智能优化算法及其应用

Intelligent Optimization Algorithms and Their Applications

龚文引 (教授、博士生导师)

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1. 大纲

- 优化（Optimization）
- 智能优化（Intelligent Optimization）
- 算法（Algorithms）
- 智能优化方法相关应用（Applications）
- 小结

2. 优化（Optimization）

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- 智能优化（Intelligent Optimization）
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2. 优化（Optimization）

优化的重要性

- 人类的一切活动都是认识世界和改造世界的过程。
- 一切学科都是建模与优化在某个特定领域中的应用。

2. 优化（Optimization）

(a) 共振 (b) 坍塌 (c) 新桥

塔科马大桥共振坍塌事故

- 一座雄伟的单跨桥，居然被阵并不太大风吹得像波浪一样起伏。1940年11月7日，美国华盛顿州塔科马大桥因风振致毁。该于1940年7月1日建成通车。
- 机械结构模态分析、谐响应分析、各种工况下结构的强度分析

2. 优化（Optimization）

无处不在的优化问题

优化问题普遍存在：

- 和朋友到鲁磨路吃饭，选择哪家饭点最好？
- 怎样找到最好的女/男朋友？
- 有 10 万元，现要投资 5 支股票，怎样的投资策略才能获得最佳收益？
- 怎样设计跑车的外形才能以最大程度减小空气阻力，同时最大程度增加附着力？

2. 优化（Optimization）

一般形式

许多生产计划与管理问题都可以归纳为最优化问题，其内容包括线性规划、整数线性规划、非线性规划、动态规划、变分法、最优控制等。

其中，函数/连续优化问题（如结构设计问题）的一般形式为：

$$\min \quad \mathbf{f}(\mathbf{x}) = \{f_1(\mathbf{x}), \cdots, f_k(\mathbf{x})\}^{\mathsf{T}} \tag{1}$$

满足

$$\begin{cases} g_i(\mathbf{x}) \le 0, i = 1, \cdots, p \\ e_j(\mathbf{x}) = 0, j = 1, \cdots, q \end{cases}$$

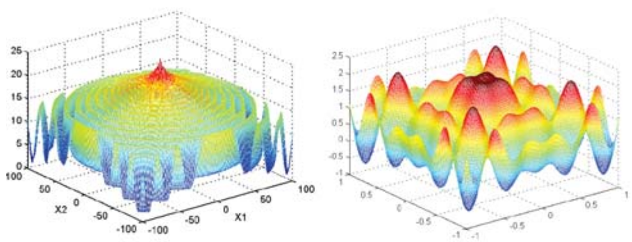
其中 $\mathbf{x} = \{x_1, \cdots, x_n\}^{\mathsf{T}}$，$n$ 是自变量个数，k 是目标函数个数，p 是不等式约束个数，q 是等式约束个数。

2. 优化（Optimization）

函数优化（Function optimization）

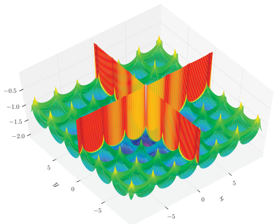
令 $\mathbb{S}$ 是 $\mathbb{R}^n$ 上的有界子集，$f: \mathbb{S} \to \mathbb{R}$ 为 n 维实数函数，所谓函数 f 在 $\mathbb{S}$ 上的最大值就是寻找点 $\mathbf{x}_{\max} \in \mathbb{S}$ 使得：

$$\forall \mathbf{x} \in \mathbb{S}: \quad f(\mathbf{x}_{\max}) \ge f(\mathbf{x})$$



2. 优化（Optimization）

$$f(x,y) = -0.0001\left[\left|\sin(x)\sin(y)\exp\left(\left|100-\frac{\sqrt{x^2+y^2}}{\pi}\right|\right)\right|+1\right]^{0.1}, \quad x,y\in[-10,10]$$



$$\text{min} = \begin{cases} f(1.34941,-1.34941) & = -2.06261 \\ f(1.34941,1.34941) & = -2.06261 \\ f(-1.34941,1.34941) & = -2.06261 \\ f(-1.34941,-1.34941) & = -2.06261 \end{cases}$$

https://en.wikipedia.org/wiki/Test_functions_for_optimization

2. 优化（Optimization）

一般形式

组合/离散优化问题（如物流、背包、TSP问题）的一般形式为：
Find:

$$s^*, \forall s\in\Omega, C(s^*) = \min C(s), \Omega = \{s_1, s_2, \cdots, s_n\} \tag{2}$$

2. 优化（Optimization）

组合优化（Combinational optimization）

所谓组合优化，是指在离散的、有限的数学结构上，寻找一个（或一组）满足给定约束条件并使其目标函数值达到最大或最小的解。

一般来说，组合优化问题通常带有大量的局部极值点，往往是不可微的、不连续的、多维的、有约束条件的、高度非线性的 NP 完全（难）问题，因此，精确地求解组合优化问题的全局最优解的“有效”算法一般是不存在的。

2. 优化（Optimization）

组合优化分类

- 集覆盖问题（set-covering problem）
- 装箱问题（bin-packing problem）
- 背包问题（knapsack problem）
- 指派问题（assignment problem）
- 旅行商问题（traveling salesman problem）
- 影片递送问题（film delivery problem）
- 最小生成树问题（minimum span tree problem）
- 图划分问题（graph partitioning problem）
- 车间调度问题（job-shop scheduling problem）

2. 优化（Optimization）

旅行商问题，即TSP问题（Traveling Salesman Problem）又称货郎担问题，是数学领域中著名问题之一。假设有一个旅行商人要拜访 n 个城市，他必须选择所要走的路径，路径的限制是每个城市只能拜访一次，而且最后要回到原来出发的城市。路径的选择目标是要求得的路径路程为所有路径之中的最小值。

https://en.wikipedia.org/wiki/Travelling_salesman_problem

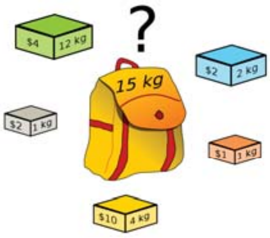
2. 优化（Optimization）

TSP 问题的数学模型

- min $\sum_{i \neq j} d_{ij} \cdot x_{ij}$ // 优化目标
- 满足：
  - $\sum_{j=1}^{n} x_{ij} = 1, i = 1, \cdots, n$ // 只从 i 城市出发一次
  - $\sum_{i=1}^{n} x_{ij} = 1, j = 1, \cdots, n$ // 只走入 j 城市一次
  - $\sum_{i,j \in s} x_{ij} \leq |s| - 1, 2 \leq |s| \leq n - 1, s \subset \{1, \cdots, n\},$ // 在任意城市子集中不形成回路
  - $x_{ij} \in \{0, 1\}, i, j = 1, \cdots, n, i \neq j$ // 决策变量
- 其中：
  - d_{ij} 是城市 i 与城市 j 之间的距离
  - $x_{ij} = 1$ 表示走城市 i 与城市 j 之间的路径，反之亦然
- 对称距离 TSP: $d_{ij} = d_{ji}, \forall i, j$
- 非对称距离 TSP: $d_{ij} \leq d_{ji}, \exists i, j$

