Negatively Correlated Search as a Parallel Exploration Search Strategy

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Abstract

Parallel exploration is a key to a successful search. The recently proposed Negatively Correlated Search (NCS) achieved this ability by constructing a set of negatively correlated search processes and has been applied to many real-world problems. In NCS, the key technique is to explicitly model and maximize the diversity among search processes in parallel. However, the original diversity model was mostly devised by intuition, which introduced several drawbacks to NCS. In this paper, a mathematically principled diversity model is proposed to solve the existing drawbacks of NCS, resulting a new NCS framework. A new instantiation of NCS is also derived and its effectiveness is verified on a set of multi-modal continuous optimization problems.

Section I Introduction

Negatively Correlated Search (NCS) [1] is a recently proposed Evolutionary Algorithm (EA) [2] of iteratively searching for optimal solutions. Driven by that a properly diversified population can be more beneficial to search [3], NCS explicitly models the population diversity, and adaptively finds the trade-off between exploitation (by maximizing the fitness function) and exploration (by maximizing the diversity model). NCS is featured in explicitly modeling the diversity of the next population at the current iteration, thus is capable of capturing the on-going interactions between successive iterations and introducing manageable diversity to guide the generation of the next population, distinguishing itself from traditional EAs who can only measure the diversity of sampled population [3]. Given this feature, NCS has shown very promising performance on standard benchmark suites [1], and has been frequently applied to real-world problems [4]-[8].

Although the basic idea of NCS has attracted increasing research interests [9]-[12], the original implementation of NCS [1] was mostly motivated by intuition, which lacked mathematical foundations and thus maybe sub-optimal. Specifically, in order to form a parallel exploration, the original NCS presented a decentralized diversity model for the next population. That is, the diversity was modeled separately at each exclusive sub-set of population, i.e., sub-population. Then the diversity model could only be maximized by individually comparing the zero-order of the sub-population diversity model between its parents and offsprings and selecting the larger ones. As the candidates were randomly sampled, the comparisons might involve considerable noise, leading to possibly inaccurate directions of maximizing the sub-population diversity. Even worse, such heuristic comparisons introduced

1 Without loss of generality, the maximization problems is taken for examples in this paper.
interdependencies among sub-populations that maximizing the diversity of one sub-population may deteriorate the others, finally resulting in a less controllable diversity of the population.

In this paper, a mathematically principled NCS is proposed to address the above issues. In the new NCS, a centralized model is presented to measure the diversity of the next population, which can be maximized by gradient descending along its negative first-order direction. Since the mathematical gradient is naturally the optimal direction to maximizing a function, the interactions between successive iterations are captured and no more heuristic comparison is needed. As a result, the sampling noise of each individual comparison can be greatly eliminated and the interdependencies among sub-populations are removed by exactly calculating the diversity gradient. Basically, the centralized diversity model is built in a sequential manner. Fortunately, by utilizing the gradient, such sequential process can be mathematically re-implemented in parallel. As a result, it is easy to scale-up the new NCS with respect to computing resources for parallel exploration.

Given that the maximization of the fitness function can be modeled as the gradient descent of the averaged fitness values of the population [13], the new NCS is thus able to simultaneously calculate the gradient of both the fitness function and the diversity model. The former gives ways to quickly find the optimum via exploitation, while the latter provides possibilities of avoiding early convergence through exploration. Note that, NCS is a general framework, thus an instantiation is needed for applications. As searching by fitness gradient has already been realized by Natural Evolution Strategy (NES) [13], we adopt it for simplicity. Thus, the resultant algorithm, i.e., Negatively Correlated Natural Evolution Strategy (NCNES), can be regarded as a new variant of NES equipped with parallel exploration capability.

The reminder of this paper is as follows. In Section II, the weakness of the original NCS is discussed to motivate the proposal of the new NCS. An instantiation of the new NCS framework, i.e., NCNES, is detailed in Section III. In Section IV, the effectiveness of the new diversity model, as well as NCNES, is verified on a set of multi-modal continuous optimization benchmark problems. The conclusions and discussions are given in the Section V.

**Section II A Centralized Diversity Model for Parallel Exploration**

NCS stems from re-thinking of “how does population facilitate the search?” Although it has been widely acknowledged that effective information sharing among population is the key to successful cooperative search, an open question remains what information to share and how [14]. By mimicking the cooperation in human, NCS asks the individuals in a population to have different search behaviors, so as to avoid repetitively searching a same region of solution space. Similar idea has also been adopted in machine learning [15]. Each search behavior is defined as how the offsprings will be sampled based on their parents, and usually can be represented as a probabilistic distribution. The mathematical correlation among distributions is utilized to statistically model the diversity among the population. As a result, by explicitly driving multiple probabilistic distributions to be negatively correlated, NCS suffices to maximize the diversity of the next population (will be generated by those distributions) for exploration.

