Massachusetts Institute of Technology

Genetic Programming

A Tutorial Introduction

Una-May O'Reilly, Erik Hemberg
The ALFA Group: AnyScale Learning for All
CSAIL, MIT
unamay@csail.mit.edu, hembergerik@csail.mit.edu
http://groups.csail.mit.edu/ALFA

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Instructor: Una-May O'Reilly

- Leader: AnyScale Learning For All Group, MIT CSAIL
- Experience solving real world, complex problems requiring **AI/machine learning** where **evolutionary computation** is a core capability
- Applications include
  - Cybersecurity
  - Waveform data mining – medical applications
  - Behavioral data mining – MOOC
  - Circuits, network coding
  - Sparse matrix data mapping on parallel architectures
  - Finance
  - Flavor design
  - Wind energy
    - Turbine layout
    - Resource assessment
- Focus on innovation in genetic programming
  - coevolution
  - Improving its competence
  - Program synthesis

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Instructor: Erik Hemberg

- Research Scientist: AnyScale Learning For All Group, MIT CSAIL
- Experience solving complex problems requiring **AI and machine learning** with **evolutionary computation** as a core capability, Bronze HUMIE 2018
- Applications include
  - Cybersecurity
  - Behavioral data mining – MOOC
  - Pylon design
  - Network controllers
  - Tax avoidance
- Focus on innovation and implementation in genetic programming
  - Grammatical representation
  - Coevolution
  - Estimation of Distribution

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About You

- EA experience?
  - ES? GA? EDA? PSO? ACO? EP?
- CS experience?
- Programming? algorithms?
- Teacher?
- Native English speakers?

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Tutorial Goals

- Introduction to GP algorithm, given some knowledge of genetic algorithms or evolutionary strategies
  - provide Black box demonstration of GP symbolic regression
- Become familiar with GP design properties and recognize them
  - ponygp in python
- You could teach it in an undergrad lecture
- Use it "out of the box"
- Set groundwork for advanced topics
  - Theory, other tutorials
  - Specialized workshops (Genetic improvement etc)
  - GP Track talks at GECCO, Proceedings of EuroGP, Genetic Programming and Evolvable Machines

Agenda

1. Context: Evolutionary Computation and Evolutionary Algorithms
2. GP is the genetic evolution of executable expressions
   - Black box example of GP symbolic regression
3. Nuts and Bolts Description of Algorithm Components
4. pony_gp.py demonstration from project PonyGP
5. Resources and reference material

Neo-Darwinian Evolution

- Survival and thriving in the environment
- Offspring quantity - based on survival of the fittest
- Offspring variation: genetic crossover and mutation
- Population-based adaptation over generations
- Genotype-phenotype duality
- Complex and non-deterministic

EA Generation Loop

Each generation

- **select**
- **breed**
- **replace**

```
population = random_pop_init()
generation = 0
while needToStop == false
    generation++
    solution = bestOf(population)
    phenotypes =decoder(genotypes)
    calculateFitness(phenotypes)
    parents = select (phenotypes)
    offspring = breed(parents.genotypes)
    population = replace(parents, offspring)
    recheck(needToStop)
```

Problem Domains where EAs are Used

- Where there is need for complex solutions
  - evolution is a process that gives rise to complexity
  - a continually evolving, adapting process, potentially with changing environment from which emerges modularity, hierarchy, complex behavior and complex system relationships
- Combinatorial optimization
  - NP-complete and/or poorly scaling solutions via LP or convex optimization
  - unyielding to approximations (SQP, GEO-P)
  - eg. TSP, graph coloring, bin-packing, flows
  - for: logistics, planning, scheduling, networks, bio gene knockouts
  - Typified by discrete variables
  - Solved by Genetic Algorithm (GA)

Problem Domains where EAs are Used

- Continuous Optimization
  - non-differentiable, discontinuous, multi-modal, large scale objective functions 'black box'
  - applications: engineering, mechanical, material, physics
  - Typified by continuous variables
  - Solved by Evolutionary Strategy (ES)
- Program Search
  - program as s/w system component, design, strategy, model
  - common: system identification aka symbolic regression, modeling
  - Symbolic regression is a form of supervised machine learning
    - GP offers some unsupervised ML techniques as well
      - Clustering
  - will show a blackbox GP example soon
    - http://flexgp.github.io/gp-learners/sr.html
    - http://flexgp.github.io/gp-learners/blog.html