2. 优化（Optimization）

背包问题(Knapsack problem)是一种组合优化的NP完全问题。问题可以描述为：给定一组物品，每种物品都有自己的重量和价格，在限定的总重量内，我们如何选择，才能使得物品的总价格最高。



https://en.wikipedia.org/wiki/Knapsack_problem

2. 优化（Optimization）

背包问题的数学模型

- max $\sum_{i=1}^{n} w_i \cdot x_i$ // 优化目标
- 满足：
  - $\sum_{i=1}^{n} w_i \cdot x_i \leq W$ // 约束条件
  - $x_i \in \{0, 1\}, i = 1, \cdots, n$ // 决策变量

2. 优化（Optimization）

单车间调度问题（Job-shop scheduling problem, JSP）是NP难问题，无最优解精确算法。一般类型的JSP问题可表达为：n个工件在m台机器上加工，每个工件有特定的加工工艺，每个工件加工的顺序及每道工序所花时间给定，安排工件在每台机器上工件的加工顺序，使得某种指标最优。

https://en.wikipedia.org/wiki/Job_shop_scheduling

2. 优化（Optimization）

优化的定位

优化技术是一种以数学为基础，用于求解各种工程问题优化解的应用技术。任何控制与决策问题本质上都是优化问题！

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优化问题的三要素

1. 决策变量：决定优化问题的影响因素
2. 约束条件：问题优化时的一些约束限制
3. 优化目标：拟达到的目标（目标函数）

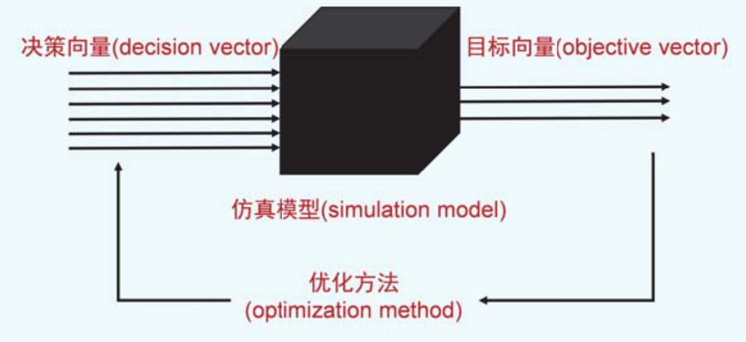
2. 优化（Optimization）

实际优化问题的特点

- 目标函数和约束函数不可微（non-differentiable）
- 约束函数非线性（nonlinear）
- 搜索空间离散或非连续（discrete/discontinuous）
- 混合变量（整型、实型、布尔等）
- 大量约束和变量
- 目标函数多峰（multimodal）
- 目标函数和约束函数计算昂贵（computationally expensive）

2. 优化（Optimization）

实际优化问题的特点



2. 优化（Optimization）

优化问题的复杂性

- 工程优化问题存在诸多复杂性
- 传统优化方法质量差、效率低、对初值依耐性强
- 实现全局、高效、鲁棒优化极其困难

3. 智能优化（Intelligent Optimization）

为什么研究智能优化方法？

传统最优化面临新挑战：实际问题

- 离散性（discrete）问题–主要指组合优化
- 不确定性（uncertain）问题–随机性数学模型
- 大规模（large-scale）问题：超高维
- 动态优化（dynamic optimization）问题
- 容易陷入局部最优解
- 需要知道目标函数和约束函数的一阶或二阶导数

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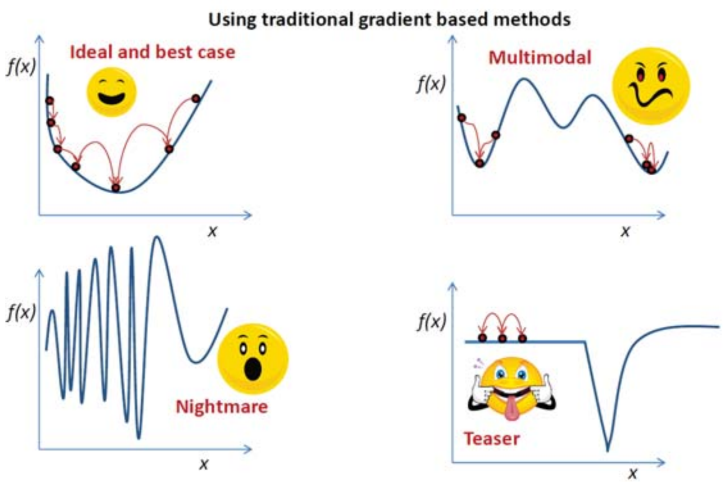
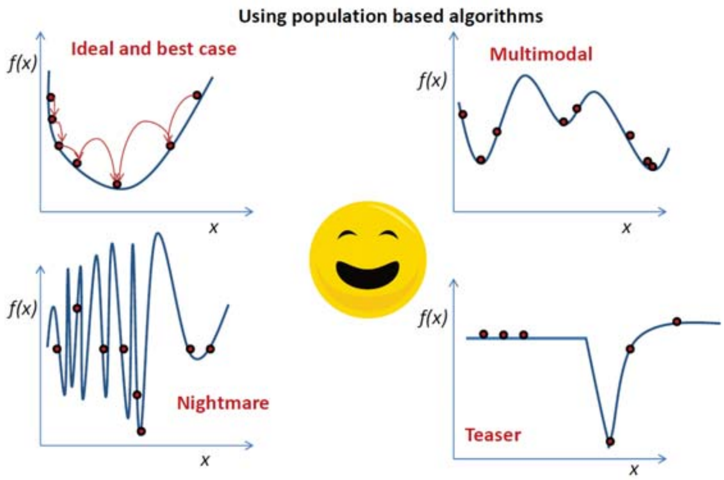
智能优化方法

- 追求满意–近似解（approximate solution）
- 实用性强–解决实际问题

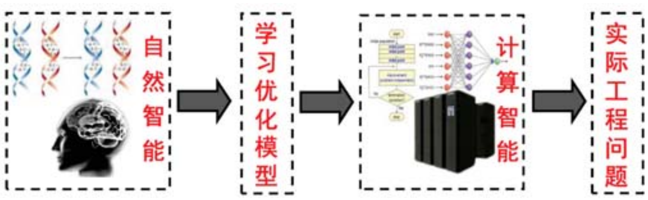
3. 智能优化（Intelligent Optimization）



3. 智能优化（Intelligent Optimization）



3. 智能优化（Intelligent Optimization）



人工智能研究的重要途径和科学研究的前沿

- 欧盟第七框架计划 2011 年启动“自然启发的计算"项目
- 俄罗斯 2011 年启动“2045 人造大脑计划"
- 美国 2013 年启动新一轮的“脑研究计划"
- 国家中长期科技发展规划（2006-2020）重点领域（“智能信息处理"、“脑科学与认知科学"）

