Particle Swarm Optimization for Nano-Particles Extraction from Supporting Materials

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Abstract

Evolutionary computation for image processing is an encouraging research area. Transmission electron microscopy (TEM) images when used to characterize metallic and non-metallic nano-particles (size, morphology, structure, or composition), need such advanced image processing algorithms. This paper presents an efficient evolutionary computational method, particle swarm optimization (PSO), for automatic segmentation of nano-particles. A threshold-based segmentation technique is applied, where image entropy is attacked as a minimization problem to specify local and global thresholds. We are concerned with reducing wrong characterization of nano-particles due to concentration of liquid solutions or supporting material within the acquired image. The obtained results are compared with manual techniques and with previous researches in this area.

Keywords: Particle Swarm Optimization, TEM Images Scanning, Threshold Segmentation, Nano-Particles.

1. INTRODUCTION

Evolutionary computation algorithms (genetic-algorithms, genetic programming, or particle swarm optimizations) and data mining tools (neural network or decision tree) since introduced in image processing, have leaded to significant results [1-2-3]. In medical data classifications, neural networks [4–5] and linear programming models [6] obtained high classification accuracy rate, however their decision process was poor. Better results were achieved when using hybrid computation techniques, i.e. fuzzy-genetic, or neuro-fuzzy. In [7], a hybrid model was developed by introducing PSO for medical data classification.

Particle Swarm Optimization (PSO) is a relatively recent optimization method based on the idea of birds' swarming. PSO is similar to the Genetic Algorithm (GA) in the sense that they are both population-based search approaches. They both depend on information sharing among their population members to enhance their search processes. GA converges towards high quality solutions but within many and many iterations. PSO is easy to be implemented, have few parameters to be adjusted, and is more computationally efficient. This superior computational efficiency makes PSO more consistent in future image processing optimization problems [8].

From image processing point of view, TEM images characterization could be either manual or automatic. Existing techniques are facing different problems: illumination changes across the image, intensity variation of similar nano-particles due to diffraction contrast and/or liquids, and weak signal-to noise-ratio. TEM images contents' usually investigate binary or multi-class classifications [9]. Thresholding is an efficient image classifier tool, especially when real time processing is needed. Threshold selection can be either global or local. A global thresholding technique is one that segments the entire image with a single threshold value, whereas a local thresholding technique is one that partitions a given image into subimages and determines a threshold for each subimage [10]. Global techniques are further classified into point-dependent or region-dependent methods. When the threshold value is determined from the pixel gray tone independently from the gray tone of its neighborhood pixels, the thresholding method is point-dependent. On the other hand, a method is called region-dependent if the threshold value is determined from the local property within a neighborhood of a pixel.

1.1 Particle Swarm Optimization

PSO was originally introduced by Eberhart and Kennedy in 1995 [11]. In PSO algorithm, birds in a flock are our particles, where these particles are considered as simple agents through a problem space (food). PSO could be considered as an optimization technique. The algorithm starts by initializing a group of randomly distributed particles. These particles freely fly across the concerned space. During their flight, each initial particle should update its own velocity and position based on the experience of its own and the entire population. Instant particles' location in the multi-dimensional problem space represents one of the assumed solutions for the problem. When these particles move to new locations, another solution is generated. The velocity and direction of each particle will be recorded then altered in each generation. In any iteration, the particle's new location is computed by adding the particle's current velocity to its location. A fitness function is calculated for each solution and is to be minimized via further population of the swarms [8]. The PSO algorithm could better be summarized by means of a descriptive block diagram in the next section.

1.2 Nano-Particle Characterization Techniques in TEM Images

In [12], we have introduced a new fast Transmission Electron Microscopy (TEM) images clustering technique. In this research, analysis of particle sizes and shapes from two-dimensional TEM images were attacked. The hybrid method consisted of: an automatic segmentation and nano-particles counting. The automatic segmentation has assumed what we called "Automatic Threshold Generator" (ATG) towards a high efficient multiple- regions segmentation technique. ATG generated a vector of bi-threshold values used for electronic microscopic input image segmentation. This ATG gave good results when compared with existing algorithms [13]. However, TEM images where concentration of liquid solutions or supporting material affects image intensities failed to be counted via ATG correctly. Results were not comparable to manual results in these TEM images. This could be referred to wrong classification of supporting materials as nano particles.

