3. Local optima network

Fitness landscape analysis for understanding and designing local search heuristics

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Outline of this part

- Basis of fitness landscape :
  - introductory example *(Done)*
  - brief history and background of fitness landscape *(Done)*
  - fundamental definitions *(Done)*
- Geometries of fitness landscapes :
  - multimodality *(Done)*
  - ruggedness *(Done)*
  - neutrality *(Done)*
  - neutral networks *(Done)*
- **Local optima network** :
  - Definition inspired by complex systems science
  - Features of the network, design and performance
  - Performance prediction and portfolio

Join work

Gabriela Ochoa, University of Stirling, Scotland,
Marco Tomassini, University of Lausanne, Switzerland,
Fabio Daolio, University of Stirling, Scotland,

Key idea : Complex system tools

Principle of variables aggregation

A model for dynamical systems with two scales (time/space)

- Split the state space according to the different scales
- Study the system at the large scale

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$$X \xrightarrow{op} X$$

Variables aggregation for fitness landscape

- At solutions level (small scale) :
  - Stochastic local search operator,
  - Exponential number of solutions,
  - Exponential size of the stochastic matrix of the process (Markov chain)
- Projection on a relevant space :
  - Reduce the size of state space
  - Potentially loose some information
  - Relevant information remains when :

$$p(op(x)) \approx op^{'}(p(x))$$

Key idea : Complex system tools

Principle of variables aggregation

A model for dynamical systems with two scales (time/space)

- Split the state space according to the different scales
- Study the system at the large scale

$$\begin{array}{ccc} X & \xrightarrow{op} & X \\ \downarrow p & & \downarrow p \\ E & \xrightarrow{op'} & E \end{array}$$

Variables aggregation for fitness landscape

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    $$p(op(x)) \approx op'(p(x))$$

Key idea : Complex system tools

Complex network

Bring the tools of *complex networks* analysis to the study the structure of combinatorial fitness landscapes

Methodology

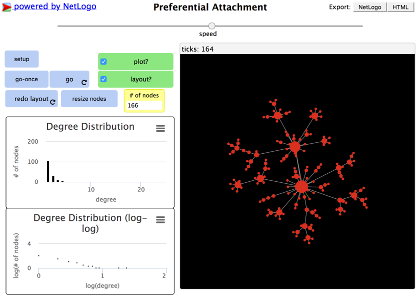
- **Design a network** that represents the landscape
  - Vertices : local optima
  - Edges : a notion of adjacency between local optima
- **Extract features** :
  "complex" network analysis
- **Use the network features** :
  search algorithm design, difficulty, etc.

J. P. K. Doye, The network topology of a potential energy landscape : a static scale-free network., *Phys. Rev. Lett.*, 88 :238701, 2002. [Doy02]

Complex networks

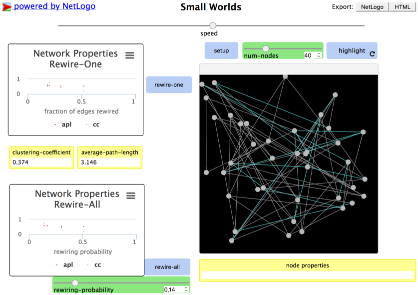
Scale free network

(Watts and Strogatz, 1998 [WS98])



Small world network

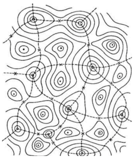
(Barabasi and Albert, 1999 [BA99])



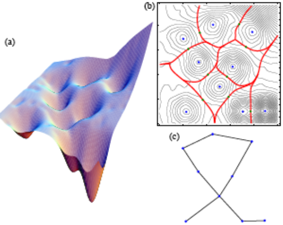
Energy surface and inherent networks

Inherent network

- **Nodes** : energy minima
- **Edges** : two nodes are connected if the energy barrier separating them is sufficiently low (transition state)



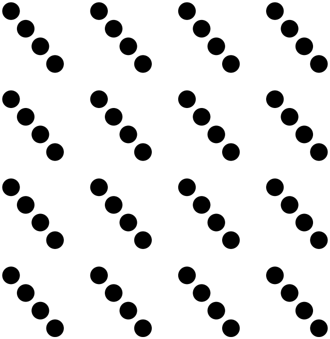
(a) Energy surface
(b) Contours plot :
partition of states space into basins of attraction
(c) Landscape as a network