EA Individual Examples

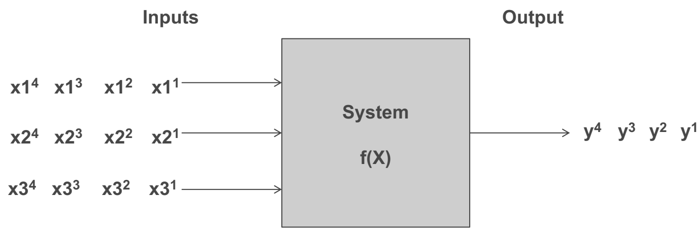
Problem	Gene	Genome	Phenotype	Fitness Function
TSP	110	sequence of cities	tour	tour length
Function optimization	3.21	variables $\underline{x}$ of function	f($\underline{x}$)	|min-f($\underline{x}$)|
graph k-coloring	permutation element	sequence for greedy coloring	coloring	# of colors
investment strategy	rule	agent rule set	trading strategy	portfolio change
Regress data	Executable sub-expression	Executable expression	model	Model error on training set (L1, L2)

Blackbox Example of GP Symbolic Regression

http://flexgp.github.io/gp-learners/sr.html
http://flexgp.github.io/gp-learners/blog.html

S/W by ALFA Group's FlexGP team
Special recognition to Ignacio Arnaldo, PhD who prepared SR Learner tutorial and blog post

Regression



AKA
Explanatory variables
Independent variables
Manipulated variables
Control variables
Decision variables
Features

Response variable
Dependent variable
Label

GOAL: FIND F(X) THAT GENERATES Y

Regression

- Regress a relationship between a set of explanatory variables and a response variable
- Linear regression:
  - Assume linear model: y=ax+b
  - Optimize parameters (a,b) so data best fits model
- Logistic regression for classification
  - Maps linear model into sigmoid family

$$F(x) = \frac{1}{1+e^{-(\beta_0+\beta_1 x)}}$$

- Symbolic regression does NOT assume a model
  - Not parameter search
  - Model is intrinsic in GP solutions

FlexGP's SR Learner

- Targeted partly to be black-box for non-researchers
- sr.jar is available for download
  - Only supported for Debian linux
  - Source is on
    - http://flexgp.github.io
- functionality both for performing Symbolic regression on numerical datasets and for testing the retrieved models
- Referred to as our baseline in time-aligned ALFA group publications
  - Bring Your Own Learner! A cloud-based, data-parallel commons for machine learning, Ignacio Arnaldo, Kalyan Veeramachaneni, Andrew Song, Una-May O'Reilly. IEEE Computational Intelligence Magazine. Special Issue on Computational Intelligence for Cloud Computing (Feb. 2015), Vol 10, Issue 1, pp 20-32.
  - Multiple regression genetic programming, Ignacio Arnaldo, Krzysztof Krawiec, Una-May O'Reilly, GECCO '14, pp 879--886.
- Option to accelerate runs with C++ optimized execution
  - Requires gcc and g++ compilers, configuring Linux kernel parameter governing the maximum size of shared memory segments
- Option to accelerate runs with CUDA (GPU)
  - Added requirement of nvcc compiler
  - append the *-cuda* flag, make some extra directories…
- Easy parameter changing through a central file

DEMONSTRATION

- http://flexgp.csail.mit.edu -> LEARNERS
- http://flexgp.github.io/gp-learners/sr.html INSTRUCTIONS
- http://flexgp.github.io/gp-learners/blog.html EXAMPLE

Agenda

HOW DOES IT WORK UNDER THE HOOD?

WHAT IS THIS EXECUTABLE EXPRESSION?

Koza's Executable Expressions

Pioneered circa 1988

- Lisp S-Expressions
  - Composed of primitives called 'functions' and 'terminals'
  - Aka operators and variables/operands

Example:

- primitives: + - * div a b c d 4
- (*(- (+ 4 c) b) (div d a))

In a Lisp interpreter:

1. bind a b c and d
2. Evaluate expressions

```
% Lisp interpreter
(set! a 2) -> 2
(set! b 4) -> 4
(set! c 6) -> 6
(set! d 8) -> 8
(*(- (+ 4 c) b) (div d a)) -> 12
; Rule Example
(if (= a b) c d) -> 8
;Predicate:
(> c d) -> nil
```


A Lisp GP system

A Lisp GP system is a large set of functions which are interpreted by evaluating the entry function

- Some are definitions of primitives you write!
  - » (defun protectedDivide ...)
- Rest is software logic for evolutionary algorithms

Any GP system has a set of functions that are pre-defined (by compilation or interpretation) for use as primitives also has software logic that handles

- Population initialization, iteration, selection, breeding, replacement, fitness evalution*

GP expressions are first class objects in LISP so the GP software logic can manipulate them as data/variables as well as have the interpreter read and evaluate them

