

大规模多目标进化 优化: 算法与应用

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大规模多目标优化

Large-scale multi-objective optimization



大规模多目标进化算法

Large-scale multi-objective evolutionary algorithms



大规模多目标优化应用

Applications of large-scale multi-objective optimization

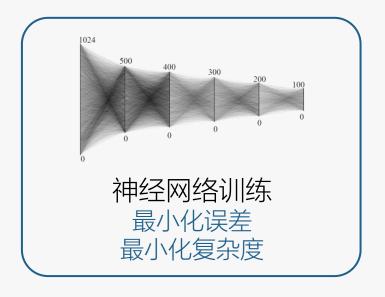


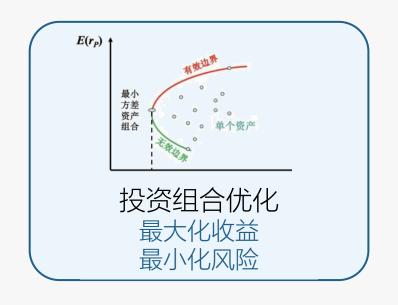


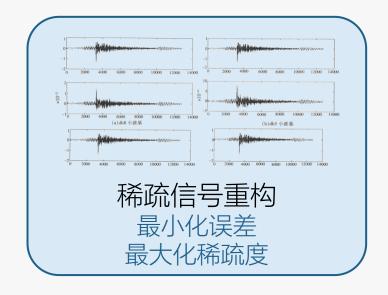
问题定义

•有多个优化目标、大量优化变量的问题, 称为大规模多目标优化问题

目标向量
$$\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), ..., f_M(\mathbf{x}))$$
 共 $M \geq 2$ 个目标函数 决策向量 $x_i \in [l_i, u_i]$ 共 $D \geq 100$ 个决策变量







问题定义



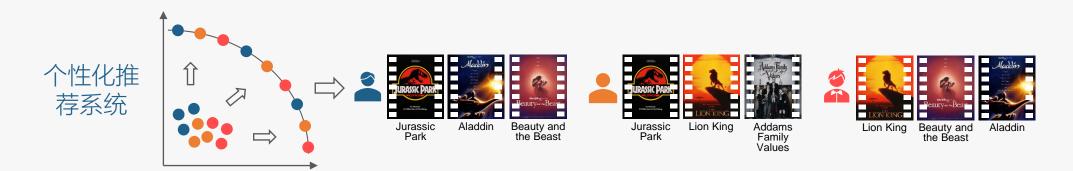
•目标间具有矛盾,量级不同,难以加权

训练误差 vs 网络复杂度

预期收益 vs 预期风险

重构误差 vs 信号稀疏度

•问题建模不精准,决策者需要多样化的解决方案供备选



现有算法

优势

大规模多目标上劣势

数学规划

大规模单目标收敛快

无法求解黑盒问题,多目标必 须加权,只能得到一个解

贝叶斯优化

小规模问题评价少

难以对许多变量拟合模型,数据不足

强化学习

优化过程中学习到经验

无法求解黑盒问题,无法求解连续优化问题(无法定义状态)

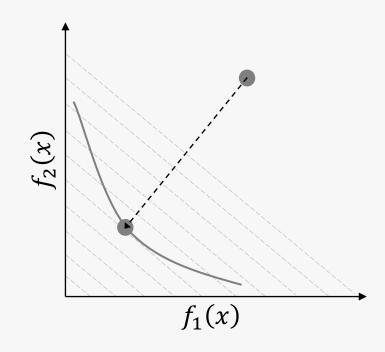
进化算法

通用性强

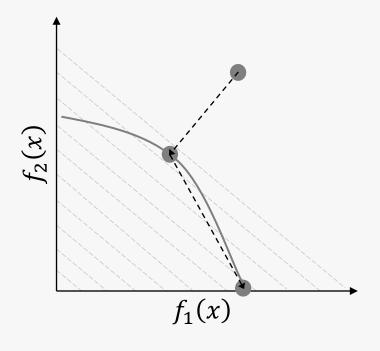
大规模空间收敛速度太慢

现有算法

? 为什么不能加权



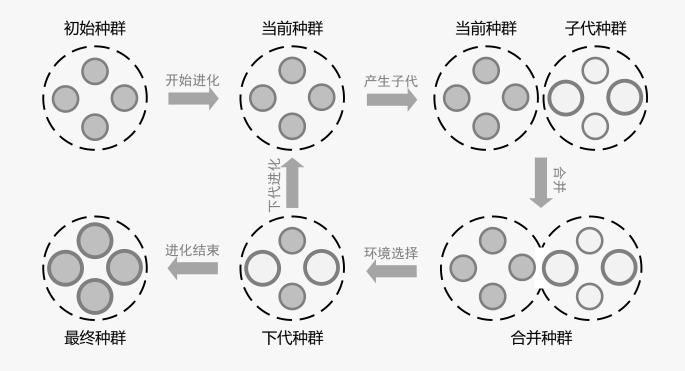
当最优前沿为凸时,最优解 位于权重向量与前沿的交点



当最优前沿为凹时, 最优解始终位于边界

解决方案

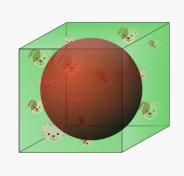
- 采用进化算法作为基本框架
 - ✓ 无需目标加权
- ✓ 直接求解黑盒问题
- ✓ 得到一组多样化解
- ✓ 适用复杂前沿

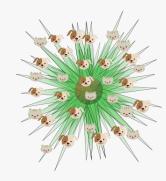


解决方案

•进化算法在大规模空间中会遭遇"维数灾难问题",收敛过慢







•针对不同类型问题设计不同策略, 提升进化算法收敛速度

变量聚类

问题重构

稀疏搜索

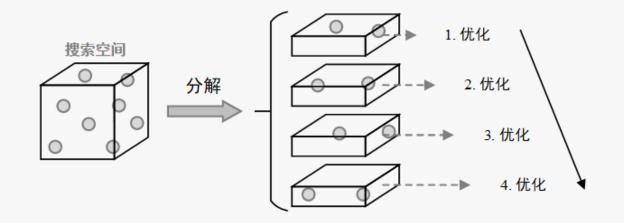
硬件加速

梯度辅助



变量聚类

•对大量决策变量进行分组并分别优化,分而治之



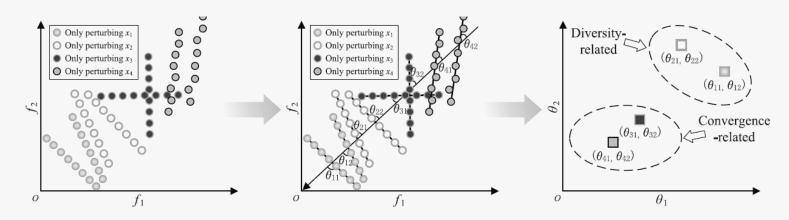


变量聚类



如何划分变量

• 将变量聚类为收敛性相关和多样性相关, 并分别优化



- 收敛性相关变量 → 收敛性优化
- 多样性相关变量 → 多样性优化

• 将收敛性相关变量进一步划分为不相关的多组,并分别优化

若变量 x_1 和 x_2 不相关,则一定存在 a_1 , a_2 , b_1 , b_2 满足

$$\begin{cases} f(\mathbf{x})|_{x_i = a_1, x_j = b_1} > f(\mathbf{x})|_{x_i = a_2, x_j = b_1} \\ f(\mathbf{x})|_{x_i = a_1, x_j = b_2} < f(\mathbf{x})|_{x_i = a_2, x_j = b_2} \end{cases}$$

(1) X. Zhang, Y. Tian, R. Cheng*, and Y. Jin, A decision variable clustering-based evolutionary algorithm for large-scale many-objective optimization, *IEEE Transactions on Evolutionary Computation*, 2018, 22(1): 97-112.