2. The Proposed Nano-particle Segmentation Algorithm

In this paper we are attacking threshold-segmentation problem as a minimization problem, where both local and global minima are to be detected via an evolutionary computational method (PSO). The objective is to search for a better classifier that differentiates between nano-particles and their supporting materials.

2.1 PSO Algorithm

Figure (1) presents a summary of the PSO steps. Equation (1) refers to a number 'rand' which is a generated positive random number les than unity. As we are dealing with computer based simulation, the variable Δt is generally referred to the iterations span that could be considered unity. Thus, X^i_0 is limited between a minimum and a maximum value. The second step is the particles velocity update through the iterative procedure. In equation (2), the particles velocities are updated (V_{k+1}^i) looking towards the initial velocity (V_k^i) and influences emerging from: the particle itself (p_i) and the swarm (p_k^g); where pi denotes the best position required from the fitness function for the particle itself and p_k^g is the best position obtained globally for any particle within the whole swarm towards the desired minimum. The values of w, c_1, and c_2 are all knowledge based constants that take values from experience knowledge. Equation (3) explains the position updates. Equation (4) deals with the memory update for the fittest position and velocity. Finally, equation (5) concerns with the stopping criteria. The algorithm could stop in one of two conditions: either the error obtained is less than the required error, or the algorithm undergoes successive iterations without any improvement in the error.

2.2 Entropy- Based Segmentation

The motivation of application of the maximum entropy method to solve threshold selection has been started since 1989 [14]. The maximum entropy principle states that, for a given amount of information, the probability distribution which best describes our knowledge is the one that maximizes the Shannon entropy subjected to a set of constrains [15]. The Entropy mathematical model could be summarized as figure (2). This model assumes first the number of classes required for the nano-particles image. We have selected two thresholds in order to compare the obtained results with the ATG previously presented in

[12]. Selecting two threshold means that we have three classes: [0, t_1] where we will define an entropy H_0; from [t_1, t_2] where entropy H_1 is defined, and finally [t_2, L] where H_2 is calculated. ‘L’ represents the maximum grayscale obtained during histogram analysis.

2.3 Thresholds Generation

The previously discussed PSO algorithm is included within a segmentation procedure, as shown in figure (3). This algorithm starts with a histogram generator, a PSO implemented algorithm where the target function is the entropy and the output is the threshold vector. Images are then segmented to separate the nano-particles from the TEM image. Swarming, the PSO technique generates a vector of bi-threshold values used for electronic microscopic input image segmentation.

Generating Particles:

$$X_0^i = X_{\min} + rand\,.[X_{\max} - X_{\min}]$$
$$V_0^i = \frac{X_0^i}{\Delta t} \qquad (1)$$

↓

Velocity Update:

$$V_{k+1}^i = w.V_k^i + c_1.rand\,.[\frac{p_i - X_k^i}{\Delta t}] + c_2.rand\,.[\frac{p_k^g - X_k^i}{\Delta t}] \qquad (2$$

↓

Position Update:

$$X_{k+1}^i = X_k^i + V_{k+1}^i.\Delta t \qquad (3)$$

↓

Memory Update:

$$p_{i,best} = p_i \qquad \text{if } f(p_i) > f(p_{i,best})$$
$$g_{i,best} = g_i \qquad \text{if } f(g_i) > f(g_{i,best}) \qquad (4)$$

↓

Stopping Criteria:

$$\left| f(p_k^g) - f(p_{k-q}^g) \right| \le \varepsilon \qquad q = 1,2,\ldots S \qquad (5)$$

The advantage of the PSO when compared to other existing techniques concerns with the dimensionality broadband of the PSO. This means that PSO could generate a multi-threshold values vector with ***n***-dimensions according to the type of images to be segmented. The vector length is related to the entropy equation applied which in turns is related to the degree of the image classifier.

$$f(t) = H_0 + H_1 + H_2$$

$$P_i = \frac{h(i)}{N} \qquad (6)$$

$h(i)$: The number of pixels in gray level (i)

N : The total number of pixels in the TEM image

$$w_0 = \sum_{0}^{t_1 - 1} P_i \qquad w_1 = \sum_{t_1}^{t_2 - 1} P_i$$

$$w_2 = \sum_{t_2}^{L} P_i \qquad (7)$$

$$H_0 = \frac{-1}{w_0} \sum_{0}^{t_1 - 1} P_i \log(P_i) + \log(w_0)$$

$$H_1 = \frac{-1}{w_1} \sum_{t_1}^{t_2 - 1} P_i \log(P_i) + \log(w_1)$$

$$H_2 = \frac{-1}{w_2} \sum_{t_2}^{L} P_i \log(P_i) + \log(w_2) \qquad (8)$$

FIGURE 2: Entropy Calculations of TEM Image.

