Promoting Diversity in Evolutionary Optimization: Why and How

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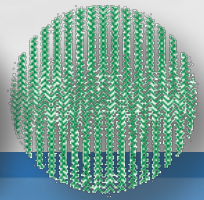


INRA

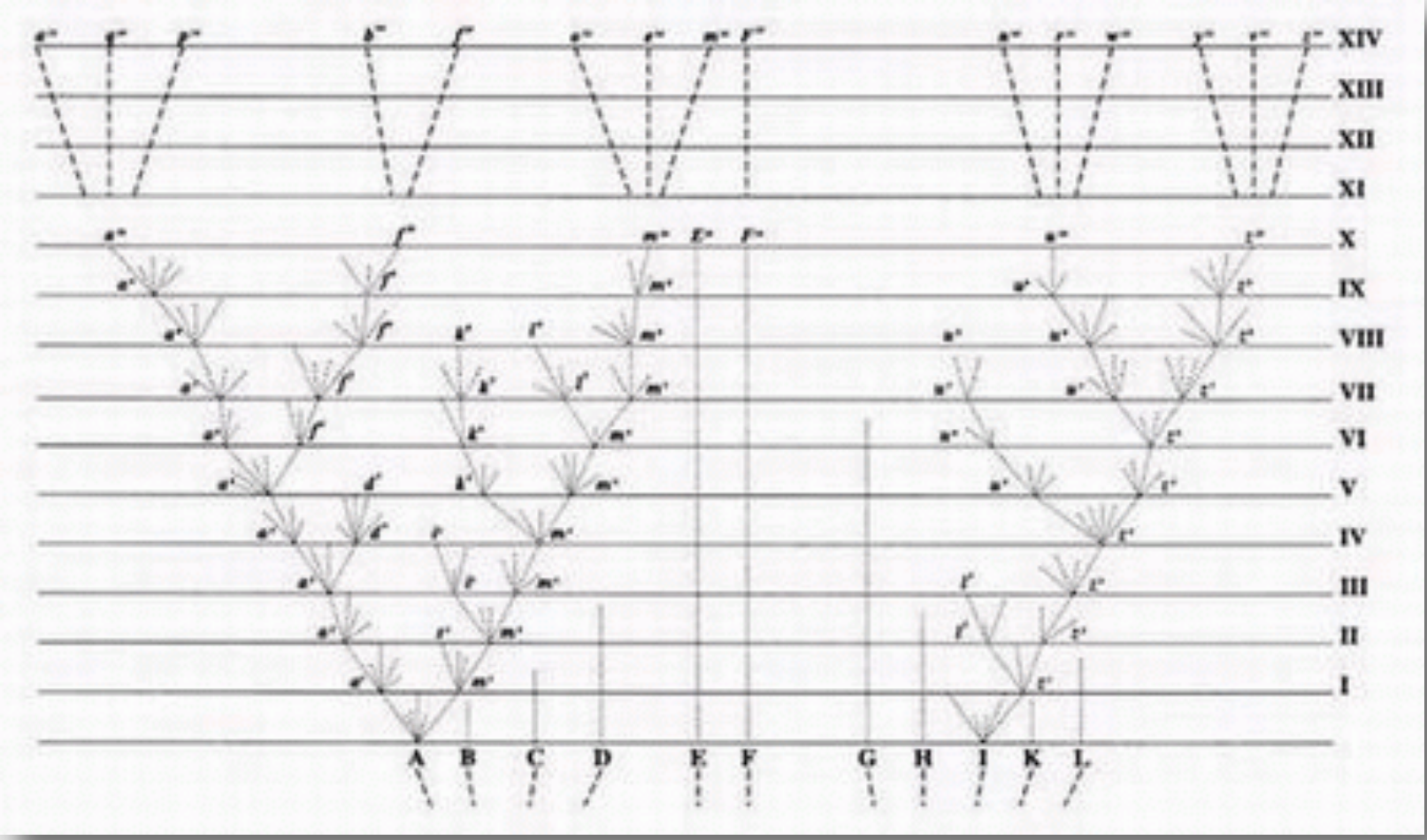
Saturday, September 17th 2016

Outline

- Generic EA
- Divergence of character in natural and artificial evolution
- Background (diversity and similarity, …)
- Mechanisms for promoting diversity
- Hints and tips
- Conclusion

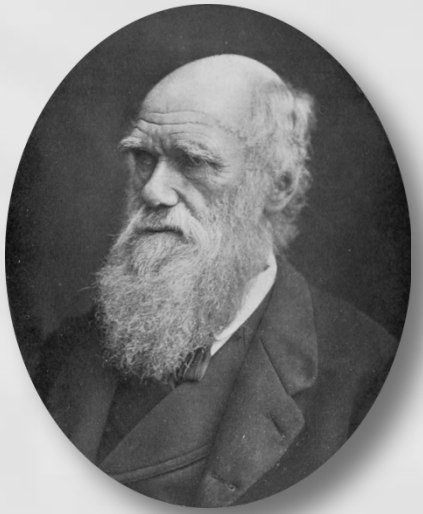
Real world (Galapagos)

Darwin's tree of life



The only illustration in *On the Origin of Species by Natural Selection* (1859)

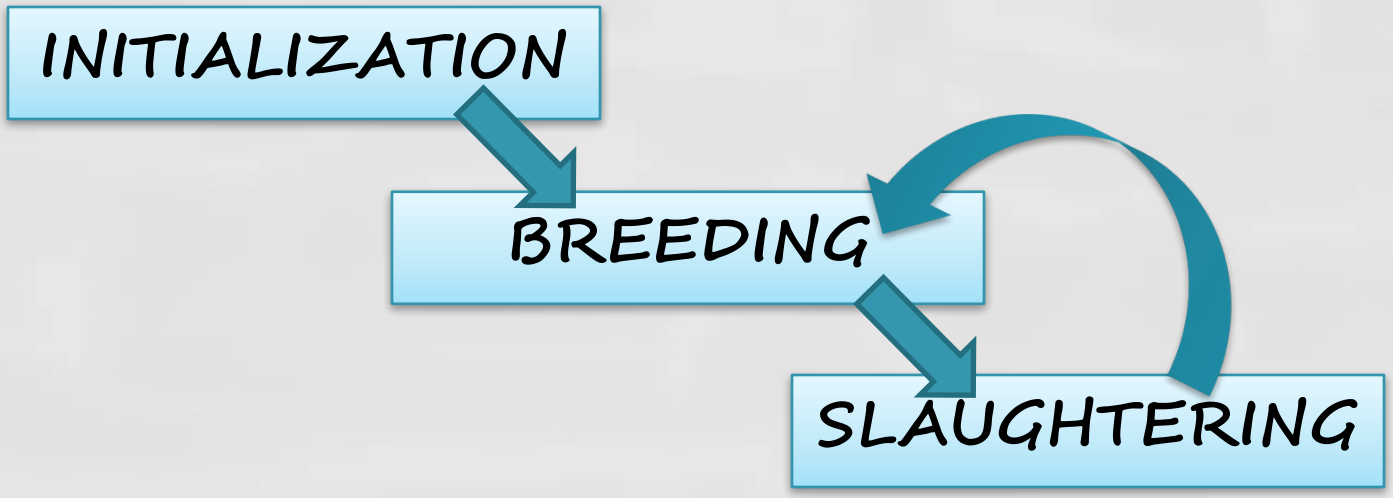
Divergence of character



- *"Great diversity of forms in nature"*
- *"The principle, which I have designated by this term, is of high importance, and explains, as I believe, several important facts"*
  - *"The principle of divergence causes differences, at first barely appreciable, to steadily to increase, and the breeds to diverge in character, both from each other and from their common parent"*
  - *"The varying descendants of each species try to occupy as many and as different places as possible in the economy of nature"*

Evolutionary computation

- A rough idea about “what” an evolutionary algorithm is



- Note: Optimization, not artificial life!

