The Road to VEGAS: Guiding the Search over Neutral Networks

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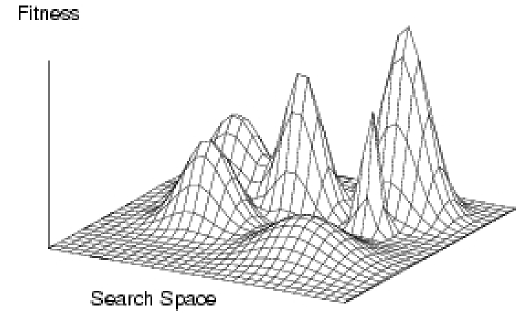
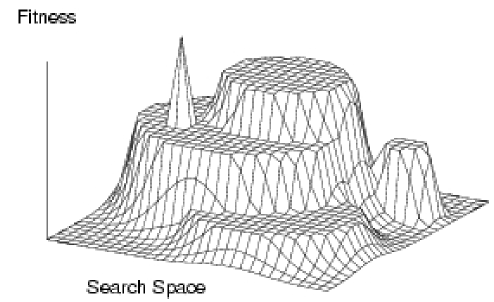
Motivations



- 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?



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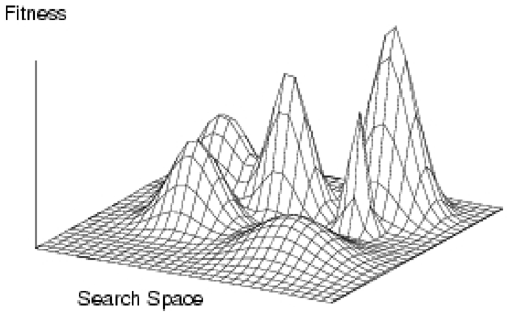

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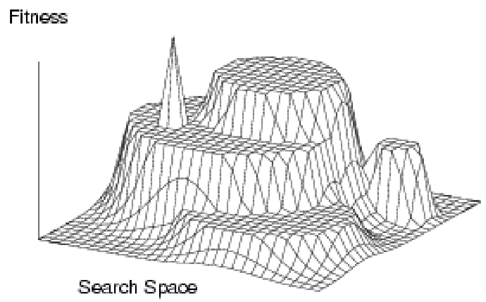
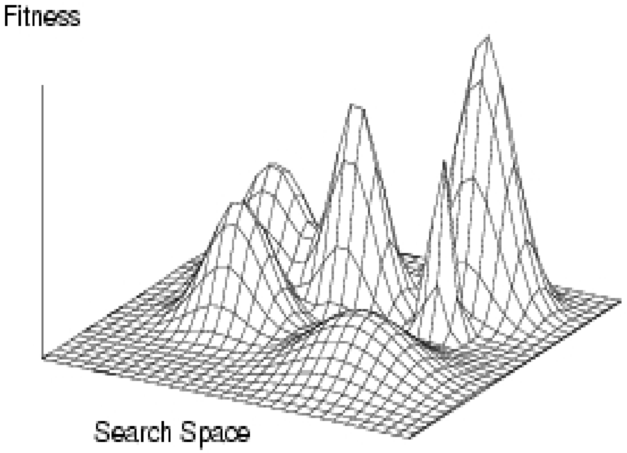


Objectives

- 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



<u>FiL</u> (S, N, f)

- S   Search space

  all feasible solutions

- $N : S \rightarrow 2^S$ Neighborhood relation

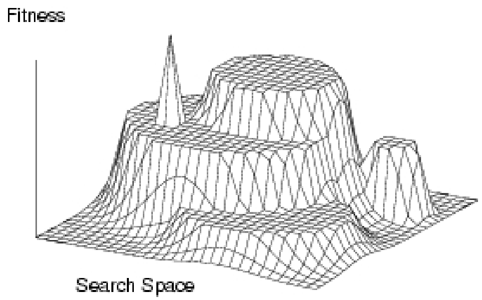
  N(s) : neighborhood, $s' \in N(s)$: neighbor of s