变量聚类

•基于变量聚类的进化算法LMEA,在变量相关性弱的大规模多目标优化问题上,可收敛至全局最优

算法主流程

Algorithm 1: Main Framework of LMEA

Input: *N* (population size), *nSel* (number of selected solutions for decision variable clustering), *nPer* (number of perturbations on each solution for decision variable clustering), *nCor* (number of selected solutions for decision variable interaction analysis)

Output: *P* (final population)

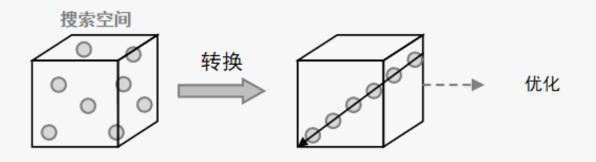
- 1 $P \leftarrow Initialize(N)$;
- $[DV, CV] \leftarrow VariableClustering(P, nSel, nPer);$
- $subCVs \leftarrow InteractionAnalysis(P, CV, nCor);$
- 4 while termination criterion not fulfilled do
- $P \leftarrow ConvergenceOptimization(P, subCVs);$
- P ← DiversityOptimization(P, DV);

对比实验结果

Problem	Obj.	Dec.	MOEA/D	NSGA-III	KnEA	MOEA/DVA	LMEA	
		100	4.5161e-2(9.31e-7)-	1.4957e-1(2.58e-2)-	2.7185e-1(4.11e-2)-	2.0440e-1(5.06e-4)-	4.1162e-3(1.44e-4)	
	5	500	4.5161e-2(1.04e-6)-	1.9413e-1(1.78e-2)-	3.1740e-1(6.11e-2)-	2.0469e-1(5.20e-8)-	4.0861e-3(1.48e-4)	
DTLZ5		1000	4.5162e-2(3.32e-7)-	2.0606e-1(1.10e-2)-	3.8913e-1(6.77e-2)-	2.0461e-1(1.36e-4)-	4.0729e-3(9.90e-5)	
		100	4.9994e-2(2.41e-4)-	3.1946e-1(2.03e-2)-	3.6432e-1(5.71e-2)-	1.8877e-1(1.87e-4)-	2.3954e-3(6.95e-5)	
	10	500	5.0407e-2(4.16e-4)-	5.2642e-1(2.04e-2)-	3.6389e-1(5.43e-2)-	1.8866e-1(3.30e-4)-	2.2721e-3(4.47e-5)	
		1000	5.0759e-2(2.12e-5)-	6.2093e-1(1.14e-2)-	4.1806e-1(5.07e-2)-	1.8880e-1(2.03e-4)-	2.0713e-3(6.98e-5)	
		100	1.4970e-1(3.14e-2)-	2.5642e-1(2.29e-2)-	5.8811e-1(1.34e-1)-	1.8236e-1(2.43e-6)-	3.9943e-3(2.14e-4)	
	5	500	1.3010e+0(1.04e-1)-	4.9939e-1(1.89e-2)-	7.2754e-1(1.43e-1)-	1.8236e-1(4.25e-7)-	4.5127e-3(1.22e-3)	
DTLZ6		1000	2.7140e+0(1.97e-1)-	6.5774e-1(2.19e-2)-	1.5085e+0(4.53e-1)-	1.8236e-1(5.91e-7)-	3.9747e-3(2.29e-4)	
		100	6.7510e-2(1.85e-2)-	7.2120e+0(1.35e+0)-	3.7560e+0(9.56e-1)-	1.6531e-1(4.09e-2)-	2.4477e-3(5.11e-4)	
	10	500	1.1735e+0(2.52e-1)-	8.7171e+1(4.88e+0)-	6.3085e+0(2.18e+0)-	1.2750e-1(5.33e-2)-	3.0711e-3(7.20e-4)	
		1000	2.6191e+0(5.73e-1)-	1.9202e+2(9.83e+0)-	4.8989e+0(2.54e+0)-	1.1844e-1(2.26e-2)-	3.7077e-3(1.66e-3)	
		100	2.0705e+0(8.91e-2)-	7.7137e-1(3.83e-2)-	6.2696e-1(4.24e-1)-	2.3769e+0(7.55e-3)-	1.2581e-1(2.91e-2)	
	5	500	2.2789e+0(6.03e-2)-	8.6982e-1(2.37e-2)-	2.2284e-1(2.56e-2)-	2.4699e+0(9.15e-3)-	1.1736e-1(3.58e-2)	
WFG3		1000	2.3370e+0(8.10e-2)-	8.8753e-1(2.53e-2)-	4.6414e-1(1.49e-1)-	2.4410e+0(3.52e-2)-	1.2493e-1(2.41e-2)	
		100	3.4569e+0(1.29e-1)-	3.0344e+0(5.71e-2)-	2.2907e+0(7.93e-1)-	3.4846e+0(2.45e-2)-	1.8542e-1(5.96e-2)	
	10	10	500	3.8106e+0(8.24e-2)-	3.1112e+0(5.04e-2)-	1.6148e+0(5.53e-1)-	3.5264e+0(9.75e-2)-	4.8685e-1(5.49e-2)
		1000	3.9456e+0(7.23e-2)-	3.1454e+0(4.20e-2)-	1.9861e+0(1.27e+0)-	3.5070e+0(1.17e-1)-	6.9330e-1(1.16e-1)	
		100	2.9851e-1(1.58e-2)-	2.2030e-1(9.19e-2)-	5.3546e-1(1.39e-1)-	4.3517e-2(2.50e-6)+	5.7008e-2(8.91e-3)	
UF9	3	500	3.1975e-1(2.92e-2)-	3.1029e-1(7.27e-2)-	4.6017e-1(1.19e-1)-	4.3516e-2(9.76e-7)+	5.3626e-2(6.94e-3)	
		1000	3.0557e-1(8.39e-2)-	3.7850e-1(4.21e-2)-	5.3607e-1(8.03e-2)-	4.3516e-2(7.00e-7)+	5.1231e-2(4.50e-3)	
		100	5.9354e-1(1.50e-1)-	3.3482e-1(8.13e-2)-	7.5510e-1(1.49e-1)-	1.1024e-1(2.92e-3)+	1.6632e-1(1.45e-2)	
UF10	3	500	6.3119e-1(1.92e-1)-	3.6779e-1(8.36e-2)-	1.3142e+0(8.69e-1)-	1.0158e-1(8.55e-4)+	1.5547e-1(4.99e-3)	
		1000	5.6232e-1(2.48e-1)-	4.2148e-1(1.10e-1)-	9.1794e-1(1.35e-1)-	1.0277e-1(1.01e-3)+	1.6924e-1(9.48e-3)	
+/	′ – / ≈		0/24/0	0/24/0	0/24/0	6/18/0		

问题重构

• 对大规模搜索空间直接进行降维,从而减小问题难度



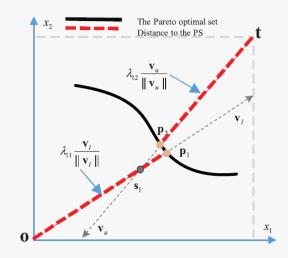


问题重构

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如何降维

•对于一个当前最优解,仅在穿过其的两个直线方向上进行搜索



$$\mathbf{x}_{i}^{l} = \mathbf{o} + w_{i}^{l} \frac{\mathbf{x}_{i} - \mathbf{o}}{\|\mathbf{x}_{i} - \mathbf{o}\|} \|\mathbf{t} - \mathbf{o}\|$$

$$\mathbf{x}_i^u = \mathbf{t} - w_i^u \frac{\mathbf{t} - \mathbf{x}_i}{\|\mathbf{t} - \mathbf{x}_i\|} \|\mathbf{t} - \mathbf{o}\|$$

•同时优化 k 个解 x 的HV值,则降维后仅优化 2k 个权重 w

$$\max f(w_1^l, w_1^u, w_2^l, w_2^u, \dots, w_k^l, w_k^u) = H(\mathbf{x}_1^l, \mathbf{x}_1^u, \mathbf{x}_2^l, \mathbf{x}_2^u, \dots, \mathbf{x}_k^l, \mathbf{x}_k^u)$$

问题重构

•基于问题重构的进化框架LSMOF,在评价次数很少时可快速收敛至局部最优

算法主流程

Algorithm 1 Main Framework of the Proposed LSMOF

Input: Z (original LSMOP), FE_{max} (total FEs), Alg (embedded MOEA), N (population size for Alg), r (number of reference solutions), tr (threshold).