Expressions are data and are executed

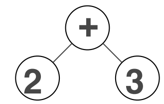
How to Evaluation an Expression

- interpreter beneath your code
  - Lisp example
- interpreter within your code
  - typical,
  - examples: SR.jar or ponygp.py
- compile then execute on your OS
  - older system in existence

How to Manipulate Expressions as Data

- for Crossover and Mutation we want
  - offspring can be different size and structure than parents
  - syntactic correctness
  - randomness in replication and variation
- GP solution
  - reference the parse tree
  - XO - swap subtrees between trees of parents
  - Mutation: insert, subst or delete from a parse tree (PT)
- A picture tells a 1000 words…

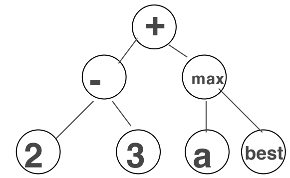
Parse Trees



Inorder: 2+3

preorder: + 2 3

Post-order: 2 3 +



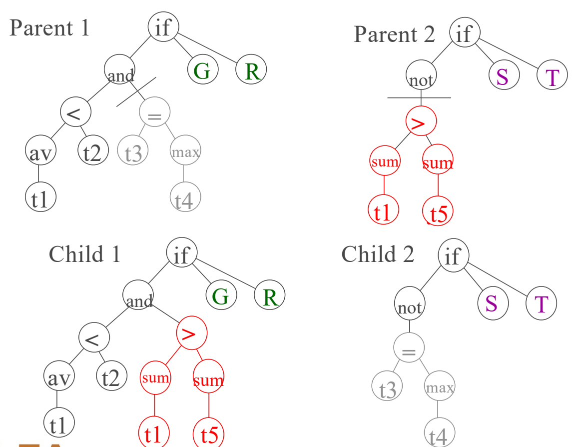
Inorder: (2-3) + (a max best)

preorder: (+ (-2 3) (max a best))

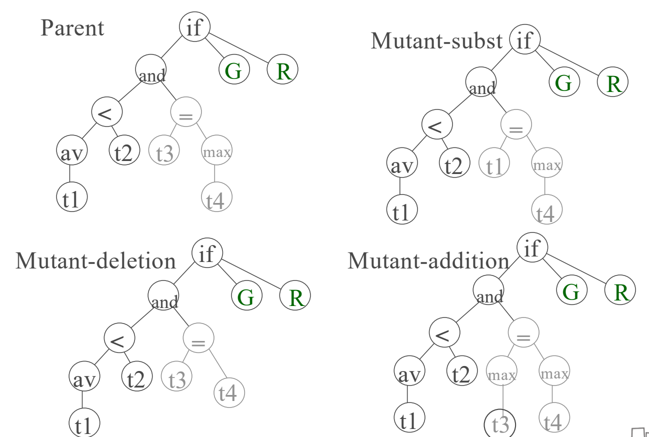
Post-order: (2 3 -) (a best max) +)

- Whether parsed preorder (node, left-child, right-child) or postorder (left-child, right-child, node) or inorder (left, node, right) the expression evaluates to the same result
- (tree)GP uses an expression tree as its genotype structure

GP Tree Crossover



HVL-Mutation: substitution, deletion, insertion



GP Preparatory Steps

Assume we have a GP system with internal expression evaluator.

1. Decide upon functions and terminals
   – Terminals bind to decision variables in problem
   – Combinatorial expression space defines the search space
2. Set up the fitness function
   – Translation of problem goal to GP goal
   – Minimization of error between desired and evolved expression when executed
   – Maximization of a problem based score
   – Construct test cases for program (input examples, desired output)
3. Decide upon run parameters
   – Population size is most important
   – GP is robust to many other parameter choices
4. Determine a halt criteria and result to be returned
   – Maximum number of fitness evaluations
   – Time
   – Minimum acceptable error
   – Good enough solution (satisficing)

Top Level GP Algorithm

```
Begin
    pop = random programs from a  set of operators and operands
    repeat
        execute each program in pop with each set of inputs
        measure each program's fitness
        repeat
            select 2 parents
            copy 2 offspring from parents
                crossover
                mutate
            add to new-pop
        until pop-size
    pop = new-pop
    until max-generation
        or
      adequate program found
End
```


Population Initialization

- Fill population with random expressions
  – Create a function set Φ and a corresponding argument-count set
  – Create an terminal set (arg-count = 0), T
  – draw from Φ with replacement and recursively enumerate its argument list by additional draws from Φ U T.
  – Recursion ends at draw of a terminal
  – requires closure and/or typing
- maximum tree height parameter
  – At max-height-1, draw from T only
- "ramped half-half" method ensures diversity
  – equal quantities of trees of each height
  – half of height's trees are full
    » For full tree, only draw from terminals at max-height-1