- $f : S \rightarrow R$ 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

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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 fitness values from the neighborhood
- Probability to increase
- Neutral degree…

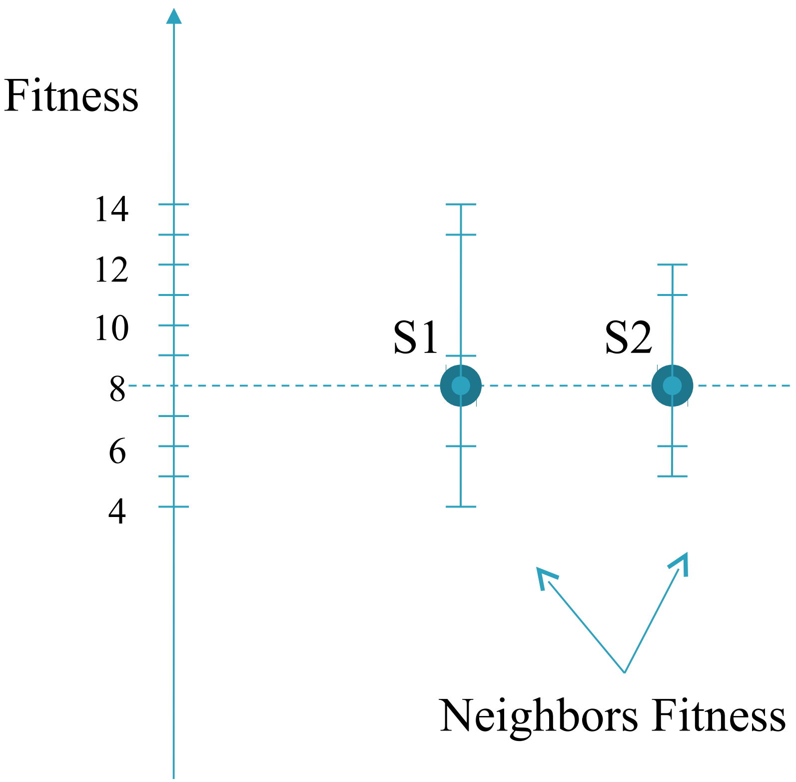
Our approach

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

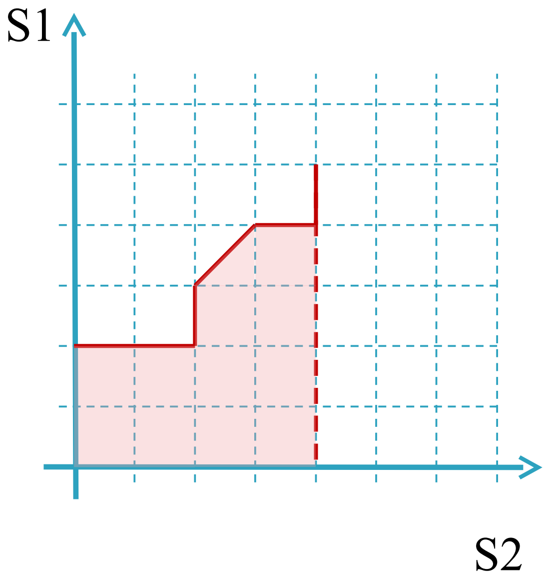
*Altenberg, L.: **The evolution of evolvability in genetic programming**. In Kinnear, Jr., K.E., ed. : Advances in Genetic Programming. MIT Press (1994) 47–74*

*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



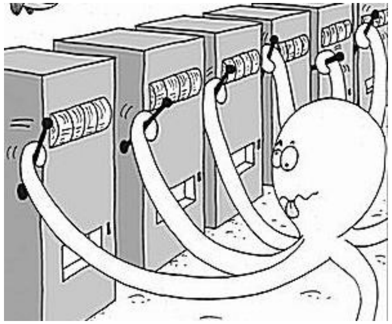
Fitness	Solution
14	S1
13	S1
12	S2
11	S2
9	S1
6	S1
6	S2
5	S2
4	S1



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 :