F. H Stillinger, T. A Weber. Packing structures and transitions in liquids and solids. *Science*, 225.4666 , p. 983-9, 1984.[SW84]
J. P. K. Doye, The network topology of a potential energy landscape : a static scale-free network., *Phys. Rev. Lett.*, 88 :238701, 2002.[Doy02]

Basins of attraction in combinatorial optimization

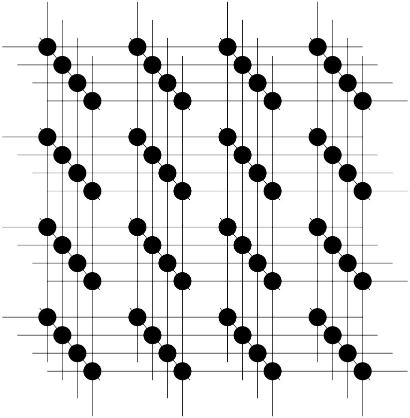
Example of small NK landscape with $N = 6$ and $K = 2$



- Bit strings of length $N = 6$
- $2^6 = 64$ solutions
- one point = one solution

Basins of attraction in combinatorial optimization

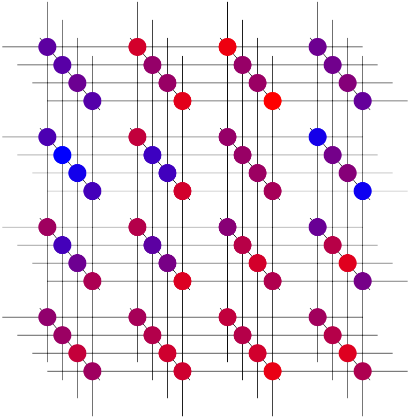
Example of small NK landscape with $N = 6$ and $K = 2$



- Bit strings of length $N = 6$
- Neighborhood size $= 6$
- Line between points $=$ solutions are neighbors
- Hamming distances between solutions are preserved (except for at the border of the cube)

Basins of attraction in combinatorial optimization

Example of small NK landscape with $N = 6$ and $K = 2$

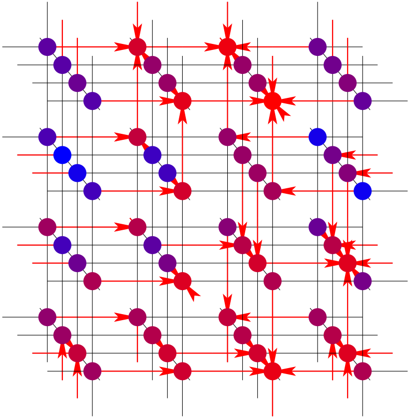


Color represent fitness value

- high fitness
- low fitness

Basins of attraction in combinatorial optimization

Example of small NK landscape with $N = 6$ and $K = 2$



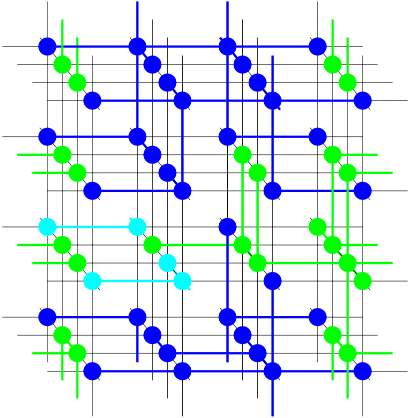
- Color represent fitness value
  - high fitness
  - low fitness
- → point towards the solution with highest fitness in the neighborhood

Exercise :

Why not make a Hill-Climbing walk on it ?

Basins of attraction in combinatorial optimization

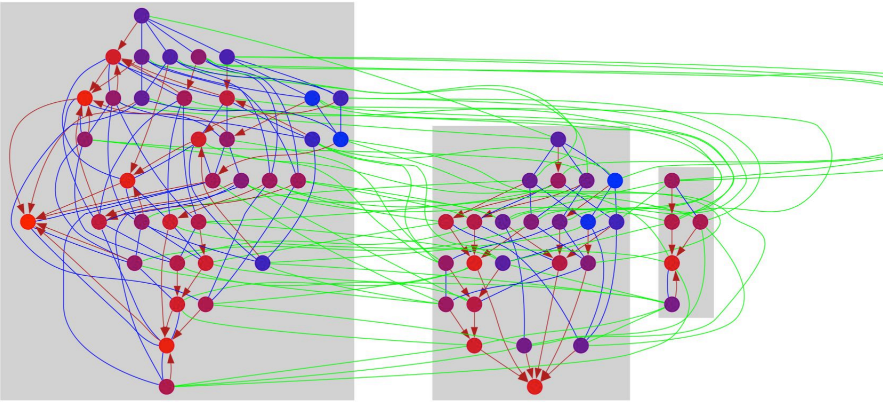
Example of small NK landscape with $N = 6$ and $K = 2$



