Non-negative Matrix Factorization for Derivation of Search Objectives in GP

Paweł Liskowski   Krzysztof Krawiec

Computational Intelligence Group
Institute of Computing Science
Poznan University of Technology, Poland

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Fitness Evaluation

Observation 1

GP algorithms do not let programs know **which** tests they solve.

Typical fitness function in GP *aggregates* program's behavior on *tests* by

- counting the number of passed tests (discrete domains).

$$f(p) = |\{y_i \neq \hat{y}_i(p)\}|_i \tag{1}$$

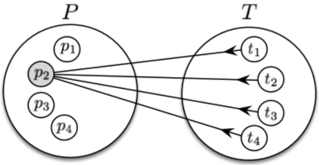
- summing the errors on individual tests (continuous domains).

$$f(p) = \sum_i (y_i - \hat{y}_i(p))^2 \tag{2}$$

Test-based Genetic Programming

Observation 2

Detailed information on particular interactions **is available** in GP.



$$g : P \times T \rightarrow [0, 1]$$

G	t_1	t_2	t_3	t_4
p_1	1	1	0	0
p_2	0	1	0	1
p_3	1	1	1	0
p_4	0	1	1	0

- P: set of m programs,
- T: set of n tests (fitness cases)
- $g(p, t)$: interaction function between $p \in P$ and $t \in T$
- G: $m \times n$ matrix of interaction outcomes between P and T
- Test-based problems (Pollack, Bucci, de Jong, Popovici)

Fitness Evaluation

Observation 3

Interaction outcomes for particular tests are *partially* dependent.

Can be used to **estimate** program-test interactions in G:

- Surrogate Fitness via Factorization of Interaction Matrix (*SFIMX*) (Liskowski & Krawiec, EuroGP 2016)

Fitness Evaluation

Observation 3

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Hypothesis

- $g(p, t)$ can be *explained* by decomposition into a set of **factors**,
- These factors can be used as **search drivers**.

The idea

Use **matrix factorization** to extract the factors from patterns in G.

Non-negative matrix factorization (NMF)

Given G, find W and H such that

$$G \approx WH \;\; s.t. \;\; W, H \geq 0,$$

or more precisely:

$$\underset{W,H}{min}\, f(W,H) \equiv \frac{1}{2}||G - WH||_F^2 \;\; s.t. \;\; W, H \geq 0,$$

- Effective, gradient-based algorithms exist (e.g., multiplicative update rule).
- Intensely used in machine learning (recommender systems, Netflix contest)

NMF: Example 1

$$G = \begin{array}{c c} & \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{array}{c} p_1 \\ p_2 \\ p_3 \end{array} & \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \end{array}$$

$$W \times H = \begin{array}{c c} & \begin{array}{cc} f_1 & f_2 \end{array} \\ \begin{array}{c} p_1 \\ p_2 \\ p_3 \end{array} & \begin{pmatrix} 0.70 & 2.05 \\ 0.73 & 0.66 \\ 0.35 & 1.02 \end{pmatrix} \end{array} \times \begin{array}{c c} & \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{array}{c} f_1 \\ f_2 \end{array} & \begin{pmatrix} 0.70 & 0.70 & 2.70 & 2.70 \\ 0.74 & 0.74 & 0.06 & 0.06 \end{pmatrix} \end{array}$$

NMF: Example 2

$$G' = \begin{array}{c c} & \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{array}{c} p_1 \\ p_2 \\ p_3 \end{array} & \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ \color{blue}{2} & 1 & 1 & 1 \end{pmatrix} \end{array}$$

$$W' = \begin{array}{c c} & \begin{array}{cc} f_1 & f_2 \end{array} \\ \begin{array}{c} p_1 \\ p_2 \\ p_3 \end{array} & \begin{pmatrix} 0.96 & 1.51 \\ 0.39 & 1.84 \\ 0.86 & 0.38 \end{pmatrix} \end{array}, \quad H' = \begin{array}{c c} & \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{array}{c} f_1 \\ f_2 \end{array} & \begin{pmatrix} 2.16 & 1.20 & 0.72 & 0.72 \\ 0.05 & 0.35 & 0.90 & 0.90 \end{pmatrix} \end{array}$$

$$W' \times H' = \begin{array}{c c} & \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{array}{c} p_1 \\ p_2 \\ p_3 \end{array} & \begin{pmatrix} 2.17 & 1.70 & 2.07 & 2.07 \\ 0.95 & 1.13 & 1.96 & 1.96 \\ 1.88 & 1.17 & 0.97 & 0.97 \end{pmatrix} \end{array}$$

DOF: Discovery of Search **O**bjectives by **F**actorization

Algorithm

1. Calculate $m \times n$ interaction matrix G between P and T,
2. Factorize G into non-negative components W and H,
3. Define the derived objectives f'_j based on W and H,
4. Use f'_js for multiobjective evaluation/selection.