$\longrightarrow$ Arms = sampling from NN

K : sample size

$\longrightarrow$ Credit assignement based on evolvability

$\hat{r}_i$: AUC of solution i

$\longrightarrow$ Number of sampled neighbors

n_i : evaluated neighbor

$\longrightarrow$ Exploitation / Exploration trade-off parameter

C : small (exploitation), large (exploration)

Management of the NN sample:

- Add equivalent solutions
- Delete solutions when n_i = |N(s)|

VEGAS

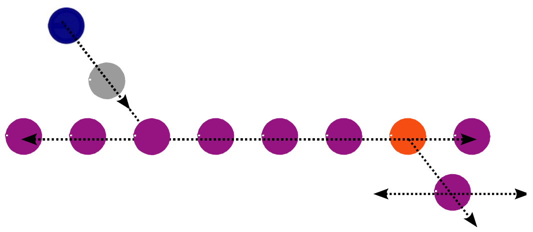
$S=\{s_0\}$

WHILE $\exists\ s \in S$ such that s is not visited do

- s ← **select(S)**
- Choose a solution $s' \in N(s)$ at random (no repetition)
- IF $f(s) < f(s')$ THEN
  - S ← {s'}
- ELSE IF $f(s)=f(s')$ THEN
  - $S \leftarrow S \cup \{s'\}$
- END IF
- Update **rewards(s,s')**

END WHILE

Return $s \in S$



NKq fitness landscapes

$$f(x) = \frac{1}{N} \sum_{i=1}^{N} f_i(x_i, x_{i1}, \ldots, x_{ik})$$

- N : length of the bit string, $x_i \in \{0, 1\}$
- $K \le N-1$ 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

$x_1 x_2 x_4$	f_1
000	2
001	1
010	0
011	0
...	...

$x_1 x_2 x_3$	f_2
000	1
001	2
010	2
011	0
...	...

$x_2 x_3 x_4$	f_3
000	2
...	...
101	0
110	1
111	1

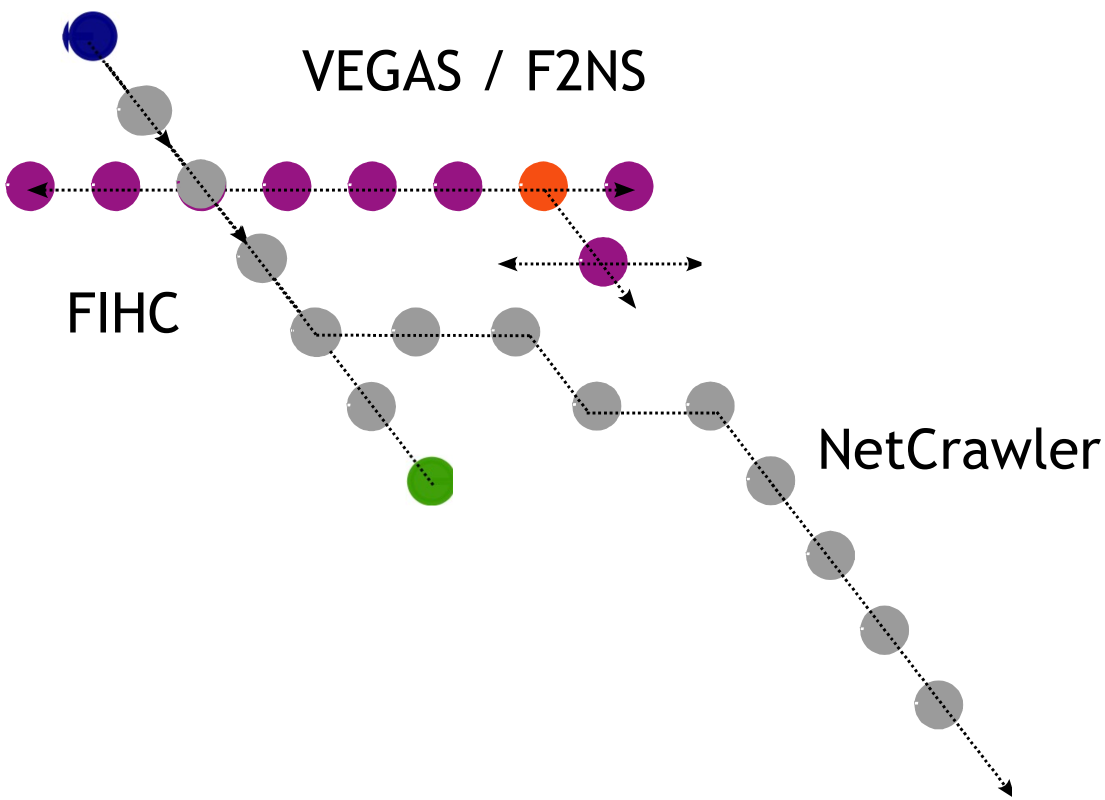
$x_1 x_2 x_4$	f_4
000	0
001	2
010	1
011	0
...	...