Evolutionary algorithms

Premature convergence

- I.e., the tendency of an algorithm to converge towards a point where it was not supposed to converge to in the first place
- Probably an oxymoron
- Holland's "Lack of speciation"
- EAs general inability to exploit environmental niches

divergence of character

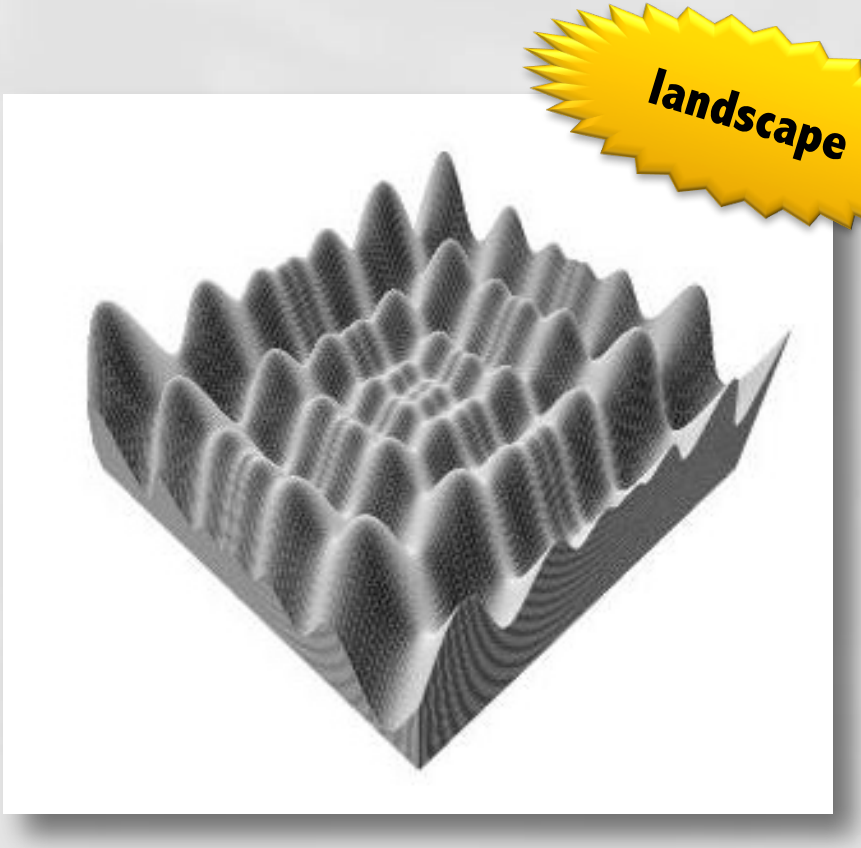
vs.

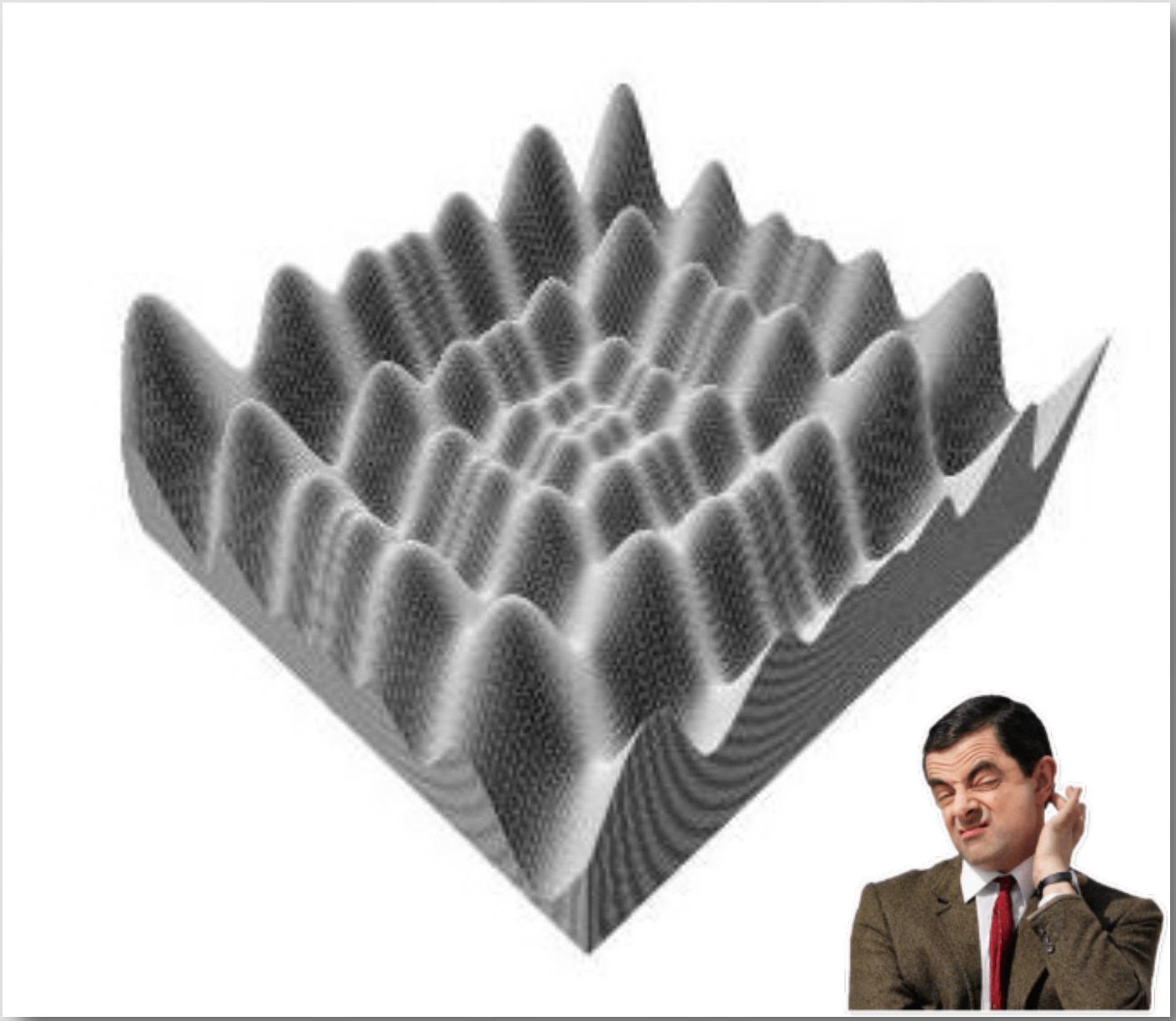
premature convergence

Divergence of character

- *"The basic point of the principle of divergence is **simplicity itself**: the more the coinhabitants of an area differ from each other in their ecological requirements, the less they will compete with each other; therefore natural selection will tend to favor any variation toward greater divergence."*