3. 智能优化（Intelligent Optimization）

Science AAAS

A Biological Solution to a Fundamental Distributed Computing Problem
Yehuda Afek *et al.*
Science **331**, 183 (2011);
DOI: 10.1126/science.1193210

A Biological Solution to a Fundamental Distributed Computing Problem

Yehuda Afek,[1*] Noga Alon,[1,2*] Omer Barad,[3*] Eran Hornstein,[3] Naama Barkai,[3†] Ziv Bar-Joseph[4†]

Computational and biological systems are often distributed so that processors (cells) jointly solve

while only using one-bit messages. Our findings suggest that simple and efficient algorithms can be developed on the basis of biologically derived insights.

selection, we derived a fast algorithm for MIS selection that combines two attractive features. First,
processors do not need to know their degree; second
while only using one-bit messages. Our findings sugg
can be developed on the basis of biologically derive

普林斯顿高等研究院、卡耐基梅隆大学等机构的科学家2011年在《Science》的论文指出，从生物启发的角度可以建立简单、高效的算法

3. 智能优化（Intelligent Optimization）

Science AAAS

Learning from Nature
Jeffrey O. Kephart
Science **331**, 682 (2011);
DOI: 10.1126/science.1201003

COMPUTER SCIENCE

Learning from Nature

Jeffrey O. Kephart

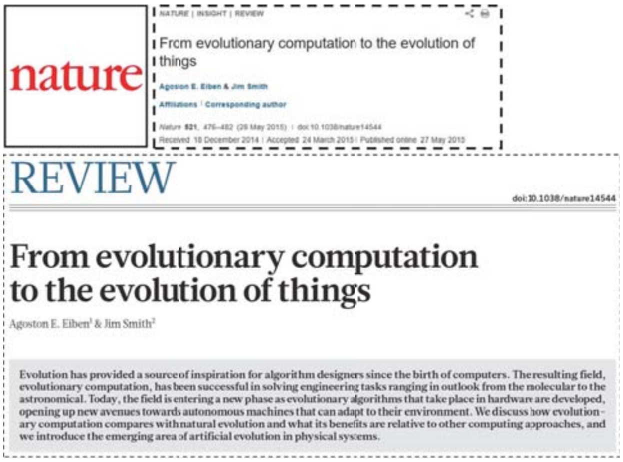
The tradition of biologically inspired computing extends back more than half a century to the original musings of Alan Turing about artificial intelligence and John von Neumann's early work on self-replicating cellular automata in the 1940s. Since then, computer scientists have frequently turned to biological processes for inspiration. Indeed, the names of major subfields of computer science—such as artificial neural networks, genetic algorithms, and evolutionary computation—attest to the influence of biological analogies.

Recently, Afek *et al.* (1) offered an example of how biology can inform computer sci-

computer viruses. In both cases, harnessing a biological analogy—and treating it with both respect and some skepticism—led to very effective computer algorithms. Apparently, to truly profit from the lessons of Mother Nature, we must be judicious, not slavish, in applying analogies.

IBM自主计算技术的负责人Kephart发表在《Sceince》的论文认为，通过模拟生物可以建立非常高效的计算机算法

3. 智能优化（Intelligent Optimization）


nature

NATURE | INSIGHT | REVIEW

From evolutionary computation to the evolution of things

Agoston E. Eiben & Jim Smith

Affiliations | Corresponding author

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REVIEW

doi:10.1038/nature14544

From evolutionary computation to the evolution of things

Agoston E. Eiben[1] & Jim Smith[2]

Evolution has provided a source of inspiration for algorithm designers since the birth of computers. The resulting field, evolutionary computation, has been successful in solving engineering tasks ranging in outlook from the molecular to the astronomical. Today, the field is entering a new phase as evolutionary algorithms that take place in hardware are developed, opening up new avenues towards autonomous machines that can adapt to their environment. We discuss how evolutionary computation compares with natural evolution and what its benefits are relative to other computing approaches, and we introduce the emerging area of artificial evolution in physical systems.

3. 智能优化（Intelligent Optimization）

启发（Inspiration）

受自然界中各种现象（生物、物理、化学、艺术等）的启发来设计元启发式（meta-heuristic）算法，将是求解实际复杂问题的有效途径。

自然界中的优化

- 鸟：最小化飞行阻力
- 座头鲸：最大化机动性
- 硬鳞鱼：最小化阻力、最大化外骨骼坚硬度
- 翠鸟：最小化微压力波

3. 智能优化（Intelligent Optimization）

智能优化（Intelligent optimization）定义

智能优化方法是基于计算智能 (Computation Intelligence) 的机制求解复杂优化问题最优解或满意解的方法。学术界也称之为 meta-heuristics.

王凌. 中国大百科全书（第三版）. 2018.

3. 智能优化（Intelligent Optimization）

智能优化原理

智能优化方法通过对生物、物理、化学、社会、艺术等系统或领域中的相关行为、功能、经验、规则、作用机理的认知，揭示优化算法的设计原理，在特定问题特征的导引下提炼相应的特征模型，设计智能化的迭代搜索性优化方法。

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智能优化目标

通过智能化的搜索方式，力争取得优化性能的“稳、快、准"，即优化结果的一致性、优化效率的快速性、优化质量的全局性。

3. 智能优化（Intelligent Optimization）

智能优化方法主要特点

1) 基于群体的搜索
2) 个体之间相互共享信息，同时相互竞争资源
3) 优胜劣汰，适者生存
4) 隐并行性

4. 算法（Algorithms）

优化（Optimization）

智能优化（Intelligent Optimization）

算法（Algorithms）

智能优化方法相关应用（Applications）

小结

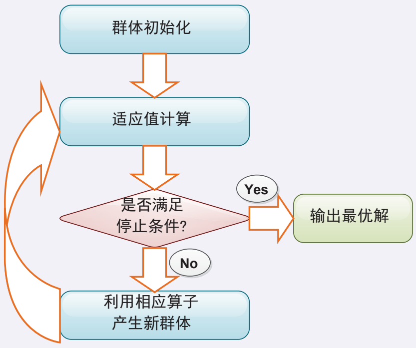
4. 算法（Algorithms）

智能优化步骤

- 建模（特征/知识）
  - 决策变量、目标函数、约束条件、问题知识
- 框架设计
- 操作设计
- 参数设置
- 策略设计
- 试验设计
- 测试比较与应用

4. 算法（Algorithms）

基于群体的智能优化算法基本框架



4. 算法（Algorithms）

进化（演化）算法 (Evolutionary algorithms)