- Each color corresponds to one basin of attraction
- Basins of attraction are interlinked and overlapped
- Basins have no "interior"

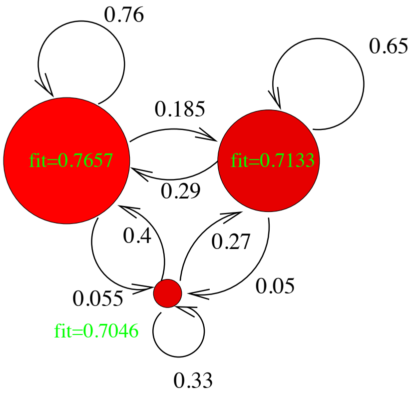
Basins of attraction in combinatorial optimization

Example of small NK landscape with $N = 6$ and $K = 2$



- Basins of attraction are interlinked and overlapped !
- Most neighbors of a given solution are outside its basin

Local optima network



- **Nodes** :
  local optima
- **Edges** :
  transition probabilities

Basin of attraction

Hill-Climbing algorithm (best-improvement)

Choose initial solution $x \in X$
repeat
  choose $x^{'} \in \mathcal{N}(x)$ such that $f(x^{'}) = max_{y \in \mathcal{N}(x)} \; f(y)$
  if $f(x) < f(x^{'})$ **then**
    $x \leftarrow x^{'}$
  end if
until x is a Local optimum

Basin of attraction of x^* :

$$b_{x^*} = \{x \in X \mid HillClimbing(x) = x^*\}.$$

local optima network

Definition : Local Optima Network (LON)

Orienter weighted graph (V, E, w)

- Notes V : set of local optima $\{LO_1, \ldots, LO_n\}$
- Edges E : notion of connectivity between local optima

local optima network

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2 possible definitions of edges

- **Basin-transition edges** :
  transition between random solutions from basin b_i to basin b_j
  ([OTVD08], [VOT08], [TVO08], [VOT10])
- **Escape edges** :
  transition from Local Optimum i to basin b_j
  (EA 2011, GECCO 2012, PPSN 2012, EA 2013 [DVOT13])

Basin-transition edges : random transition between basins

Edges

e_{ij} between LO_i and LO_j if $\exists\ x_i \in b_i$ and $x_j \in b_j : x_j \in \mathcal{N}(x_i)$

Prob. from solution x to solution $x^{'}$

$$p(x \rightarrow x^{'}) = \Pr(x^{'} = op(x))$$

Prob. from solution s to basin b_j

$$p(x \rightarrow b_j) = \sum_{x^{'} \in b_j} p(x \rightarrow x^{'})$$

Weights : Transition prob. from basin b_i to basin b_j

$$w_{ij} = p(b_i \rightarrow b_j) = \frac{1}{\sharp b_i} \sum_{x \in b_i} p(s \rightarrow b_j)$$

Basin-transition edges : random transition between basins

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Prob. from solution x to solution $x^{'}$

$$p(x \rightarrow x^{'}) = \Pr(x^{'} = op(x))$$

For example, $X = \{0,1\}^N$ and bit-flip operator
if $x^{'} \in \mathcal{N}(x)$, $p(x \rightarrow x^{'}) = \frac{1}{N}$, otherwise $p(x \rightarrow x^{'}) = 0$

Prob. from solution s to basin b_j

$$p(x \rightarrow b_j) = \sum_{x^{'} \in b_j} p(x \rightarrow x^{'})$$

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LON with Escape edges

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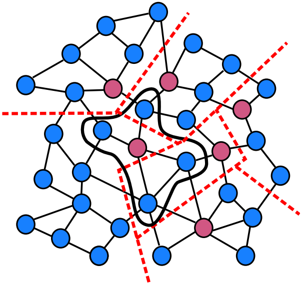
Escape edges

Edge e_{ij} between LO_i and LO_j
if $\exists x$: $distance(LO_i, x) \leqslant D$ and $x \in b_j$.