By implementing the above idea, one should instantiate a way for modeling the diversity and maximizing it. In the original NCS, such steps are mainly motivated by intuition, lacking mathematic foundations for
in-depth analysis and shown to be sub-optimal. In this section, we provide an integrated solution for these issues by presenting the centralized diversity model.

Section II.A Two Drawbacks of the Original Decentralized Model

Basicallly, the idea of NCS requires the population being exclusively grouped into $\lambda$ sub-populations, each of which is then evolved by a traditional EA, preferably those who sample solutions from an explicit probabilistic distribution [16]. At each iteration, each sub-population will be “pushed” away from the others to maximize the diversity of the population. In order for parallel acceleration, the original NCS heuristically proposed a decentralized model to measure the diversity. That is, the diversity of each sub-population was modeled individually and maximized separately.

To be specific, the diversity model of the $i$-th sub-population, denoted as $\tilde{d}(\theta_i)$, was defined as the minimum of the negative correlation between its distribution and the distributions of the other sub-populations, shown as Eq.(1),

$$\tilde{d}(\theta_i) = \min\{-C(\theta_i, \theta_j)\} \quad \forall \ i,j \in \{1, \ldots, \lambda\} \quad (1)$$

where $\theta_i$ denotes the parameters of the distribution $p(\theta_i)$ of the $i$-th sub-population$^2$, and $C(\theta_i, \theta_j)$ means the correlation between the distributions of the $i$-th and the $j$-th sub-populations. To maximize each $\tilde{d}(\theta_i)$, the original NCS proposed to compare the diversity values of the parents and offsprings belonging to the sub-population, and select the larger ones for the next iteration. In order to obtain good balance between exploration and exploitation for an effective search, the fitness values are also considered during the maximization of diversity. Let $x_i$ be the parents in the $i$-th sub-population, and $x'_i$ be their offsprings. Then the comparison goes as Eq.(2),

$$\begin{cases} \text{discard } x_i \text{ and } \theta_i, & \text{if } f(x_i) + \varphi \cdot \tilde{d}(\theta_i) < f(x'_i) + \varphi \cdot \tilde{d}(\theta'_i) \\ \text{discard } x'_i \text{ and } \theta'_i, & \text{otherwise} \end{cases} \quad (2)$$

where $\varphi \in (0, +\infty)$ is a trade-off parameter, and $f(x_i)$ is the fitness values of $x_i$. For more details of the original NCS, please refer to [1].

It is clear in Eqs.(1)-(2) that the maximization of diversity highly depends on the samplings of the candidate solutions. However, existing sampling techniques in EAs are usually randomized and thus may involve significant noise, which may mislead the maximization of diversity. Another drawback is that, the above heuristic comparisons introduces the interdependencies among sub-populations. Specifically, by substituting Eq.(1) to Eq.(2), it can be seen that the heuristic comparison in the $i$-th subpopulation explicitly requires the offspring distribution $\theta'_j$ from all other $j$-th sub-populations as the input for outputting its own offspring distribution $\theta'_i$, while the other sub-populations also require doing so. Thus, it appears that the heuristic comparison in one sub-population interacts with that in the other sub-populations. As a result, the de-centralized diversity model may not be maximized by maximizing the diversity of each sub-population one-by-one, making the idea of NCS ineffective.

Section II.B Gradient Descending a Centralized Diversity Model

$^2$ For simplicity, in this paper, we assume all the distributions are with the same type, e.g., Gaussian distribution, while the parameters of the distribution, e.g., mean and covariance, can be different.
To re-design NCS, let us start a thought game from what kind of probabilistic distribution can facilitate the evolutionary search better by generating new solutions. It is usually straightforward to have a simple well-defined distribution like Gaussian distribution and Cauchy distribution [16]. Unfortunately, such distribution may not be complicated enough to capture the problem characteristic like the multi-modality [17]. Usually, it is non-trivial to properly setup one complicated distribution. Similar to Gaussian Mixture Model [18], we can have multiple distributions instead of one complicated distribution. Another advantage of setting up multiple distributions is that we can explicitly sample different solutions herefrom for the purpose of finding multiple optima [19].

Then the problem turns into how we can add new simple distributions to the first simple distribution. Clearly, the new distribution should be able to sample new solutions with high fitness values. Moreover, the new distribution should have fewer “overlaps” (correlations) with existing ones, so that it can be used to sample a different region of the solution space.