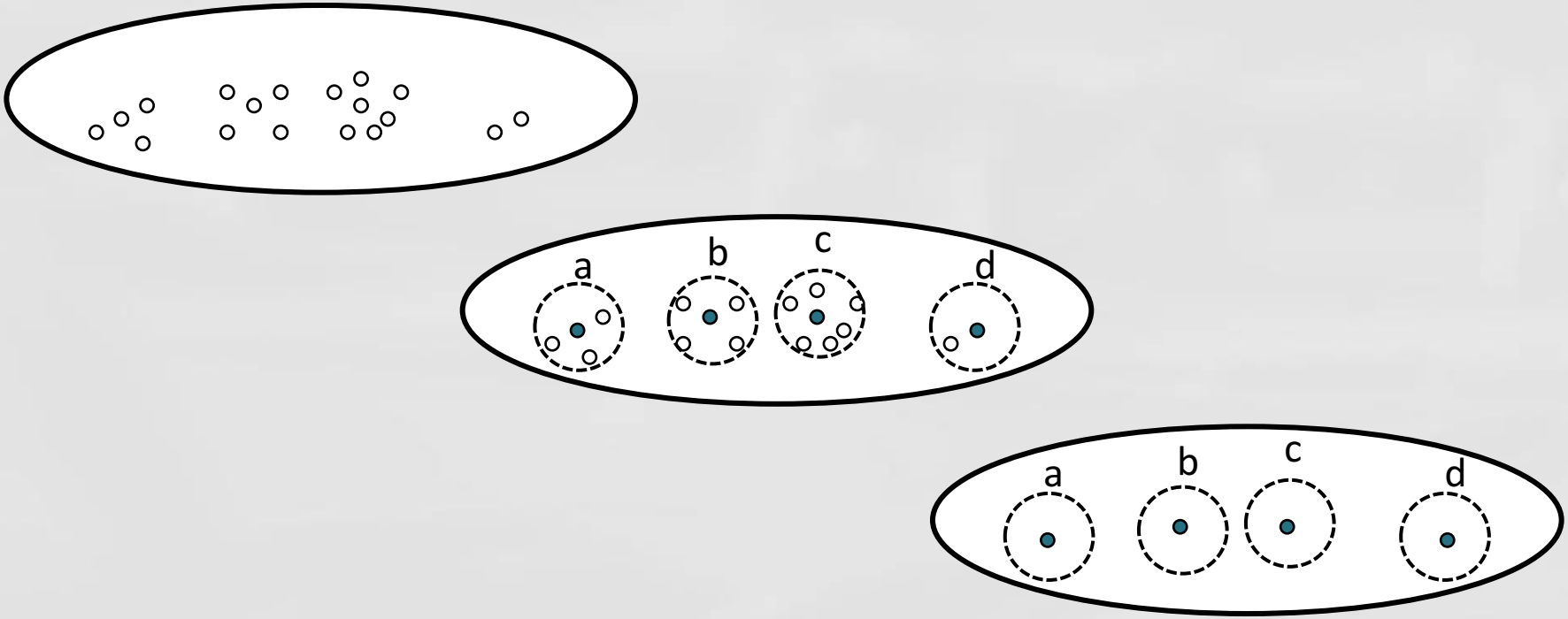
Environment vs. Fitness function





Niches

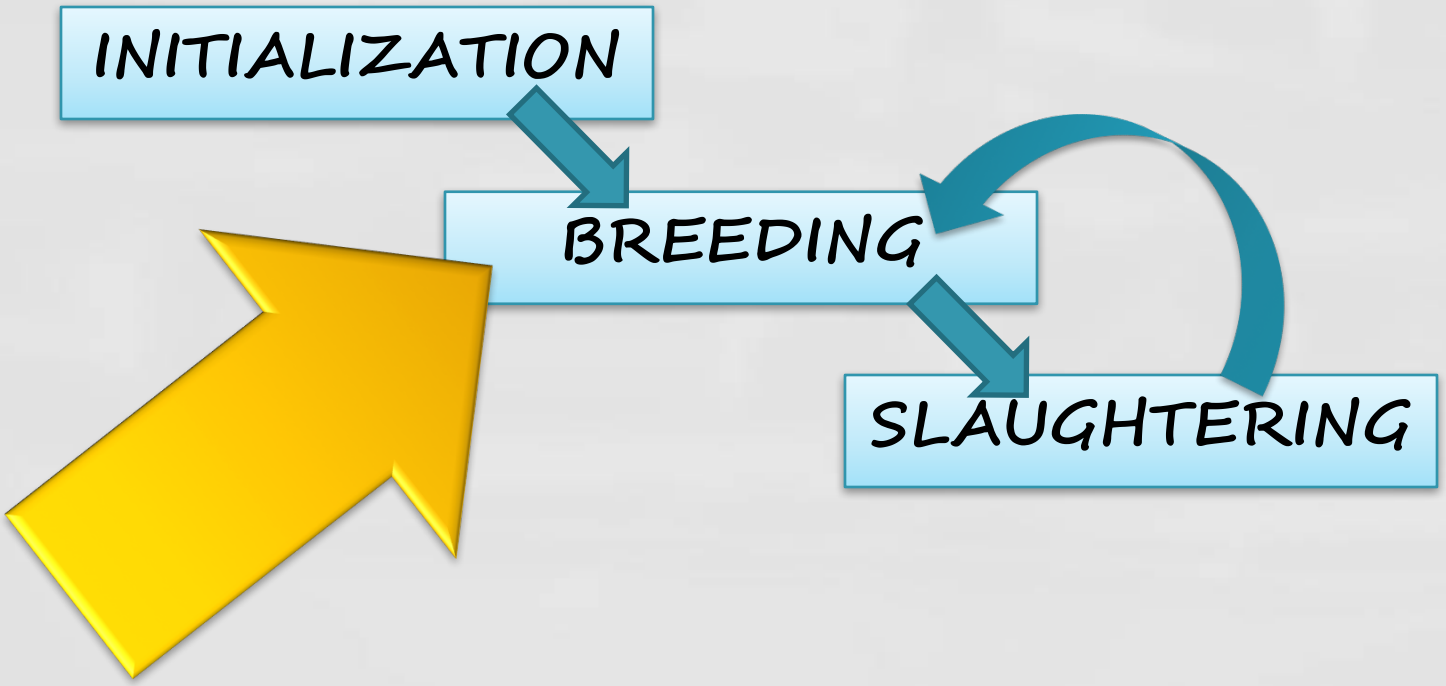
- Niche: subspace in the environment with a finite amount of physical resources that can support different types of life



Niches

- Niches favor the divergence of character
- Niches and speciation
- How to create “niches” in EAs since the environment is missing?

A Very Generic EA



Exploration vs. Exploitation

- Recombination
  - mixes together two or more solutions to create the offspring
  - associated with the idea of *exploration*
- Mutation
  - performs a (usually small) change in an individual
  - associated with the idea of *exploitation*

Exploration vs. Exploitation

- When all parents are very similar, the effectiveness of recombination is limited
- The ability to explore remote parts of the search space is impaired
- “Conventional wisdom suggests that increasing diversity should be generally beneficial”

Exploration vs. Exploitation

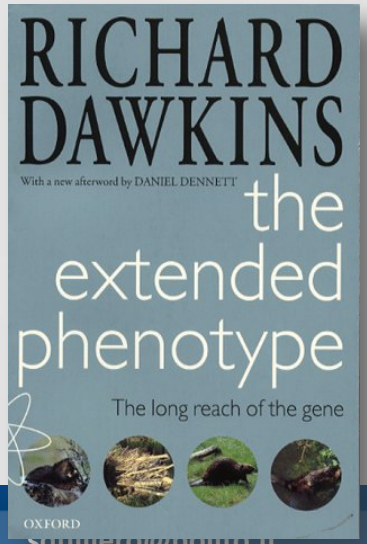
- When all parents are very similar, the effectiveness of recombination is limited
- The ability to explore remote parts of the search space is impaired
- "Conventional wisdom suggests that increasing diversity should be generally beneficial"

what is the definition of "similar"?

and the definition of "diversity"?