Weights

$w_{ij} = \sharp\{x \in X \mid d(LO_i, x) \leqslant D,\ x \in b_j\}$
can be normalized by the number of solutions at

distance D



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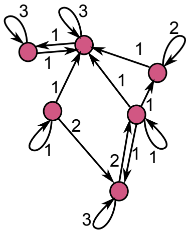


Basins of attraction features

- **Basin of attraction** :
  - Size :
    average, distribution, etc.
  - Fitness of local optima :
    average, distribution, correlation, etc.

NK-landscapes

[Kauffman 1993] [Kau93]

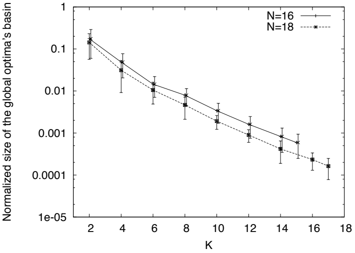
$$x \in \{0,1\}^n \qquad f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x_j, x_{i_1}, \ldots, x_{i_k})$$

Two parameters

- Problem size n
- Non-linearity k $<$ n
  (multi-modality, epistatic interactions)
  - $k = 0$: linear problem, one single maxima
  - $k = n - 1$: random problem, number of local optima $\frac{2^N}{N+1}$

remarks : "same" results with QAP, flow shop.

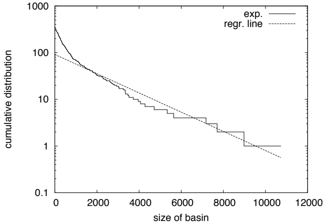
Global optimum basin size *vs.* non-linearity degree k



Size of the global maximum basin as a function of non-linearity degree k

- Basin size of maximum decreases exponentially with non-linearity degree
- $\Rightarrow$ Difficulty of (best-improvement) hill-climber from a random solution

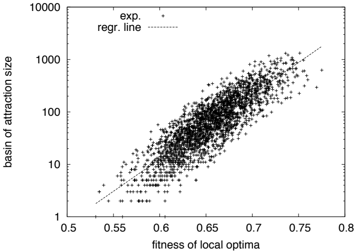
Distribution of basin sizes



Cumulative distribution of basins sizes for $n = 18$ and $k = 4$

- Log-normal cumulative distribution (**not uniform !**) :
  - large number of small basins,
  - small number of large basins.
- Effect of non-linearity :
  the distribution becomes more uniform with non-linearity degree k

Fitness of local optima *vs.* basin size

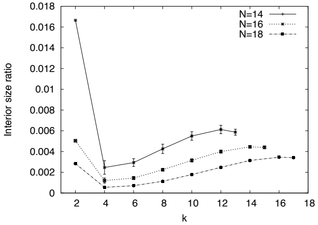


Correlation fitness of local optima *vs.* their corresponding basins sizes

The highest, the largest !

- On average, the global optimum easier to find than one given other local optimum
- But more difficult to find, as the number of local optima increases exponentially with increasing K

Basin : Interior and border sizes



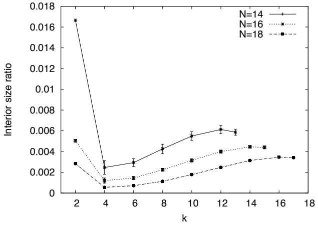
Average of basins interior size ratio

Question :

Do basins look like a "mountain" with interior and border ?

solution ∈ interior
if all neighbors are in the same basin

Basin : Interior and border sizes



Average of basins interior size ratio

Question :

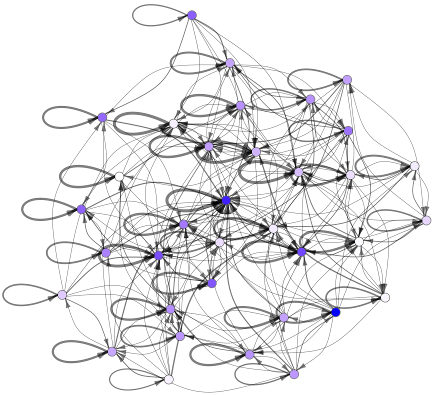
Do basins look like a "mountain" with interior and border ?

solution $\in$ interior
if all neighbors are in the same basin

Answer

- Interior is very small
- Nearly all solutions $\in$ border

Features of local optima network



- nv : ♯vertices
- lv : avg path length
  $d_{ij} = 1/w_{ij}$
- lo : path length to best
- fnn : fitness corr.
  $(f(x), f(y))$ with $(x, y) \in E$
- wii : self loops
- wcc : weighted clust. coef.
- $zout$: out degree
- $y2$: disparity
- knn : degree corr.
  $(deg(x), deg(y))$ with $(x, y) \in E$

