Taxonomy and Coarse Graining in Evolutionary Computation



A Tale of Elephants, Blind Men and Soup!

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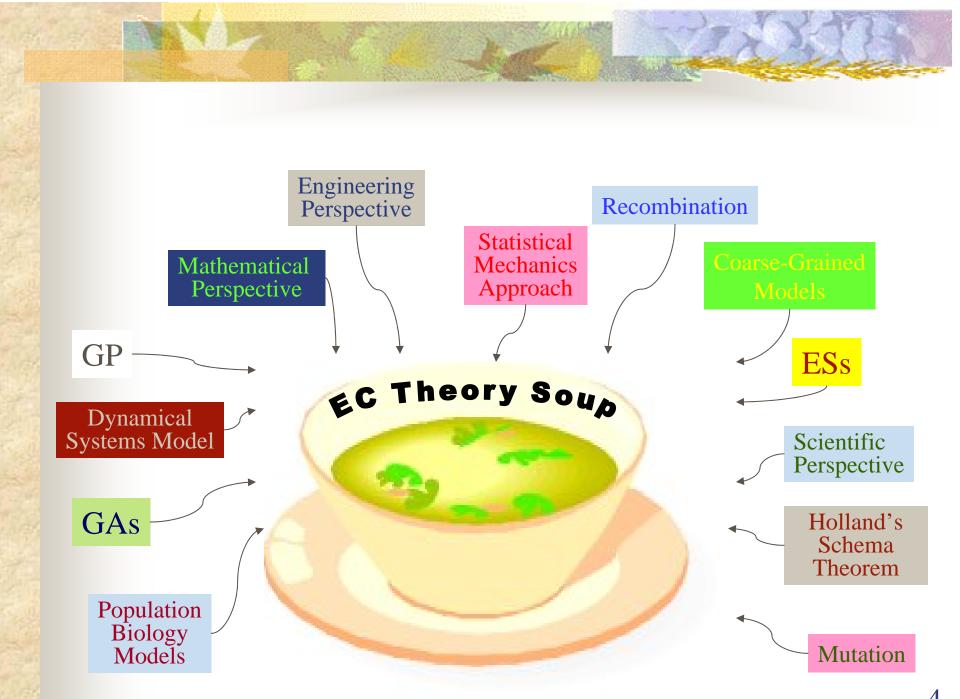
WARNING

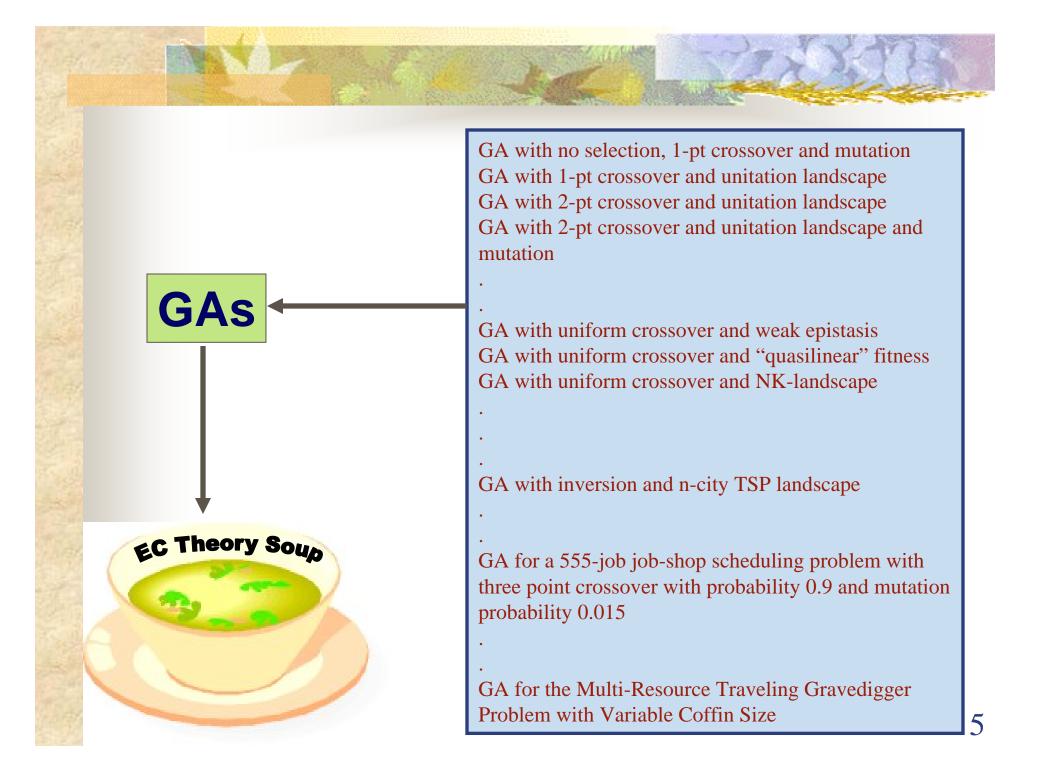
EQUATIONS

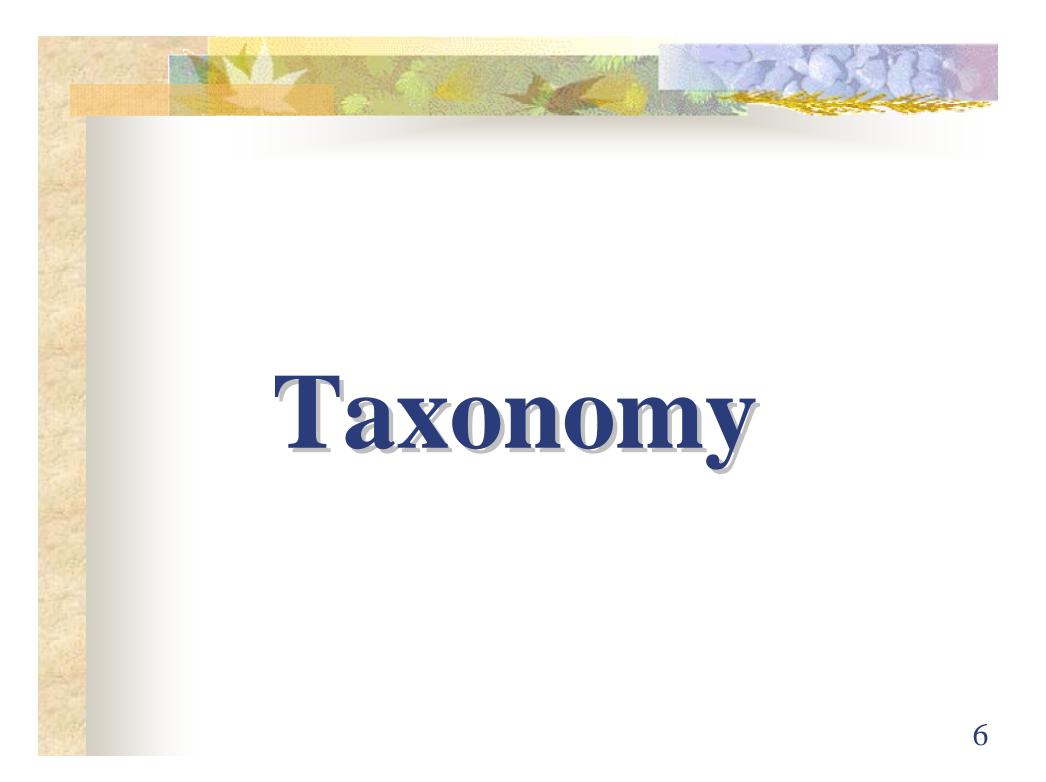
G Slides suitable for a general audience

