The Road to VEGAS: Guiding the Search over Neutral Networks

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Motivations

• Fitness landscapes
  • To analyze the structure of the search space
  • Understanding the problem structure to design efficient search methods

• Many combinatorial optimization problems involve neutrality (robot controller, planning problem, learning problem, protein folding...)

• Can we and how to exploit this neutrality?
Motivations

- **Fitness landscapes**
  - To analyze the structure of the search space
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- Many combinatorial optimization problems involve **neutrality** (robot controller, planning problem, learning problem, protein folding...)

- Can we and how to exploit this neutrality?
Objectives

- How to exploit neutrality?
- How to guide the search adaptively over a neutral network?
- What is Exploration / Exploitation tradeoff of neutral networks?

→ VEGAS: Varying Evolvability Guided Adaptive Search
**Fitness Landscape**

\( \text{FiL} (S, N, f) \)

- **S** \hspace{1cm} \text{Search space}
  - all feasible solutions

- **N : S → 2^S** \hspace{1cm} \text{Neighborhood relation}
  - \( N(s) : \text{neighborhood, } s' \in N(s) \): neighbor of \( s \)

- **f : S → R** \hspace{1cm} \text{Evaluation function}
  - Fitness values assigned to solution

*local optima, ruggedness, etc.*
Neutrality properties

- **Neutral Network (NN) - Plateau**
  - Connected sub-graph
    - Vertices: equivalent solutions (same fitness value)
    - Edges: Neighborhood structure

- **Degree of neutrality**
  - Number of neighbors with the same fitness value
  \[
  \mathcal{N}_n(s) = \{ s' \in \mathcal{N}(s) \mid f(s') = f(s) \}
  \]

- **Portal (exit solution)**
  - Solution from NN with at least one improving neighbor
Guiding the search on NN

- How to guide the search?
  - Consider all solutions with the same fitness
  - Estimate the evolvability of solutions
  - Select the most promising solution
Estimate Evolvability

Altenberg: the ability of random variations to sometimes produce improvement

Existing measures of evolvability:
- Average, max fitness values from the neighborhood
- Probability to increase
- Neutral degree...

Our approach
- Inspired by the « Area Under Curve » (AUC) scheme used for operator selection
- Neighborhood sampling

Altenberg, L.: The evolution of evolvability in genetic programming. In Kinnear, Jr., K.E., ed.: Advances in Genetic Programming. MIT Press (1994) 47–74

Álvaro Fialho, Marc Schoenauer and Michele Sebag. Toward Comparison-based Adaptive Operator Selection. In J. Branke et al., eds.: "GECCO'10: Proc. 12th Annual Conference on Genetic and Evolutionary Computation", ACM Press: p. 767-774. July 2010
Estimate Evolvability

Fitness

| Fitness | Solution |
|---------|----------|
| 14      | S1       |
| 13      | S1       |
| 12      | S2       |
| 11      | S2       |
| 9       | S1       |
| 6       | S1       |
| 6       | S2       |
| 5       | S2       |
| 4       | S1       |

AUC(S1)=11.5
Select the most promising solution

- Exploration vs. exploitation
  - Multi-armed bandit
  - Upper Confidence Bound strategy (UCB)

\[
\arg \max_{i=1..K} \left( \hat{r}_{i,t} + C \sqrt{\frac{\log \sum_{k} n_{k,t}}{n_{i,t}}} \right)
\]

- \( K \) : number of arms
- \( \hat{r}_{i} \) : credit of arm \( i \)
- \( n_{i} \) : number of applications of arm \( i \)
- \( C \) : controls the trade-off (exploitation vs. exploration)

Álvaro Fialho, Marc Schoenauer and Michele Sebag. *Toward Comparison-based Adaptive Operator Selection*. In J. Branke et al., eds.: "GECCO'10: Proc. 12th Annual Conference on Genetic and Evolutionary Computation", ACM Press: p. 767-774. July 2010
Select the most promising solution

\[ \arg \max_{i=1..K} \left( \hat{r}_{i,t} + C \sqrt{\frac{\log \sum_k n_{k,t}}{n_{i,t}}} \right) \]