Some formal definitions

Weighted clustering coefficient

local density of the network

$$c^w(i) = \frac{1}{s_i(k_i - 1)} \sum_{j,h} \frac{w_{ij} + w_{ih}}{2} a_{ij} a_{jh} a_{hi}$$

where $s_i = \sum_{j \neq i} w_{ij}$, $a_{nm} = 1$ if $w_{nm} > 0$, $a_{nm} = 0$ if $w_{nm} = 0$ and $k_i = \sum_{j \neq i} a_{ij}$.

Disparity

dishomogeneity of nodes with a given degree

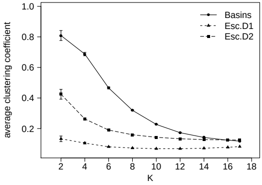
$$Y_2(i) = \sum_{j \neq i} \left(\frac{w_{ij}}{s_i} \right)^2$$

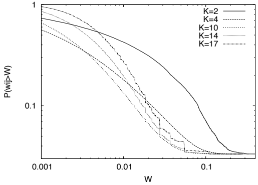
A fitness landscape analysis approach

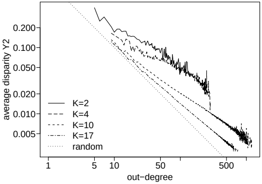
- Link between LON features and difficulty :
  small size instances of NK-landscapes
- Analysis of the LON structure :
  small size instances of NK-landscapes, QAP and FSSP
- Design of one local search component :
  small size instances of NK-landscapes and FSSP
- Explication de performance avec les propriétés du ROL :
  corrélation simple, petites instances, NK et QAP
  corrélation multi-linéaire, petites instances, FSSP
- Prédiction de performance basée sur le ROL :
  grandes instances NK et QAP
- Portfolio d'algorithmes :
  grandes instances NK et QAP

Structure of Local Optima Network

- NK-landscapes (small instances) :
  Most of the features are correlated with K
  relevance of LON definition

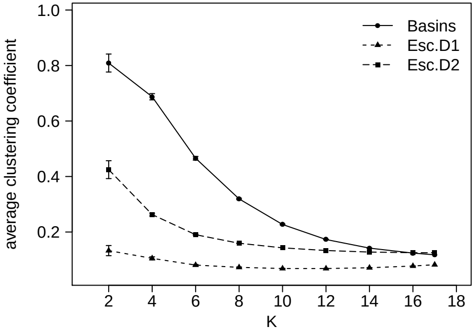






- LON is **not a random** network (NK, QAP, FSSP) :
  Highly clustered network,
  Distribution of weights and degrees have long tail, etc.

Example : clustering coefficient for NK-landscapes



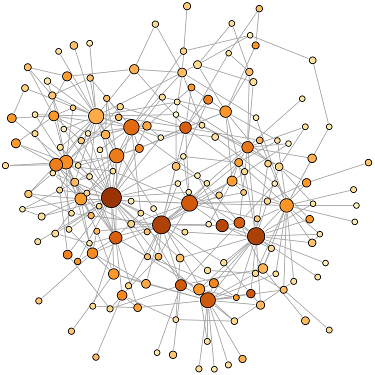
- Network highly clustered
- Clustering coefficient decreases with the degree of non-linearity

LON to compare of problem difficulty

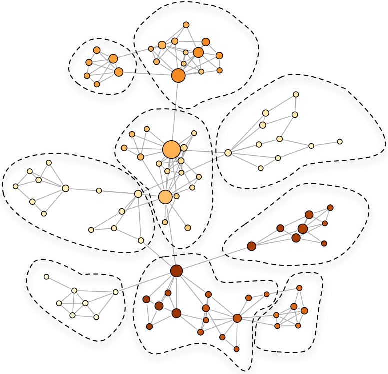
Local Optima Network for Quadratic Assignment Problem (QAP) [DTVO11]

→ Community detection in LON for

Random instance



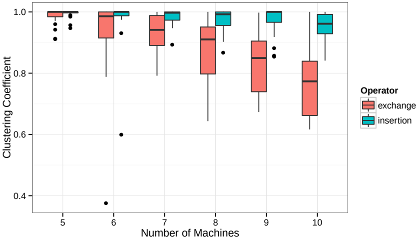
Real-like instance

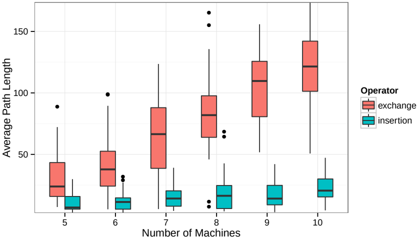


Structure of the LON related to **problem difficulty**

LON to compare algorithm components (1)