A Slides suitable only for those accompanied by someone with knowledge of arithmetic and elementary linear algebra
 AA Slides only for those not shocked by a coordinate transformations and giving new names to things that previously had other names
 X No X rated slides – no mention of the words "Theorem",
 "Lemma" or "Proof"

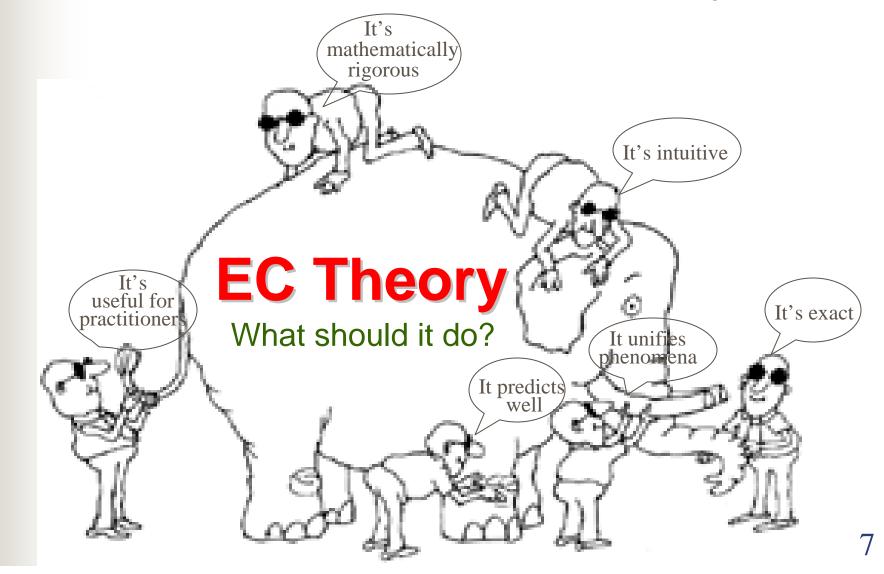
ALL CLEAR!



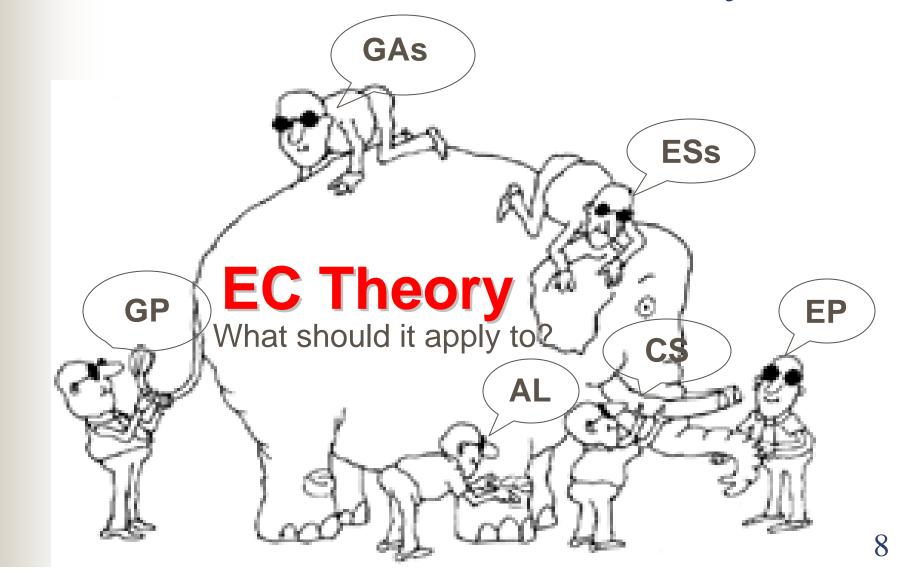




The Problem of Taxonomy...

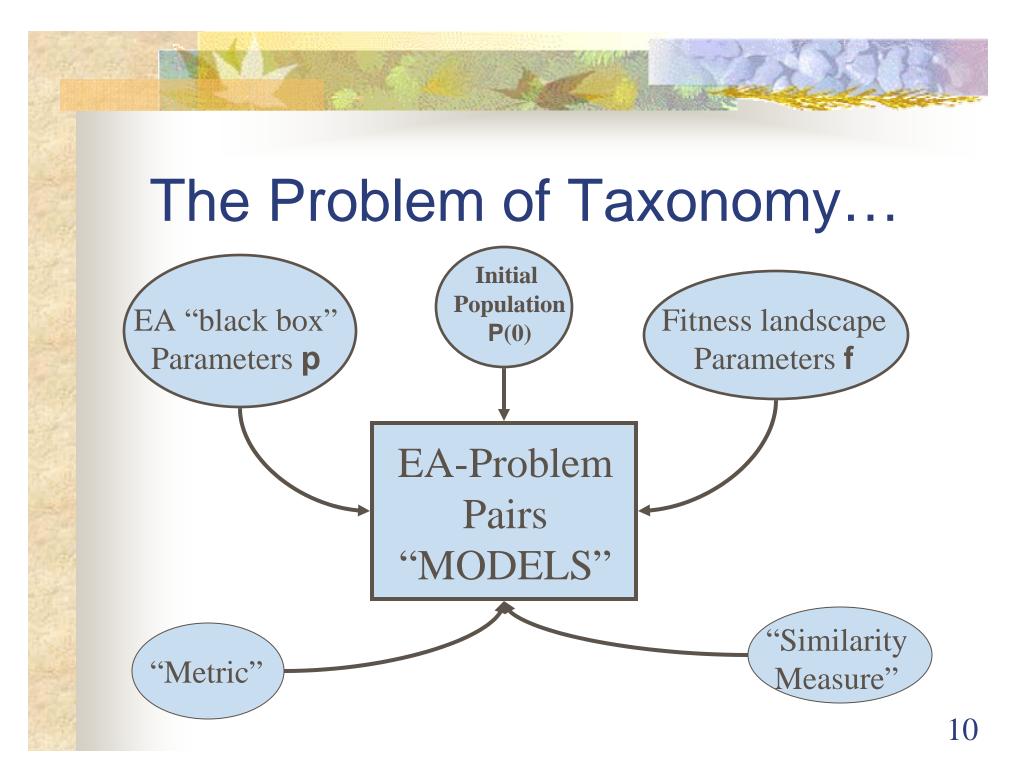


The Problem of Taxonomy...



The Problem of Taxonomy...





The Space of EAs

How "far apart" are a GA with one-point crossover, pc=0.8, mutation, p=0.08, and a NK fitness landscape, N=27, K=3 and GP for K-SAT, K=4, sub-tree crossover, pc=0.5, mutation, p=0.05?

How "far apart" are a giraffe and a grasshopper?

How "far apart" are hydrogen and uranium?