For simplicity, let us setup the multi-distribution model from scratch. If we only have one distribution \( p_1 \), there is no worry of “overlap”, so it will only be required to sample solutions with higher enough fitness values. Mathematically, this objective \( J \) (to be maximized) can be modeled as the expectation of fitness values of the solutions \( x \) sampled from \( p(\theta_1) \) [13], shown as Eq.(3).

\[
J = \int f(x)p(x|\theta_1)dx \tag{3}
\]

Suppose we want to add a new distribution \( p(\theta_2) \) to \( p(\theta_1) \), we have to minimize the correlation between them, as well as maximizing the expected fitness value of \( p(\theta_2) \). For that purpose, the following Eq.(4) should be maximized.

\[
J = \int f(x)p(x|\theta_1)dx + \int f(x)p(x|\theta_2)dx + (-C(\theta_1, \theta_2) - C(\theta_2, \theta_1)) \tag{4}
\]

Now if \( \lambda \) distributions are considered, Eq.(4) can be readily extended to Eq.(5).

\[
J = \sum_{i=1}^{\lambda} \int f(x)p(x|\theta_i)dx + \sum_{i=1}^{\lambda} \sum_{j=1}^{\lambda} (-C(\theta_i, \theta_j)) \tag{5}
\]

Consequently, to have \( \lambda \) distributions searching different regions of the solution space for high fitness values, we need to maximize the objective function \( J \) in Eq.(5). To take a closer look at the right side of Eq.(5), the first additive term describes that all the distributions should be able to sample solutions with high fitness values. For the second additive term, it means that all the distributions should be mutually negatively correlated, by which the information entropy among \( \lambda \) distributions will be maximized [1]. Given that the distributions reflect how new solutions are generated, the second additive term is thus capable of modeling the diversity of the next population. As a result, a centralized diversity model \( D \) for all \( \lambda \) distributions is defined as Eq.(6).
\[ D = \sum_{i=1}^{\lambda} \sum_{j=1}^{\lambda} -C(\theta_i, \theta_j) = \sum_{i=1}^{\lambda} d(\theta_i) \]  

where \( d(\theta_i) = \sum_{j=1}^{\lambda} -C(\theta_i, \theta_j) \) is the derived diversity component for the \( i \)-th sub-population, which is also different from the original one \( d(p_i) \) in Eq.(1). By further denoting the first additive term as \( F \) and its \( i \)-th component as \( f(\theta_i) = \int f(x)p(x|\theta_i)dx \), Eq.(5) can be re-written as Eq.(7) for clarity.

\[ J = F + D = \lambda \sum_{i=1}^{\lambda} f(\theta_i) + \sum_{i=1}^{\lambda} d(\theta_i) \]  

It is highly desired that \( J \) can be maximized in parallel to enjoy the computational acceleration. Since the distribution of each sub-population is independent from each other by definition, one way to achieve the parallel maximization of \( J \) is to apply the gradient descent to \( J \) with respect to each \( \theta_i \). The gradient of Eq.(7) can be calculated as Eq.(8).

\[ \nabla_{\theta_i}J = \nabla_{\theta_i}F + \nabla_{\theta_i}D = \nabla_{\theta_i}f(\theta_i) + \nabla_{\theta_i}d(\theta_i) \]  

Clearly, by applying the gradient descent to the centralized diversity model, the diversity of each distribution can be independently maximized to enable NCS a parallel exploration, avoiding the random noise of samplings and the interdependencies among sub-populations introduced by using heuristic comparisons. Hence, the proposed centralized diversity model has successfully addressed the two issues of the original NCS, and brings a clear mathematical explanation to NCS.

**Section II.C The New NCS Framework**

To implement Eq.(8), it is required to know how to obtain \( \nabla_{\theta_i}f(\theta_i) \) and \( \nabla_{\theta_i}d(\theta_i) \), and how to update \( \theta_i \) based on them.

For \( \nabla_{\theta_i}f(\theta_i) \), [13] has derived the following formulation (Eq.(9)) that we can directly employ.

\[ \nabla_{\theta_i}f(\theta_i) = \nabla_{\theta_i} \int f(x)p(x|\theta_i)dx = \mathbb{E}_{\theta_i}[f(x)\nabla_{\theta_i}\log p(x|\theta_i)] \approx \frac{1}{\mu} \sum_{k=1}^{\mu} f(x_i^k)\nabla_{\theta_i}\log p(x_i^k|\theta_i) \]  

where \( x_i^k \) indicates the \( k \)-th solution in the \( i \)-th sub-population and \( \mu \) is the number of the solutions in the \( i \)-th sub-population. For more details, please refer to [13].

To calculate \( \nabla_{\theta_i}d(\theta_i) \), by Eq.(6), a correlation measurement \( C(\theta_i, \theta_j) \) should be specified for a pair of distributions \( \theta_i \) and \( \theta_j \). Following that of the original NCS, let the Bhattacharyya distance [20] be the negative correlation measurement, i.e., \( C(\theta_i, \theta_j) = -\log \left( \int \sqrt{p(x|\theta_i)p(x|\theta_j)}dx \right) \) for continuous distributions and \( C(\theta_i, \theta_j) = -\log \left( \sum_{x \epsilon X} \sqrt{p(x|\theta_i)p(x|\theta_j)} \right) \) for discrete distributions, respectively.