Levels in biology

- **Genotype**: the genetic constitution of an organism
- **Phenotype**: the composite of the organism's observable characteristics or traits
- **Fitness**: individual's ability to propagate its genes (well, almost)



Richard Dawkins

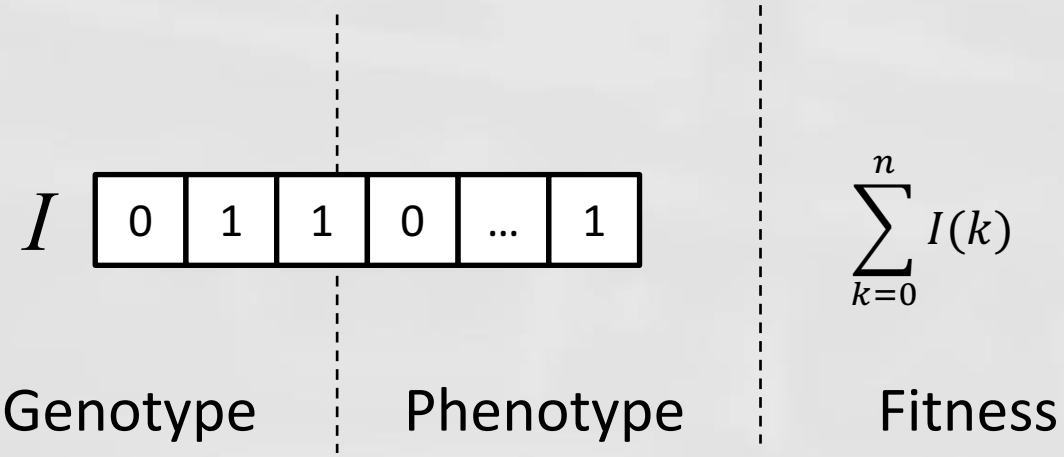
The Extended Phenotype: The Long Reach of the Gene

Oxford University Press, 1982 (revised ed. 1999)

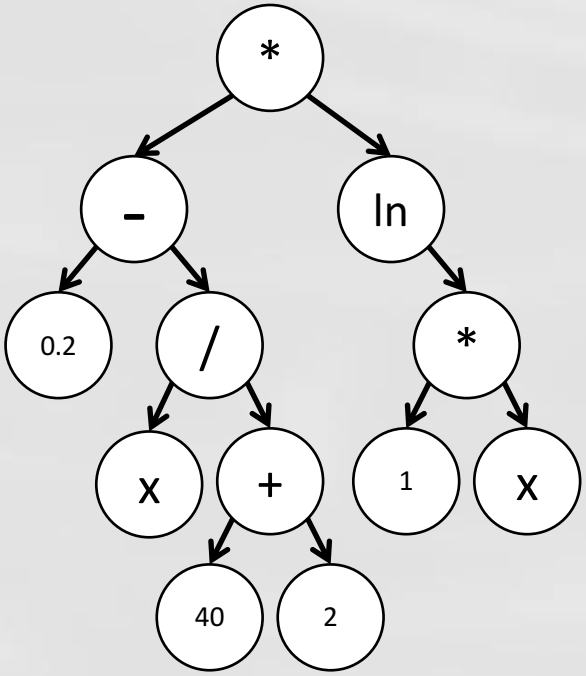
Levels in EC (a modest proposal)

- **Fitness**: how well the candidate solution is able to solve the target problem
- **Genotype**: the internal representation of the individual, i.e., what is directly manipulated by genetic operators
- **Phenotype**: the candidate solution that is encoded in the genotype
  - the intermediate form in which the genotype needs to be transformed into for evaluating fitness
  - if genotype can be directly evaluated: genotype and phenotype coincide

Levels in EC (GA)

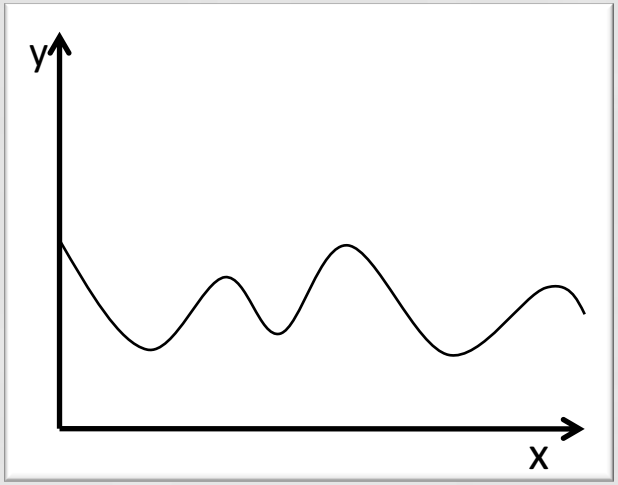


Levels in EC (GP & LGP)



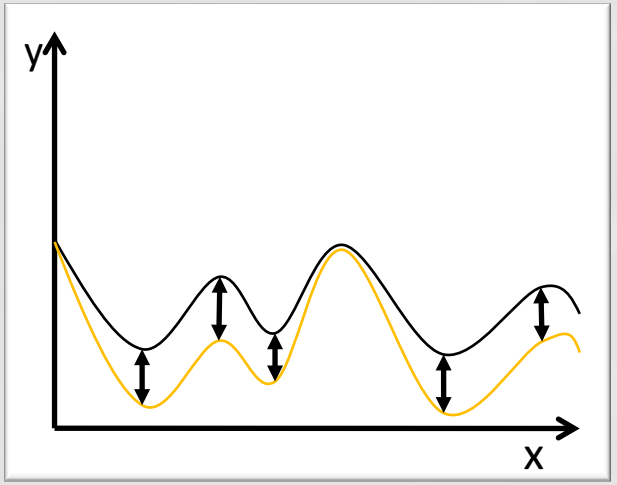
Genotype

$$f(x) = \left(0.2 - \frac{x}{42}\right) \cdot \ln(x)$$



Phenotype

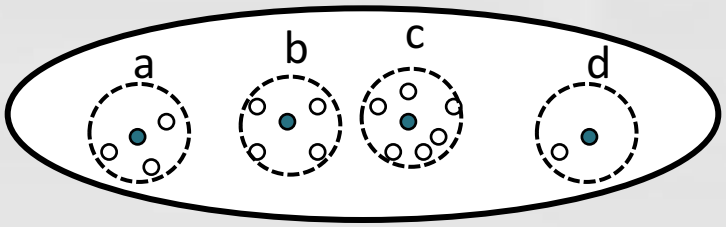
$$\text{Fitness} \approx \int_{x=0}^{E} |f(x) - g(x)|$$



Fitness

Niches in EA

- Niching: grouping similar individual
  - similar spatial positions (i.e., islands)
  - similar genotypes (i.e., niching)
  - similar phenotypes
- Several approaches are based on niching



Detecting clones

- Detecting whether two individuals are clones, i.e., identical, is often an easy task at any level

Measuring diversity

- Diversity $\Rightarrow$ distance metric: *how far* the individual is
  - from (a subset of) the whole population
  - from a single individual
- Diversity $\Rightarrow$ property of the population
- But, at what level?
  - Phenotype
  - Genotype
  - Fitness