How "far apart" are a GA with one-point crossover, pc=0.8, mutation, p=0.08, and a NK fitness landscape, N=27, K=3 and a GA with one-point crossover, pc=1, mutation, p=0.1, and a NK fitness landscape, N=35, K=3?

How "far apart" are a giraffe and a horse?

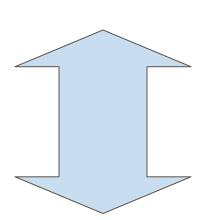
How "far apart" are sodium and potassium?

Taxonomy is easier with "distance" measures

Taxonomy

Theory – what can it tell us? E.g. "electronic structure"

Phenomenology – we want more of that! e.g. "periodic table"



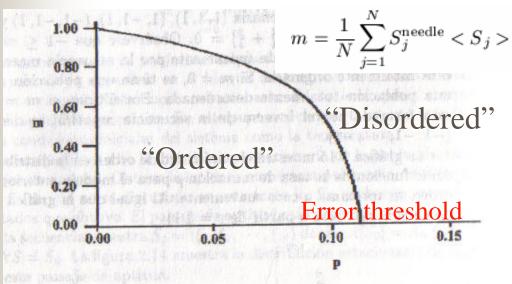
History – contingency, that's what we've had

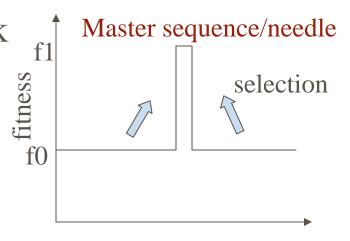
Universality

Phenomenology

Eigen model/Needle-in-a-haystack Characteristic of viruses and real world BRITTLE problems (it works or it doesn't!)

Qualitative behavior dominated by existence of error threshold – doesn't depend on "details" - **UNIVERSAL**

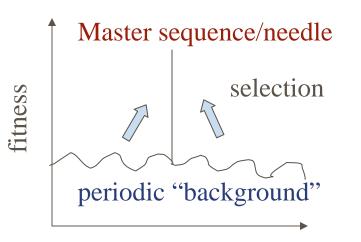




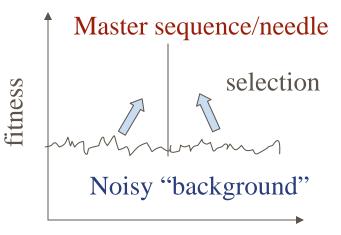
genotype

Value of critical mutation rate does depend on details (N, f1, f0 ...) – **NON-UNIVERSAL**

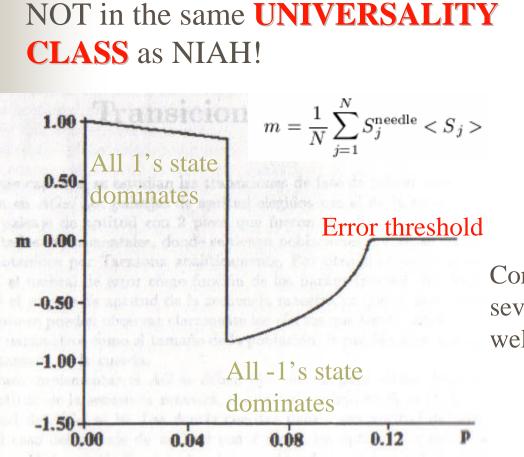
Same **UNIVERSALITY CLASS** as NIAH

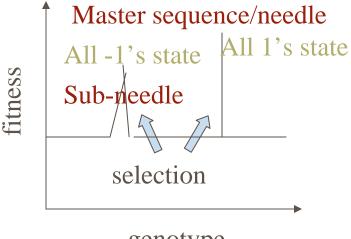


genotype



genotype





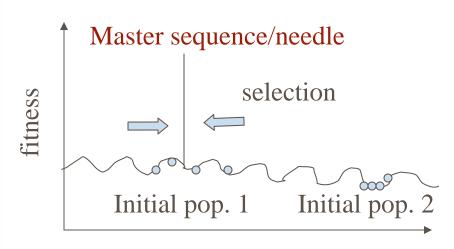
genotype

Corresponds to a system where there's several "it kind of works" states as well as a "it definitely works" state

fitness

Same **UNIVERSALITY CLASS** as NIAH? YES

What typically happens?



genotype

Master sequence/needle selection initial population genotype

Phase transition for K-SAT

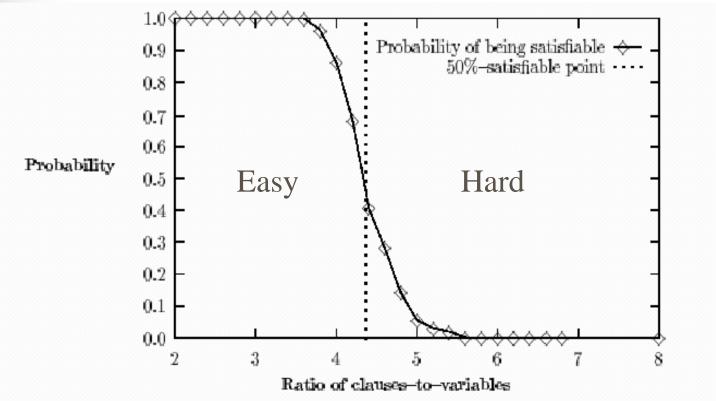


Figure 4: Probability of satisfiability of 50-variable formulas, as a function of the ratio of clauses-to-variables.

From: Mitchell et al.(1992) Hard and easy distributions of SAT problems

Similarity measures

Need objective criteria by which to judge the degree of affinity between different models. There are many possibilities...e.g.

- Average population fitness vs. time
- Best in population versus time
- Diversity versus time
- "Order parameter" (e.g. % of population that is optimal as function of EA parameters)
- Time to find optimum
- "Hardness"
- "Robustness"
- Fixed points (asymptotic behaviour)

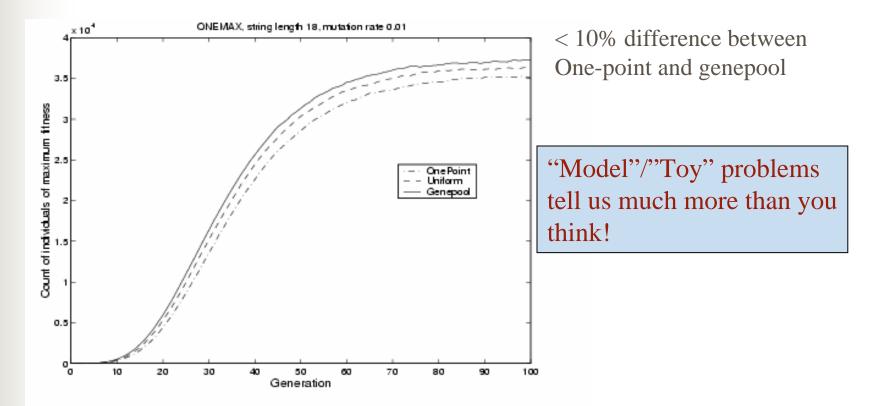
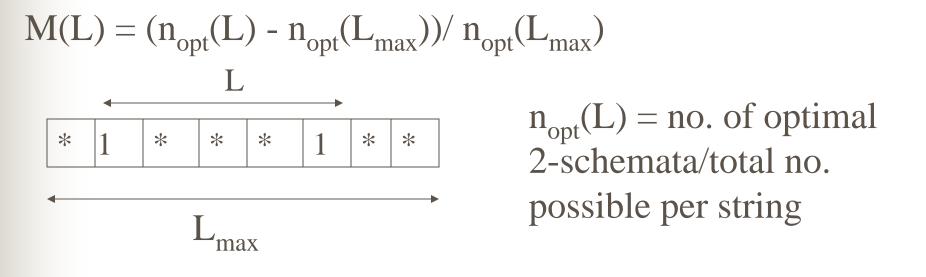