Then we can have \( \nabla_{\theta_i}d(\theta_i) \) as Eq.(10) shows.
\[ \nabla_{\theta_i}d(\theta_i) = \sum_{j=1}^\lambda \nabla_{\theta_j}\log(\int p(x|\theta_j)p(x|\theta_i)dx) \]

\[ \nabla_{\theta_i}f(\theta_i) = \sum_{j=1}^\lambda \nabla_{\theta_j}\log(\sum_{x} p(x|\theta_j)p(x|\theta_i)) \]  

(10)

In case that the probability density function \( p \) is not explicitly known, one can randomly sample a set of candidate solutions for both distributions and estimate \( \nabla_{\theta_i}d(\theta_i) \) using Eq.(10).

Given \( \nabla_{\theta_i}f(\theta_i) \) and \( \nabla_{\theta_i}d(\theta_i) \) are ready, it is straightforward to obtain \( \nabla_{\theta_i}J \) by Eq.(8). Alternatively, we can inject a parameter \( \varphi \) to trade-off \( \nabla_{\theta_i}f(\theta_i) \) and \( \nabla_{\theta_i}d(\theta_i) \) for a more subtle \( \nabla_{\theta_i}J \) using Eq.(11).

\[ \nabla_{\theta_i}J = \nabla_{\theta_i}f(\theta_i) + \varphi \cdot \nabla_{\theta_i}d(\theta_i) \]  

(11)

Similar to standard gradient descent methods [21], the objective function \( J \) can be maximized using Eq.(12).

\[ \theta_i = \theta_i + \eta \cdot \nabla_{\theta_i}J \]  

(12)

where \( \eta \) is a step-size parameter for the gradient descent.

Based on the discussions above, the new NCS framework is listed in Algorithm I and described as follows. At the beginning stage, \( \lambda \) probabilistic distributions are initialized to form a set of parallel search processes. For each iteration, the following steps are executed in parallel: 1) each search process first generate \( \mu \) candidates solutions according to its probabilistic distribution \( p(\theta_i) \) at step 6; 2) the fitness values of all \( \mu \) newly generated solutions are evaluated with respect to the fitness function \( f \) at step 7; 3) the gradient of the fitness function \( f \) locally approximated by the \( i \)-th sub-population, i.e., \( \nabla_{\theta_i}f(\theta_i) \), is calculated according to Eq.(9) at step 9; the gradient of the centralized diversity model with respect to the \( i \)-th distribution, i.e., \( \nabla_{\theta_i}d(\theta_i) \), is calculated according to Eq.(10) at step 10; then the gradient of

**Algorithm I: The New NCS Framework**

1. **Input:** \( f, d, \lambda, \mu, \eta, \varphi \)
2. **Begin:**
3. Initialize \( \lambda \) search processes defined by probabilistic model \( p(\theta) \);
4. **While** stopping-criteria not met do:
5. **For** each \( i \)-th search process:
6. Generate \( \mu \) solutions according to \( p(\theta_i) \);
7. Evaluate the fitness of all \( \mu \) generated solutions;
8. Update \( x^* \) as the best solution ever found.
9. Calculate the gradient of fitness as \( \nabla_{\theta_i}f(\theta_i) \);
10. Calculate the gradient of diversity as \( \nabla_{\theta_i}d(\theta_i) \);
11. \( \nabla_{\theta_i}J \leftarrow \nabla_{\theta_i}f(\theta_i) + \varphi \cdot \nabla_{\theta_i}d(\theta_i) \);
12. \( \theta_i \leftarrow \theta_i + \eta \cdot \nabla_{\theta_i}J \);
13. **Output** \( x^* \), \( f(x^*) \).
the general objective function, i.e., $\nabla_{\theta_i} J$, can be accumulated based on Eq. (11) at step 11; the general objective function $J$ is thus maximized by using gradient descent method (see Eq. (12)), as shown in step 12. Finally, the best ever-found solution $x^*$ that is iteratively recorded (see step 8) will be output as the result of NCS before its halting (see step 13).

Section III Negatively Correlated Natural Evolution Strategies

Basically, the new NCS is a framework. To implement it as an executable algorithm, the type of probabilistic distribution $p(\theta_i)$ should be specified. In this paper, the Gaussian distribution is employed, i.e., $p(\theta_i) = N(m_i, \Sigma_i)$. The underlying reason is three-folds: 1) the Gaussian distribution is the most commonly used distribution in EA [16]; 2) by using the Gaussian distribution, $\nabla_{\theta_i} f(\theta_i)$ has an analytic closed form for efficient computation [13]; 3) the Bhattacharyya distance is also analytic based on the Gaussian distribution [1].