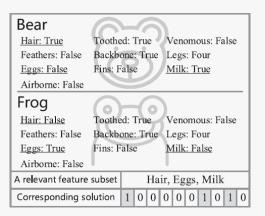
Output: *P* (final population).

- 1: $P \leftarrow \text{Initialization}(N, Z)$
- 2: /*********First Stage*********/
- 3: while $t \le tr \times FE_{max}$ do
- 4: $Z' \leftarrow \text{Problem_Reformulation}(P, r, Z)$
- 5: $A, \Delta t \leftarrow \text{Single_Objective_Optimization}(Z')$
- 6: $P \leftarrow \text{Environmental_Selection}(A \cup P, N)$
- 7: $t \leftarrow t + \Delta t$
- 8: end while
- 9: /*******Second Stage*******/
- 10: $P \leftarrow \text{Embedded_MOEA}(P, N, Alg, Z)$

对比实验结果

Problem	M	D	MOEA/DVA	WOF-NSGA-II	LS-NSGA-II
LSMOP1	2	200 500 1000	8.66E+0(8.04E-1)- 1.91E+1(1.00E+0)- 2.39E+1(7.84E-1)-	6.30E-1(9.36E-2)- 6.58E-1(6.11E-2)- 6.79E-1(4.22E-2)-	5.78E-1(5.32E-2) 6.14E-1(2.54E-2) 6.37E-1(1.97E-2)
	3	200 500 1000	6.26E+0(4.62E-1)- 9.42E+0(2.89E-1)- 1.08E+1(3.22E-1)-	6.95E-1(1.32E-1)— 7.09E-1(8.36E-2)— 8.01E-1(7.05E-2)—	5.24E-1(1.35E-2) 5.96E-1(1.08E-2) 6.33E-1(1.34E-2)
LSMOP2	2	200 500 1000	1.51E-1(6.75E-4)— 7.27E-2(2.30E-4)— 4.04E-2(3.87E-4)—	7.46E-2(4.63E-4)— 3.30E-2(3.91E-4)— 1.92E-2(3.40E-4)—	3.85E-2(1.08E-3) 2.32E-2(6.90E-4) 1.81E-2(5.41E-4)
	3	200 500 1000	1.23E-1(2.61E-3)+ 7.89E-2(2.63E-3)+ 6.48E-2(2.46E-3)+	1.36E-1(3.84E-3)≈ 8.54E-2(3.82E-3)≈ 7.00E-2(4.28E-3)≈	1.38E-1(2.76E-3) 8.71E-2(3.29E-3) 7.05E-2(3.08E-3)
LSMOP3	2	200 500 1000	1.71E+1(1.30E+0)- 2.87E+1(8.26E-1)- 3.36E+1(6.07E-1)-	1.50E+0(6.88E-2)≈ 1.57E+0(1.47E-3)− 1.58E+0(1.61E-3)−	1.54E+0(1.43E-3 1.57E+0(1.05E-3 1.57E+0(2.28E-4
	3	200 500 1000	2.30E+1(3.53E+0)- 3.60E+1(2.95E+0)- 4.02E+1(2.09E+0)-	8.61E-1(3.38E-4)— 8.61E-1(1.30E-4)— 8.61E-1(7.28E-4)≈	8.40E-1(2.51E-2) 8.59E-1(3.26E-3) 8.61E-1(7.03E-5)
LSMOP4	2	200 500 1000	6.56E-1(9.76E-3)— 5.44E-1(1.90E-3)— 4.61E-1(6.97E-4)—	1.33E-1(1.51E-2)— 8.74E-2(6.83E-3)— 5.99E-2(5.57E-3)—	9.87E-2(1.69E-3) 5.05E-2(1.14E-3) 3.20E-2(9.49E-4)
	3	200 500 1000	3.26E-1(2.31E-3)— 1.94E-1(5.71E-4)+ 1.20E-1(1.96E-4)+	3.15E-1(9.10E-3)— 2.14E-1(6.87E-3)≈ 1.39E-1(5.80E-3)≈	2.92E-1(8.37E-3) 2.13E-1(4.72E-3) 1.41E-1(3.63E-3)
LSMOP5	2	200 500 1000	1.42E+1(6.21E-1)- 2.09E+1(5.02E-1)- 2.41E+1(3.40E-1)-	7.42E-1(1.14E-6)≈ 7.42E-1(1.14E-6)≈ 7.42E-1(1.14E-6)≈	7.42E-1(1.14E-6) 7.42E-1(1.14E-6) 7.42E-1(1.14E-6)
	3	200 500 1000	1.17E+1(9.27E-1)- 1.70E+1(6.15E-1)- 1.91E+1(5.97E-1)-	5.41E-1(1.02E-3)— 5.41E-1(4.66E-5)— 5.41E-1(7.27E-5)≈	4.88E-1(5.13E-2) 5.35E-1(1.23E-2) 5.49E-1(2.83E-2)

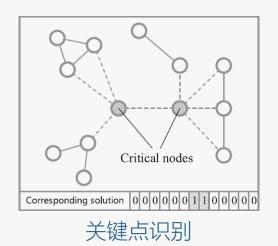
•很多大规模多目标优化问题是稀疏的, 即最优解中有大量为零的变量



特征选择



模式挖掘



Weights Weights

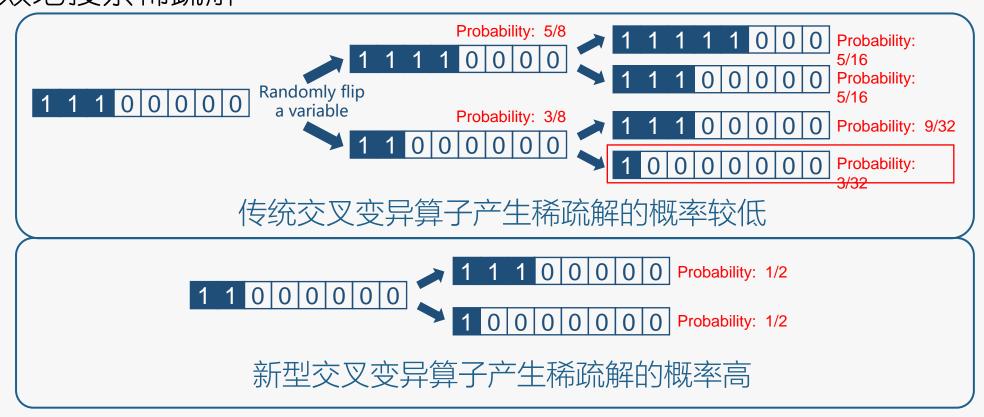
Corresponding solution 0.3 0 0 0 0.1 0.1 0.4 0 0.2 0 0 0.1