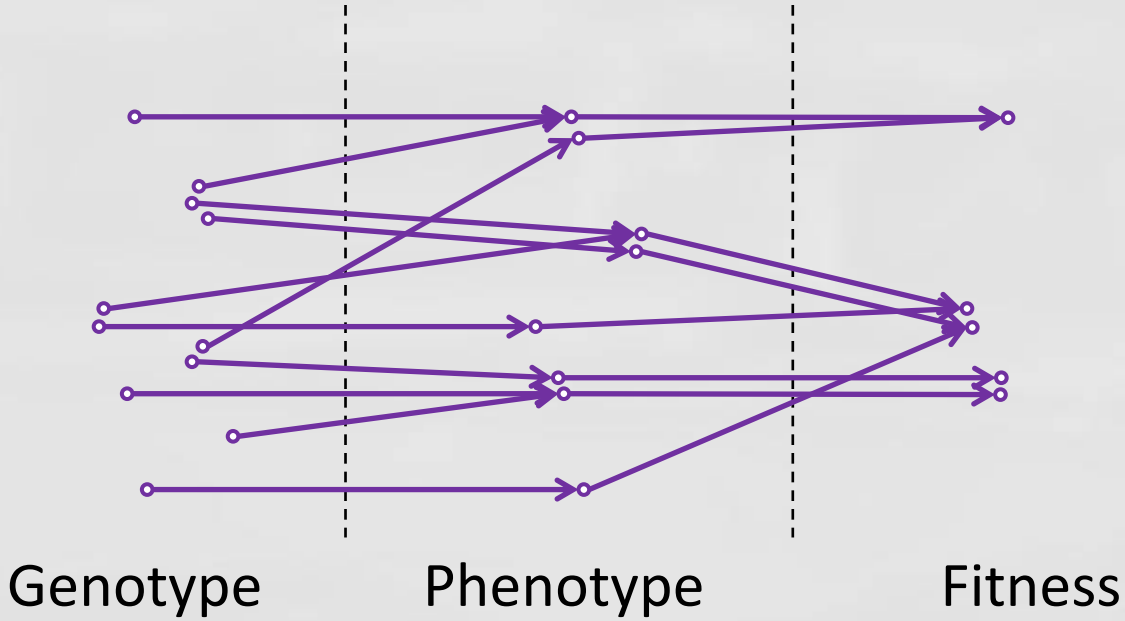
Measuring diversity

- Different fitness values imply different phenotypes, different phenotypes imply different genotypes

$$F_x \neq F_y \Rightarrow P_x \neq P_y \Rightarrow G_x \neq G_y$$

Measuring diversity

- What about “diversity”?
- Locality principle
- Rechenberg’s *strong causality*



Measuring diversity

- Fitness
  - Usually trivial
- Phenotype
  - Usually ad-hoc
- Genotype
  - Different genotypes in the population
  - GP subtree frequency
  - Edit distance (a.k.a., Levenshtein distance)
  - Entropy and free energy

Outline

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What has been proposed to alleviate it?

End goal vs. Means goal

- The **end goal** in optimization is reaching better solutions in less time
- Promoting diversity has often been seen as the key factor to improve performances
- Promoting diversity is a mere **means goal** (yet a quite important one)
- No distinction is made here whether the means goal is
  - preserve existing diversity
  - increase diversity

How diversity is promoted (practice)

- Fitness scaling
- Fitness holes
- Tweaking selection mechanism
- Adding selection mechanism
- Multiple populations
- Population topologies
- …

In theory there is no difference between theory and practice

How diversity is promoted (theory)

- A methodology for promoting diversity alters the selection probability of individuals

$$\bar{p}_{x|\Psi} = p_{x|\Psi} \cdot \xi(x, \Psi)$$

- **Mere definition**: we do not imply that a mechanism operates *explicitly* on the selection operators
- **But** the *effects* on selection probabilities are assessed to classify it

How diversity is promoted (theory)

individual

set of individuals (may be empty)

$$\bar{p}_{x|\Psi} = p_x \cdot \xi(x, \Psi)$$

selection probability of individual x given that all individuals in set Ψ are also chosen

corrective factor

selection probability of individual x

Relevant characteristic

- Lineage (**LIN**)
- Phenotype (**PHE**)
- Genotype (**GEN**)
- ~~Fitness~~ (used as a proxy for either phenotype or genotype)

$$\xi(x, \Psi)$$

Lineage-based methodologies

- The value of $\xi(\circ)$ does not depend on individual structure nor behavior, but it can be determined considering circumstances of its birth (e.g., time, position)
- LBMs can be applied to any kind of problem, even in addition to other diversity preservation methods

Genotype-based methodologies

- Particularly effective when it is possible to define a sensible distance between genotypes
- Often used to
  - avoid overexploitation of peaks in the fitness landscape
  - promote the generation of new solutions very far from the most successful ones
  - preserve variability in the gene pool

Phenotype-based methodologies

- Usually impractical
- Sometimes fitness distance can be used as a proxy for phenotype distance (multi objective EAs, or many objective EAs)

Type of selection

- Parent selection (α or $\not\alpha$)
  - Usually non-determinstic
- Survival selection (ω or $\not\omega$)
  - Usually deterministic

$$\bar{p}_{x|\Psi}$$

Diversity Promotion in EA

ELSEVIER

Information Sciences

Volume 329, 1 February 2016, Pages 782–799

Special issue on Discovery Science

Divergence of character and premature convergence: A survey of methodologies for promoting diversity in evolutionary optimization ☆

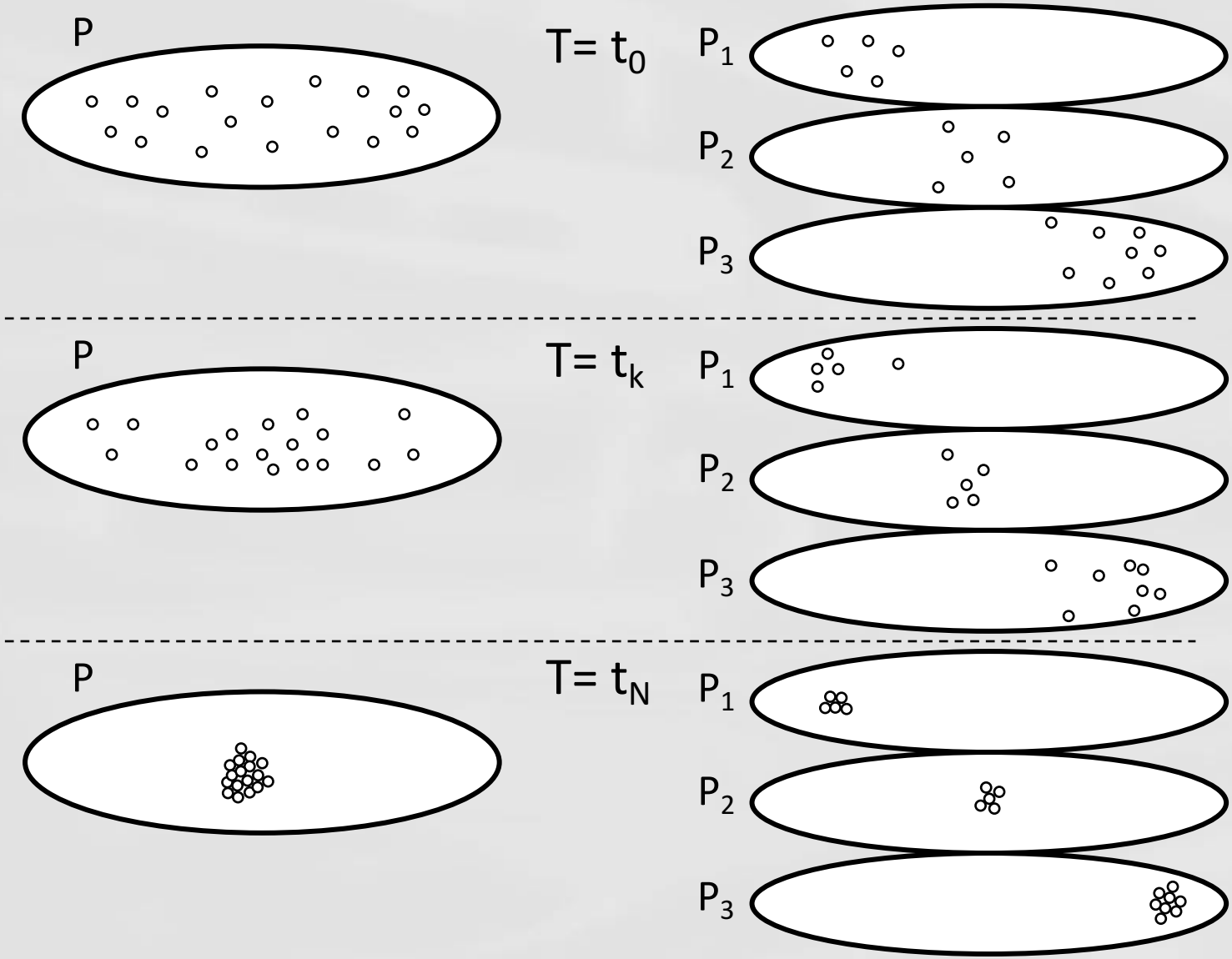
Giovanni Squillero [a], Alberto Tonda [b]