- 遗传算法（genetic algorithm）
- 遗传编程（genetic programming）
- 进化规划（evolutionary programming）
- 进化策略（evolution strategy）
- 差分进化（differential evolution）
- 分布估计算法（estimation of distribution algorithm）
- 人工免疫系统（artificial immune systems）

- https://en.wikipedia.org/wiki/Evolutionary_algorithm
- https://en.wikipedia.org/wiki/Evolutionary_computation
- https://en.wikipedia.org/wiki/Estimation_of_distribution_algorithm

4. 算法（Algorithms）

基于 metaphor 的元启发式方法

- 模拟退火（simulated annealing）
- 蚁群优化（ant colony optimization）
- 粒子群优化（particle swarm optimization）
- 人工蜂群算法（artificial bee colony algorithm）
- 和声搜索（harmony search）

- https://en.wikipedia.org/wiki/List_of_metaphor-based_metaheuristics
- https://arxiv.org/abs/1307.4186
- S. Salcedo-Sanz, “Modern meta-heuristics based on nonlinear physics processes: A review of models and design procedures,” *Physics Reports*, vol. 655, pp. 1-70, 2016.

4. 算法（Algorithms）

Swarm intelligence based algorithms			Bio-inspired (not SI-based) algorithms		
Algorithm	Author	Reference	Algorithm	Author	Reference
Accelerated PSO	Yang et al.	[69], [71]	Atmosphere clouds model	Yan and Hao	[67]
Ant colony optimization	Dorigo	[15]	Biogeography-based optimization	Simon	[56]
Artificial bee colony	Karaboga and Basturk	[31]	Brain Storm Optimization	Shi	[55]
Bacterial foraging	Passino	[46]	Differential evolution	Storn and Price	[57]
Bacterial-GA Foraging	Chen et al.	[6]	Dolphin echolocation	Kaveh and Farhoudi	[33]
Bat algorithm	Yang	[78]	Japanese tree frogs calling	Hernández and Blum	[28]
Bee colony optimization	Teodorović and Dell'Orco	[62]	Eco-inspired evolutionary algorithm	Parpinelli and Lopes	[45]
Bee system	Lucic and Teodorovic	[40]	Egyptian Vulture	Sur et al.	[59]
BeeHive	Wedde et al.	[65]	Fish-school Search	Lima et al.	[14], [3]
Wolf search	Tang et al.	[61]	Flower pollination algorithm	Yang	[72], [76]
Bees algorithms	Pham et al.	[47]	Gene expression	Ferreira	[19]
Bees swarm optimization	Drias et al.	[16]	Great salmon run	Mozaffari	[43]
Bumblebees	Comellas and Martinez	[12]	Group search optimizer	He et al.	[26]
Cat swarm	Chu et al.	[7]	Human-Inspired Algorithm	Zhang et al.	[80]
Consultant-guided search	Iordache	[29]	Invasive weed optimization	Mehrabian and Lucas	[42]
Cuckoo search	Yang and Deb	[74]	Marriage in honey bees	Abbass	[1]
Eagle strategy	Yang and Deb	[75]	OptBees	Maia et al.	[41]
Fast bacterial swarming algorithm	Chu et al.	[8]	Paddy Field Algorithm	Premaratne et al.	[48]
Firefly algorithm	Yang	[70]	Roach infestation algorithm	Havens	[25]
Fish swarm/school	Li et al.	[39]	Queen-bee evolution	Jung	[30]
Good lattice swarm optimization	Su et al.	[58]	Shuffled frog leaping algorithm	Eusuff and Lansey	[18]
Glowworm swarm optimization	Krishnanand and Ghose	[37], [38]	Termite colony optimization	Hedayatzadeh et al.	[27]
Hierarchical swarm model	Chen et al.	[5]	Physics and Chemistry based algorithms		
Krill Herd	Gandomi and Alavi	[22]	Big bang-big Crunch	Zandi et al.	[79]
Monkey search	Mucherino and Seref	[44]	Black hole	Hatamlou	[24]
Particle swarm algorithm	Kennedy and Eberhart	[35]	Central force optimization	Formato	[21]
Virtual ant algorithm	Yang	[77]	Charged system search	Kaveh and Talatahari	[34]
Virtual bees	Yang	[68]	Electro-magnetism optimization	Cuevas et al.	[13]
Weightless Swarm Algorithm	Ting et al.	[63]	Galaxy-based search algorithm	Shah-Hosseini	[53]
Other algorithms			Gravitational search	Rashedi et al.	[50]
Anarchic society optimization	Shayeghi and Dadashpour	[54]	Harmony search	Geem et al.	[23]
Artificial cooperative search	Civicioglu	[9]	Intelligent water drop	Shah-Hosseini	[52]
Backtracking optimization search	Civicioglu	[11]	River formation dynamics	Rabanal et al.	[49]
Differential search algorithm	Civicioglu	[10]	Self-propelled particles	Vicsek	[64]
Grammatical evolution	Ryan et al.	[51]	Simulated annealing	Kirkpatrick et al.	[36]
Imperialist competitive algorithm	Atashpaz-Gargari and Lucas	[2]	Stochastic difusion search	Bishop	[4]
League championship algorithm	Kashan	[32]	Spiral optimization	Tamura and Yasuda	[60]
Social emotional optimization	Xu et al.	[66]	Water cycle algorithm	Eskandar et al.	[17]