Selection in GP

- Proceeds in same manner as evolutionary algorithm
  – Same set of methods
  – Conventionally use tournament selection
  – Also see fitness proportional selection
  – Cartesian genetic programming:
    » One parent: generate 5 children by mutation
    » Keep best of parents and children and repeat
      ▪ If parent fitness = child fitness, keep child

Determining a Expression's Fitness

- One test case:
  - Execute the expression with the problem decision variables (ie terminals) bound to some test value and with side effect values initialized
  - Designate the "result" of the expression
- Measure the error between the correct output values for the inputs and the result of the expression
  - Final output may be side effect variables, or return value of expression
  - Eg. Examine expression result and expected result for regression
  - Eg. the heuristic in a compilation, run the binary with different inputs and measure how fast they ran.
  - EG, Configure a circuit from the genome, test the circuit with an input signal and measure response vs desired response
- Usually have more than one test case but cannot enumerate them all
  - Use rational design to create incrementally more difficult test cases
  - Use class balanced data for classification

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Details When Using Executable Expressions

- Closure
  - Design functions with wrappers that accept any type of argument
  - Often types will semantically clash…need to have a way of dealing with this

Practicality/Solution Feasibility

- Sufficiency
  - Make sure a correct solution can be plausibly expressed when choosing your primitive set
    - » Functions must be wisely chosen but not too complex
    - » General primitives: arithmetic, boolean, condition, iteration, assignment
    - » Problem specific primitives
  - Can you handcode a naïve solution?
  - Balance flexibility with search space size

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Tree Crossover Details

- Crossover point in each parent is picked at random
- Conventional practices
  - All nodes with equal probability
  - leaf nodes chosen with 0.1 probility and non-leaf with 0.9 probability
- Probability of crossover
  - Typically 0.9
- Maximum depth of child is a run parameter
  - Typically ~ 15
  - Can be size instead

Crossover Properties

- Two identical parents rarely produce offspring that are identical to them
- Tree-crossover produces great variations in offspring with respect to parents
- Crossover, in addition to preserving syntax, allows expressions to vary in length and structure (sub-expression nesting)

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GP Tree Mutation

- Often only crossover is used
- But crossover behaves often like macro-mutation
- Mutation can be better tuned to control the size of the change
- A few different versions

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Other Sorts of Tree Mutation

- Koza:
  - Randomly remove a sub-tree and replace it
  - Permute: mix up order of args to operator
  - Edit: + 1 3 -> 4, and(t t) -> t
  - Encapsulate: name a sub-tree, make it one node and allow re-use by others (protection from crossover)
    - » Developed into advanced GP concept known as
      - Automatic module definition
      - Automatically defined functions (ADFs)
- Make your own
  - Could even be problem dependent (what does a subtree do? Change according to its behavior)

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Top Level GP Algorithm

Begin

pop = random programs from a set of operators and operands

repeat

execute each program in pop with each set of inputs

measure each program's fitness

repeat

select 2 parents

copy 2 offspring from parents

crossover

mutate

add to new-pop

until pop-size

pop = new-pop

until max-generation

or

adequate program found

End

Grow or Full

Ramped-half-half

Max-init-tree-height

•Tournament selection
•Fitness proportional selection
•Your favorite selection

Tournament size

Prepare input data
Designate solution
Define error between actual and expected

•HVL-mutate
•Subtree subst
•Permute
•Edit
•Your own

Mutation probs

Sub-tree crossover

Prob to crossover

Max-tree-height

Leaf:node bias

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GP Parameters

- Population size
- Number of generations
- Max-height of trees on random initialization
  - Typically 6
- Probability of crossover
  - Higher than mutation
  - 0.9
  - Rest of offspring are copied
- Probability of mutation
  - Probabilities of addition, deletion and insertion
- Population initialization method
  - Ramped-half-half
  - All full
  - All non-full
- Selection method
  - Elitism?
- Termination criteria
- Fitness function
- what is used as "solution" of expression

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GP Software Deep Dive

- flexgp.csail.mit.edu
- http://flexgp.github.io/gp-learners/

Basic:

- https://flexgp.github.io/pony_gp/
- https://github.com/flexgp/pony_gp

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PonyGP: Simple Symbolic Regression