DOI: 10.1016/j.ins.2015.09.056

Island model

- Recipe [LIN αω]
  - The population is partitioned into sub-populations
  - Only local interactions are allowed
  - Periodically, individuals are moved between sub-populations (**migrants**)
- Rationale
  - Different populations may explore different parts of the search space
  - … but global interactions can be useful

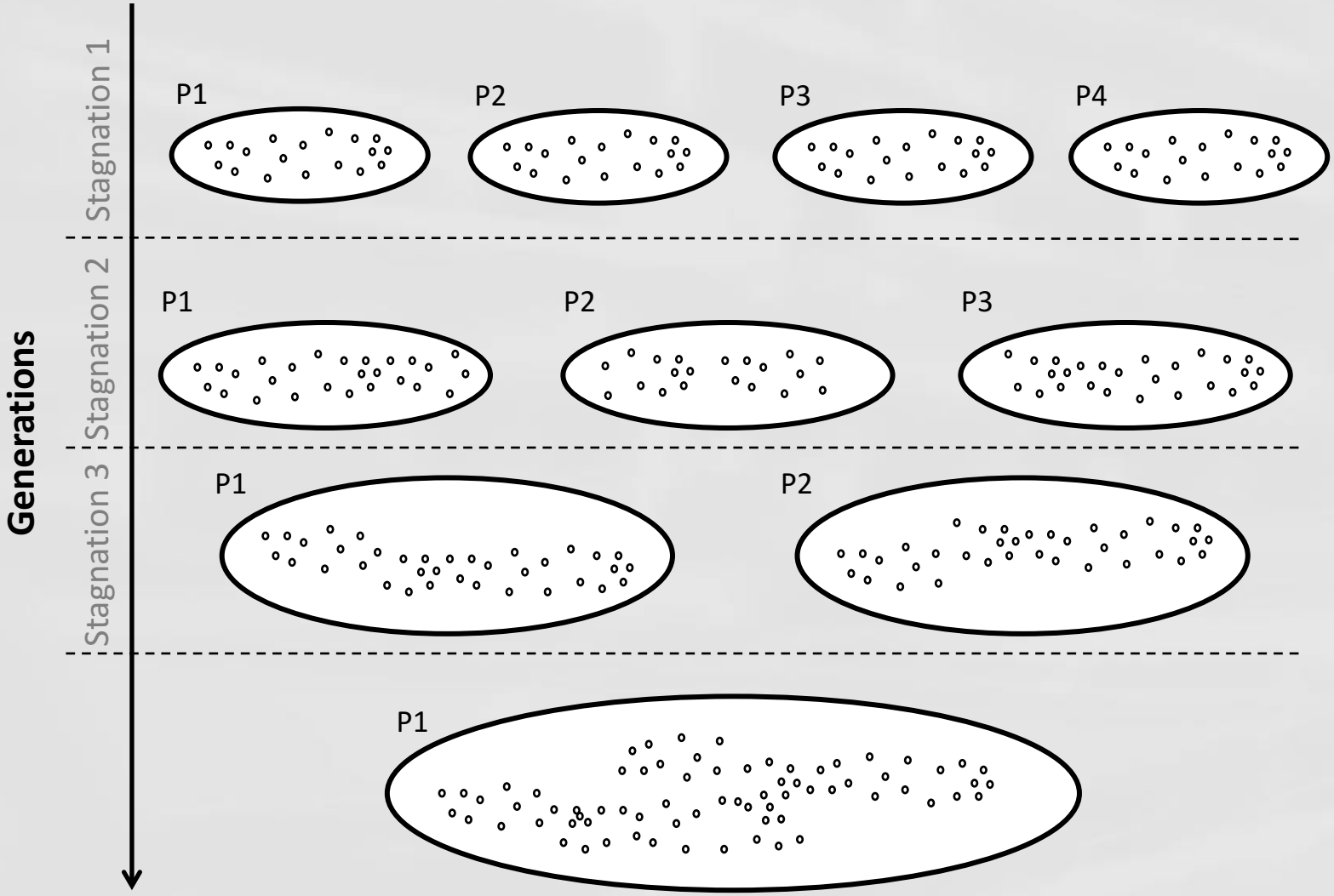
Island model



Segregation

- Recipe [LIN αω]
  - The population is partitioned into *N* sub-populations
  - Only local interactions are allowed
  - Upon stagnation, the *N* sub-populations are merged into *N*-1 sub-populations
- Rationale
  - Same as island models
  - The selective pressure decreases during evolution

