

Electronic Supplementary Material

Multiple input self-organizing-map ResNet model for optimization of petroleum refinery conversion units

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Optimization algorithms

Meta-heuristics, which is also called the intelligent optimization algorithm, is a kind of popular optimization method for solving complex linear and nonlinear problems. The typical algorithms include particle Swarm Optimization (PSO), Genetic Algorithm (GA), Differential Evolution (DE), Artificial Immune Algorithm (AIS), Simulated Algorithm (SA) etc. The methods adopted in the present work are mainly PSO and DE, which are classified as a swarm intelligence (SI) approach and an evolutionary computing (EC) technique, respectively.

Particle swarm optimization is a robust method for optimization based on the movement and intelligence of swarms. It was inspired by the swarms in nature, such as swarms of birds, fish, etc. It was developed in 1995 by James Kennedy and Russ Eberhart and later has been applied successfully to a wide variety of search and optimization problems. The basic concept of PSO lies in accelerating each particle toward the best position found so far (p-best) and the global best position(g-best)

obtained so far by any particle, with a random weighted acceleration at each time step.

The formula of updating velocity and the position of the particles are listed:

$$v_{t+1} = \frac{W}{t} \times v_t + c_1 \times rand(0,1) \times (pbest - x_t) + c_2 \times rand(0,1) \times (gbest - x_t) \quad (1)$$

$$x_{t+1} = x_t + v_{t+1} \quad (2)$$

where, v_t is the velocity of the particle, x is the position, t is the iteration, c_1 and c_2 are the acceleration factors. $pbest$ is the best solution that a particle has achieved until now, and global value($gbest$) is the best value obtained among all particles up till that step.

The PSO method can traverse a search space and converge rapidly but easily fall into the local optimum. Hence, the Multi-Round-PSO method is used in this work as the main scheme to find the global optimum as far as possible. The flowchart of this method is shown in Fig. 1. In each round of PSO, all particles are continuously updated according to their previous values until the targeted criteria are complied with in classical PSO applications. When the current round reaches the predetermined number of steps, the results will be recorded, and a new round of PSO will start with the brand new random initialized particle population. Until the target round criterion is reached, this reviving is repeated. The best results of the rounds of PSO will be selected.

In this work, the Multi-Round-PSO algorithm will be used as the main method and the DE algorithm will also be applied to verify the optimization results.