By using the Gaussian distribution, $\nabla_{\theta_i} f(\theta_i)$ can be further represented by $\nabla_{m_i} f(\theta_i)$ and $\nabla_{\Sigma_i} f(\theta_i)$, as proposed in NES [13].

$$\nabla_{m_i} f(\theta_i) = \frac{1}{\mu} \sum_{k=1}^{\mu} \Sigma_i^{-1} (x_i^k - m_i) \cdot f(x_i^k)$$

$$\nabla_{\Sigma_i} f(\theta_i) = \frac{1}{\mu} \sum_{k=1}^{\mu} \frac{1}{2} \Sigma_i^{-1} (x_i^k - m_i)(x_i^k - m_i)^T \Sigma_i^{-1} - \frac{1}{2} \text{tr} \Sigma_i^{-1} \cdot f(x_i^k) \tag{13}$$

Similarly, by using the Gaussian distribution, $\nabla_{\theta_i} d(\theta_i)$ can be further represented by $\nabla_{m_i} d(\theta_i)$ and $\nabla_{\Sigma_i} d(\theta_i)$. Given $d(\theta_i)$ can be analytically represented as Eq. (14) [1]. $\nabla_{m_i} d(\theta_i)$ and $\nabla_{\Sigma_i} d(\theta_i)$ can be obtained using Eq. (15).

$$d(\theta_i) = \sum_{j=1}^{J} \frac{1}{8} (m_i - m_j)^T \left( \frac{\Sigma_i + \Sigma_j}{2} \right)^{-1} (m_i - m_j) + \frac{1}{2} \log \left( \frac{\Sigma_i + \Sigma_j}{2 |\Sigma_i|} \right) \tag{14}$$

$$\nabla_{m_i} d(\theta_i) = \frac{1}{8} \sum_{j=1}^{J} \left( \frac{\Sigma_i + \Sigma_j}{2} \right)^{-1} (m_i - m_j)$$

$$\nabla_{\Sigma_i} d(\theta_i) = \frac{1}{4} \sum_{j=1}^{J} \left( \frac{\Sigma_i + \Sigma_j}{2} \right)^{-1} - \frac{1}{4} \left( \frac{\Sigma_i + \Sigma_j}{2} \right)^{-1} (m_i - m_j)(m_i - m_j)^T \left( \frac{\Sigma_i + \Sigma_j}{2} \right)^{-1} - \Sigma_i^{-1} \tag{15}$$

Thus, $\nabla_{m_i} J$ and $\nabla_{\Sigma_i} J$ can be readily obtained by considering Eqs. (11), (13) and (15). Nevertheless, [13] notices that if the above $\nabla_{m_i} J$ and $\nabla_{\Sigma_i} J$ are used as the gradients for $J$, there is an issue for directly updating $m_i$ and $\Sigma_i$ with respect to Eq. (12). To be specific, it can be observed that $\nabla_{m_i} J \propto \frac{1}{\Sigma_i}$ and $\nabla_{\Sigma_i} J \propto \frac{1}{\Sigma_i^2}$, which means a large $\Sigma_i$ can make the learning steps of $m_i$ and $\Sigma_i$ insignificant, while a small $\Sigma_i$ can result in a significant update of $m_i$ and $\Sigma_i$. This can lead to an unstable search and thus become impossible to precisely locate the optimum [13]. To address this issue, NES derives the Fisher information matrix $F$ from the natural gradient of a population. We extend it to the Gaussian distribution based multi-population cases where each pair of $F_{m_i}$ and $F_{\Sigma_i}$ is respectively assigned for a sub-
population, shown as Eq.(16).

\[
\begin{align*}
F_{m_i} & = \frac{1}{\mu} \sum_{k=1}^{\mu} (x_k^i - m_i)(x_k^i - m_i)^T \Sigma_i^{-1} \\
F_{\Sigma} & = \frac{1}{4\mu} \sum_{k=1}^{\mu} \left( \Sigma_i^{-1} (x_k^i - m_i)(x_k^i - m_i)^T \Sigma_i^{-1} - \Sigma_i^{-1} \right) \left( \Sigma_i^{-1} (x_k^i - m_i)(x_k^i - m_i)^T \Sigma_i^{-1} - \Sigma_i^{-1} \right)^T
\end{align*}
\]  

(16)

With the Fisher information matrix, \( m_i \) and \( \Sigma_i \) are updated using Eq.(17).

\[
\begin{align*}
m_i & = m_i + \eta_m \cdot F_{m_i} \cdot \nabla m_i \theta_j \\
\Sigma_i & = \Sigma_i + \eta_\Sigma \cdot F_{\Sigma} \cdot \nabla \Sigma_j \theta_k
\end{align*}
\]

(17)

where \( \eta_m \) and \( \eta_\Sigma \) are step-size parameters for updating \( m_i \) and \( \Sigma_i \), respectively. Intuitively, since \( F_{m_i}^{-1} \propto \Sigma_i^2 \) and \( F_{\Sigma}^{-1} \propto \Sigma_i^2 \), it turns out that \( F_{m_i}^{-1} \cdot \nabla_m \theta_j \propto \Sigma_i \) and \( F_{\Sigma}^{-1} \cdot \nabla_\Sigma \theta_k \propto \Sigma_i^2 \) are no longer to be oscillating for convergence.