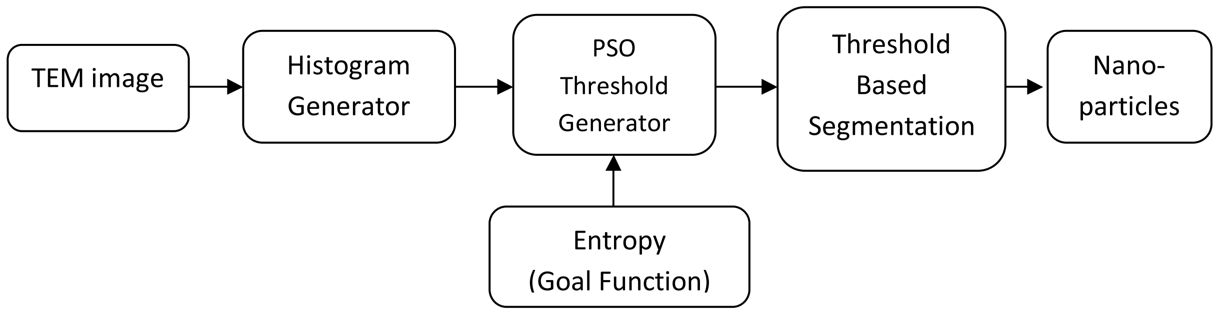


FIGURE 3: The Segmentation Technique: The PSO uses entropy as a goal function.

3. Results and Discussion

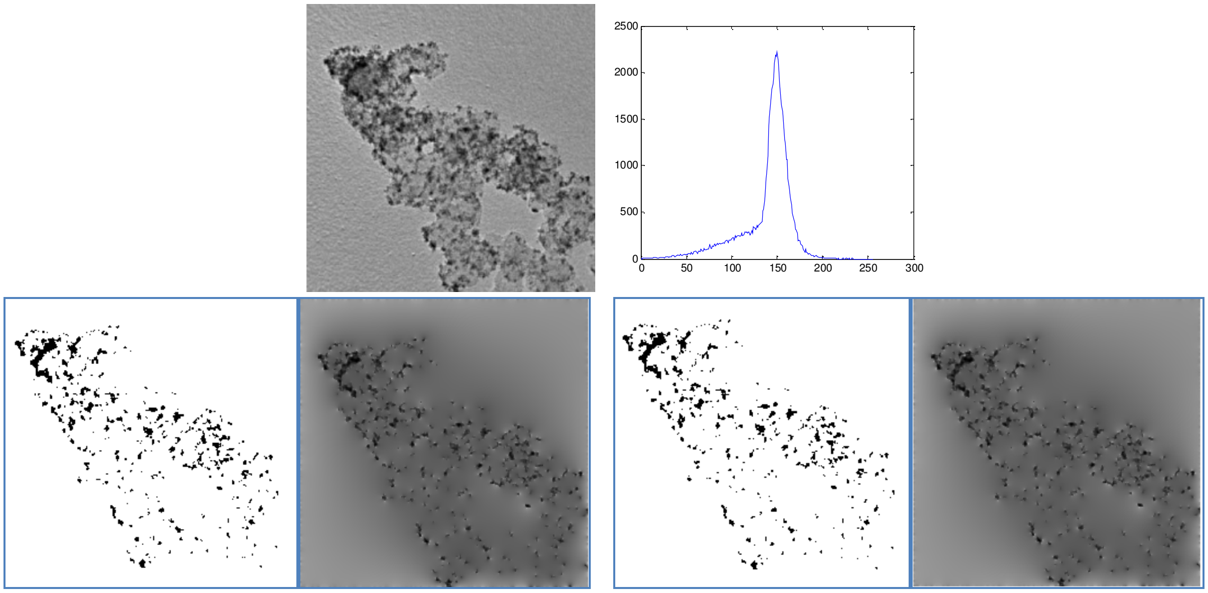
The introduced algorithm is applied to a wide TEM data set. Comparison starts with cases described in [12] to evaluate the improvement gained. Table (1) shows a comparison between this PSO based segmentation and the previous presented ATG method [12] for four different selected cases: nano1- nano2- nano3- nano4. Table (2) shows the ratio of nano-particles characterized by means of two different algorithms. The improvement in the PSO method is remarkable in cases: nano3 and nano4. Figures (4 and 5) show a comparison between two easy segmented cases. PSO gives results approximately equal to those obtained in [12].