- Given a set of independent decision variables and corresponding values for a dependent variable
- Want: a model that predicts the dependent variable
  - Eg: linear model with numerical coefficients
    - » Y= aX1 + bX2 + c(X1X2)
  - Eg: non-linear model
    - » y= a x1^2 + bx2^3
  - Prediction accuracy: minimum error between model prediction and actual samples
- Usually: designer provides a model and a regression (ordinary least squares, Fourier series) determines coefficients
- With genetic programming, the model (structure) and the coefficients can be learned

- Test problem:
  - f(x)=(X0 * X0) + (X1 * X1)
- Domain of X0 and X1 [-5.0,5.0]
- Choose the 4 operands (terminals)
  - X0, X1, 1.0, 0
- Choose the 4 operators (functions)
  - +, - , *, / (protected)
  - protected divide: if denom==0, return numerator
- Fitness function: sum of mean squared error between y_i, and expression's return values
- Prepare 121 randomized points for testing
- Out of sample training:testing ratio is 70:30, random selection of points as training or test

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GP Examples

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Agenda

Context: Evolutionary Computation and Evolutionary Algorithms

1. GP is the genetic evolution of executable expressions
2. Nuts and Bolts Descriptions of Algorithm Components
3. Resources and reference material

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Agenda

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Reference Material

Online Material
- http://geneticprogramming.com/

Where to search for conference and journal publications
- Genetic Programming Bibiliography
  - https://liinwww.ira.uka.de/bibliography/Ai/genetic.programming.html

Digital Libraries
- ACM digital library: http://portal.acm.org/
  - GECCO conferences
  - GP conferences (pre GECCO),
- IEEE digital library: http://www.computer.org/portal/web/csdl/home
  - Congress on Evolutionary Computation (CEC)
- Springer digital library: http://www.springerlink.com/
  - European Conference on Genetic Programming: "EuroGP"

JOURNALS
- Evolutionary Computation Journal (MIT Press)
- Genetic Programming and Evolvable Machines Journal (Springer)
- ACM Transactions on Evolutionary Learning and Optimization (ACM)
- IEEE Transactions on Evolutionary Computation

Software
- https://github.com/search?q=genetic+programming

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Genetic Programming Benchmarks

Genetic programming needs better benchmarks
- James McDermott, David R. White, Sean Luke, Luca Manzoni, Mauro Castelli, Leonardo Vanneschi, Wojciech Ja´skowski, Krzysztof Krawiec, Robin Harper, Kenneth De Jong, and Una-May O'Reilly.
- In Proceedings of GECCO 2012, Philadelphia, 2012. ACM.

- **Related benchmarks wiki**
  - http://GPBenchmarks.org

- **GP Program Synthesis Benchmarks**
  - http://thelmuth.github.io/GECCO_2015_Benchmarks_Materials/
  - Thomas Helmuth, Lee Spector

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Software Packages for Symbolic Regression

No Source code available

- Datamodeler - mathematica, Evolved Analytics
- Eureqa II/ Formulize - a software tool for detecting equations and hidden mathematical relationships in data
  - http://creativemachines.cornell.edu/eureqa
  - Plugins to Matlab, mathematica, Python
  - Convenient format for data presentation
  - Standalone or grid resource usage
  - Windows, Linux or Mac
  - http://www.nutonian.com/ for cloud version
- Discipulus™ 5 Genetic Programming Predictive Modelling

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Reference Material - Books

- Genetic Programming, James McDermott and Una-May O'Reilly, In the Handbook of Computational Intelligence, Topic Editors: Dr. F. Neumann and Dr. K Witt, Editors in Chief Prof. Janusz Kacprzyk and Prof. Witold Pedrycz.
- Essentials of Metaheuristics, Sean Luke, 2010
- Genetic Programming: From Theory to Practice
  - 10 years of workshop proceedings, on SpringerLink, edited
- A Field Guide to Genetic Programming, Poli, Langdon, McPhee, 2008, Lulu and online digitally
- Advances in Genetic Programming
  - 3 years, each in different volume, edited
- John R. Koza
  - Genetic Programming: On the Programming of Computers by Means of Natural Selection, 1992 (MIT Press)
  - Genetic Programming II: Automatic Discovery of Reusable Programs, 1994 (MIT Press)
  - Genetic Programming III: Darwinian Invention and Problem Solving, 1999 with Forrest H Bennett III, David Andre, and Martin A. Keane, (Morgan Kaufmann)
  - Genetic Programming IV: Routine Human-Competitive Machine Intelligence, 2003 with Martin A. Keane, Matthew J. Streeter, William Mydlowec, Jessen Yu, and Guido Lanza
- Linear genetic programming, Markus Brameier, Wolfgang Banzhaf, Springer (2007)
- Genetic Programming: An Introduction, Banzhaf, Nordin, Keller, Francone, 1997 (Morgan Kaufmann)

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