Comparaison of **operators** for Flow Shop Scheduling Problem





LON to compare algorithm components (2)

Comparaison of **pivot rule** in hill-climbing for NK-landscapes

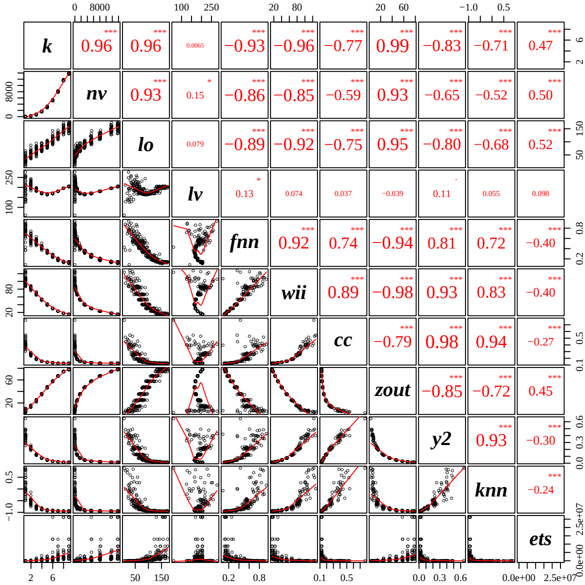
K	$\bar{n}_e / \bar{n}_v^2$		$\bar{Y}$		$\bar{d}$		$\bar{d}_{best}$	
	b-LON	f-LON	b-LON	f-LON	b-LON	f-LON	b-LON	f-LON
2	0.81	0.96	0.326	0.110	56	39	16	12
4	0.60	0.92	0.137	0.033	126	127	35	32
6	0.32	0.79	0.084	0.016	170	215	60	70
8	0.17	0.65	0.062	0.011	194	282	83	118
10	0.09	0.53	0.050	0.009	206	340	112	183
12	0.05	0.44	0.043	0.008	207	380	143	271

Information given by the local optima network

Advanced questions

- Can we explain the performance from the LON features ?
- Can we predict the performance from the LON features ?
- Can we select the relevant algorithm based on the LON features ?

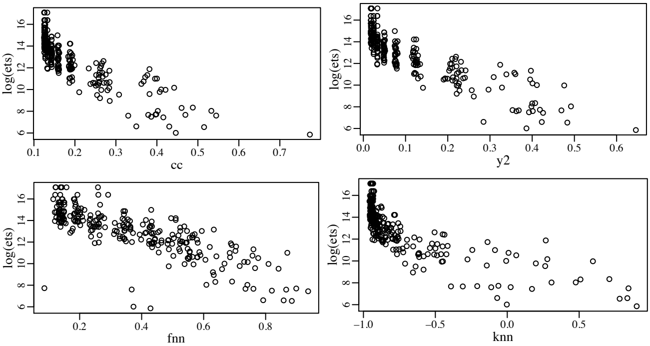
Correlation Matrix



LON features *vs.* performance : simple correlation

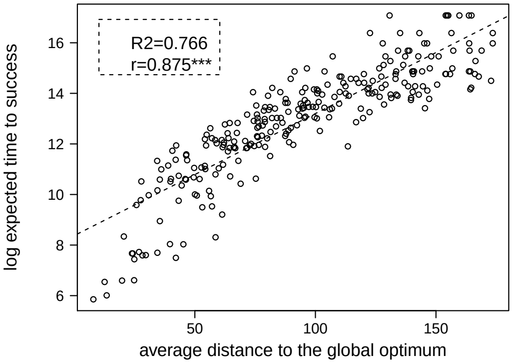
Algorithm : Iterated Local Search on NK-landscapes with $N = 18$
Performance : $ert = \mathbb{E}(T_s) + \left(\frac{1-p_s}{p_s}\right) T_{max}$

n_v	$\bar{d}_{best}$	$\bar{d}$	fnn	w_{ii}	$\bar{C}^w$	zout	$\bar{Y}$	knn
0.885	0.915	0.006	-0.830	-0.883	-0.875	0.885	-0.883	-0.850