Figure 2: The number of optimal individuals for different types of recombination

Wright, Rowe, Poli and Stephens – GECCO2002

Stephens, Waelbroeck and Aguirre – FOGA 7



Interested in whether short or long building blocks are preferred. M(L) > 0 preference for short blocks, M(L) < 0 preference for long blocks

Experiment: popsize = 5,000; $L_{max} = 8$; 30 runs

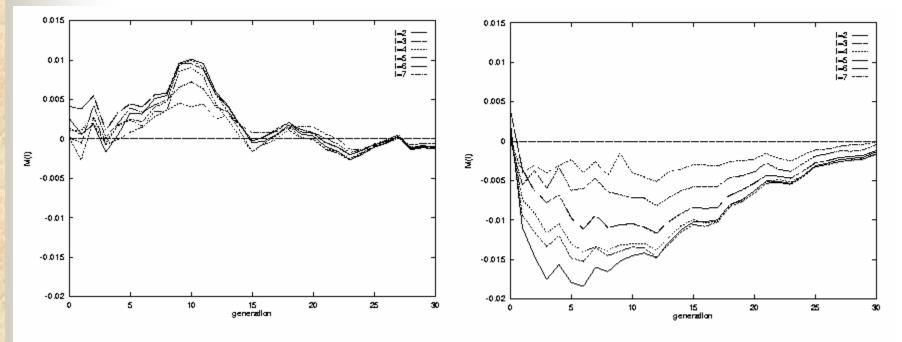


Figure 1: Graph of M(l) versus t in the unitation model with $p_c = 0$.

Figure 2: Graph of M(l) versus t in unitation model with $p_c = 1$.

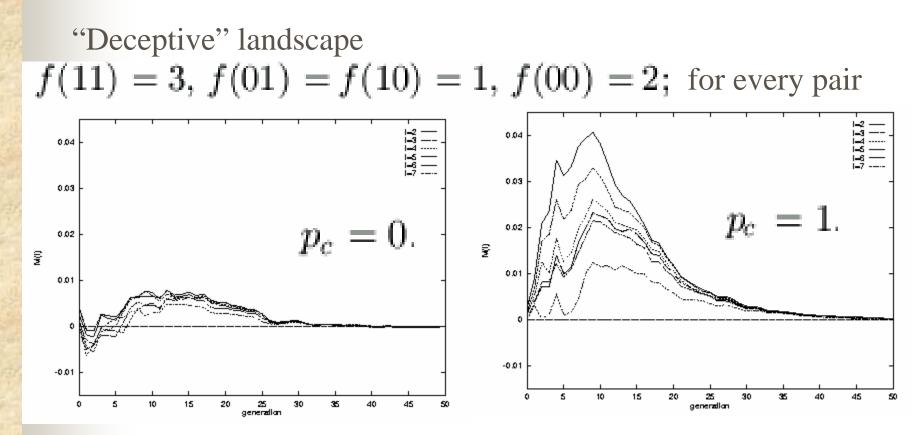
Without crossover – no preference for one size versus another

With crossover – large schemata grow, short schemata diminish – opposite of Building Block Hypothesis

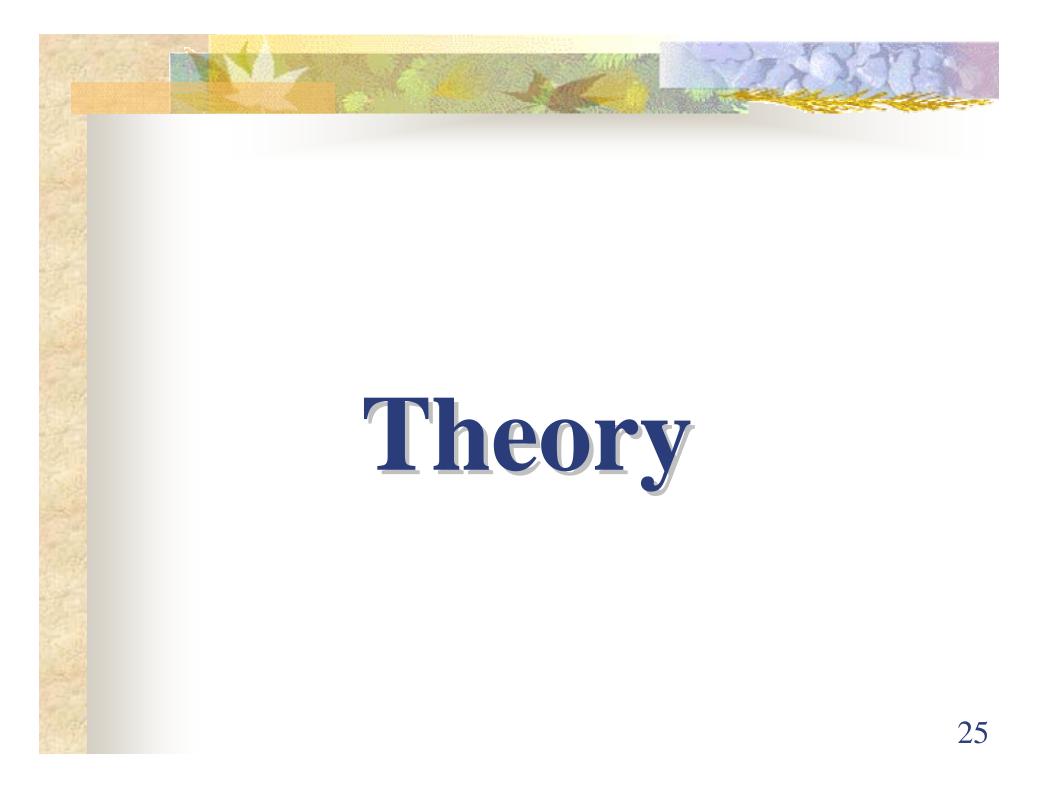
Example of a similarity measure $f(C_i) = \sum_j 1_j + \frac{\epsilon}{N^{\pm}} \sum_{jk \in C_i} l_{jk}^{\pm 1}$ Add pair epistasis: $+ \rightarrow$ repulsion; \rightarrow attraction 0.01 0.0 0.005 0.005 $\epsilon = 0.75$ -0.005 -0.005 ŝ Ş $\epsilon = 0.3$ -0.01 "Attraction" -0.01 "Repulsion" -0.015 -0.015 $p_c = 1.$ $p_c = 0.$ -0.02 -0.02 -0.025 L 0 -0.025 Ô. 20 15 20 25 generation generation

Results for $p_c = 1$ with no epistasis are similar to those with $p_c = 0$ and an epistatic repulsion between bits Results for $p_c = 0$ with no epistasis are similar to those with $p_c = 1$ and an epistatic attraction between bits