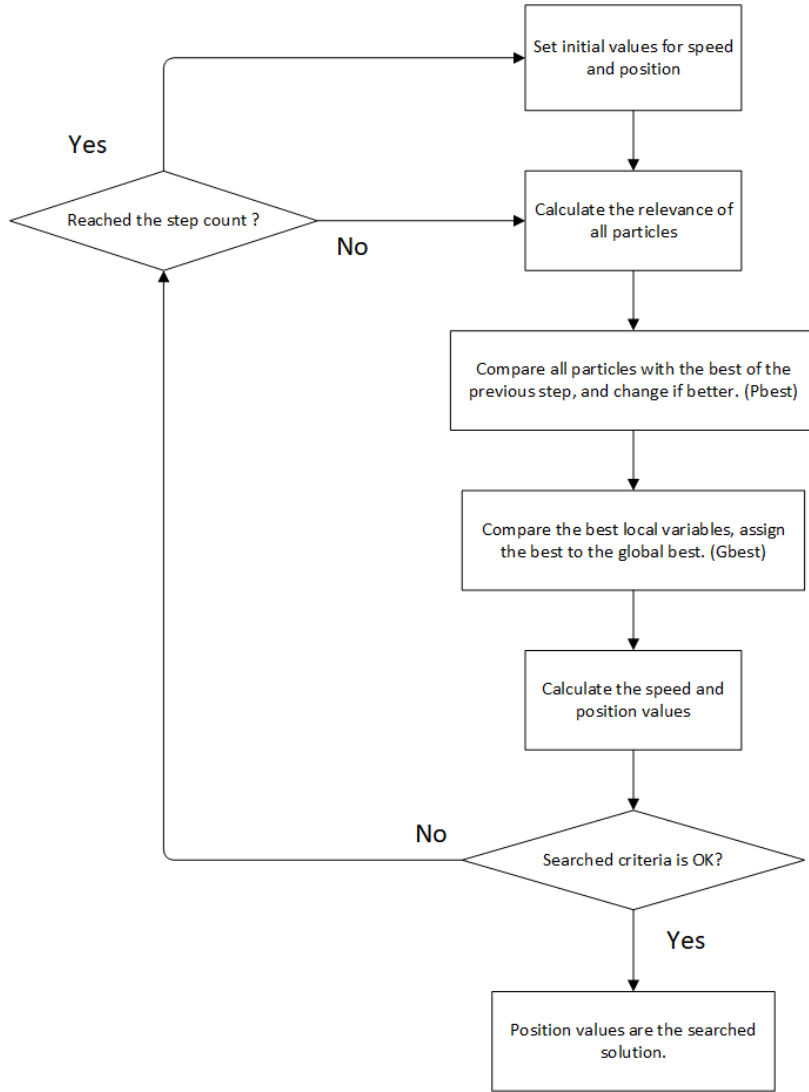


Fig. 1. The flow diagram of the hierarchical structure of the Multi-Round-PSO method

Table 1. The input output variables used in the work

Input or output	category	definition	number
Input	Feed 1 (VGO)	true boiling points	9
		density	1
		sulfur content	1

Input or output	category	definition	number
		nitrogen content	1
	Feed 2 (FCC diesel)	true boiling points	9
		density	1
		sulfur content	1
		nitrogen content	1
	Operating conditions	feed ratio	1
		hydrogen to oil ratio	2
		reactor pressure	1
		inlet temperatures	8
Output	Sour gas	yield	1
	LPG	yield	1
		density	1
	Light naphtha	yield	1
		density	1
		PNA contents	3
		TBP (5%-95%)	7
		RON	1
	Heavy naphtha	yield	1
		density	1
		PNA contents	3
		TBP (5%-95%)	7
		RON	1
	Kerosene	yield	1
		density	1
		PNA contents	3
		TBP (0%-100%)	9
		flash point	1
		freeze point	1
		smoke point	1
	Diesel	yield	1
		density	1
		PNA contents	3
		TBP (0%-100%)	9
		flash point	1
		cetane number	1
		pour point	1
	Bottom oil	yields	1
		density	1
		PNA contents	3
		TBP (0%-100%)	9
		flash point	1

Input or output	category	definition	number
		BMCI	1

Comments:

PNA contents represent the paraffin content, naphthenic content and aromatic content.

80 output parameters include:

The yield of 8 products(H₂S, dry gas, LPG, light naphtha, heavy naphtha, kerosene, diesel, tailoil)

LPG: density

LN: density, paraffin, naphthenic, aromatic, RON, 5%, 10%, 30%, 50%, 70%, 90%, 95% TBP

HN: density, paraffin, naphthenic, aromatic, RON, 5%, 10%, 30%, 50%, 70%, 90%, 95% TBP

Kerosene: density, flash point, freeze point, smoke point, paraffin, naphthenic, aromatic, 0%, 5%, 10%, 30%, 50%, 70%, 90%, 95%, 100% TBP

Diesel: density, flash point, cetane number, pouring point, paraffin, naphthenic, aromatic, 0%, 5%, 10%, 30%, 50%, 70%, 90%, 95%, 100% TBP

Bottom oil: density, flash point, BMCI, paraffin, naphthenic, aromatic, 0%, 5%, 10%, 30%, 50%, 70%, 90%, 95%, 100% TBP

Table 2. Statistics Related to Performances of Different Structures (80 outputs)

Index	FNN	SOM-CNN	3c-SOM-CNN	MISR(3 residual blocks)
Loss(train)	0.00606	0.00509	0.00402	0.00157
Loss(test)	0.00576	0.00489	0.00351	0.00278
Iterations	10000	5000	5000	5000
Total time(min)	10.83	19.20	20.32	61.37
Correlation coefficient R ² (total outputs)	0.7624	0.7869	0.8112	0.8681
R ² (properties only)	0.7403	0.7670	0.8279	0.8562
Number of which R ² ≥0.9	26	30	40	44
MRE (test samples)	1.8436	1.6998	1.3598	1.1702
MAE (test samples)	0.9741	0.9375	0.7495	0.6323