ILS Performance vs LON Metrics

NK-landscapes [DVOT12]



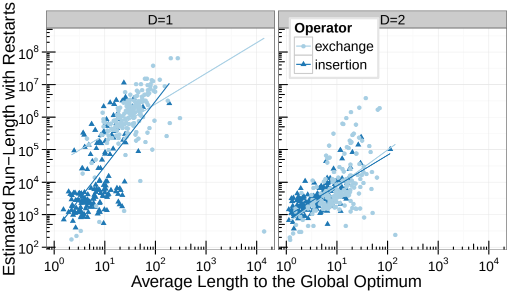
Expected running times

vs.

Average shortest path to the global optimum.

ILS Performance vs LON Metrics

Flow-Shop Scheduling Problem [EA'13]



Expected running times

vs.

Average shortest path to the global optimum.

LON features *vs.* performance : multi-linear regression

1. Multiple **linear** regression on all possible predictors :

$$\log(ert) = \beta_0 + \beta_1 k + \beta_2 \log(nv) + \beta_2 lo + \cdots + \beta_{10} knn + \varepsilon$$

2. Step-wise **backward elimination** of each predictor in turn.

Predictor	$\widehat{\beta_i}$	Std. Error	p-value
(Intercept)	10.3838	0.58512	$9.24 \cdot 10^{-47}$
lo	0.0439	0.00434	$1.67 \cdot 10^{-20}$
zout	-0.0306	0.00831	$2.81 \cdot 10^{-04}$
y2	-7.2831	1.63038	$1.18 \cdot 10^{-05}$
knn	-0.7457	0.40501	$6.67 \cdot 10^{-02}$

Multiple R-squared : 0.8494, Adjusted R-squared : 0.8471.

LON features *vs.* performance : multi-linear regression

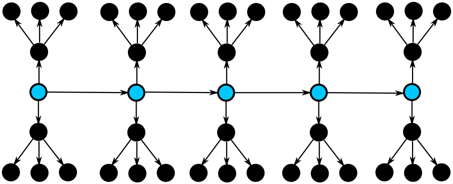
For **Flow Shop Scheduling Problem** using exhaustive selection

$\sharp P$	$\log(N_V)$	CC^w	F_{nn}	k_{nn}	r	$\log(L_{opt})$	$\log(L_V)$	w_{ii}	Y_2	k_{out}	C_p	$adjR^2$
1						2.13					265.54	0.574
2		−5.18				1.43					64.06	0.675
3						1.481	0.895			−0.042	16.48	0.700
4		−2.079				1.473	0.540			−0.032	8.75	0.704
5		−2.388			−1.633	1.470	0.528			−0.030	5.97	0.706

Sampling methodology for large size instances

From the sampling of large-size complex network :

- Random walk on the network
- Breadth-First-Search



Procedure LONSampling(d, m, l)
$x_0 \leftarrow hc(x)$ with x random solution
for $t \leftarrow 0, \ldots l-1$ **do**
  Snowball(d, m, x_t)
  $x_{t+1} \leftarrow$ RandomWalkStep(x_t)
end for

Set of estimated LON features for large size instances

	LON metrics
fit	Average fitness of local optima in the network.
wii	Average weight of self-loops.
zout	Average outdegree.
y_2	Average disparity for outgoing edges.
knn	Weighted assortativity.
wcc	Weighted clustering coefficient.
fnn	Fitness-fitness correlation on the network.
	Metrics from the sampling procedure
lhc	Average length of hill-climbing to local optima.
mlhc	Maximum length of hill-climbing to local optima.
nhc	Number of hill-climbing paths to local optima.

Performance prediction based on estimated features

- Optimization scenario using off-the-shelf metaheuristics :
  TS, SA, EA, ILS on 450 instances for NK and QAP.
- Performance measures :
  average fitness / average rank
- Model of regression :
  linear model / random forest
- Set of features :
  - *basic* : 1st autocorr. coeff. of fitness (rw of length 10^3),
    Avg. fitness of local optima (10^3 hc),
    Avg. length to reach local optima (10^3 hc).
  - *lon* : see previous,
  - *all* : *basic* and *lon* features
- Quality measure of regression :
  R^2 on cross-validation (repeated random sub-sampling)

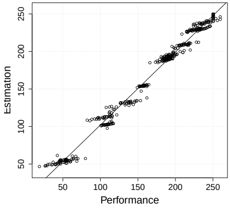
R^2 on cross-validation for NK-landscapes and QAP