*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 $N=64$, $K \in \{2,4,6,8\}$, $q \in \{2,3,4\}$
- Neighborhood
  - 1 bit-flip
- Comparisons with
  - FIHC: First Improvment Hill-Climbing
  - NC: NetCrawler (HC which accepts if $f(s) \leq f(s')$)
  - 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



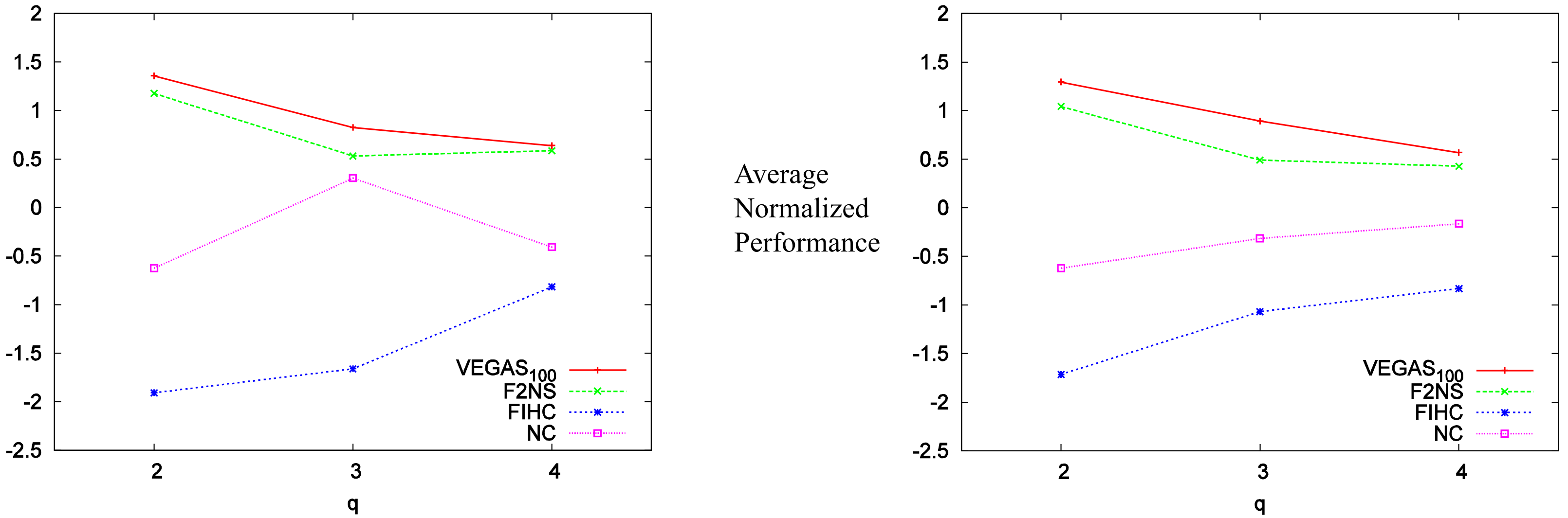
FIHC
- Without neutrality

NetCrawler
- With Neutrality
- NN sample size =1

F2NS