Case	ATG [12]		Proposed PSO	
Nano1	T1 = 0	T2 = 73.5	T1 = 0.0441	T2 = 70.1350
Nano2	T1 = 0	T2 = 83.5	T1 = 1.0643	T2 = 70.449
Nano3	T1 = 0	T2 = 127	T1 = 1.1497	T2 = 50.1398
Nano4	T1 = 0	T2 = 64	T1 = 0.1290	T2 = 30.1241

TABLE 1: Comparison between the two entropy-based segmentation techniques.

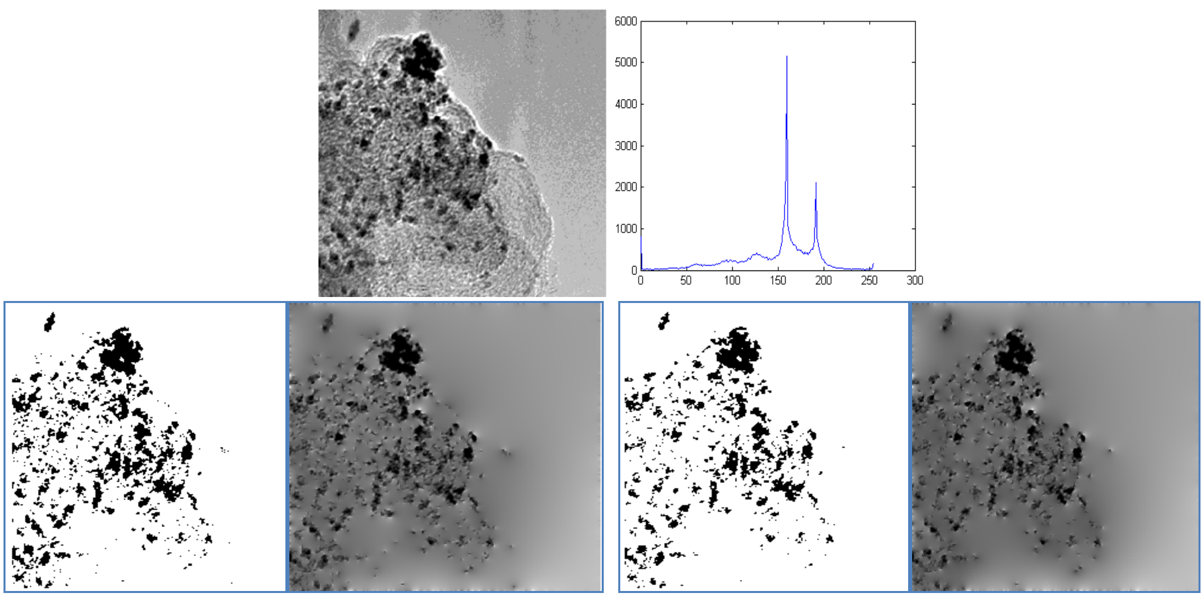
Case	Ratio of nano-particles extracted		Improvement
	ATG [12]	Proposed PSO	
Nano1	0.0401	0.0356	0.4532
Nano2	0.1015	0.0771	2.4475%
Nano3	0.2527	0.0358	21.6934%
Nano4	0.2843	0.0133	27.1027%

TABLE 2: Nano-particles extraction effectiveness of the proposed method.