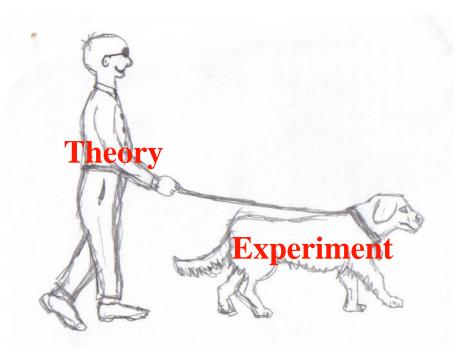
UNIVERSALITY



Without crossover - no preference for one size versus another With crossover – short blocks preferred

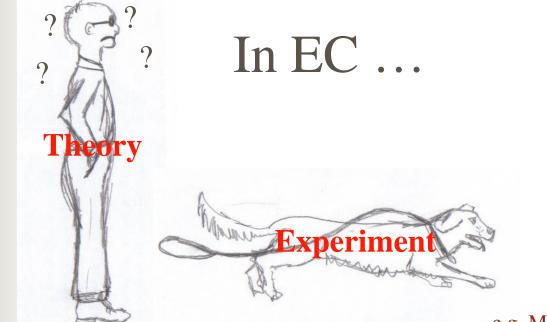


The Problem of Theory...

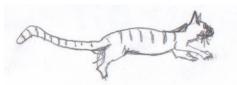


The "ideal"

The Problem of Theory...



New Applications New Algorithms



e.g. Multi-Resource Traveling Gravedigger Problem with Variable Coffin Size

"Most algorithms are NEVER used (except by the people who created them)" - Darrell Whitley, GECCO 2003 tutorial

The Problem of Theory... The EC Expectation Gap



What theoreticians think practitioners are and what practitioners think theoreticians should be

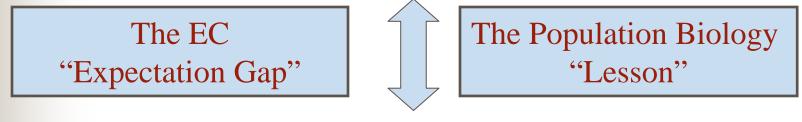
What practitioners think theoreticians are and what theoreticians think practitioners should be

The Problem of Theory...

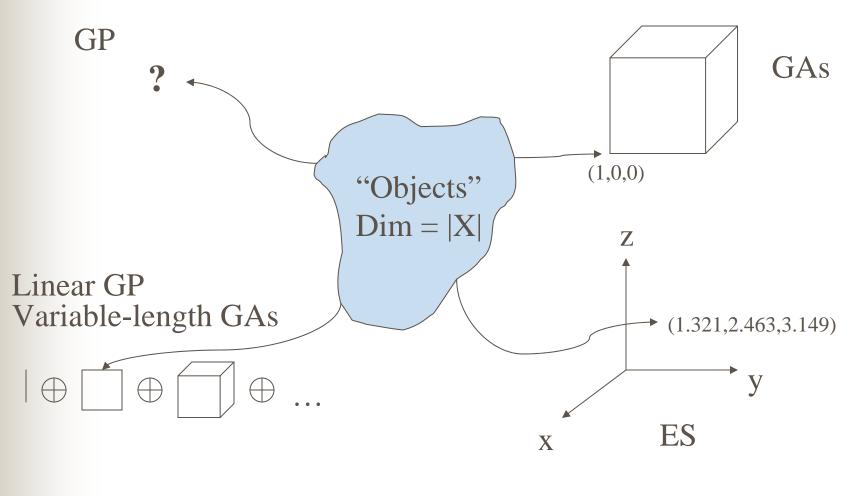
"Professors in every branch of the sciences prefer their own theories to truth; the reason is that their theories are private property, but truth is common stock" – Charles Caleb Colton, Lacon (1825).

"It is the nature of an hypothesis, when once a man has conceived it, that is assimilates everything to itself as proper nourishment, and, from the first moment of your begetting it, it generally grows the stronger by everything you see, hear, read, or understand" – Laurence Sterne, Tristram Shandy (1767).

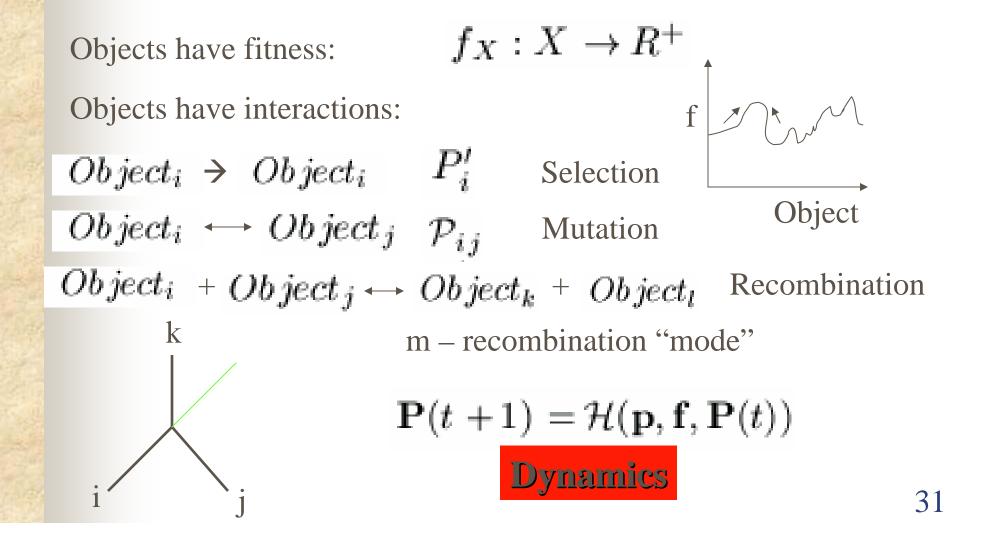
"EC theory is hard!" - Chris Stephens (most weeks).



"How does this help practitioners...?" – most referees



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$$P_{I}(t+1) = M_{I}^{J} \left((1-p_{c})P_{J}' + p_{c} \sum_{M} \sum_{K,L} \frac{1}{2} (p(M) + p(\bar{M})) \lambda_{J}^{KL}(M) P_{K}' P_{L}' \right)$$

- Probability to find "object" I

 $P_{I}(t+1)$

 $\lambda_I^{KL}(M).$

 P'_J

 M_I^J

p(M)

 $p_{c_{\perp}}$

- Probability to select "object" J
- Probability to mutate "object" J to "object" I
- Probability for recombination mask/mode M
- Probability to implement recombination
- Probability that given "objects" K and L and mode M "object" J is created (= 0, 1).