Hidden layer

稀疏神经网络

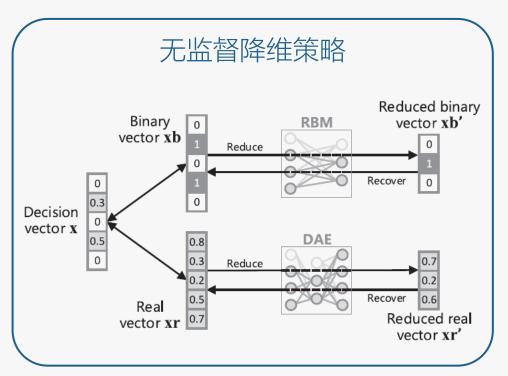
•若能快速识别其中为零的变量,则可大幅减小搜索空间、提升收敛速度

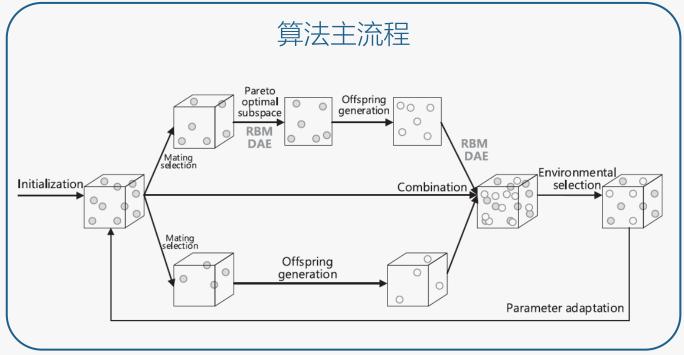
•首个面向稀疏优化的进化算法SparseEA,提出新型交叉变异算子以更高效地搜索稀疏解



(3) Y. Tian, X. Zhang*, C. Wang, and Y. Jin, An evolutionary algorithm for large-scale sparse multiobjective optimization problems, *IEEE Transactions on Evolutionary Computation*, 2020, 24(2): 380-393.

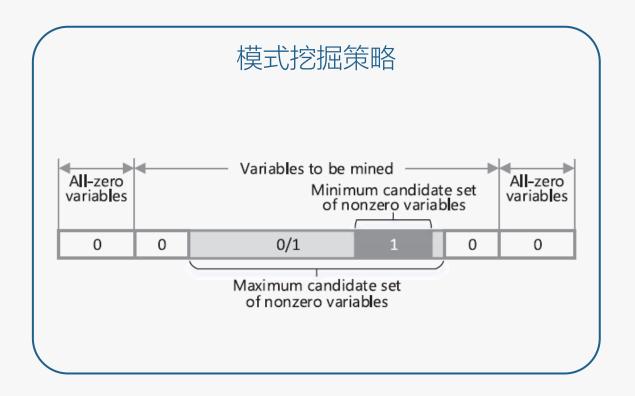
•基于无监督神经网络的进化算法MOEA/PSL,提出无监督降维策略以 压缩稀疏搜索空间、提升收敛速度

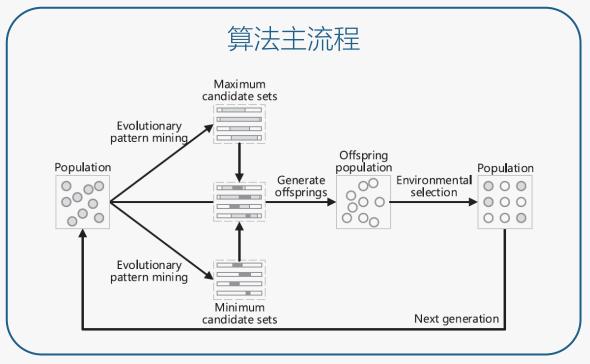




(4) Y. Tian, C. Lu, X. Zhang*, K. C. Tan, and Y. Jin, Solving large-scale multiobjective optimization problems with sparse optimal solutions via unsupervised neural networks, *IEEE Transactions on Cybernetics*, 2021, 51(6): 3115-3128.

•基于模式挖掘的进化算法PM-MOEA,提出进化模式挖掘策略以发现非稀疏搜索子空间、提升收敛速度



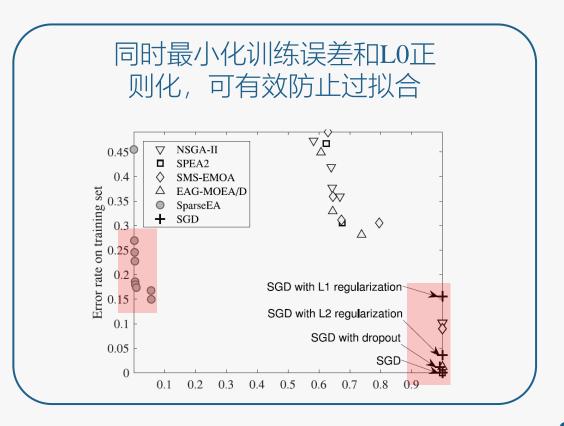


(5) Y. Tian, C. Lu, X. Zhang*, F. Cheng, and Y. Jin, A pattern mining based evolutionary algorithm for large-scale sparse multi-objective optimization problems, *IEEE Transactions on Cybernetics*, 2022, 52(7): 6784-6797.