AGT PSO

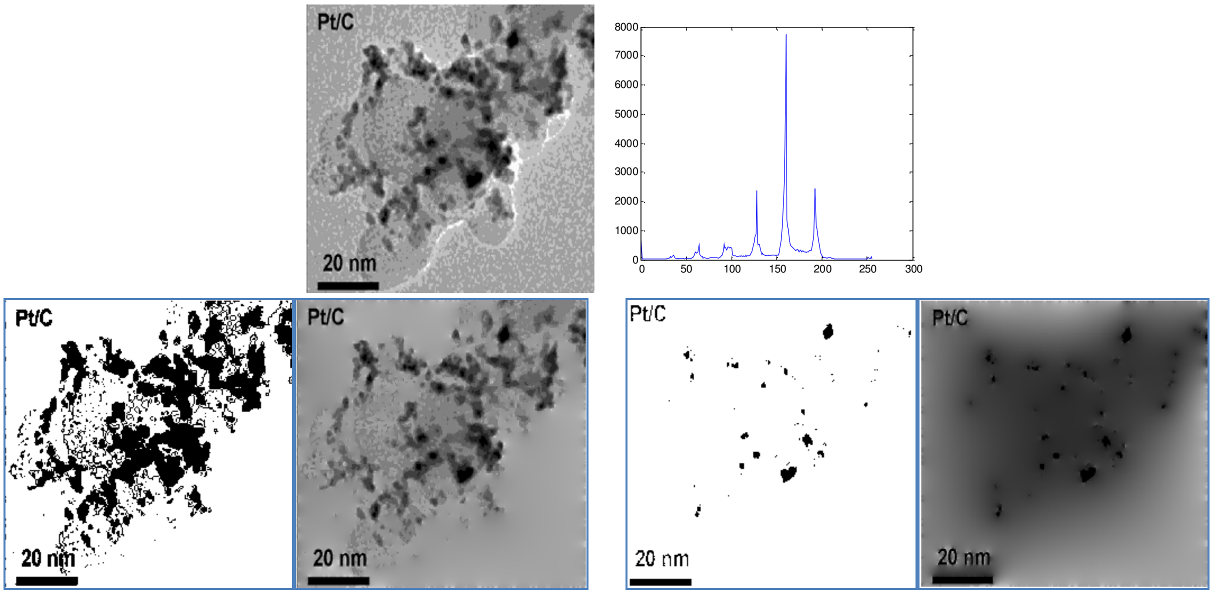
FIGURE 4: Nano1 case: Original image- Histogram- AGT results- PSO results



AGT PSO

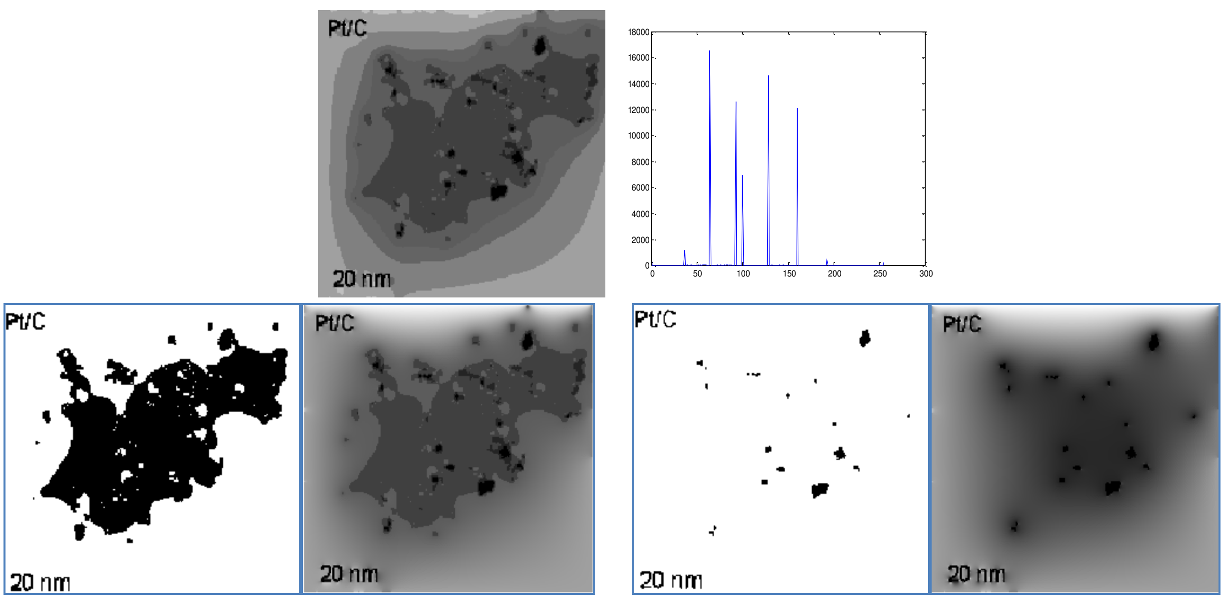
FIGURE 5: Nano2 case: Original image- Histogram- AGT results- PSO results.