4. 算法（Algorithms）

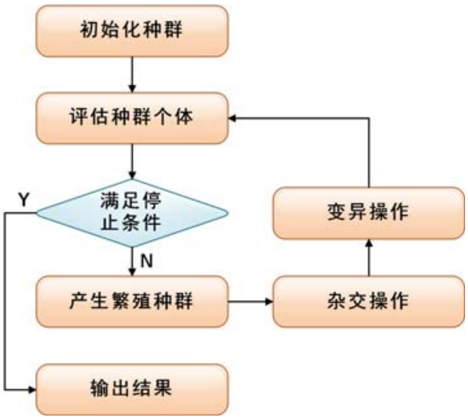


Figure: 遗传算法框架

4. 算法（Algorithms）

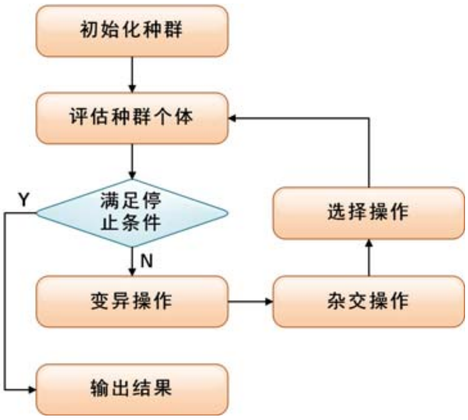


Figure: 差分进化算法框架

4. 算法（Algorithms）

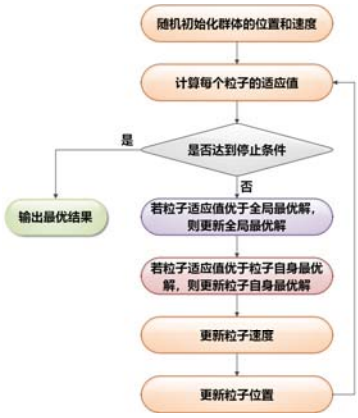


Figure: 粒子群优化框架

4. 算法（Algorithms）

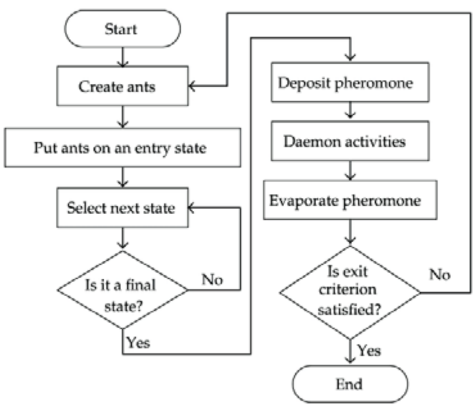


Figure: 蚁群优化框架

4. 算法（Algorithms）

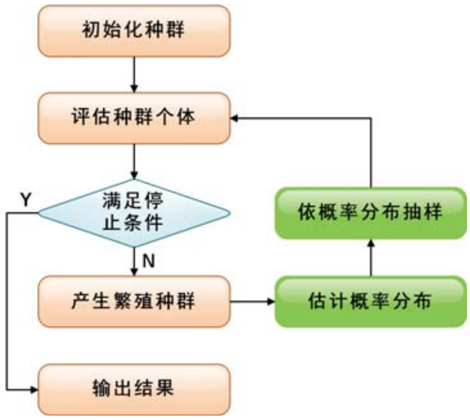


Figure: 分布估计算法框架

4. 算法（Algorithms）

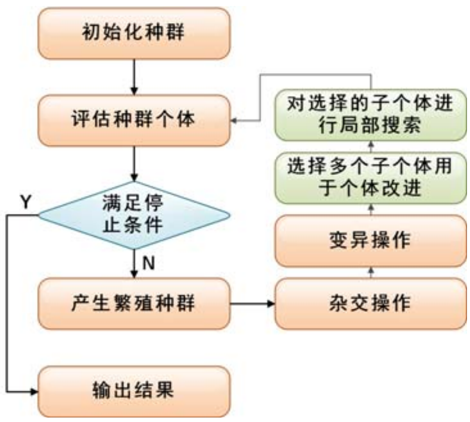


Figure: Memetic 算法框架

4. 算法（Algorithms）

为什么有如此多的智能优化方法？

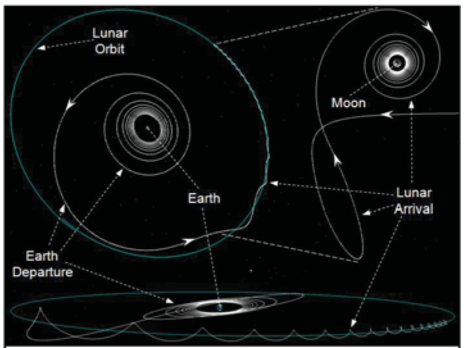
尺有所短，寸有所长！

优化中的“没有免费午餐（No free lunch）”理论：对于所有的优化问题，任何两个算法的性能都是等效的。换言之，没有一个算法能对所有的优化问题能优于另外一个算法。

D. H. Wolpert and W. G. Macready, “No free lunch theorems for optimization," *IEEE Transactions on Evolutionary Computation*, vol. 1, no. 1, pp. 67-82, 1997.

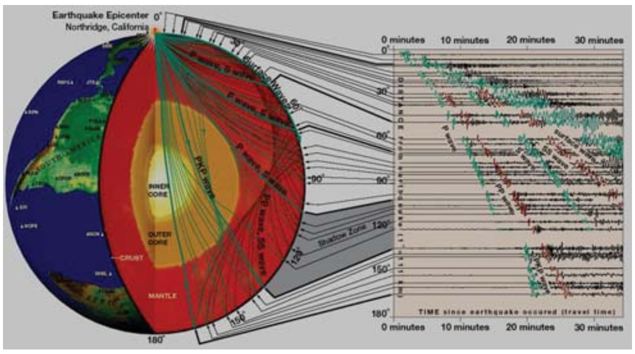
5. 智能优化方法相关应用（Applications）

5. 智能优化方法相关应用（Applications）

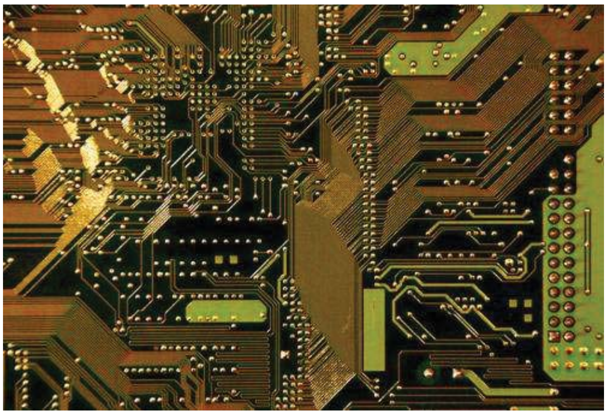


MAPS is Capable of Robustly Optimizing Multi-Spiral, Low-Thrust, Inter-Body Trajectories Such as This Low-Thrust, Earth-Orbit to Lunar Polar Orbit (LPO) Example Mission Scenario