•实验结果表明,以上进化算法在稀疏大规模多目标优化问题上,可大幅提升优化性能

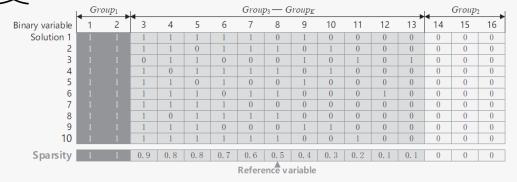
对比实验结果

Problem (D)	NSGA-II	MOEA/D-DE	MOEA/DVA	LMEA	WOF- SMPSO	LSMOF- NSGA-II	IM-MOEA	LMOCSO	SparseEA	MOEA/PSL	PM-MOEA
SMOP1 (100)	1.9337e-1	4.3614e-1	7.8851e-1	5.9369e-1	2.3918e-1	1.4151e-1	3.7767e-1	4.1068e-1	6.9883e-2	4.8689e-2	9.4315e-2
SMOP2 (100)	3.0427e-1	6.8635e-1	8.1987e-1	6.7602e-1	3.7089e-1	2.4525e-1	5.4250e-1	6.5158e-1	1.3044e-1	5.5829e-2	9.0096e-2
SMOP3 (100)	2.9980e-1	3.3553e-1	6.9653e-1	4.9054e-1	2.5190e-1	2.0252e-1	5.7921e-1	3.5256e-1	8.6080e-2	7.0560e-2	1.0548e-1
SMOP4 (100)	1.6997e-1	6.4059e-1	7.5967e-1	5.4760e-1	3.3175e-1	1.1802e-1	3.4479e-1	5.2913e-1	6.5248e-2	4.9980e-2	5.6740e-2
SMOP5 (100)	1.4063e-1	3.7059e-1	6.1990e-1	4.6552e-1	1.4168e-1	9.6309e-2	3.0165e-1	2.4447e-1	4.6993e-2	4.4203e-2	3.7296e-2
SMOP6 (100)	1.3167e-1	4.6350e-1	7.2521e-1	6.0050e-1	1.7961e-1	8.8620e-2	2.7609e-1	3.4374e-1	4.4372e-2	4.7910e-2	4.8082e-2
SMOP7 (100)	7.6009e-1	8.7693e-1	1.6762e+0	1.3955e+0	4.1530e-1	6.1877e-1	1.1281e+0	9.0127e-1	2.1786e-1	1.0306e-1	2.4001e-1
SMOP8 (100)	1.0803e+0	1.3295e+0	1.8521e+0	1.6576e+0	7.8605e-1	8.5502e-1	1.4568e+0	1.2191e+0	3.2522e-1	1.5662e-1	2.9235e-1
SMOP1 (500)	2.0078e-1	4.7565e-1	6.5680e-1	5.2181e-1	2.5840e-1	1.4826e-1	3.8710e-1	4.1421e-1	7.7962e-2	6.8524e-2	7.4613e-2
SMOP2 (500)	2.2361e-1	5.3837e-1	6.2014e-1	4.9237e-1	1.7649e-1	1.3007e-1	4.0178e-1	5.1778e-1	6.1991e-2	4.6055e-2	7.5849e-2
SMOP3 (500)	2.1226e-1	2.2364e-1	4.5775e-1	3.1473e-1	1.6350e-1	1.1170e-1	3.8878e-1	2.2364e-1	5.4376e-2	5.0797e-2	5.1477e-2
SMOP4 (500)	2.9639e-1	7.4486e-1	8.4093e-1	5.4238e-1	2.4601e-1	1.9151e-1	4.1929e-1	6.3857e-1	9.1078e-2	6.0793e-2	1.3729e-1
SMOP5 (500)	1.5555e-1	3.6846e-1	6.8601e-1	5.8986e-1	1.0433e-1	1.5748e-1	4.2196e-1	2.7542e-1	4.7540e-2	5.6343e-2	4.0170e-2
SMOP6 (500)	1.3524e-1	4.9684e-1	5.8008e-1	4.4997e-1	1.8761e-1	8.2919e-2	2.7406e-1	3.5664e-1	5.9739e-2	4.7825e-2	3.3376e-2
SMOP7 (500)	2.9905e-1	3.5295e-1	9.4878e-1	7.4620e-1	1.6603e-1	2.4426e-1	5.9310e-1	4.1848e-1	8.1813e-2	5.2182e-2	1.0454e-1
SMOP8 (500)	3.6262e-1	5.0656e-1	9.3498e-1	7.8791e-1	1.8598e-1	3.0491e-1	6.5754e-1	4.3061e-1	1.0165e-1	7.5297e-2	8.8172e-2
SMOP1 (1000)	1.5571e-1	3.5225e-1	5.2676e-1	4.3443e-1	1.9660e-1	1.0731e-1	3.1717e-1	3.3554e-1	4.8398e-2	5.3307e-2	5.3906e-2
SMOP2 (1000)	2.5495e-1	5.2097e-1	5.9670e-1	4.9781e-1	2.0615e-1	1.5315e-1	4.0175e-1	5.3552e-1	9.2543e-2	7.0190e-2	4.0488e-2
SMOP3 (1000)	2.5065e-1	2.5065e-1	4.6366e-1	3.4697e-1	1.9917e-1	1.4570e-1	4.0951e-1	2.5065e-1	7.5598e-2	6.2881e-2	5.5213e-2
SMOP4 (1000)	2.9679e-1	7.9097e-1	8.7980e-1	5.8962e-1	2.4536e-1	1.9047e-1	4.0549e-1	6.9149e-1	1.0773e-1	5.3168e-2	1.4350e-1
SMOP5 (1000)	1.8111e-1	3.9310e-1	5.8350e-1	5.9136e-1	1.2368e-1	1.4881e-1	4.1826e-1	2.8160e-1	4.8329e-2	7.0232e-2	3.6738e-2
SMOP6 (1000)	1.3829e-1	4.9495e-1	5.5872e-1	5.1353e-1	1.9575e-1	8.9246e-2	2.7406e-1	3.5636e-1	5.7827e-2	5.0686e-2	3.5731e-2
SMOP7 (1000)	3.0360e-1	3.5633e-1	9.0563e-1	7.2155e-1	1.7128e-1	2.4907e-1	5.8356e-1	4.1170e-1	6.9131e-2	6.6191e-2	1.1651e-1
SMOP8 (1000)	3.6972e-1	5.6807e-1	9.0280e-1	7.3794e-1	1.7119e-1	3.0418e-1	7.2364e-1	4.2391e-1	8.5294e-2	5.5697e-2	7.7375e-2
SMOP1 (5000)	3.0581e-1	4.3757e-1	7.1662e-1	6.5268e-1	2.5393e-1	2.0094e-1	4.3473e-1	4.3757e-1	1.1666e-1	8.4255e-2	7.2000e-2
SMOP2 (5000)	2.3548e-1	3.9400e-1	4.1265e-1	5.3216e-1	1.3689e-1	1.8393e-1	3.8831e-1	3.9517e-1	6.6315e-2	5.1404e-2	6.6043e-2
SMOP3 (5000)	2.0494e-1	2.0494e-1	4.0782e-1	3.3496e-1	1.5823e-1	1.6087e-1	3.9645e-1	2.0494e-1	8.5894e-2	4.6221e-2	6.6826e-2
SMOP4 (5000)	2.9513e-1	6.3529e-1	7.4225e-1	6.3870e-1	2.0108e-1	2.4033e-1	3.9630e-1	5.7324e-1	8.9054e-2	7.9108e-2	1.4608e-1
SMOP5 (5000)	1.8998e-1	3.9632e-1	4.8896e-1	6.4584e-1	1.3207e-1	1.3989e-1	4.4364e-1	2.8988e-1	4.8379e-2	8.3544e-2	4.6288e-2
SMOP6 (5000)	2.1177e-1	4.6564e-1	5.0253e-1	7.2834e-1	1.4962e-1	1.2542e-1	2.8417e-1	3.6945e-1	6.1343e-2	6.5937e-2	3.5237e-2
SMOP7 (5000)	3.7257e-1	2.9600e-1	1.0383e+0	9.1123e-1	1.5326e-1	2.3453e-1	5.0184e-1	3.1529e-1	1.1192e-1	7.0545e-2	1.1669e-1
SMOP8 (5000)	2.7640e-1	4.3124e-1	1.0415e+0	9.3653e-1	1.7614e-1	2.2673e-1	5.5521e-1	3.2799e-1	1.1516e-1	7.5387e-2	4.4007e-2
Average ranking	5.7500	8.3125	10.6875	9,4688	4,8438	4,4688	7.9375	7,7500	2,4375	1,5313	2,0313



硬件加速

- •对于超大规模问题(一百万变量),不仅要考虑算法的收敛速度,更要考虑算法的执行效率
- •首个超大规模进化算法SLMEA中,提出快速聚类的策略对所有变量进行分组,该策略具有线性时间复杂度

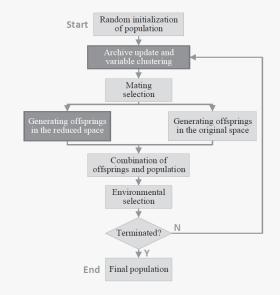


•对每组变量赋予相同的值并优化,可达到大幅减小搜索空间的目的

Algorithm 3: Clustering(A, K)

Input: *A* (current archive), *K* (number of groups) **Output**: *Group* (groups of variables)

- 1 $B \leftarrow A \ |A| \times D$ matrix containing the binary vectors of all solutions in A; //D denotes the number of variables
- 2 $Sparsity \leftarrow \operatorname{sum}(B)$; //sum of each column of B
- $c \leftarrow \operatorname{argmin}_b |Sparsity_b 0.5|;$
- 4 $B' \leftarrow \operatorname{repmat}(B_{\cdot c}, D)$; //Repeat the c-th column of B for D columns
- $5 Sim \leftarrow \text{sum}\left(\frac{(1-B) \cdot B' + B \cdot (1-B')}{(1-B) \cdot B' + B \cdot (1-B') + B \cdot B'}\right);$
- $6 \ rank \leftarrow sort(Sim)$; //Rank of variables in Sim
- 7 $Group_1 \leftarrow \{b|Sparsity_b = 1\};$
- s $Group_2 \leftarrow \{b|Sparsity_b = 0\};$
- 9 $rank \leftarrow rank \setminus Group_1 \setminus Group_2$;
- 10 $l \leftarrow \left| \frac{|rank|}{K-2} \right|$;
- 11 for i=3 to K do
- 12 $Group_i \leftarrow \{rank_{1+(i-3)l}, \cdots, rank_{\min(|rank|, (i-2)l)}\};$
- 13 return Group;

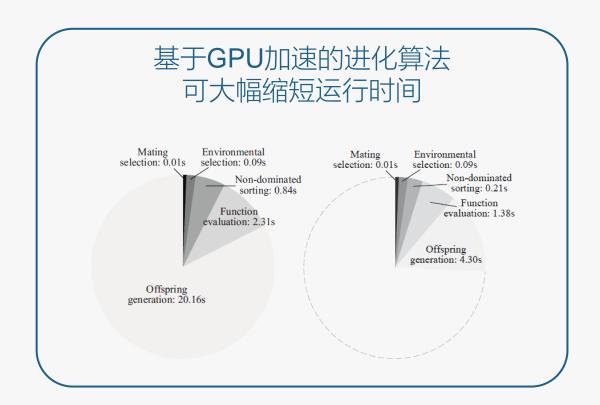


(6) Y. Tian, Y. Feng, X. Zhang*, and C. Sun, A fast clustering based evolutionary algorithm for super-large-scale sparse multi-objective optimization, *IEEE/CAA Journal of Automatica Sinica*, 2022, 9(4): 1-16.