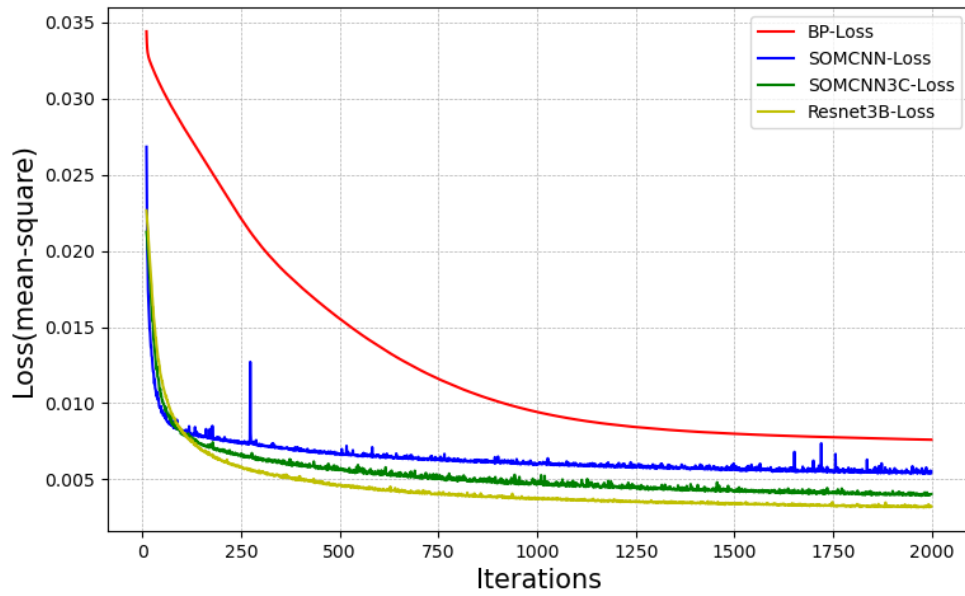


Fig. 2. The test loss curves of different structures

Table 2. Statistics Related to Performances of MISR with Different Number of Residual Blocks(80 outputs)

Index	2 residual blocks	3 residual blocks	4 residual blocks	5 residual blocks
Loss(train)	0.001732	0.00157	0.00179	0.000580
Loss(test)	0.003142	0.00278	0.00247	0.00249
Iterations	5000	5000	5000	5000
Total time(min)	48.07	61.37	81.33	178.54
Correlation coefficient				
R^2 (total outputs)	0.8472	0.8681	0.8941	0.8983
R^2 (properties only)	0.8333	0.8562	0.8846	0.8894
Number of which $R^2 \geq 0.9$	41	44	50	53
MRE (test samples)	1.3146	1.1702	1.0356	0.9974
MAE (test samples)	0.7054	0.6323	0.5517	0.5103

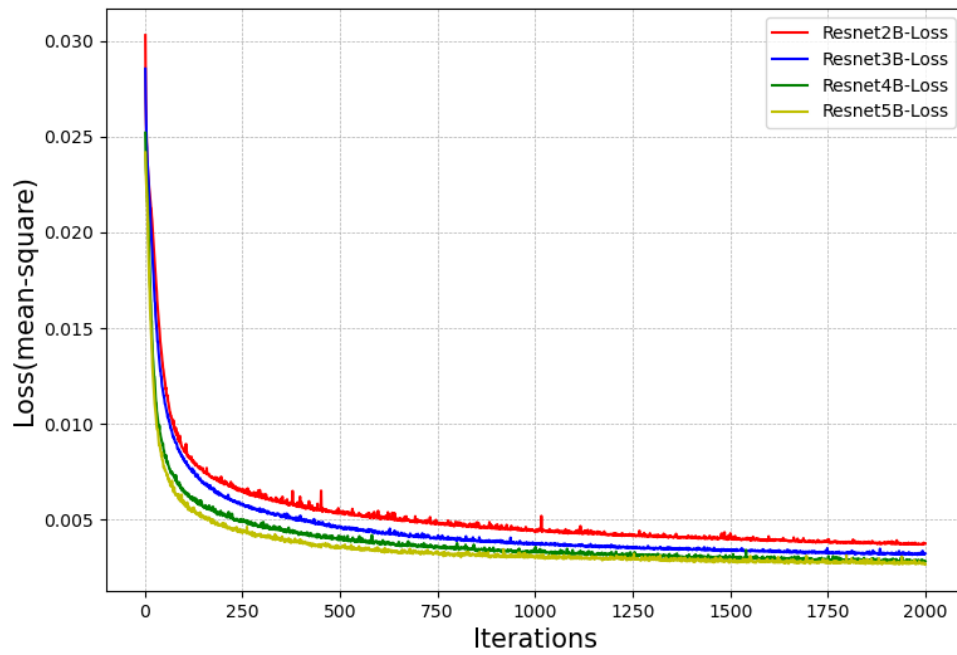


Fig. 3. The test loss curve of SOM-Residual net with different residual blocks

Test environment:

Linux system

CPU: Intel Xeon gold 6240 2.60GHz

GPU: 2080ti