Sums are over all possible recombination modes and all objects J and K. e.g. for GA and homologous crossover 2^{3N} terms

$$P_{I}(t+1) = M_{I}^{J} \left((1-p_{c})P_{J}^{\prime} + p_{c} \sum_{M} \sum_{K,L} \frac{1}{2} \left(p(M) + p(\bar{M}) \right) \lambda_{J}^{KL}(M) P_{K}^{\prime} P_{L}^{\prime} \right)$$

Probability that "object" J is mutated to "object" I

Probability that "object" J is cloned

Probability that parent "objects" K and L are selected and "mixed" to form child "object" J via mode M

Example: 2-bit GA with p(M) = 1/4 for all M, I = (11) $\lambda_{(11)}((00)) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix}$ $\lambda_{(11)}((01)) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix}$ Ugly! $\lambda_{(11)}((11)) = \lambda_{(11)}((00))^T$ $\lambda_{(11)}((10)) = \lambda_{(11)}((01))^T$

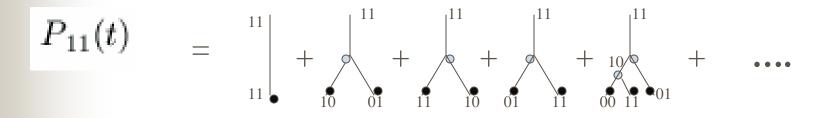
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Can integrate the equation and represent the solution graphically -

$$\begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{J} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{t} \\ \mathbf{J} & \mathbf{I} \end{bmatrix} = \begin{bmatrix} \mathbf{G}_{IJ}(t, t') & \mathbf{T} \end{bmatrix}$$
 Probability that object J propagates from t to t' and converts to I on the way
$$\mathbf{O} = \frac{1}{2} \left(p(M) + p(\bar{M}) \right) \lambda_J^{KL}(M) \frac{f_K}{\bar{f}(t)} \frac{f_L}{\bar{f}(t)}$$
 Measures strength of interaction between objects J, K and L

$$\mathbf{K} \bullet = \mathbf{P}_I(t)$$

Iterate ... by recursively substituting for • until get to t = 0Example – 2-bits 1-point crossover



Each tree tells us the probability of forming 11 by a given process. In principle can see which processes are most important. But ... Tree depth bounded only by t! COMPLICATED!

EC Theory – the "Bare Necessities"

General (Feynman) rules:

- 1) Draw all possible tree diagrams that contribute to creation of "object"
- 2) For each internal line attach a propagator $G_{IJ}(t,t') = (1-p_c)^{t-t'} \frac{(\mathbf{FM})_{IJ}^{t-t'}}{\sum_{I} (\mathbf{FM})_{IJ}^{t-t'} P_J(t')}$
- 3) To each vertex \bigcirc attach a weight $\frac{1}{2} (p(M) + p(\bar{M})) \lambda_J^{KL}(M) \frac{f_K}{\bar{f}(t)} \frac{f_L}{\bar{f}(t)}$
- 4) To each root attach a factor $P_I(t')$
- 5) Carry out integration over time for all vertices

ALL CLEAR!

EC Theory – the "Bare Necessities"

So what do we have so far from the "microscopic" theory?

Exact Mathematically rigorous Unifies Phenomena Intuitive Predicts well Useful for Practitioners Yes Yes? Yes/No No No No

EC Theory – the "old stuff"

Let's compare with the old Schema theorem and Building Block Hypothesis approach

Exact Mathematically rigorous Unifies Phenomena Intuitive Predicts well Useful for Practitioners

No Yes ?? Yes/No Yes/No No ? Yes/No

Coarse Graining

Coarse Graining

Why?

What?

How?

Coarse Graining Why?

1. Emergence of "Effective Degrees of Freedom" (EDOF)/Collectivity/Universality

2. Curse of dimensionality/intractable dynamics

Coarse-grained degrees of freedom are combinations of the underlying "microscopic" degrees of freedom. EDOF are those coarse-grained degrees of freedom that are important for the dynamics

Coarse Graining What?

- 1. "Direct" dimensional reduction
- 2. Phenotypes
- 3. Schemata
- 4. Hyperschemata
- 5. Building Blocks
- 6. Lowest cumulants of fitness distribution
- 7. "Normal (e.g. Walsh) modes"
- 8. Others

What is the most natural coarse graining depends on the operators and their corresponding parameters, the fitness landscape and the population.

Coarse Graining How?

- 1. Phenotype Dynamics
- 2. Schemata Dynamics
- 3. Hyperschemata Dynamics
- 4. Building Block Dynamics
- 5. Aggregation of Markov chain
- 6. Truncation of cumulants
- 7. Walsh analysis
- 8. Others



Coarse Graining By Coordinate Transformations

Identifying "Effective Degrees of Freedom"



$$P_{I}(t+1) = M_{I}^{J} \left((1-p_{c})P_{J}' + p_{c} \sum_{M} \sum_{K,L} \frac{1}{2} (p(M) + p(\bar{M})) \lambda_{J}^{KL}(M) P_{K}' P_{L}' \right)$$

is COVARIANT, i.e. has the same content in ANY coordinate system $\mathbf{P}(t)$ is INVARIANT in any coordinate system, its components $P_I(t)$ however, do change

$$P_{I} = \sum_{J} \Lambda_{I}^{J} P_{J}$$

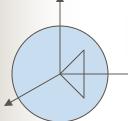
$$Y$$

$$A = \sum_{J} \Lambda_{I}^{J} P_{J}$$

$$X = \sum_{J} \Lambda_{J}^{J} P_{J}$$

$$X = \sum_{J} \Lambda_{J}^{J}$$

• Appropriate choice of coordinate system can make manifest the **Effective Degrees of Freedom** and greatly facilitate calculations



 $\begin{array}{ll} (x,y,z) \rightarrow (R,\theta,\phi) & & & & & \\ \hline \end{array}$ Exploit spherical symmetry $u(k) = \frac{1}{\sqrt{2}} \sum_{x_i} \exp(ikx_i)u(x_i) \end{array}$

Normal modes - waves

Coordinate system used up to now is the "object" system – e.g. strings, trees etc. \bigcirc OK when EDOF are strings, trees etc. **Appropriate in "strong" selection regime**

Coarse graining via Coordinate Transformations <u>Mutation</u>...

Walsh basis (for fixed length binary strings)

Coordinate transformation matrix is orthonormal

$$\mathbf{M} = \begin{pmatrix} (1-p)^2 & p(1-p) & p(1-p) & p^2 \\ p(1-p) & (1-p)^2 & p^2 & p(1-p) \\ p(1-p) & p^2 & (1-p)^2 & p(1-p) \\ p^2 & p(1-p) & p(1-p) & (1-p)^2 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-2p) & 0 & 0 \\ 0 & 0 & (1-2p) & 0 \\ 0 & 0 & (1-2p)^2 \end{pmatrix}$$

"Frequencies" of normal modes

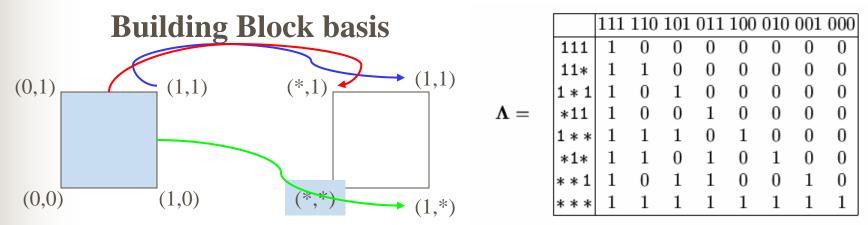
EDOF are discrete versions of normal modes

In Walsh basis ...