硬件加速

•SLMEA减少复杂逻辑判断,并将所有操作矩阵化,从而可以支持GPU 加速

对比实验结果 NSGA-II MOEA/PSL SLMEA 8.5255e-1 (2.11e-2) - 1.1139e+0 (4.97e-2) - 7.1073e-1 (1.53e-2) - 2.2035e-1 (3.09e-2)-SMOP1 100000 13335e+0 (4.90e-3) = 11403e+0 (1.04e-2) = 7.2615e-1 (1.19e-2) = 3.2690e-1 (1.90e-2) = 6.5167e-1 (7.39e-3) = 10,000 1,6723e+0 (6,57e-3) = 2,1214e+0 (6,69e-2) = 2,0303e+0 (4,06e-3) = 3,4487e-1 (1,34e-1) = 8,1988e-1 (1,14e-2) = $2.0483e + 0 \; (5.26e - 3) - \\ 2.1093e + 0 \; (3.35e - 3) - \\ 2.0365e + 0 \; (1.24e - 2) - \\ 1.0149e + 0 \; (2.34e - 1) - \\ 1.0585e + 0 \; (2.90e - 3) - \\ 1.0586e + 0 \; (2.90e - 3) - \\ 1.05$ 1000 000 22175e+0 (1.01e-3) - 2.1489e+0 (0.00e+0) - 2.0289e+0 (0.00e+0) - 1.0516e+0 (1.07e-1) - 1.1651e+0 (0.00e+0) - $10\,000 \quad 2.0604 \\ e+0 \quad (1.82 \\ e-2) \\ - \quad 2.1404 \\ e+0 \quad (3.97 \\ e-2) \\ - \quad 1.7561 \\ e+0 \quad (1.44 \\ e-2) \\ - \quad 7.0353 \\ e-1 \quad (2.06 \\ e-3) \\ - \quad 2.5800 \\ e+0 \quad (1.41 \\ e-2) \\ - \quad 4.7620 \\ e-2 \quad (7.74 \\ e-3) \\ - \quad (1.41 \\ e-2) \\ - \quad (1.41 \\$ SMOP3 100 000 2.4274e+0 (3.41e-3) - 2.1163e+0 (3.13e-3) - 1.7635e+0 (3.95e-3) - 7.0114e-1 (2.24e-4) - 2.8156e+0 (3.18e-3) -1000000 2.5806e+0 (3.95e+4) - 2.1367e+0 (0.00e+0) - 1.7673e+0 (0.00e+0) - 7.0095e+1 (1.02e+6) - 2.9037e+0 (3.47e+4) - 2.9037e+010 000 8,2280e-1 (3.57e-3) - 1.0483e+0 (4.56e-2) - 1.0378e+0 (1.60e-2) - 2.8248e-2 (3.98e-2) - 2.6116e-1 (4.86e-3) -SMOP4 100 000 1.0069e+0 (3.79e-3) - 1.0606e+0 (1.37e-3) - 1.0321e+0 (1.54e-2) - 3.4081e-1 (5.82e-2) - 3.7765e-1 (2.23e-3) - $1.000\ 0.00 \quad 1.0912e + 0\ (8.23e - 4) - 1.0829e + 0\ (0.00e + 0) - 1.0447e + 0\ (0.00e + 0) - 3.5733e - 1\ (0.00e + 0) - 4.2600e - 1\ (3.24e - 5) - 1.0829e - 1.082$ 10 000 6.0886e-1 (4.25e-3) - 6.8227e-1 (2.28e-2) - 4.5992e-1 (5.44e-4) - 3.5439e-1 (2.99e-3) - 2.2960e-1 (4.32e-3) -SMOP5 100 000 9.1117e-1 (3.27e-3) - 6.8136e-1 (3.42e-3) - 4.6135e-1 (3.70e-4) - 3.6432e-1 (2.40e-3) - 3.8880e-1 (4.04e-3) -1000 000 1.0934e+0 (9.99e-4) - 7.0471e-1 (0.00e+0) - 4.6270e-1 (0.00e+0) - 9.7012e-2 (0.00e+0) - 4.9411e-1 (4.01e-4) - 1.6188e-2 (3.59e-4) -10 000 2.5603e-1 (3.54e-3) - 3.5305e-1 (2.27e-2) - 2.2085e-1 (1.68e-3) - 5.8457e-2 (1.27e-2) - 1.0191e-1 (2.31e-3) -SMOP6 100 000 4.1137e-1 (2.87e-3) - 3.4831e-1 (2.71e-3) - 2.2544e-1 (2.19e-3) - 9.7341e-2 (4.84e-4) - 1.8529e-1 (1.42e-3) - $1\,000\,000 \qquad 4.9367 \\ e^{-1}\,(5.62 \\ e^{-4}) - \qquad 3.6337 \\ e^{-1}\,(0.00 \\ e^{+0}) - \qquad 2.3002 \\ e^{-1}\,(0.00 \\ e^{+0}) - \qquad 1.9822 \\ e^{-1}\,(2.80 \\ e^{-3}) - \qquad 2.3038 \\ e^{-1}\,(0.00 \\ e^{+0}) - \qquad 2.3002 \\ e^{-1}\,(0.00 \\ e^{-1}) - \qquad 2.3002 \\ e^{-1}\,$ 10 000 1.6126e+0 (8.31e-2) - 1.7815e+0 (5.99e-2) - 8.3812e-1 (6.25e-2) - 8.1614e-2 (8.87e-3)-SMOP7 100 000 2.4672e+0 (4.29e-2) - 1.8551e+0 (2.73e-2) - 8.4147e-1 (2.25e-2) - 2.1584e-1 (1.02e-2) - 1.5216e+0 (1.24e-2) - $1\,000\,000 \quad 3.0333 \\ e+0 \ (5.11 \\ e-3) - \quad 1.9036 \\ e+0 \ (0.00 \\ e+0) - \quad 8.6488 \\ e-1 \ (0.00 \\ e+0) - \quad 5.4422 \\ e-1 \ (1.77 \\ e-2) - \quad 1.8954 \\ e+0 \ (1.61 \\ e-3) - \quad 1.8954 \\ e+0 \ ($ $10\,000 \quad 3.0912e + 0 \, (3.35e - 2) - \quad 3.6289e + 0 \, (4.72e - 2) - \quad 3.0709e + 0 \, (1.05e - 1) - \quad 5.7141e - 1 \, (2.35e - 2) - \quad 2.1975e + 0 \, (2.09e - 2) - \quad 3.0709e + 0 \, (2.09e - 2)$ $1\,000\,000 \quad 3.7057 \\ e+0\,\, (9.92 \\ e+4) \\ - \quad 3.6743 \\ e+0\,\, (0.00 \\ e+0) \\ - \quad 3.2062 \\ e+0\,\, (0.00 \\ e+0) \\ - \quad 4.2363 \\ e+1\,\, (0.00 \\ e+0) \\ - \quad 2.8873 \\ e+0\,\, (4.24 \\ e+3) \\ - \quad 2.8873 \\ e+0\,\, (4.24 \\ e+3) \\ - \quad 3.2062 \\ e+0\,\, (0.00 \\ e+0) \\ - \quad 4.2363 \\ e+0\,\, (0.00 \\ e+0$