Two variants:

- DOF-W: $f_j(p) = w_{pj}$
- DOF-WH: $f_j(p) = w_{pj} \sum_{t \in T} h_{jt}$

The matrix G can be **sparse** (see Liskowski & Krawiec, EuroGP 2016)

- $\alpha \in (0, 1]$ - density of partial interaction matrix

Example

Example: $P = \{s_1, s_2, s_3\}$, $T = \{t_1, \dots, t_4\}$

$$G = \begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \end{array} \xrightarrow[rank(G)=2]{NMF \quad k=2} W \times H = \begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cc} f_1 & f_2 \end{array} \\ \begin{pmatrix} 0.70 & 2.05 \\ 0.73 & 0.66 \\ 0.35 & 1.02 \end{pmatrix} \end{array} \times \begin{array}{c} \\ f_1 \\ f_2 \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{pmatrix} 0.70 & 0.70 & 2.70 & 2.70 \\ 0.74 & 0.74 & 0.06 & 0.06 \end{pmatrix} \end{array}$$

$p_1 \succ p_2, \quad p_2 \succ p_3, \quad p_1 \succ p_3$

$p_1 \succ p_3$

	s_1	s_2	s_3
fitness:	4	2	0
ranking:	1	2	3

	s_1	s_2	s_3
ranking f_1	2	1	3
ranking f_2	1	3	2
average ranking	1.5	2	2.5

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$$G' = \begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ 2 & 1 & 1 & 1 \end{pmatrix} \end{array} \xrightarrow[rank(G)=3]{NMF \quad k=2} W' \times H' = \begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{pmatrix} 2.17 & 1.70 & 2.07 & 2.07 \\ 0.95 & 1.13 & 1.96 & 1.96 \\ 1.88 & 1.17 & 0.97 & 0.97 \end{pmatrix} \end{array}$$

$$= \begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cc} f_1 & f_2 \end{array} \\ \begin{pmatrix} 0.96 & 1.51 \\ 0.39 & 1.84 \\ 0.86 & 0.38 \end{pmatrix} \end{array} \times \begin{array}{c} \\ f_1 \\ f_2 \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & t_3 & t_4 \end{array} \\ \begin{pmatrix} 2.16 & 1.20 & 0.72 & 0.72 \\ 0.05 & 0.35 & 0.90 & 0.90 \end{pmatrix} \end{array}$$

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	s_1	s_2	s_3
fitness:	4	2	1
ranking:	1	2	3

$$\begin{array}{c} \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} \begin{array}{cc} f'_1 & f'_2 \end{array} \\ \begin{pmatrix} 4.61 & 3.22 \\ 1.87 & 4.05 \\ 4.13 & 0.84 \end{pmatrix} \end{array}$$

	s_1	s_2	s_3
ranking f'_1	1	3	2
ranking f'_2	2	1	3
average ranking	1.5	2	2.5

Experiment

- GP: 'vanila' GP, $|P| = 1000$
- DOF: Derived Objectives via Factorization
  - $\mathrm{DOF\text{-}W}$: derived objectives taken directly from W
  - $\mathrm{DOF\text{-}WH}$: weights features in H by program's factors in W
  - $|P|$ increased $(1 - \alpha)$ times $\implies$ same budget
  - Multiobjective selection: NSGA-II (Deb et al. 2002)
- DOC: Discovery of Objectives by Clustering
- $k \in 2, 3$ $\alpha \in 0.4, 0.6, \ldots, 1.0$

Domain	Instruction set	Problem	Variables	#tests
Boolean	and, nand or, nor	Cmp6	6	64
		Cmp8	8	256
		Par5	5	32
		Mux6	6	64
		Maj6	6	64
Algebras	$a_i(x, y)$	Disc-a1...a5	3	27
	$a_i(x, y)$	Malcev-a1...a5	3	15

Experiment

Average ranks on success rate (Friedman's $p \ll 0.001$)

	DOF		DOC	GP
	W	WH		
All problems	1.97	2.03	2.9	3.10
Boolean	2.4	2.6	3.15	4.4
Categorical	1.90	1.75	2.5	4.25

- Best results for DOF-W and DOF-WH,
- Pays off to derive objectives based on both W and H,
- High compression of G without affecting the performance
  - Interaction outcomes are indeed correlated.
- Low k $\rightarrow$ low computational overhead of factorization
  - only 6% of the total cost of $1,000|T|$ interactions

Conclusions

- A way to multiobjectivize GP,
- Applicable beyond GP:
  - Evolving controllers, two-player games, image analysis, ...
- Works with sparse interaction marices,
- Computationally efficient,
- Promising results for symbolic regression.

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Thank You