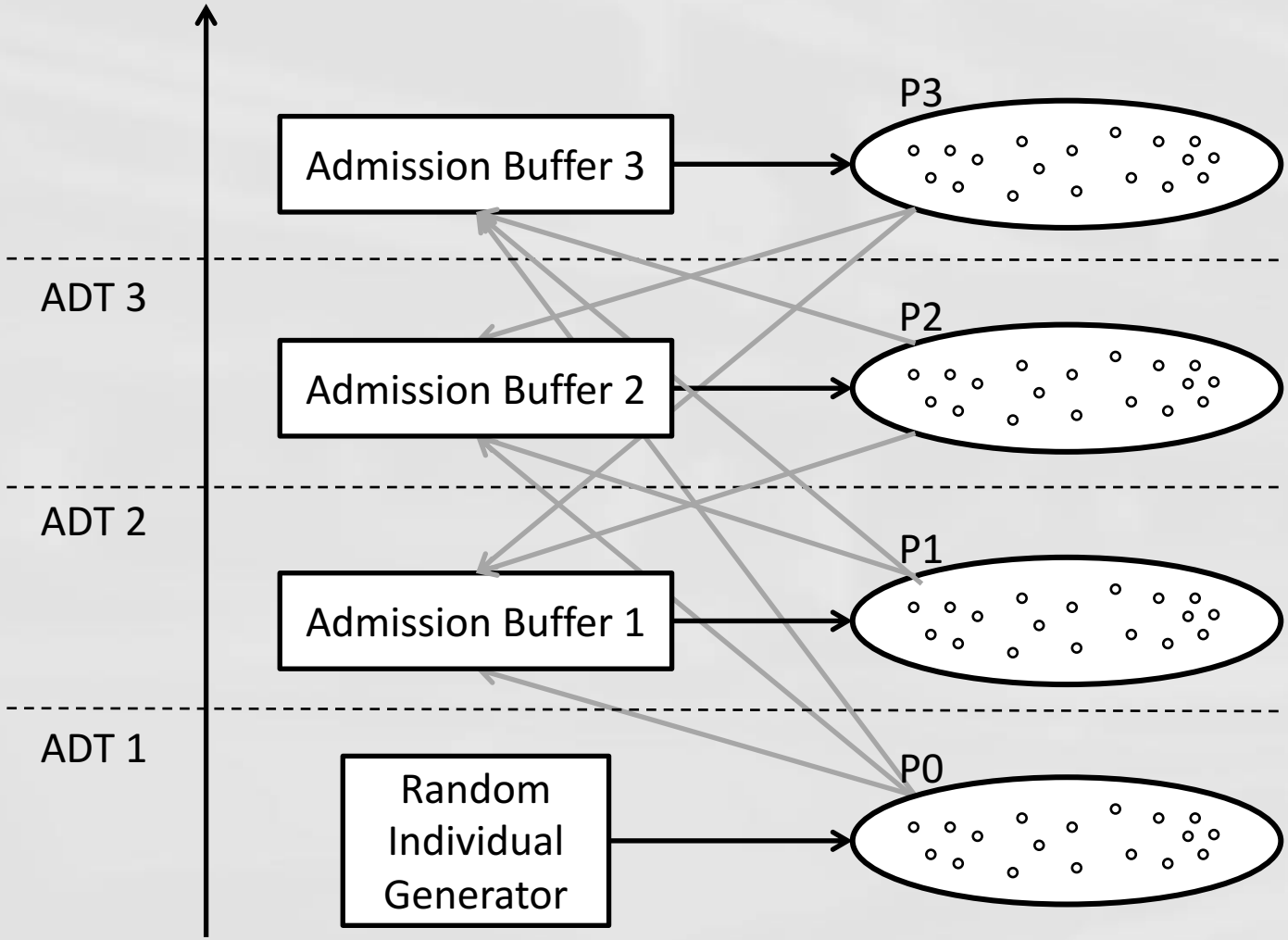
Segregation



Hierarchical fair competition

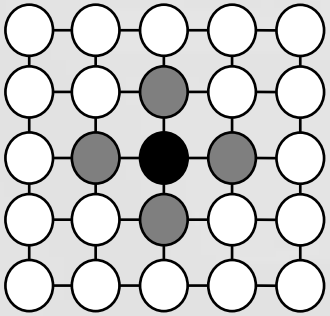
- Recipe [PHE αω]
  - The population is partitioned into sub-populations with similar fitness
  - Only local interactions are allowed
  - The offspring is promoted or demoted according to fitness
  - New random individuals are constantly generated
- Rationale
  - Hard niching with implicit neighborhood
  - Reduce competition between newborns and already optimized individuals (ladder)

Hierarchical fair competition

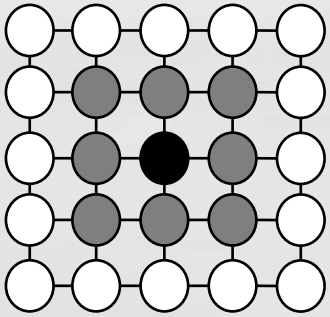


Cellular EA

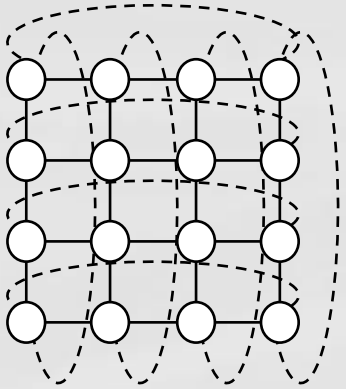
- Recipe [LIN αω]
  - Fixed topology (lattice)
  - Only interactions between neighbors are allowed
- Rationale
  - Limiting interaction could defer the takeover of the population by clones of the fittest individual



Linear-5 (L5)



Compact-9 (C9)



Deterministic crowding

- Recipe [LIN αω]
  - Offspring compete against parents for survival
- Rationale
  - Flexible niching with implicit neighborhood
  - Parents and offspring occupy the same niche
  - No need for evaluating the similarity

Allopatric selection

- Recipe [LIN $\varepsilon\omega$]
  - The whole offspring compete for survival
- Rationale
  - Flexible niching with implicit neighborhood
  - No need for evaluating the similarity
  - Genetic operators that create large offspring can be exploited without the risk for the offspring to invade the population

Fitness Sharing

- Recipe [GEN αω]
  - Scale down individual fitness

$$\bar{f}(I_k) = \frac{f(I_k)}{\sum_i sh(I_k, I_i)}$$

  - with *sh*(*x*, *y*) depending on the distance between the individuals, and is 0 beyond a fixed radius
- Rationale
  - Flexible niching with explicit neighborhood
  - Reduce attractiveness of densely populated area

Clearing

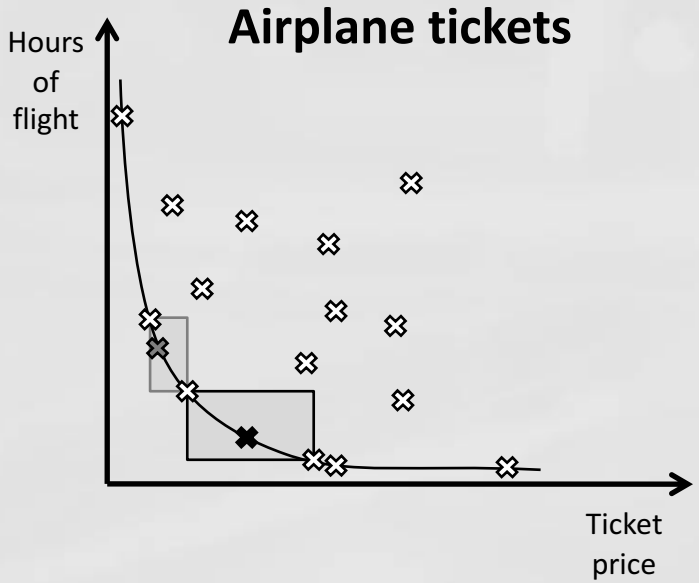
- Recipe [GEN αω]
  - Inside niches of a certain radius, the best *k* individuals retain their fitness while the rest are zeroed
- Rationale
  - Flexible niching with explicit neighborhood
  - Set a hard limit to population density

Standard crowding

- Recipe [GEN ≠ω]
  - New individuals replace the most similar individual in a random niche of size CF
- Rationale
  - Flexible niching with explicit neighborhood
  - Favor novelty (generational approach)

Crowded-comparison operator

- Recipe [PHE αττ]
  - Estimate the *free territory* around solutions and favor solutions less crowded regions
- Rationale
  - Smart implementation of artificial niches
  - Requires a strong correlation between phenotype and fitness
  - NSGA-III introduces ε-domination (adaptive discretization)



Reference points partitioning

- Recipe [GEN $\not\in\omega$]
  - Population is partitioned using in clusters centered around a set of reference points
  - Reference points are initially chosen by the user, then can be dynamically updated
  - New individuals compete for survival inside their own niche
- Rationale
  - Flexible niching with explicit neighborhood

Vector evaluated genetic algorithm

- Recipe [PHE αtt]
  - Divide the mating pool in *N* parts, each one filled with individual selected on their *i*-th component of the fitness
  - Alternative: select on a weighted sum, but use different weight sets for the different parts
- Rationale
  - Increase the push towards specialization
- Caveats
  - Only applicable to MOEAs, or when using an aggregate fitness

Lexicase selection

- Recipe [PHE αtt]
  - Before selection, re-arrange the components of the fitness
  - Compare individual fitnesses lexicographically
- Rationale
  - Increase the push towards specialization
- Caveats
  - Only applicable when using an aggregate fitness