5. 智能优化方法相关应用（Applications）



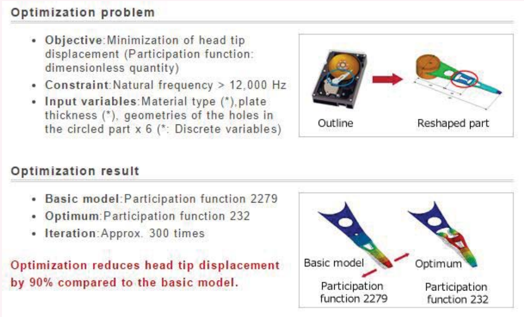
5. 智能优化方法相关应用（Applications）



5. 智能优化方法相关应用（Applications）

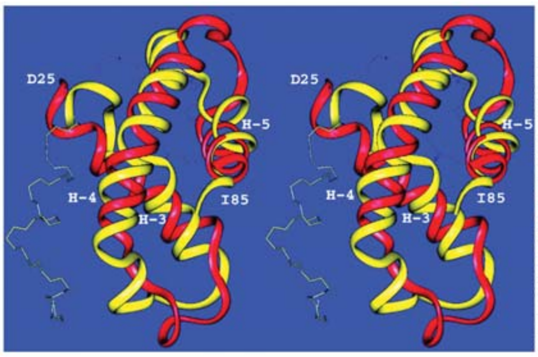
5. 智能优化方法相关应用（Applications）

基于差分演化的硬盘磁头优化



http://www.cybernet.co.jp/english/products/mds/solutions/sol3.html

5. 智能优化方法相关应用（Applications）



化学领域

Conclusions

We have provided an overview of some selected recent developments in the field of global optimization as applied to clusters, crystals, and biomolecules. For atomic and molecular clusters the basin-hopping approach coupled to search strategies based on Monte Carlo sampling or genetic algorithms seems to work well. Unbiased algorithms can often treat systems with at least 100 atoms or molecules reliably, and we expect biased or seeded approaches to be useful for significantly larger systems.

David J. Wales and Harold A. Scheraga. *Science*, 285:1368-1372, 1999.

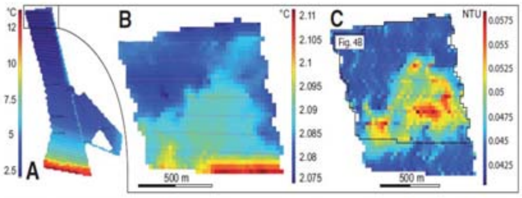


Figure 4. Anomalies in water turbidity and water temperature logged by autonomous underwater vehicle. A: Complete water temperature record showing expected stratification with depth. B: Detailed map of water temperature (rectangle in A) from planar lower detachment. C: Corresponding turbidity map represented in NTU (nephelometric turbidity unit) in ocean bottom water above lower detachment.

地学领域

Genetic algorithm inversion of seismic reflection data parallel to the MSD shows a layer with seismic velocities of ~4.3 km^{-1} at 4–5 km depth, including isolated zones with velocities as low as ~1.7 km^{-1} (Floyd et al., 2001). This inversion suggests that high fluid pressures and hydrothermal flow may be actively weakening the MSD. Therefore the MSD must be weakly coupled, either due to low-friction fault-zone materials or fluid overpressure, or both. The bot-

R. Speckbacher, J. H. Behrmann, T. J. Nagel, M. Stipp, and C. W. Devey. *Geology*, 39(7):651–654, 2011.

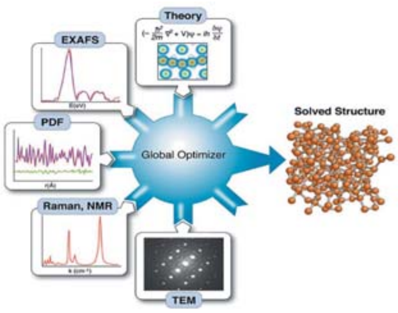


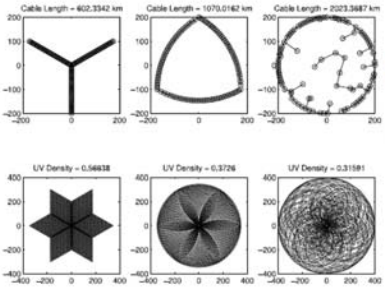
Figure 1
Complex modeling feeds all available data sets and theoretical constraints into a global optimizer to produce a unique structure solution for a new material. Reproduced from Billinge (2010).

物理学领域

algorithm to 'cook' the fit recipe is of particular importance; a simple least-squares algorithm may be appropriate for a fit with relatively few free variables and a good starting model, whereas a more complicated procedure, such as a Monte Carlo method, or an evolutionary algorithm, may be required for a recipe with a large number of variables. Viewed this way, the regression interface is simply another modular unit in the complex modeling framework that can be changed or adapted as necessary such that different regression algorithms may be inserted, or even nested together into a hybrid regression scheme.

P. Juhas, *et al.* *ACTA Crystallographica Section A.* A71: 562–568, 2015.

5. 智能优化方法相关应用（Applications）



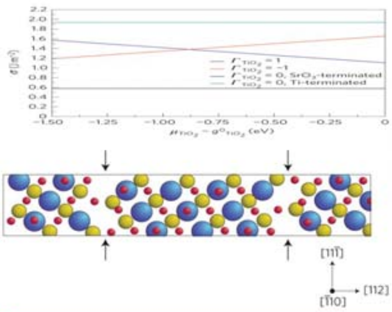
天文学领域

ABSTRACT

The next generation of radio telescope interferometric arrays requires careful design of the array configuration to optimize the performance of the overall system. We have developed a framework, based on a genetic algorithm, for rapid exploration and optimization of the objective space pertaining to multiple objectives. We have evaluated a large space of possible designs for 27, 60, 100, and 160 station arrays. The 27 station optimizations can be compared to the well-known VLA case, and the larger array designs apply to arrays currently under design such as LOFAR, ATA, and the SKA. In the initial implementation of our framework we evaluate designs with respect to two metrics, array imaging performance and the length of cable necessary to connect the stations. Imaging performance is measured by the degree to which the sampling of the u-v plane is uniform. For the larger arrays we find that well-known geometric designs perform well and occupy the Pareto front of optimum solutions. For the 27 element case we find designs, combining features of the well-known

B. E. Cohanim and J. N. Hewitt. *The Astrophysical Journal Supplement Series*, 154:705–719, 2004.

5. 智能优化方法相关应用（Applications）



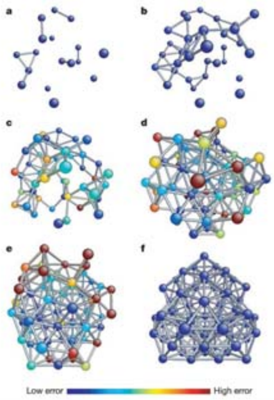
工程与材料科学领域

Abstract

Recent years have seen great advances in our ability to predict crystal structures from first principles. However, previous algorithms have focussed on the prediction of bulk crystal structures, where the global minimum is the target. Here, we present a general atomistic approach to simulate in multicomponent systems the structures and free energies of grain boundaries and heterophase interfaces with fixed stoichiometric and non-stoichiometric compositions. The approach combines a novel genetic algorithm using empirical interatomic potentials to explore the configurational phase space of boundaries, and thereafter refining structures and free energies with first principles electronic structure methods. We introduce a structural order parameter to bias the genetic algorithm search away from the global minimum (which would be bulk crystal), while not favouring any particular structure types, unless they lower the energy. We demonstrate the power and efficiency of the algorithm by considering nonstoichiometric grain boundaries in a ternary oxide, $SrTiO_3$.