- Mutation matrix is diagonal
- Selection matrix is non-diagonal
- Crossover O(n) Walsh coefficients made up from crossing O(m) and O(n-m) coefficients
- "Normal modes" not simply interpretable
- Useful for landscape analysis
- Gives exact solution for mutation only

Appropriate in "strong" mutation regime

Coarse graining via Coordinate Transformations <u>**Crossover**</u>...



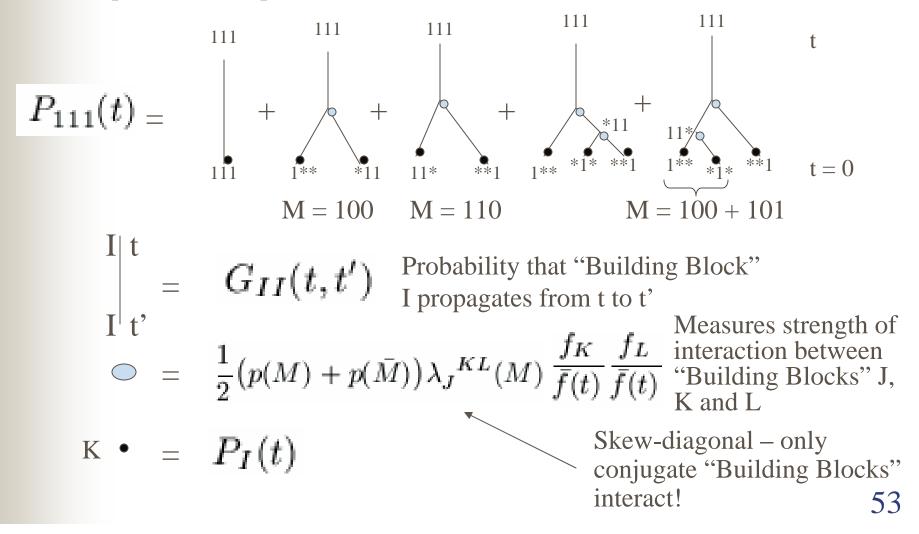
 $\tilde{\lambda}_{\alpha\beta\gamma}(m) = \Lambda_{\alpha i} \lambda_{ijk} \Lambda_{\beta j}^{-1} \Lambda_{\gamma k}^{-1} = 0$ unless γ is the complement of β with respect to α and β is equivalent to mExample: 2-bit GA with p(M) = 1/4 for all M, I = (11)

$$\lambda_{(11)}^{\rm m} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

• In Building Block basis interaction matrix is skew diagonal

• Mask simply tells you which skew diagonal elements interact, e.g. mask 101011 points to building block 1*1*11 which interacts with *1*1** to give 111111

Iterate ... by recursively substituting for • until get to t = 0Example – 3-bits 1-point crossover



Each tree tells us the probability of forming 111 by a given process. In principle can see which processes are most important. Tree depth bounded by N. MUCH SIMPLER THAN STRING (OBJECT) BASIS!

For a particular recombination "channel" (mode) whether recombination contributes positively or negatively to the effective fitness is determined by

$$\Delta(m) = P'_{i}(t) - P'_{i_{m}}(t)P'_{i_{\bar{m}}}(t)$$

$$\overset{\text{SWLD (Selection Weighted Linkage Disequilibrium)}}{\underset{\text{BBs of i}}{\overset{\text{SWLD (Selection Weighted Linkage Disequilibrium)}}}$$

If $\Delta(m) < 0$ "channel" is non-deceptive \Box long schemata preferred (see page 21)

If $\Delta(m) > 0$ "channel" is deceptive; deception – just like BBs - is dynamic

Standard Two-bit deception: $f(0^*) > f(1^*) \qquad \square \Delta(m) > 0$

i.e. $P'_{11}(t) - P'_{1*}(t)P'_{*1}(t) > 0$

ALL CLEAR!

Coarse graining via Coordinate Transformations In Building Block basis ...

- Building Blocks schemata are the natural EDOF for recombination
- They are dynamical and not necessarily "short" or "fit"
- They are the ONLY way in which higher order "objects" can be built up by recombination
- Generically, the "construction" term dominates
- BBB is complete but not orthonormal
- There are |X| equivalent BBB (related by simple permutations)
- Only "dual" objects (i.e. conjugate BBs) interact, e.g. line and plane intersect at a point
- Gives exact solution for recombination only

Appropriate in "strong" crossover regime

Coarse Graining By Projections

Making intractable dynamics more tractable



Introduce a general coarse-graining operator $\mathcal{R}(\eta, \eta')$ Which coarse grains from the variables $\eta \in X_{\eta}$ to the variables $\eta' \in X_{\eta'} \subset X_{\eta}$ Given two such coarse grainings:

 $\mathcal{R}(\eta, \eta') P_{\eta}(t) = P_{\eta'}(t) \qquad \qquad \mathcal{R}(\eta, \eta'') P_{\eta}(t) = P_{\eta''}(t)$

but
$$\mathcal{R}(\eta', \eta'')P_{\eta'}(t) = P_{\eta''}(t)$$

hence

$$\mathcal{R}(\eta,\eta'') = \mathcal{R}(\eta,\eta')\mathcal{R}(\eta',\eta'')$$

i.e. coarse grainings form a semi-group – **"Renormalization Group"** 60

Dynamics coarse grains via

$$\mathcal{R}(\eta, \eta') \mathcal{H}(\mathbf{p}, \mathbf{f}, \mathbf{P}_{\eta}(t))$$

If this can be written in the form

$$\mathcal{H}(\mathbf{p}',\mathbf{f}',\mathbf{P}_{\eta'}(t))$$

with suitable "renormalizations"

$$f \longrightarrow f'$$
 and $p \longrightarrow p'$

then the dynamics is form covariant or invariant under the coarse graining. If $\mathbf{f} = \mathbf{f}'$ and $\mathbf{p} = \mathbf{p}'$ dynamics is "compatible"

Examples: Compatible Coarse grainings

- 1. Selection and Phenotypes
 - Unitation, e.g. $(2^N \text{ genotypes} \rightarrow (N+1) \text{ phenotypes})$
 - Eigen model (NIAH), e.g. (2^N) genotypes $\rightarrow 2$ phenotypes
- 2. Mutation and Crossover and Schemata
 - 2^N genotypes $\rightarrow 2^{N_2}$ coarse grained genotypes

Incompatible Coarse grainings

1. Selection, Mutation and Crossover and Schemata

- 2^N genotypes $\rightarrow 2^{N_2}$ coarse grained genotypes
- $f_{\alpha} = \mathcal{R}(x, \alpha) f_x = \sum_{x \in \alpha} f_x P_x(t) / \sum_{x \in \alpha} P_x(t)$. time-dependent

In BBB for 1-point crossover...