Figures (6 and 7) show how the proposed PSO segmentation succeeded in segmenting smaller regions corresponding to nano-particles areas. False areas are characterized as nano-particles due to fluids within the specimen sample. In figure (8), the false areas characterized as nano particles using the ATG [12] are shown. All these areas are not the required targeted particles. The histogram presented in figure (9) is a comparison of one manual and two automatic counting methods. The PSO presented in this work is close to the manual method especially in images that are difficult to be segmented.



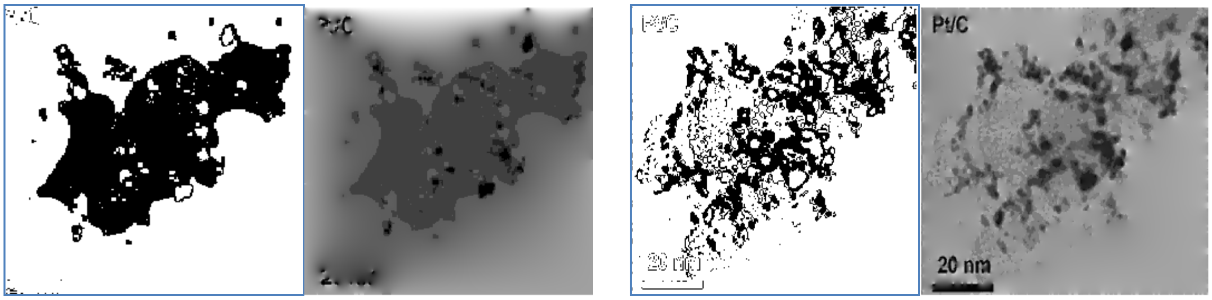
AGT PSO

FIGURE 6: Nano3 case: Original image- Histogram- AGT results- PSO results



AGT PSO

FIGURE 7: Nano4 case: Original image- Histogram- AGT results- PSO results



Nano4 nano3

FIGURE 8: PSO improvement: false Area characterized as nano-particles using ATG.

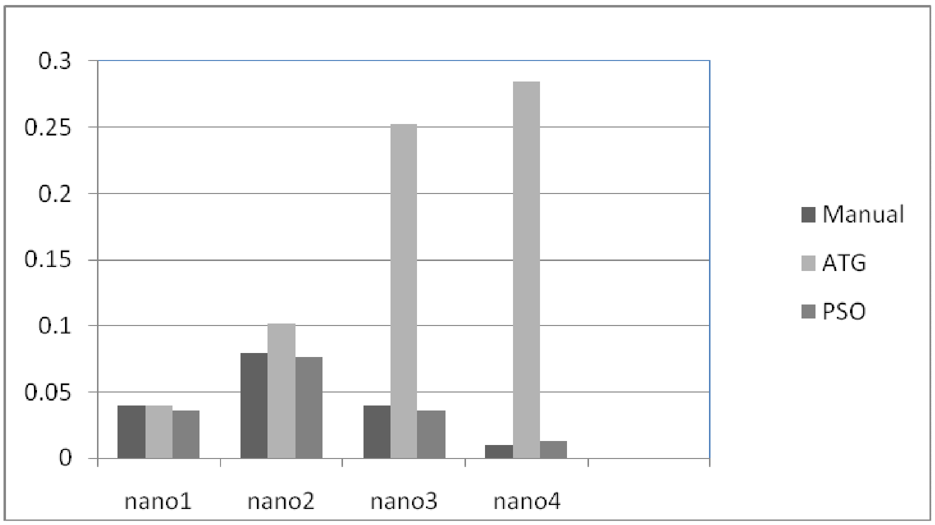


FIGURE 9: Nano-particles counting: Manual- ATG [12]- Proposed method.

CONCLUSION

The PSO- automatic segmentation presented has specified a threshold vector that clusters the nano-particles existing within the TEM image, where image entropy measure is the goal function. Obtained results show that the proposed segmentation method reduces wrong characterization of nano-particles in images where concentration of liquid solutions or supporting material affects image intensities. The PSO segmentation surpasses the ATG, presented in [12], by about 27%. Furthermore, the counted particles although comparable to manual results, the PSO presented technique has shown high computational efficiency which serves for real time characterization.

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