- With Neutrality
- NN sample size > 1

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

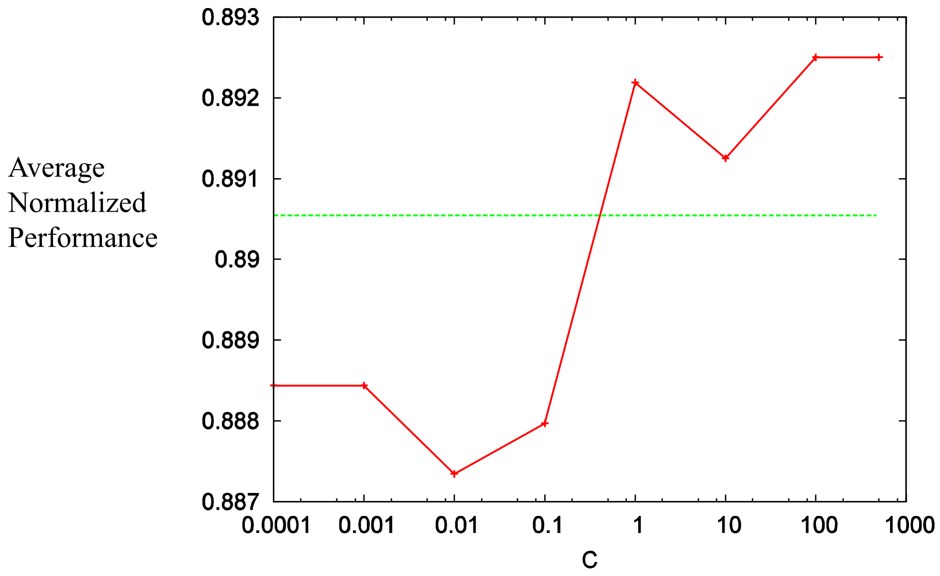
Performance

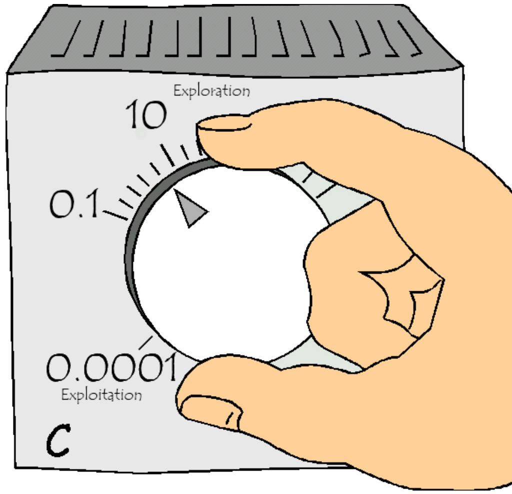


K = 4 K = 8

Neutrality ?	FIHC << NC
NN sample size > 1 ?	NC << F2NS, VEGAS
Evolvability ?	F2NS < $VEGAS_{100}$

Impact of parameter C



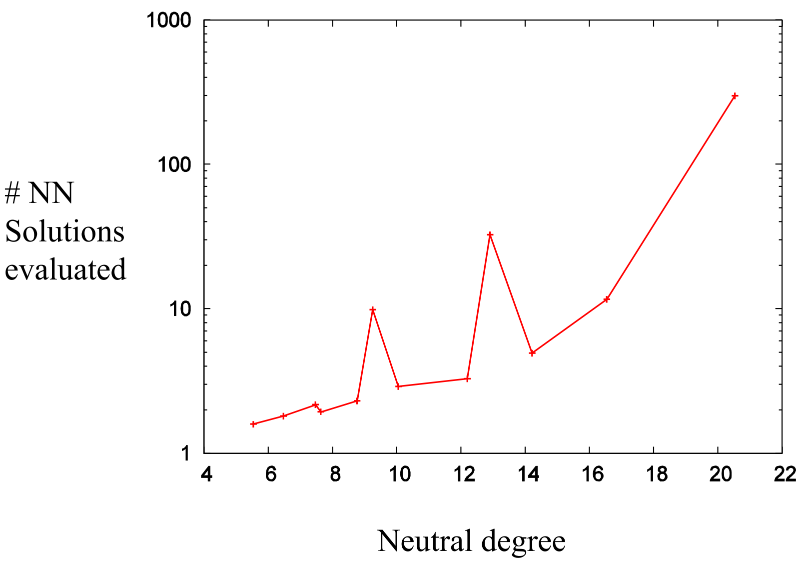


C controls the Trade-off Exploration *vs.* Exploitation?