A. Chua, N. A. Benedek, L. Chen, M. W. Finnis, and A. P. Sutton. *Nature Materials*, 9, 418-422, 2010.

5. 智能优化方法相关应用（Applications）



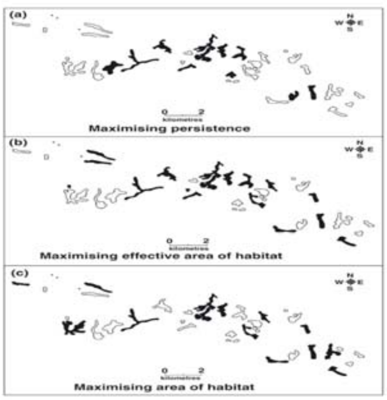
工程与材料科学领域

$N_p = N(N-1)/2$ is the number of atom pairs in the cluster, d_k is the interatomic distance of atom pair k, while the suffix m indicates the model and the suffix e indicates the experimental or target value. When $\mathrm{var}(d) = 0$, the fit is exact. The most difficult computational aspect of this problem is correctly assigning the distances between model atom pairs k to target distances $l(k)$. We first tried a simulated annealing approach[26], which was successful in finding the correct small clusters from unassigned distance data. However, this method failed for anything more complicated than a 20-atom cluster. This is presumably due to the rugged topology of the potential ($\mathrm{var}(d)$) surface.

Genetic or evolutionary algorithms have been very successful in finding the ground state of many types of clusters using theoretical interatomic potentials[23,25,27]. Based on these papers, we have developed

P. Juhás, D. M. Cherba, P. M. Duxbury, W. F. Punch & S. J. L. Billinge. *Nature*, 440, 655–658, 2006.

5. 智能优化方法相关应用（Applications）



环境科学与生态学领域

Abstract

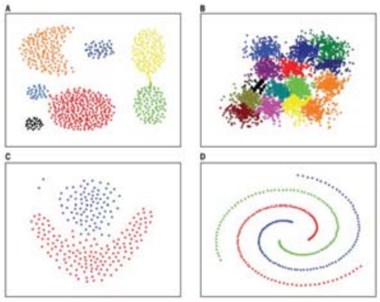
Although the aim of conservation planning is the persistence of biodiversity, current methods trade-off ecological realism at a species level in favour of including multiple species and landscape features. For conservation planning to be relevant, the impact of landscape configuration on population processes and the viability of species needs to be considered. We present a novel method for selecting reserve systems that maximize persistence across multiple species, subject to a conservation budget. We use a spatially explicit metapopulation model to estimate extinction risk, a function of the ecology of the species and the amount, quality and configuration of habitat. We compare our new method with more traditional, area-based reserve selection methods, using a ten-species case study, and find that the expected loss of species is reduced 20-fold. Unlike previous methods, we avoid designating arbitrary weightings between reserve size and configuration; rather, our method is based on population processes and is grounded in ecological theory.

Keywords

Conservation planning, metapopulation, multiple species conservation, optimization, reserve design, simulated annealing, site selection.

Emily Nicholson, *et al.* *Ecology Letters*, 9: 1049–1060, 2006.

5. 智能优化方法相关应用（Applications）



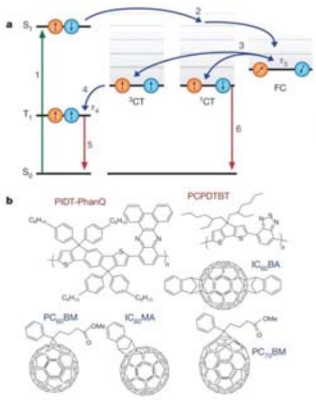
管理科学领域

DeSarbo and Grisaffe (1998) describe the NORMCLUS software system as a suite of programs for multiobjective clustering. The authors indicate that the system has considerable flexibility regarding objective criteria, multiobjective programming approach (e.g., weighted-sum, direct clustering, etc.), and algorithmic procedure (exchange heuristics, simulated annealing, tabu search, etc.). Multiobjective clustering packages have also been discussed in the pattern recognition literature and are typically based on evolutionary algorithms designed to estimate the entire Pareto frontier. For example, Handl and Knowles (2007) discuss a procedure known as MOCK (multiobjective clustering with automatic determination of the number of clusters, *K*), for which the source code is provided by Le (2007).

M. J. Brusco, D. Steinley, J. Cradit, R. Singh. *Journal of Operations Management*, 30: 454-466, 2012.

A. Rodriguez and A. Laio. *Science*, 344(6191): 1492-1496, 2014.

5. 智能优化方法相关应用（Applications）



光伏领域

The overlapping spectra of the excited states make the analysis of their kinetics difficult. To overcome this problem, we use a genetic algorithm[24] that allows us to extract the individual spectra and kinetics from the data set (Methods). Figure 2d shows the two spectra (solid lines) that the algorithm extracts from the PIDT-PhanQ:ICBA spectrum in Fig. 2c. The spectrum in blue is the charge (hole polaron) and the one in red is the triplet exciton on PIDT-PhanQ. These assignments are based on previous continuous-wave PIA experiments[18] as well as early-time transient absorption measurements (Supplementary Information).

A. Rao, P. C. Y. Chow, S. Gélinas, Cody W. Schlenker, & R. H. Friend. *Nature*, 500: 435-439, 2013.

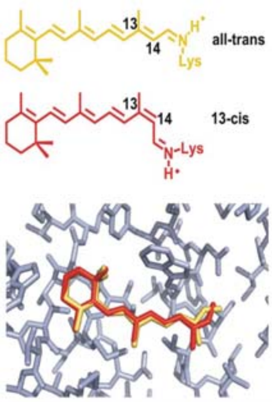
5. 智能优化方法相关应用（Applications）

计算生物物理学领域

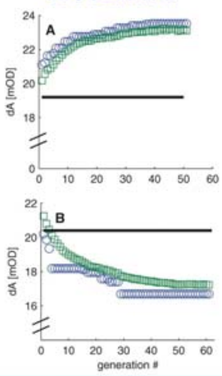
terns from those generated with our CA simulations. However, one could argue that the real and simulated labyrinthine patterns might exhibit some degree of universality, that is, many statistical CA transition rules (with colour-change probabilities potentially very different from those shown in Fig. 4d) might generate patterns that cannot be distinguished from ocellated lizard real patterns. We tested this hypothesis by implementing a genetic algorithm to optimize colour-change probabilities using a bin-wise difference statistics on the scale neighbourhood spatial state distribution function (of the simulated versus real pattern) as the optimality criterion. All genetic algorithm searches systematically converged to shape distributions of scale colour change probabilities similar to those estimated from the real data, suggesting that other profiles of relative probabilities cannot generate ocellated lizard patterns.