 $P_{111}(t+1) = (1-p_c)P_{111}(t) + \frac{p_c}{2}(P_{1**}(t)P_{*11}(t) + P_{11*}(t)P_{**1}(t))$ "Zap" (projection) $111 \rightarrow 11*$ $P_{11*}(t+1) = (1-p_c)P_{11*}(t) + \frac{p_c}{2}(P_{1**}(t)P_{*1*}(t) + P_{11*}(t)P_{***}(t))$ $\implies P_{11*}(t+1) = (1-\frac{p_c}{2})P_{11*}(t) + \frac{p_c}{2}P_{1**}(t)P_{*1*}(t)$

Note – coarse grained (projected) 3-bit equation same as "microscopic" 2-bit equation with "renormalization" $p_c \rightarrow \frac{p_c}{2}$ $P_{11}(t+1) = (1-p_c)P_{11}(t) + p_cP_{1*}(t)P_{*1}(t)$

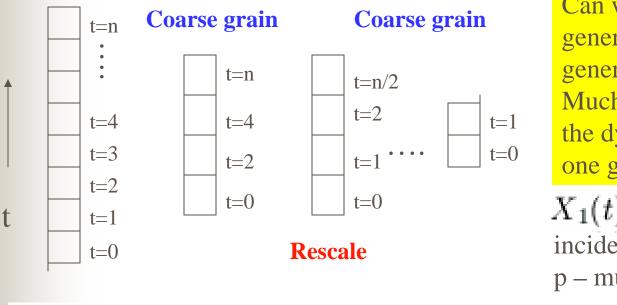
FORM INVARIANCE

• Generalizes to the case of variable-length GAs and GP; Building Block Schemata \rightarrow Building Block Hyperschemata; "form invariance" of equations over different types of EA and form invariant upon coarse graining to schemata;

• Gives exact form of the Schema Theorem and generalizes it to EAs other than GAs

• Neglecting the "construction" terms leads to standard Holland Schema Theorem as an approximation

Coarse Graining by Projection - "Divide and Conquer" Example



Example: 1-bit

Can we coarse grain an n generation problem to a one generation problem? Much easier to solve the dynamics over only one generation!

 $X_1(t)$ – unnormalized incidence vector p – mutation rate

$$\begin{pmatrix} X_1(t+2) \\ X_0(t+2) \end{pmatrix} = \begin{pmatrix} (1-p)f_1 & pf_0 \\ pf_1 & (1-p)f_0 \end{pmatrix}^2 \begin{pmatrix} X_1(t) \\ X_0(t) \end{pmatrix}$$

Evolves bit two time steps in landscape f(1), f(0) with mutation p 65

Coarse Graining by Projection - "Divide and Conquer"

$$\begin{pmatrix} X_1(t'+1) \\ X_0(t'+1) \end{pmatrix} = \begin{pmatrix} (1-p_1')f_1' & p_0'f_0' \\ p_1'f_1' & (1-p_0')f_0' \end{pmatrix} \begin{pmatrix} X_1(t') \\ X_0(t') \end{pmatrix}$$

Evolves bit one time step in "renormalized" landscape f'(1), f'(0) with asymmetric mutation rates p'(1) and p'(0)

Equivalent dynamics (all we did was "change names"!, i.e. "renormalize")

$$f_1' = (1 - p_1)f_1^2 + p_1f_0f_1$$
$$f_0' = (1 - p_0)f_0^2 + p_0f_0f_1$$
$$p_1' = p_1\left(\frac{(1 - p_1)f_1 + (1 - p_0)f_0}{(1 - p_1)f_1 + p_1f_0}\right)$$
$$p_0' = p_0\left(\frac{(1 - p_0)f_0 + (1 - p_1)f_1}{(1 - p_0)f_0 + p_0f_1}\right)$$

ALL CLEAR!

Coarse Graining by Projection - "Divide and Conquer"

Evolution of mutation/selection GA over n time steps with fitness landscape f(1), f(0) and mutation rates p(2) and p(1) is same as that of a GA with "renormalized" landscape and mutation rates, f'(1), f'(0), p'(2), p'(1) over n/2 time steps!



Fixed points of Renormalization Group transformation: $|\ln(f(1)/f(0))| = 0$, p(1) = p(0) = 0; no selection/mutation – "FERROMAGNETIC" $|\ln(f(1)/f(0))| = \text{infinity}$, p(1) = p(0) = 0; strong selection – "FROZEN" $|\ln(f(1)/f(0))| = \text{constant}$, p(1) + p(0) = 1; neutral evolution – "PARAMAGNETIC"

Coarse Graining by Projection - "Divide and Conquer"

- Iterated map takes you to a problem with fewer degrees of freedom NOT associated with "trivial" symmetries.
- Linearization around the fixed points of the equations give the late time asymptotics
- Can understand "universality" of behaviour
- Can coarse grain in both "space" and "time"
- Coarse graining can almost never be done exactly
- Have to decide what coarse graining is most appropriate for a given model

EC Theory – Coarse-grained

So what do we have so far?

Exact Mathematically rigorous Unifies Phenomena Intuitive Predicts well Useful for Practitioners Yes Yes Yes Yes No Yes/No

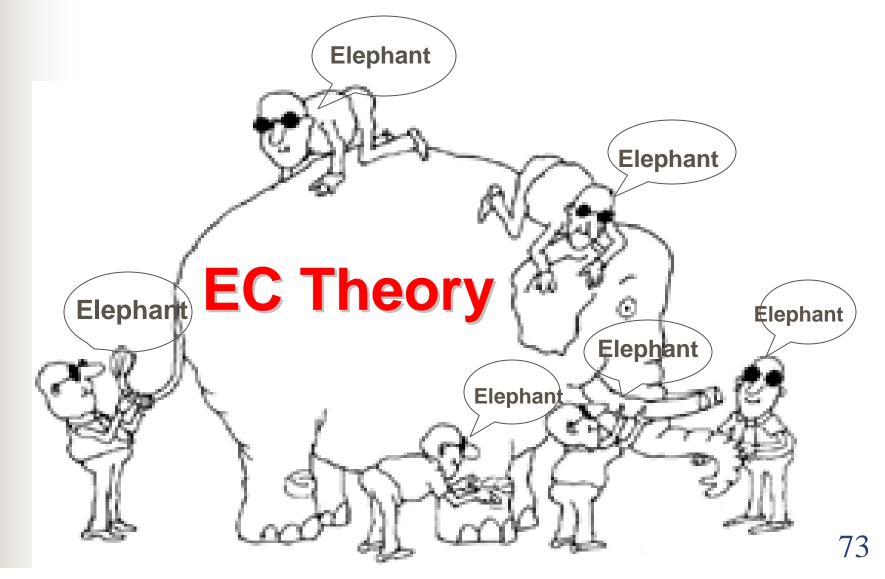
The Bottom Line ...

- Present taxonomy in EC theory is inadequate
- Taxonomy can be greatly improved by using "distance" measures
- Taxonomy and universality can also be much better understood using an appropriate coarse graining
- Coarse grained genetic dynamics unifies and makes compatible different areas of EC and different previous theoretical formulations
- GAs and GP different sides of the same coin
- Old Schema theory/BB hypothesis and Vose type models
 different sides of the same coin
- Coarse graining and the Renormalization Group offer a generic methodology for approximating genetic dynamics

The Bottom Line ...

- Theory in EC is <u>NOT</u> particularly well developed. If it was there wouldn't be such a huge expectation gap between theoreticians and practitioners. No systematic approximation techniques for attacking problems from first principles
- Practitioners have to realize what is and isn't theoretically feasible (theoretical population biologists have spent nearly a century achieving things that "practitioners" would scorn).
- Practitioners could really help by stress testing theory (too much testing of theory in the hands of people who make up the theory and too much testing of "never to be used" algorithms by practitioners)

The Bottom Line ...



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