梯度辅助

• 在梯度已知的情况下, 数学规划方法的收敛速度远超进化算法

根据梯度获得雅可比矩阵 $J_{\mathbf{f}}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \frac{\partial f_1(\mathbf{x})}{\partial x_2} & \cdots & \frac{\partial f_1(\mathbf{x})}{\partial x_D} \\ \frac{\partial f_2(\mathbf{x})}{\partial x_1} & \frac{\partial f_2(\mathbf{x})}{\partial x_2} & \cdots & \frac{\partial f_2(\mathbf{x})}{\partial x_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_M(\mathbf{x})}{\partial x_1} & \frac{\partial f_M(\mathbf{x})}{\partial x_2} & \cdots & \frac{\partial f_M(\mathbf{x})}{\partial x_D} \end{bmatrix}$

对于黑盒函数,利用有限差分估计梯度

$$\frac{\partial f_i(\mathbf{x})}{\partial x_i} \approx \frac{f_i(\mathbf{x}_{j+\epsilon}) - f_i(\mathbf{x})}{\epsilon}$$

- •利用数学规划方法辅助进化算法,可大幅提升其收敛速度
 - 数学规划 → 保证收敛性

• 进化算法 → 保证多样性

梯度辅助

? 如何避免陷入局部最优

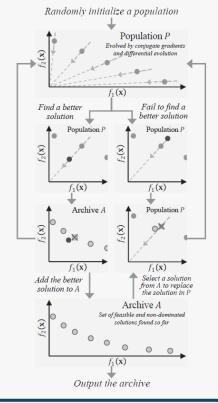
• MOCGDE建立数学规划和进化算法的联合搜索模式,利用共轭梯度法

和差分进化算法产生子代

$$\mathbf{s} = \begin{cases} -\mathbf{g}, & \text{if } \operatorname{mod}(k, D) = 0 \\ -\mathbf{g} + \frac{\mathbf{g}\mathbf{g}^T}{\mathbf{g}_0 \mathbf{g}_0^T} \mathbf{s}_0, & \text{otherwise} \end{cases}$$
$$y_i = x_i + (1 - d_i) \times 0.5^m \times s_i + d_i \times 0.5^m \times (x_i' - x_i'')$$

? 如何保证种群多样性

• MOCGDE使用小种群进化+大文档存储的结构,在快速收敛的同时保证种群多样性



(7) Y. Tian, H. Chen, H. Ma, X. Zhang*, K. C. Tan, and Y. Jin, Integrating conjugate gradients into evolutionary algorithms for large-scale continuous multi-objective optimization, *IEEE/CAA Journal of Automatica Sinica*, 2022.

梯度辅助

•MOCGDE在梯度容易计算的大规模多目标优化问题上,收敛速度提升显著

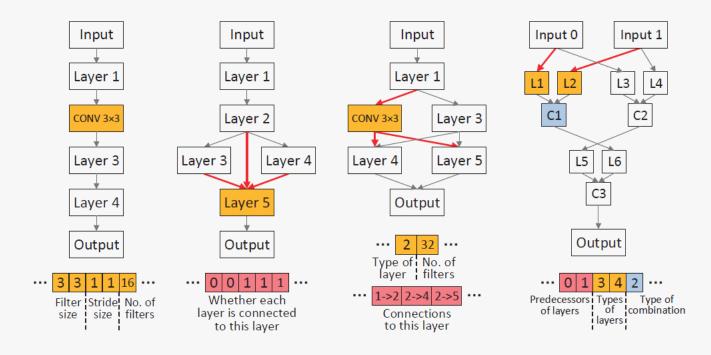
对比实验结果

ZDT1					algorithm		gradient	gSBX	MO-EGS	GPSO	SAPSO	MOCGDE
	5.6637e-1	9.9424e-3	2.1318e+0	3.1898e-1	1.2327e+0	2.6338e+0	2.0851e+0	2.0556e+0	2.2685e+0	2.3511e-1	2.5302e+0	7.5508e-3
(2,1000)	(8.74e-2) -	(4.19e-4) -	(2.01e-1) -	(9.89e-2) -	(1.84e-1) -	(2.03e-2) -	(1.18e-1) -	(1.08e-1) -	(1.02e-1) -	(9.80e-2) -	(5.57e-2) -	(8.04e-5)
ZDT1	2.0267e+0	1.0069e-2	2.7842e+0	2.6646e+0	1.1731e+0	2.9045e+0	2.7995e+0	2.6146e+0	2.7047e+0	2.1754e+0	2.8482e+0	8.0435e-3
(2,10000)	(3.85e-2) -	(3.78e-4) -	(2.32e-2) -	(4.60e-1) -	(1.38e-1) -	(2.97e-2) -	(1.41e-2) -	(9.34e-2) -	(1.52e-2) -	(9.88e-1) -	(1.43e-2) -	(5.27e-4)
ZDT2	8.1034e-1	9.8913e-3	3.1488e+0	1.1360e+0	2.2737e+0	4.0901e+0	3.5233e+0	3,3725e+0	3,9070e+0	4.5658e-1	4.2654e+0	7.6381e-3
(2.1000)	(8.38e-2) -	(4.60e-4) -	(1.48e-1) -	(1.16e-1) -	(2.85e-1) -	(5.00e-2) -				(1.32e-1) -	(1.13e-1) -	(7.67e-5)
ZDT2	3,6064e+0	1.0476e-2	3,7016e+0	4.4804e+0	2.0827e+0	4.6193e+0	4.6103e+0	4.2438e+0	4.4373e+0	6.0949e-1	4.6395e+0	7.7498e-3
(2,10000)	(5.30e-2) -	(7.57e-4) -	(2.27e-1) -	(1.03e-1) -	(8.76e-2) -	(1.85e-2) -	(1.52e-2) -	(9.90e-2) -	(1.08e-2) -	(1.17e-16) -	(1.53e-2) -	(9.62e-5)
	3.6440e-1	1.8567e-1	1.6639e+0	9,2358e-2	9.8576e-1	2.2105e+0	2.3023e+0	1.6430e+0	1.9113e+0	1.7496e+0	2.4705e+0	3.7836e-2
(2,1000)	(1.03e-1) -	(9.70e-2) -	(1.24e-1) -	(3.00e-2) -						(2.48e-1) -	(2.17e-1) -	(8.56e-2)
	1.4953e+0	4.0317e-1		3.9005e-1	7.4045e-1			2.0834e+0		2.3067e+0	2.4369e+0	
(2.10000)	(2.58e-2) -	(1.61e-1) -	(1.53e-1) -	(2.08e-1) -							(1.34e-1) -	(3.42e-2)
	3,3308e+3	6.6082e+0	2.0813e+4	8.2175e+3	2.4818e+4	1.5727e+4	7.1683e+3	1.1975e+4	1.6412e+4	1.2755e+4	1.1222e+3	4.6546e+3
				(2.42e+2) -								
	1.0087e+5	5.1586e+1		8.2703e+4	2.0777e+5		9.4186e+4		1.7454e+5	1.3836e+5	1.3476e+4	6.4416e+4
				(4.62e+2) -								
	4.8456e+0	5.3309e-1	7.2895e+0	6.4301e-1	6.6209e+0	7.6365e+0	7.5490e+0	7.3556e+0	7.0886e+0	6.0954e-1	7.6660e+0	2.3628e-1
		(9.90e-2) -								(8.94e-2) -	(2.04e-2) -	(1.14e-1)
		9.4675e-1		3.5280e+0		7.8740e+0				5.4056e-1	7.8820e+0	
	(3.65e-2) —		(1.12e-1) -							(1.76e-1) -		
	3.7988e+3		7.3815e+3	4.9581e+3		9.2265e+3				9.9829e+3	3.1072e+4	
				(2.07e+2) -								
		1.0742e+2			1.9548e+5					1.2487e+5		
				(1.41e+3) +								
DTLZ2	2.1762e-1	1.0435e-2		4.7916e-1		4.9523e+1				3.4242e-1	2.6925e+1	
				(1.84e-1) -								
		(2.90€-4) ≈ 2.7091e-2	5.0478e+1	5.4392e+1		8.0547e+2				6.0668e-1		
				(6.57e+1) —								
	9.9840e+3			1.8348e+4		2.9055e+4				1.9962e+4	8.3494e+4	
				(1.35e+4) —								
	5.1175e+5		1.6028e+5		5.3206e+5			3.2938e+5		(1.05e+4) — 2.4975e+5	8.3735e+5	
				(8.83e+4) —								
		5.2321e-1									7.4176e+1	
					3.1764e+1							
	(2.63e-1) — 4.8683e+2		(6.98e+0) — 2.7314e+2	(1.23e-1) -		(1.91e+1) — 7.1392e+2					(9.59e+0) - 5.6554e+2	
				(1.27e-11) -								
DTLZ5	3.1729e-1	1.0878e-2	4.3023e+0	5.8920e-1	1.1419e+1	4.9382e+1	8.0330e-2	3.1904e+1	7.5208e+1	3.4242e-1	3.0954e+1	1.0215e-2
				(1.78e-1) -								
	4.4325e+2		5.5592e+1		1.9391e+2					4.6010e-1		
				(7.24e+1) -								
	6.3535e+2	1.1391e+2	3.1397e+2	1.0000e+0	8.3147e+2	8.9463e+2			4.3209e+2	7.0921e+1	5.7244e+2	4.1444e-1
				(1.17e-16) -								(1.19e-4)
		3.3109e+3			8.8872e+3			8.9293e+3			8.2072e+3	4.1443e-1
				(3.73e+3) -								
	1.0665e+0	4.0072e-1		2.6633e-1	3.3289e+0	7.7334e+0		5.5639e+0	6.1115e+0	3.1983e-1	7.6237e+0	
	(1.13e-1) —		(5.27e-1) —		(6.05e-1) —							(2.79e-4)
	5.7861e+0	4.0174e-1	6.4588e+0	5.3949e-1	3.1057e+0	7.9608e+0				6.8268e-1	7.9696e+0	
				(1.96e-1) -								(9.22e-4)
+/-/≈	0/23/1	6/13/5	0/23/1	1/23/0	0/24/0	0/24/0	0/21/3	0/24/0	0/24/0	0/24/0	2/22/0	