At iteration \( t \):

\( \rightarrow \) Arms = sampling from NN

\( K \): sample size

\( \rightarrow \) Credit assignement based on evolvability

\( \hat{r}_i \): AUC of solution \( i \)

\( \rightarrow \) Number of sampled neighbors

\( n_i \): evaluated neighbor

\( \rightarrow \) Exploitation / Exploration trade-off parameter

\( C \): small (exploitation), large (exploration)

Management of the NN sample:

• Add equivalent solutions
• Delete solutions when \( n_j = |N(s)| \)
VEGAS

$S = \{s_0\}$

WHILE $\exists s \in S$ such that $s$ is not visited do
  
  $s \leftarrow \text{select}(S)$
  
  Choose a solution $s' \in N(s)$ at random (no repetition)
  
  IF $f(s) < f(s')$ THEN
    
    $S \leftarrow \{s'\}$
  
  ELSE IF $f(s) = f(s')$ THEN
    
    $S \leftarrow S \cup \{s'\}$
  
  END IF
  
  Update $\text{rewards}(s, s')$

END WHILE

Return $s \in S$
NKq fitness landscapes

\[ f(x) = \frac{1}{N} \sum_{i=1}^{N} f_i (x_i, x_{i_1}, \ldots, x_{i_k}) \]

- \( N \) : length of the bit string, \( x_i \in \{0, 1\} \)
- \( K \leq N-1 \) number of interactions (epistasis, non-linearity)
- \( q \) number of possible values (neutral degree level)
- \( \{i_1, \ldots, i_K\} \subset \{1, \ldots, i-1, i+1, \ldots, N\} \)
- \( f_i : \{0, 1\}^{K+1} \rightarrow [0,q) \cap \mathbb{N} \) chosen at random

Newman, M. And Engelhardt R.: **Effect of neutral selection on the evolution of molecular species**, In Proc. R. Soc. London B, vol. 56, 1998, 1333-1338
Experimental design

• Test problems
  • NKq N=64, K∈{2,4,6,8}, q ∈{2,3,4}
• Neighborhood
  • 1 bit-flip
• Comparisons with
  • FIHC: First Improvement Hill-Climbing
  • NC: NetCrawler (HC which accepts if f(s) ≤ f(s’))
  • F2NS: Fair Neutral Network Search (Select = random)
• Parameters
  • Stopping criteria: max number of eval.  $10^5$
  • 100 experiments/algorithm
• VEGAS
  • $C \in \{10^{-4}, 10^{-3} \ldots 10^1, 10^2, 5.10^2\}$
Dynamics of compared methods

FIHC
- Without neutrality

NetCrawler
- With Neutrality
- NN sample size = 1

F2NS
- With Neutrality
- NN sample size > 1

VEGAS
- With Neutrality
- NN sample size > 1
- With Evolvability
Neutrality?
NN sample size > 1?
Evolvability?

K = 4

FIHC << NC
NC << F2NS, VEGAS
F2NS < VEGAS\textsubscript{100}

K = 8

Average Normalized Performance
Impact of parameter \( C \)

\( C \) controls the **Trade-off** Exploration vs. Exploitation?
- small \( C \) → Importance of evolvability = **Exploitation**
- high \( C \) → Towards less visited solutions = **Exploration**
Impact of neutrality

# NN Solutions evaluated on NN increases exponentially with neutral degree
Exploration vs Exploitation

$C > 1$ (exploration) $\rightarrow$ more NN are sampled, few evaluations on NN

$C < 1$ (exploitation) $\rightarrow$ few NN are sampled, more evaluations on NN
Conclusion

- Algorithm to exploit neutrality
- Adaptive balance exploration / exploitation of neutrality
- Evolvability-guided search

→ VEGAS
  - Multi-Armed Bandit
  - Evolvability
  - A single parameter to control the exploration and exploitation trade-off of NN

- Open issues
  - Other evolvability measures?
  - Flowshop scheduling?
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