Combining Geometric Semantic GP with Gradient-descent optimization

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Outline

- Introduction
- Gradient Descent GSGP
 - Geometric Semantic Genetic Programming
 - The ADAM algorithm
 - GSGP hybridized with GD
- Experimental Settings
- Results
- Conclusion and future directions



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<u>IDEA</u>: <u>combine</u> GSGP with a well-known gradient-based optimizer, *Adam*, in order to leverage:

- the ability of **GSGP** to operate structural changes of the individuals
- the ability of gradient-based methods to optimize the parameters of a given structure.



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Geometric Semantic GP

improve the performance of GP



integration of **semantic awareness** in the evolutionary
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Geometric Semantic Genetic Programming (GSGP)

GSGP is an evolutionary technique originating from GP that directly searches the semantic space of the programs

Geometric Semantic Operators

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Geometric Semantic Crossover (GSC)

Given two parents functions $T_1, T_2 : \mathbb{R}^n \to \mathbb{R}$, **GSC** generates the real function

$$T_{XO} = (T_1 \cdot T_R) + ((1 - T_R) \cdot T_2)$$

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Geometric Semantic Mutation (GSM)

Given a parent function $T:\mathbb{R}^n \to \mathbb{R}$, **GSM** generates the real functions

$$T_M = T + ms \cdot (T_{R1} - T_{R2})$$

where T_{R1} and T_{R2} are random real functions whose output range in the interval [0,1] and ms is a parameter called mutation step.

The Adam Algorithm

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- efficient
- easy to implement
- little memory usage for its execution
- well suited for problems dealing with a vast amount of data and/or parameter



The Adam Algorithm

Algorithm 1 Pseudocode of the *Adam* algorithm.

Require: $f(\theta), \ \theta_0, \ N, \ \alpha, \ \beta_1 \in [0, 1), \ \beta_2 \in [0, 1), \ \epsilon$

```
1: m_0 \leftarrow 0
 2: v_0 \leftarrow 0
 3: for i = 0 \cdots N do
            d_{i+1} \leftarrow \nabla_{\theta} f_{i+1}(\theta_i)
 4:

    □ gradient of stochastic function f

 5:
             m_{i+1} \leftarrow \beta_1 \cdot m_i + (1 - \beta_2) \cdot d_{i+1}
                                                                                       update first moment estimates
             v_{i+1} \leftarrow \beta_2 \cdot v_i + (1 - \beta_2) \cdot d_{i+1}^2
\bar{m}_{i+1} \leftarrow m_{i+1}/(1 - \beta_1^{i+1})
 6:

    □ update second moment estimates

                                                                                  contrast intrinsic initialization bias
             \bar{v}_{i+1} \leftarrow v_{i+1}/(1-\beta_2^{i+1})
 8:
                                                                                  contrast intrinsic initialization bias
             \theta_{i+1} \leftarrow \theta_i - \alpha \cdot \bar{m}_{i+1} / (\bar{v}_{i+1})
 9:
                                                                                                          update parameters
10: end for
```

WHY?

Geometric Semantic GP

- Allows big jump on the solutions space
- New areas of the solution space can be explored

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Good jump in promising areas of the solution space (GSGP) and subsequent refinement of the solution (ADAM).

HOW?

let's consider an equivalent definition for GSOs:

- 1. **GSM**: $T_M = T + ms \cdot (R_1 R_2)$, where $0 \le m \le 1$
- 2. GSC: $T_{XO} = (T_1 \cdot \alpha) + ((1 \alpha) \cdot T_2)$, where $0 \le \alpha \le 1$

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where T, T_1 and T_2 are the parent function; R_1 and R_2 are random real functions whose output range in [0,1].

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- generate initial random population of functions
- perform evolutionary steps (GSM + GSC)
- obtain $T=(T_1,T_2,\cdots,T_N)$ new population, composed of derivable functions
- apply Adam optimizer:
 - 1. objective function $f(\theta) \to \text{the generation considered } T$
 - 2. parameter vector $\rightarrow \theta = (\alpha, \beta = (1 \alpha), ms)$

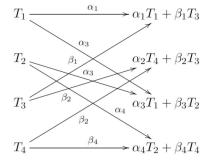


A practical example



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- initial random pop T_1, T_2, T_3, T_4
- only crossover operator
- 1. 4 new individuals created as linear combination of previous generations through parameters α_i and β_i $(i=1,\ldots,4)$
- 2. perform Adam optimization to update parameters α_i and β_i $(i=1,\ldots,4)$



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- 2. **HeH-GSGP**: (Half et Half Geometric Semantic Genetic Programming) initially, all the GSGP genetic steps are performed, followed by an equal number of Adam optimizer steps.

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Dataset

Have been considered and tested dataset:

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Dataset	Variables	Instances	Area	Task
%F	242	359	Pharmacokinetic	Regression
LD50	627	234	Pharmacokinetic	Regression
%PPB	627	131	Pharmacokinetic	Regression
yac	7	308	Physics	Regression
slump	10	102	Physics	Regression
conc	9	1030	Physics	Regression
air	6	1503	Physics	Regression



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- Total number of fitness evaluations must be equal for every method considered (200).
- 100 runs for each problem.
- 70:30 training-test partition.

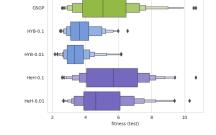


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Slump



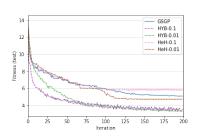
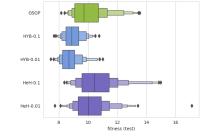


Figure: Boxplots of testing RMSE and median of the fitness over epochs obtained over 100 independent runs for **slump** problems.

Concrete



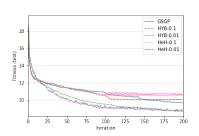
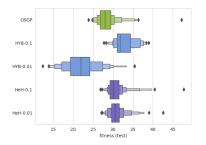


Figure: Boxplots of testing RMSE and median of the fitness over epochs obtained over 100 independent runs for **concrete** problems.

Airfoil



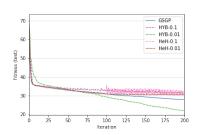


Figure: Boxplots of testing RMSE and median of the fitness over epochs obtained over 100 independent runs for **airfoil** problems.

Results

		GSGP	HYB-0.1	HYB-0.01	HeH-0.1	HeH-0.01
%F	Train	38.08	37.74	36.80	39.61	40.60
	Test	40.15	40.48	39.61	40.85	41.23
LD50	Train	2118.00	2086.56	2128.22	2144.27	2161.00
	Test	2214.78	2203.25	2229.87	2221.72	2215.09
%PPB	Train	30.15	27.00	24.32	34.79	33.26
	Test	328.1	401.43	263.81	213.86	235.53
yac	Train	11.83	11.92	12.48	12.28	12.31
	Test	11.92	11.83	12.52	12.38	12.48
slump	Train	4.56	3.47	2.92	5.19	4.41
	Test	5.08	3.63	3.32	5.77	4.76
conc	Train	9.62	8.86	8.50	10.59	10.05
	Test	9.65	8.88	8.69	10.47	10.07
air	Train	27.76	31.54	21.98	30.37	30.46
	Test	27.94	31.71	21.97	30.15	30.53

Table: Training and testing fitness (RMSE) for the considered benchmark problems. **Bold** font indicates the best results.



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Future work:

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Future work:

- to consider a different kind of crossover where more than 2 parents are involved to get a structure more similar to a neural network one.
- to test this technique considering other optimizer.

thanks for your attention!!