Notice that, the above equations are computationally intensive. Specially, the inversions of the Fisher matrix costs \( O(D^6) \) operations if the full covariance matrix are considered [13], where \( D \) indicates the dimensionality of the search space. To alleviate the computational costs, we simply restrict the covariance matrix and the Fisher matrix for each distribution to be diagonals. This means that the interdependencies among decision variables are omitted. Although it may make the algorithm less robust to non-separable problems, it is a useful way to significantly improve the computational efficiency as well as the scalability of the algorithm [22].

Another technique adopted from [13] is the normalization of the fitness values. This is motivated by the difficulty of setting a proper trade-off parameter \( \varphi \) for aggregating \( \nabla_\theta f(\theta) \) and \( \nabla_\theta d(\theta) \). As different problems may have quite varied scales of fitness values. For that purpose, the utility function in [13] is employed in this paper to reshape the fitness values in each sub-population. Specifically, for each sub-population, all \( \mu \) solutions are first ranked based on their fitness values, where \( \pi(k) \) indicates the rank of the \( k \)-th solution. Then the utility function for each \( i \)-th sub-population, denoted as \( U_i \), is carried out to re-shape the fitness of each \( k \)-th solution according to Eq.(18). After that, the utility of each solution is used by replacing the term of \( f(x_k^i) \) in Eq.(13).

\[
U_i(\pi(k)) = \frac{\max \left( 0, \log \left( \frac{\pi(k) - 1}{\mu} \right) \right)}{\sum_{k=1}^{\mu} \max \left( 0, \log \left( \frac{\pi(k) - 1}{\mu} \right) \right)} = \frac{1}{\mu}
\]

(18)

The step-size parameters \( \eta_m \) and \( \eta_\Sigma \) can be either tuned off-line or adjusted during the search. In this paper, the following strategy is used to adjust these two parameters at each iteration.

\[
\begin{align*}
\eta_m & \leftarrow \eta_m^{\text{init}} \cdot \frac{e^{-\frac{\text{FES}}{\gamma}}}{e - 1} \\
\eta_\Sigma & \leftarrow \eta_\Sigma^{\text{init}} \cdot \frac{e^{-\frac{\text{FES}}{\gamma}}}{e - 1}
\end{align*}
\]

(19)
where $MAXFES$ is the total budget of the function evaluations and $FES$ is the number of consumed function evaluations up to now. $e$ is the natural constant. $\eta_m^{\text{init}}$ and $\eta_{\Sigma}^{\text{init}}$ are the initialized values for both parameters, respectively. Then these two step-sizes decrease over iterations to gradually focus on the convergence of the search.

So far, all details are presented to instantiate a NCS algorithm. To summarize, the proposed algorithm is a multi-Gaussian distribution based EA; Each distribution drives the evolution of one sub-population with the well-established NES; Multiple Gaussian distributions are negatively correlated by the proposed centralized diversity model. As a result, the proposed algorithm can also be regarded as a new variant of

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**Algorithm II: The proposed NCNES**