L. Manukyan, S. A. Montandon, A. Fofonjka, & M. C. Milinkovitch. ***Nature***, 554, 173-179, 2017.

5. 智能优化方法相关应用（Applications）



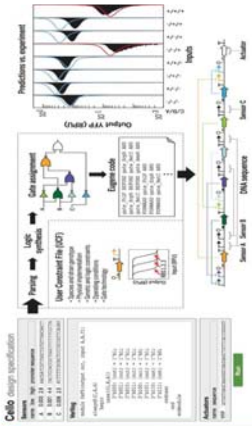
光学控制领域



yield. We then used a well-established genetic algorithm and feedback approach to solve a multivariable problem to converge toward tailored pulses that would either maximize or minimize the 630-nm induced absorption, corresponding to the respective enhancement or suppression of the isomerization yield (Fig. 2). The different excitation pulse shapes were generated by appropriate manipulation of incoming transform-limited pulses [19 fs full width at half maximum (FWHM), centered at 565 nm with a bandwidth of 60 nm] in both frequency and phase domains (*21*). Using only phase manipulation would substantially restrict the control space. In accordance with certain properties of the Fourier transform, frequency amplitude modulation is necessary to produce, for example, a comb of temporally spaced subpulses, a prominent feature of the optimal pulses derived in recent coherent control experiments (*16*, *22*).

V. I. Prokhorenko, A. M. Nagy, S. A. Waschuk, R. J. D. Mille. ***Science***, 313(5791), 1257-1261 , 2006.

5. 智能优化方法相关应用（Applications）



自动电路设计领域

Genetic circuit design automation

Alec A. K. Nielsen,[1] Bryan S. Der,[1,2] Jonghyeon Shin,[1] Prashant Vaidyanathan,[2] Vanya Paralanov,[3] Elizabeth A. Strychalski,[3] David Ross,[3] Douglas Densmore,[2] Christopher A. Voigt[1*]

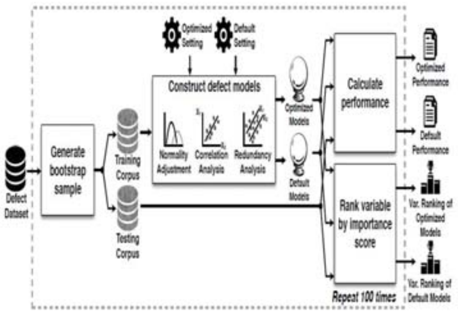
Computation can be performed in living cells by DNA-encoded circuits that process sensory information and control biological functions. Their construction is time-intensive, requiring manual part assembly and balancing of regulator expression. We describe a design environment, Cello, in which a user writes Verilog code that is automatically transformed into a DNA sequence. Algorithms build a circuit diagram, assign and connect gates, and simulate performance. Reliable circuit design requires the insulation of gates from genetic context, so that they function identically when used in different circuits. We used Cello to design 60 circuits for *Escherichia coli* (880,000 base pairs of DNA), for which each DNA sequence was built as predicted by the software with no additional tuning. Of these, 45 circuits performed correctly in every output state (up to 10 regulators and 55 parts), and across all circuits 92% of the output states functioned as predicted. Design automation simplifies the incorporation of genetic circuits into biotechnology projects that require decision-making, control, sensing, or spatial organization.

Genetic programming using Cello.

A. K. Nielsen, B. S. Der, J. Shin, P. Vaidyanathan, C. A. Voigt. *Science*, 352 (6281), aac7341, 2016.

5. 智能优化方法相关应用（Applications）

软件工程领域



The Impact of Automated Parameter Optimization on Defect Prediction Models

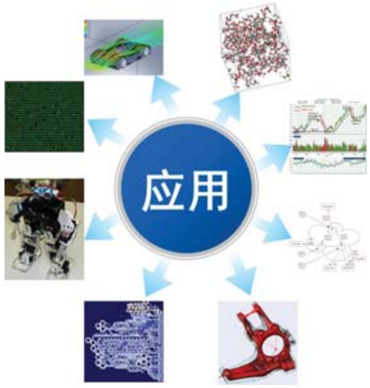
Chakkrit Tantithamthavorn, *Member, IEEE*, Shane McIntosh, *Member, IEEE*, Ahmed E. Hassan, *Senior Member, IEEE*, and Kenichi Matsumoto, *Senior Member, IEEE*

Abstract—Defect prediction models—classifiers that identify defect prone software modules—have configurable parameters that control their characteristics (e.g., the number of trees in a random forest). Recent studies show that these classifiers underperform when default settings are used. In this paper, we study the impact of automated parameter optimization on defect prediction models. Through a case study of 18 datasets, we find that automated parameter optimization: (1) improves AUC performance by up to 40 percentage points; (2) yields classifiers that are at least as stable as those trained using default settings; (3) substantially shifts the importance ranking of variables, with as few as 28% of the top-ranked variables in optimized classifiers also being top-ranked in non-optimized classifiers; (4) yields optimized settings for 17 of the 20 most sensitive parameters that transfer among datasets without a statistically significant drop in performance; and (5) adds less than 30 minutes of additional computation to 12 of the 26 studied classification techniques. While widely used classification techniques like random forest and support vector machines are not optimization-sensitive, traditionally overlooked techniques like C5.0 and neural networks can actually outperform widely-used techniques after optimization is applied. This highlights the importance of exploring the parameter space when using parameter-sensitive classification techniques.

Index Terms—Software defect prediction, search-based software engineering, experimental design, classification techniques, parameter optimization, grid search, random search, genetic algorithm, differential evolution.

C. Tantithamthavorn, et al. *IEEE Transactions on Software Engineering*, 2018, In press.

5. 智能优化方法相关应用（Applications）



https://www.brainz.org/15-real-world-applications-genetic-algorithms/

6. 小结

- 优化（Optimization）
- 智能优化（Intelligent Optimization）
- 算法（Algorithms）
- 智能优化方法相关应用（Applications）
- 小结

6. 小结

小结

- 优化问题
- 智能优化
- 代表性算法
- 典型应用

6. 小结

重要期刊和会议

1. 重要期刊
   - IEEE Transactions on Evolutionary Computation
   - IEEE Transactions on Cybernetics
   - Evolutionary Computation Journal (MIT)
   - Information Sciences
   - Swarm and Evolutionary Computation
   - ...
2. 重要会议
   - Parallel Problem Solving from Nature (PPSN)
   - Genetic and Evolutionary Computation Conference (GECCO)
   - IEEE Congress on Evolutionary Computation (CEC)
   - ...

6. 小结

进一步阅读资料

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- S. Salcedo-Sanz, “Modern meta-heuristics based on nonlinear physics processes: A review of models and design procedures,” *Physics Reports*, vol. 655, pp. 1-70, 2016.

7. 致谢

Thank you!

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