神经结构搜索

•神经网络结构搜索是一个大规模且耗时的优化问题



Softmax Normal cell Normal cell Reduction cell Normal cell Normal cell Reduction cell 0 Normal cell Hypernetwork of Hypernetwork of each reduction cell each normal cell Normal cell Image Architecture of the whole CNN

四类主流的神经网络结构编码方式

基于one-shot和block的编码方式

神经结构搜索

•建立面向多模优化的稀疏大规模多目标进化算法MP-MMEA,采用one-shot编码,同时最小化验证误差与网络复杂度

$$\begin{array}{c} \text{Minimize} \ f_1(A) = f_{valid_error}(A) \\ f_2(A) = f_{complexity}(A) \end{array}$$

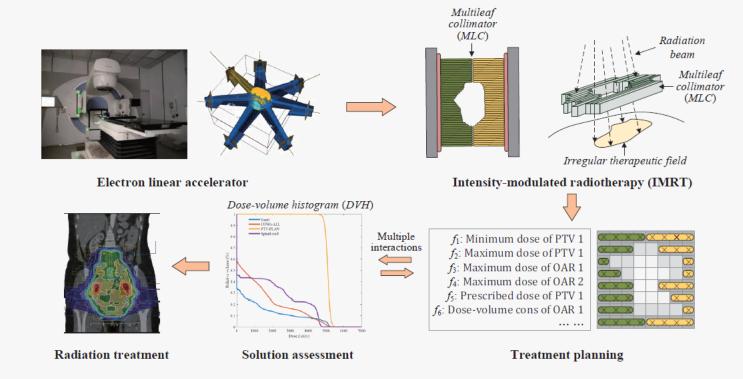
• 将得到的多样化网络结构集成,进一步提升性能

Ensemble method	Baseline 1 [47]	Baseline 2 [48]	MO_Ring_PSO_SCD	SparseEA	MP-MMEA
Best single CNN	89.47%	93.99%	93.68%	91.10%	93.91%
Unweighted average	90.19%	94.55%	94.34%	92.71%	95.03%
Majority vote	N/A	94.33%	94.11%	92.52%	94.79%
Weighted average	90.23%	N/A	94.33%	92.71%	95.03%
Rank based weight average	90.32%	N/A	94.50%	92.51%	94.97%

(8) Y. Tian, R. Liu, X. Zhang*, H. Ma, K. C. Tan, and Y. Jin, A multi-population evolutionary algorithm for solving large-scale multi-modal multi-objective optimization problems, *IEEE Transactions on Evolutionary Computation*, 2021, 25(3): 405-418.

调强放疗计划

•调强放疗计划是一个大规模超多目标的组合优化问题

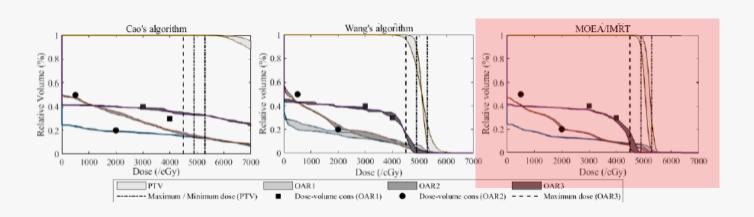


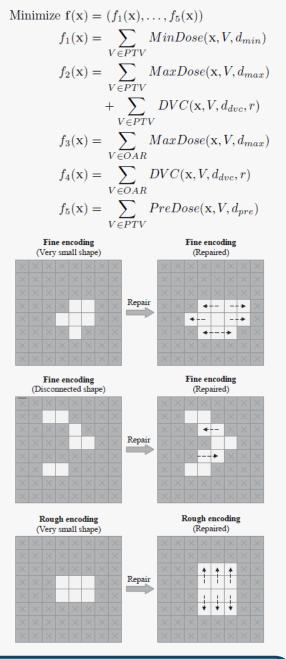
- 目标:
- 最大化癌细胞杀伤率
- 最小化正常器官损伤率

- 变量:
- 多叶准直器叶片位置 (射野形状)
- 射线强度、角度

调强放疗计划

- •建立超多目标优化模型,并设计大规模超多目标进化算法MOEA/IMRT,采用双精度编码+修正的搜索策略,以发现多样化的高效放疗方案
- •该算法可以得到比传统数学规划+贪心策略更加多样化的放疗方案,大幅降低了建模成本与人工调参耗时





(9) Y. Tian, Y. Feng, C. Wang, R. Cao, X. Zhang*, X. Pei, K. C. Tan, and Y. Jin, A large-scale combinatorial many-objective evolutionary algorithm for intensity-modulated radiotherapy planning, *IEEE Transactions on Evolutionary Computation*, 2022.



大规模多目标进化 优化 算法与应用

安徽大学 田野

ECOLE 2022, 郑州, 2022年8月3日

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