1. **Input:** $f$, $\lambda$, $\mu$, $\eta_m^{\text{init}}$, $\eta_{\Sigma}^{\text{init}}$, $\varphi$, $MAXFES$
2. **Begin:**
3.   For $i = 1$ to $\lambda$:
4.     Initialize a Gaussian distribution for the $i$-th Search Process as $N(\mu_i, \Sigma_i)$;
5.     $FES = 0$;
6.   **While** $FES < MAXFES$ **do**:
7.     $\eta_m \leftarrow \eta_m^{\text{init}} \cdot \frac{e^{-\frac{FES}{\max(1, FES)}}}{e-1}$;
8.     $\eta_{\Sigma} \leftarrow \eta_{\Sigma}^{\text{init}} \cdot \frac{e^{-\frac{FES}{\max(1, FES)}}}{e-1}$;
9.   For $i = 1$ to $\lambda$:
10.    Generate $\mu$ solutions $x_i^k \leftarrow N(\mu_i, \Sigma_i)$, $\forall k = 1, ..., \mu$;
11.    Evaluate the fitness $f(x_i^k)$, $\forall k = 1, ..., \mu$;
12.    $FES \leftarrow FES + \mu$;
13.    Update $x^*$ as the best solution ever found;
14.    Rank the $k$-th solution in terms of its fitness $f(x_i^k)$ as $\pi(k)$, $\forall k = 1, ..., \mu$;
15.    Set $U_i(\pi(k)) = \frac{\max(0, \log(\frac{\pi(k)}{\pi(k)+1})) - \log(\pi(k))}{\sum_{j=1}^{\mu} \max(0, \log(\frac{\pi(k)}{\pi(k)+1}))} - \frac{1}{\mu}$, $\forall k = 1, ..., \mu$;
16.    $\nabla_{m_i} f \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} (x_i^k - m_i) \cdot U_i(\pi(k))$;
17.    $\nabla_{\Sigma_i} f \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} (x_i^k - m_i) (x_i^k - m_i)^T \Sigma_i^{-1} (x_i^k - m_i) \cdot U_i(\pi(k))$;
18.    $\nabla_{m_i} d \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} \left( \Sigma_i^{-1} \right)^{-1} (m_i - m_i)$;
19.    $\nabla_{\Sigma_i} d \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} \left( \Sigma_i^{-1} \right)^{-1} \left( \Sigma_i^{-1} \right)^{-1} (m_i - m_i)^T (x_i^k - m_i)^T \Sigma_i^{-1}$;
20.    $F_{m_i} \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} \Sigma_i^{-1} (x_i^k - m_i) (x_i^k - m_i)^T \Sigma_i^{-1}$;
21.    $F_{\Sigma_i} \leftarrow \frac{1}{\mu} \sum_{k=1}^{\mu} \left( \Sigma_i^{-1} \right)^{-1} (x_i^k - m_i) (x_i^k - m_i)^T \Sigma_i^{-1}$;
22.    $m_i \leftarrow m_i + \eta_m \cdot F_{m_i} - \varphi \cdot \nabla_{m_i} d$;
23.    $\Sigma_i \leftarrow \Sigma_i + \eta_{\Sigma} \cdot F_{\Sigma_i} - \varphi \cdot \nabla_{\Sigma_i} d$;
24. **Output** $x^*$, $f(x^*)$. 

9 / 13
NES that has the ability of parallel exploration. Thus, it is named Negatively Correlated Natural Evolution Strategies (NCNES) for intuition. The detailed steps of NCNES is listed in Algorithm II for reference.

**Section IV Experimental Studies**

To verify the potential of the new NCS framework, experimental studies have been conducted to benchmark the search performance of NCNES. Specifically, this verification focuses on the effectiveness of the proposed centralized diversity model, as it is the key of the new NCS. For that purpose, we construct a compared algorithm called Parallel Natural Evolution Strategies (PNES), which shares the same workflow of NCNES except that the diversity model is omitted by setting $\varphi = 0.0$.

**Section IV.A Experimental Protocol**

As the first step, a set of multi-modal continuous optimization problems is considered, as the complex search space of such type of problems motivates the design of most population-based search methods. Specifically, we considered 20 multi-modal functions (Numbered $F_6 - F_{25}$) from the commonly used CEC’2005 competition on real-valued parameter optimization [23]. All 20 problems are with the dimensionality of 30. The time budget $MAXFES$ for the optimization of each problem is set to 300 thousands function evaluations, as suggested by [23]. When the time budget runs out, the search of NCNES on a problem terminates and the best solution ever found will be returned as the final solution. The quality of the final solution is measured with the function errors, i.e., the difference between the evaluated function value of the solution and that of the optimal solution to the problem (which has been known for these tested problems). In this setting, the better a solution is, the smaller its function error will be, and zero function error indicates the optimal solution. Considering that NCNES is a stochastic search method, the search for each algorithm is repeated for 25 runs, where the averaged function errors together with the standard deviations are regarded as the performance of NCNES on each problem (shown in Table I), respectively.

Through all these experimental studies, the parameters of NCNES are set as follows. As NCNES can be regarded as a multi-population based NES, the parameters corresponding to each sub-population are set the same as NES, i.e., $\mu = 4 + \lfloor 3 \log D \rfloor$, $\eta_m^{init} = 1$, $\eta_\Sigma^{init} = \frac{3+\log D}{\sqrt{D}}$. For $\lambda$, we do not wish it scales too quickly with the dimensionality, and thus set it to $\lambda = \lfloor \log D \rfloor$. $\varphi$ is an important parameter balancing the fitness gradient and diversity gradient and may vary over problems or even over search iterations. For simplicity, it is set to a fixed value $\varphi = 0.0001$ here. Intuitively, if such naïve setting of $\varphi$ can facilitate the search of NCNES, NCS can be expected as a promising framework as more sophisticated tuning techniques for $\varphi$ can be adopted. Such settings could also be regarded as a baseline for further improvements and comparisons. For illustration, the parameter settings are briefly shown in Table I. In order to study the impact of the diversity model, PNES has the same settings of NCNES, except that $\varphi$ is set to 0.0.