Sampling parameters : length $l = 100$, sampled edge $m = 30$, and deep $d = 2$

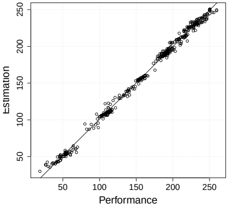
			NK					QAP				
Mod.	Feat.	Perf.	TS	SA	EA	ILS	avg	TS	SA	EA	ILS	avg
lm	basic	fit	0.8573	0.8739	0.8763	0.8874	0.8737	-38.42	-42.83	-41.63	-39.06	-40.48
lm	lon	fit	0.8996	0.9015	0.9061	0.8954	0.9007	**0.9995**	**1.0000**	**1.0000**	**0.9997**	0.9998
lm	all	fit	**0.9356**	**0.9455**	**0.9442**	**0.9501**	0.9439	**0.9996**	**0.9997**	**0.9999**	**0.9997**	0.9997
lm	basic	rank	0.8591	0.9147	0.6571	0.6401	0.7678	0.2123	0.8324	-0.0123	0.4517	0.3710
lm	lon	rank	0.9517	**0.9332**	**0.7783**	**0.7166**	0.8449	**0.7893**	**0.9673**	**0.8794**	**0.9015**	0.8844
lm	all	rank	**0.9534**	**0.9355**	**0.7809**	**0.7177**	0.8469	0.6199	0.9340	0.8577	**0.9029**	0.8286
rf	basic	fit	**0.9043**	0.9104	0.9074	**0.8871**	0.9023	0.8811	0.8820	0.8806	0.8801	0.8809
rf	lon	fit	0.8323	0.8767	0.8567	0.8116	0.8443	0.9009	0.9025	0.9027	0.9019	0.9020
rf	all	fit	0.8886	**0.9334**	**0.9196**	**0.8778**	0.9048	**0.9431**	**0.9445**	**0.9437**	**0.9429**	0.9436
rf	basic	rank	**0.9513**	0.9433	0.7729	**0.8075**	0.8687	**0.9375**	**0.9653**	0.8710	0.9569	0.9327
rf	lon	rank	0.9198	0.9291	0.7979	0.7798	0.8566	0.9308	0.9630	**0.8820**	0.9601	0.9340
rf	all	rank	**0.9554**	**0.9465**	**0.8153**	0.8151	0.8831	**0.9381**	**0.9668**	**0.8779**	**0.9643**	0.9368

Scatter plots of the observed-estimated performance

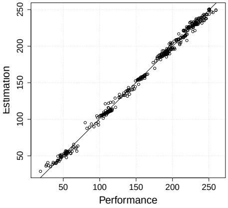
- On the 32 possibles cases (Mod. × Feat. × Algo.), the best set of features : *all* 27 times, *lon* 12 times, *basic* 6 times.
- With linear model : *basic* set is never the one of the best set,
  lon features are more linearity correlated with perf.
- Random forest model obtains higher regression quality :
  basic can be one of the best set (2 times),
  Nevertheless, 7/8 cases, *all* features are the best one.



basic, $R^2 = 0.9327$



lon, $R^2 = 0.9601$



all, $R^2 = 0.9643$

Portfolio scenario

- Portfolio of 4 metaheuristics : TS, SA, EA, ILS
- Classification task : selection of one of the best metaheuristic
- Models : logit, random forest, svm
- Quality of classification :
  error rate (algo. is not one of the best) on cross-validation.

		Avg. error rate				
Probl.	Feat.	logit	rf	svm	cst	rnd
NK	basic	0.0379	0.0278	**0.0158**	0.4711	0.6749
	lon	**0.0203**	**0.0249**	**0.0168**		
	all	0.0244	**0.0269**	**0.0165**		
QAP	basic	**0.0142**	0.0107	0.0771	0.4222	0.6706
	lon	**0.0156**	**0.0086**	**0.0456**		
	all	**0.0161**	0.0106	**0.0431**		

Conclusions and perspectives

- Structure of the local optima network
  can explain problem difficulty
- Features of LON can be used for performance prediction
- The sampling methodology gives relevant estimation of LON features for performance prediction and portfolio design

Perspectives

- Reduce the cost and improve the efficiency of the sampling
- Test on others (real world black-box) problems with others metaheuristics
- Understand the link between problem definition
  and structure of LON
- Study LON as a landscape at large scale

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