Restricted tournament selection

- Recipe [GEN ⇄ω]
  - New individuals compete with the most similar individual in a random niche of size CF
- Rationale
  - Flexible niching with explicit neighborhood

Sequential niching

- Recipe [GEN αω]
  - The most promising points in the search space after each run are altered so to become less interesting in further executions
- Rationale
  - Avoid over exploitation

Gender

- Recipe [LIN/GEN αtt]
  - Add gender to individual and enforce sexual reproduction
  - More than two sexes are possible, with different mutation probabilities
  - Gender might be part of the genome or not
- Rationale
  - Prevent crossover between clones
  - Limit interactions between related individuals

Tarpeian method

- Recipe [PHE αω]
  - Randomly kill individual who don't adhere to given standards
- Rationale
  - Note: originally used to prevent bloat
  - Creating dynamic and non-deterministic *fitness holes* may have several beneficial effects, including to promote diversity

Diversifiers

- Recipe [GEN αω]
  - Detect less populated areas in the search space and try to generate random inhabitants
- Rationale
  - Increase variability in the gene pool regardless the fitness
  - Require a reliable distance metric

Random immigrants

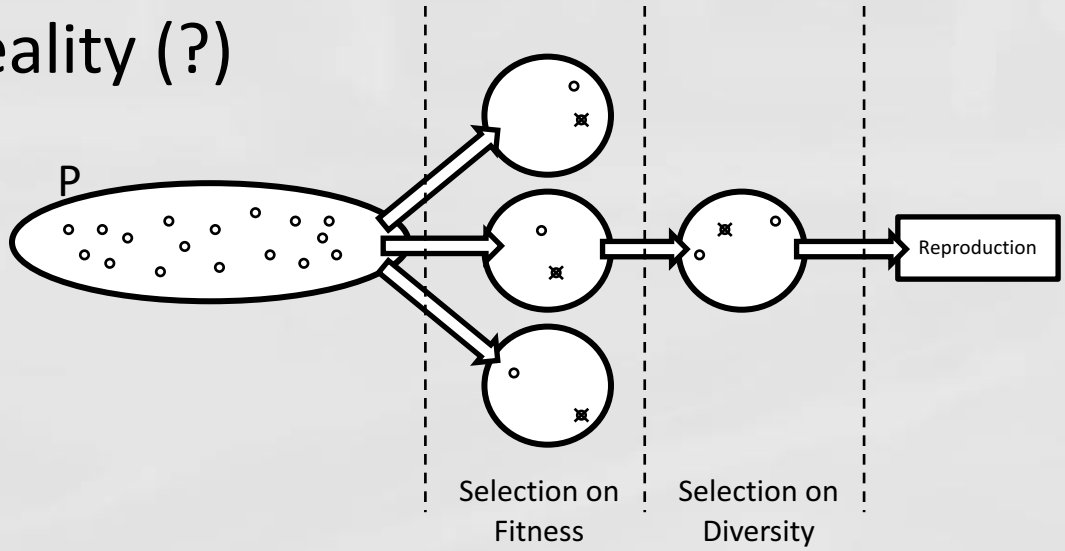
- Recipe [PHE αω]
  - Periodically insert random individuals in the population
- Rationale
  - Try to introduce novelty
- Caveats
  - Newborns may need to be artificially kept alive when competing against already optimized individuals

Extinction

- Recipe [PHE ¤ω]
  - Upon convergence (or periodically) remove a significant part of the population
  - Then fill up the population with the offspring of the survivors and/or random individuals
- Rationale
  - A gust of fresh air: already optimized individuals are not enough to occupy the whole population and newborns may start exploring new regions
- Caveat
  - Fitness variability used as phenotype variability

Two-level diversity selection

- Recipe [GEN αtt]
  - Select three individuals using fitness, then pick the two with maximum distance for reproduction
- Rationale
  - Exploit a reliable distance metric to increase the efficacy of crossover
  - Not so far from reality (?)



GDEM – Genetic Diversity Evaluation Method

- Recipe [GEN αω]
  - Add diversity as an explicit goal and go MO
- Rationale
  - Modify the domination criteria
  - Need a reliable diversity metric
- Historical note
  - See: *Find Only and Complete Undominated Sets* (FOCUS)

Delta entropy and pseudo entropy

- Recipe [GEN αtt]
  - With a certain probability select individuals on their ability to increase the global entropy of the population instead of fitness
- Rationale
  - Not-so-fit individual with peculiar traits should be preserved
  - Measuring the entropy of the population is easier than defining a distance function

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- Generic EA
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Hints and Tips

- Do you really need to promote diversity?
  - Several problems in EA are caused to ill-designed fitness functions
  - Check whether the locality principle holds true
  - Check what happen with multistart

Hints and Tips

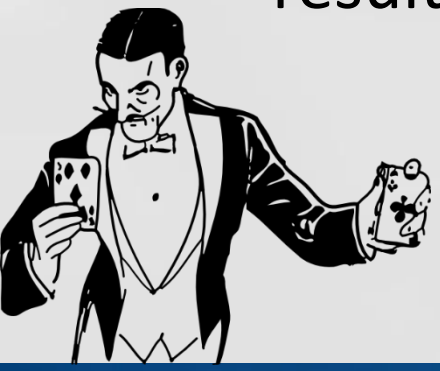
- Do you really need to promote diversity?
- Use extinction (20m)
  - Simple n’ easy

Hints and Tips

- Do you really need to promote diversity?
- Use extinction (20m)
- Use lexicase selection (20m)
  - Simple n' easy
  - Only useful for aggregate fitness (combination of several components)

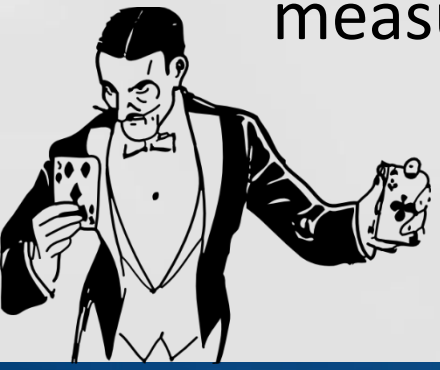
Hints and Tips

- Do you really need to promote diversity?
- Use extinction (20m)
- Use lexicase selection (20m)
- Use an island model (2h)
  - Far better than multistart (if migrations are properly handled)
  - Only useful if different experiments yield different results



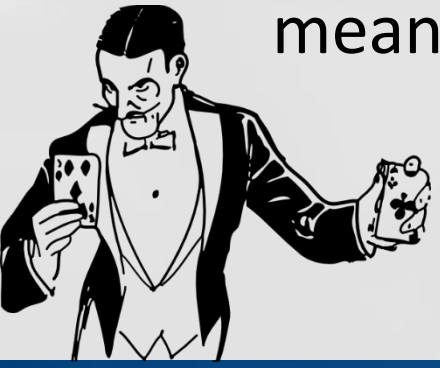
Hints and Tips

- Do you really need to promote diversity?
- Use extinction (20m)
- Use lexicase selection (20m)
- Use an island model (2h)
- Use fitness holes (20h)
  - Tweak selection operator(s)
  - Only useful if a global (and efficient) diversity measure is available



Hints and Tips

- Do you really need to promote diversity?
- Use extinction (20m)
- Use lexicase selection (20m)
- Use an island model (2h)
- Use fitness holes (20h)
- Use real niching (2-20d)
  - Only useful if the distance between genotypes is meaningful



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Conclusion

More Materials & Bibliography

- **MPDEA**: GECCO Workshop on Measuring and Promoting Diversity in Evolutionary Algorithms
- mpdea@polito.it
- https://github.com/squillero/mpdea