**Table I The parameter settings of NCNES**

| Parameter | Value       | Remarks                  |
|-----------|-------------|--------------------------|
| $\lambda$| $\lfloor \log D \rfloor$| The number of sub-populations |

10 / 13
NCNES is presented implemented in parallel. Based on this new diversity model, a new NCS framework is proposed with a key trade-off parameter for balancing the fitness gradient and the diversity gradient.

This new diversity model can not only accurately select a central diversity model which was devised by intuition. To solve these problems with a simple fixed value of \( \varphi \). The effectiveness of the proposed diversity model is thus verified as it is the only difference between NCNES and PNES.

| \( \mu \) | \( 4 + [3 \log D] \) | The size of each sub-population |
| \( \varphi \) | 0.0001 | The key trade-off parameter for balancing the fitness gradient and the diversity gradient |
| \( \eta_{m}^{\max} \) | 1 | The initial learning rate of mean vectors |
| \( \eta_{m}^{\text{init}} \) | \( 3 + \log D \) \( \frac{5\sqrt{D}}{5\sqrt{D}} \) | The initial learning rate of covariance matrix |
| MAXFES | 3E5 | The number of function evaluations (i.e., time budget for each run of NCNES). |

### Section IV.B Results

The results of the benchmark tests are shown in Table II. For each problem, the better solution quality between two algorithms is marked in bold. It can be seen that NCNES are statistically better than PNES on most of the problems with a simple fixed value of \( \varphi \). The effectiveness of the proposed diversity model is thus verified as it is the only difference between NCNES and PNES.

|       | PNES | NCNES | PNES | NCNES |
|-------|------|-------|------|-------|
| \( F_6 \) | 3.27E+09 ± 1.46E+09 | 3.24E+09 ± 9.92E+08 | F_{16} | 1.75E+02 ± 6.31E+01 | 1.09E+02 ± 7.66E+01 |
| \( F_7 \) | 7.88E+03 ± 8.37E+02 | 8.04E+03 ± 6.78E+02 | F_{17} | 2.12E+02 ± 7.07E+01 | 1.95E+02 ± 2.78E+01 |
| \( F_8 \) | 2.09E+01 ± 5.40E-02 | 2.09E+01 ± 5.40E-02 | F_{18} | 9.07E+02 ± 8.02E-01 | 9.07E+02 ± 8.84E-01 |
| \( F_9 \) | 3.06E+01 ± 6.83E+00 | 1.97E+01 ± 4.11E+00 | F_{19} | 9.07E+02 ± 5.78E-01 | 9.07E+02 ± 6.93E-01 |
| \( F_{10} \) | 1.36E+02 ± 1.11E+01 | 7.92E+01 ± 1.78E+01 | F_{20} | 9.07E+02 ± 5.68E-01 | 9.06E+02 ± 2.49E-01 |
| \( F_{11} \) | 3.95E+01 ± 8.60E-01 | 3.28E+01 ± 1.73E+00 | F_{21} | 5.01E+02 ± 9.88E-02 | 5.00E+02 ± 1.70E-01 |
| \( F_{12} \) | 7.27E+03 ± 5.49E+03 | 5.91E+03 ± 5.78E+03 | F_{22} | 8.65E+02 ± 1.18E+01 | 8.60E+02 ± 6.94E+00 |
| \( F_{13} \) | 1.12E+01 ± 9.97E-01 | 1.07E+01 ± 7.93E-01 | F_{23} | 5.34E+02 ± 4.15E-04 | 5.34E+02 ± 3.19E-04 |
| \( F_{14} \) | 1.35E+01 ± 1.64E-01 | 1.35E+01 ± 1.02E-01 | F_{24} | 2.02E+02 ± 1.38E-01 | 2.02E+02 ± 3.66E-01 |
| \( F_{15} \) | 2.79E+02 ± 7.64E+01 | 2.71E+02 ± 7.79E+01 | F_{25} | 2.01E+02 ± 1.77E-01 | 2.01E+02 ± 1.42E-01 |

### Section V Conclusions and Discussions

In this paper, we first discuss the drawbacks of the original NCS framework. The drawbacks are mainly introduced by the de-centralized diversity model which was devised by intuition. To solve these drawbacks and bring a mathematical principle for NCS, a new centralized diversity model is proposed. This new diversity model can not only accurately measure the diversity among sub-populations, but also can be maximized optimally with gradient descent techniques, by which the centralized model can be re-implemented in parallel. Based on this new diversity model, a new NCS framework is proposed with a more solid mathematical background. To assess the performance of the NCS, an instantiation called NCNES is presented. NCNES adopts the well-established NES as the search strategy of each sub-population and all the sub-populations are coordinated by explicitly maximizing the diversity model. Then NCNES is tested on 20 multi-modal continuous optimization problems selected from CEC’2005 benchmark suites against PNES, which has the same workflow as NCNES except that the diversity model is omitted. By this means, the effectiveness of the novel diversity model can be observed clearly.
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