small C → Importance of evolvability = Exploitation

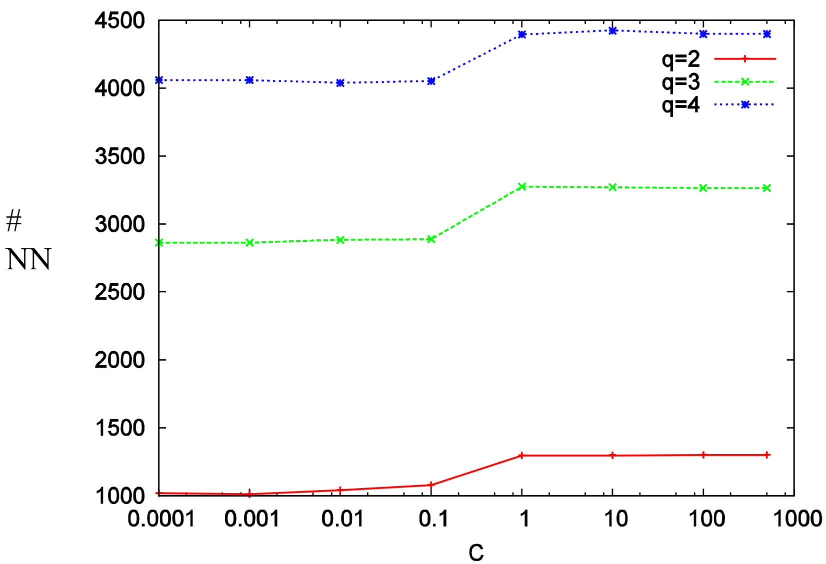
high C → Towards less visited solutions = Exploration

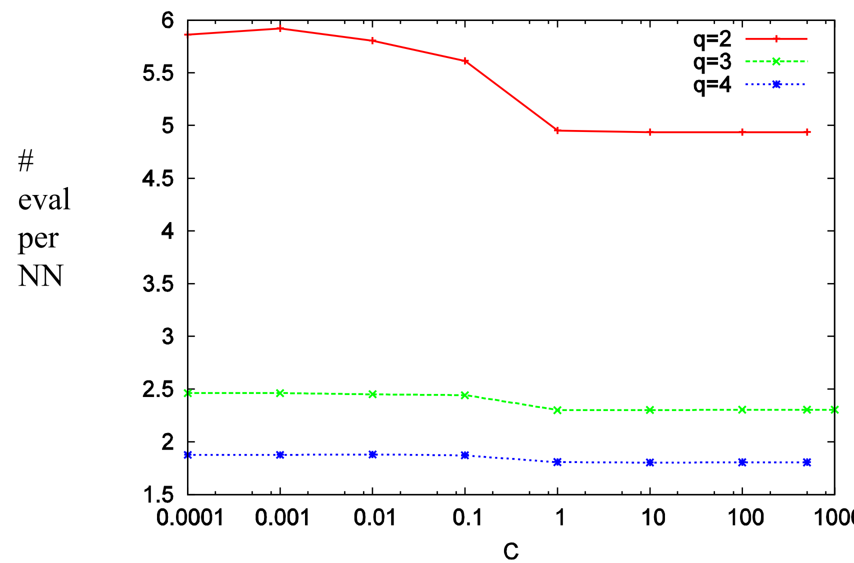
Impact of neutrality



NN Solutions evaluated on NN increases exponentially with neutral degree

Exploration vs Exploitation





C > 1(exploration) → more NN are sampled, few evaluations on NN

C < 1 (exploitation) → 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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