better representations, operators, and algorithms
  - Can tell (and has told) us useful things about how GP works...

# What *has* ST told us?

- Prediction:
  - Local estimations for schema propagation
  - Local estimations of average fitness improvement
  - Rank operators for given fitness function (derive Price's theorem)
- Explanation:
  - Understand *why* certain things happen (formally):
    - When algorithms behave differently for different initial populations
    - Rate changes of different selection operators
    - Why (and how) GP adds/removes individuals from a schema
  - Understand operator bias: ★
    - When mutation and recombination have creation/survival advantages over one another in GAs. (Spears, 2000)
    - Linear, 1-pt crossover is unbiased w.r.t. program length. (McPhee, 2001)
    - Standard crossover is biased toward longer programs, but in which primitives are uniformly distributed in quantity and position (generalized Geiringer's theorm). (Poli, 2002)
    - Combining operators *may* arrest growth from standard crossover (model validation studies). McPhee, 2002)

# What ST *hasn't* told us?

- How to build the perfect EA to solve problems of some particular problem class
- What kind of long term behaviors can we expect from our EAs
- Whether or not EAs (nearly) converge to (near) optimal solutions and under what contexts
- How long we can expect to wait for an EA to converge
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  (Omnipotence, Telepathy)

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