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Expert Habitat: A Colonization Conjecture for Exoplanetary Habitability via penalized multi-objective optimization based candidate validation

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Abstract

Colonization opportunities and interstellar trade are not remote possibilities if feasible habitable worlds are discovered. The Economics here relies heavily on the Science and the necessary conditions to be inspected when looking for life on planets beyond our solar system. The physical conditions demand structural similarity of an extra-solar planet (exoplanet) to Earth, and the necessary bio-chemical conditions needed to sustain life in the planet. These two aspects are commonly referred to as earth-similarity and habitability, respectively. We propose a novel bi-objective optimization framework as a tool to measuring Earth Similarity Score (CDHS). This is succeeded by investigating possible interactions between Earth-similarity and habitability. The investigation is conducted via two variants of penalized multi-objective particle swarm optimization: Speed Constrained Multi-objective PSO (SMPSO) and a novel variant of Multi-Objective Quantum PSO (MOQPSO). The optimization framework dispenses of classical gradient descent/ascent approach (GD/GA) by replacing it with SMPSO and MOQPSO. The approach to the production relations com-

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monly adopted in production economics can be a natural influence for modeling habitability in exoplanets. An insightful demonstration establishes this claim. The scores reveal potentially habitable planets for interstellar trade. An analytical model of colonization in an exoplanet is also presented where we derive conditions for interstellar migration using the time to travel to such a planet (if possible) as one of the key parameters.

Keywords: Exoplanetary Habitability Score, Particle Swarm Optimization, Multi-Objective Optimization, Interstellar Trade, Game Theory, Production Economics

1. Introduction

The search for planets outside our solar system [1] and the possibility of life on such planets has been an international venture since Frank Drake's attempt with Project Ozma [2] in the mid 20th Century. The discovery of the first extrasolar planet in 1991 started a trend that has lasted over 25 years and yielded over 3700 confirmed exoplanets. Many attempts have been made to model the habitability of these planets via a score based on their similarities to Earth. One such habitability score is the Cobb-Douglas Habitability score (CDHS) [3, 4] that models a planet's habitability using established planetary parameters as inputs. These inputs are the radius, density, escape velocity and surface temperature of an exoplanet. Estimating this score requires maximizing a production function by finding an optimal solution in the feasible region of a constrained search space.

The idea behind using a production function to quantify habitability is that production functions help us with the optimization of an objective whose inputs may inherently need to be balanced. In potentially habitable exoplanets, there are various physical factors that must be carefully balanced and these include the mass of a planet, the distance of the planet from its parent star, the presence of the planet within its parent star's habitable zone, etc. A majority of the observed exoplanets have extreme attributes that are unsuitable for life the way it is on Earth; for example, a planet may have an enormous mass, or the temperature of the surface may be too cold for harboring life, as some examples of extreme conditions. A very small portion of the exoplanets that we know today have well-balanced physical attributes in a manner that leads us to believe in the possibility of life, the way it is on Earth, in planets outside our solar system.

In this respect, the Cobb-Douglas Habitability Production Function (CD-HPF) is a method that can quickly provide a *score* that is representative of the potential of habitability of an exoplanet. The inputs of the CD-HPF are in Earth Units (EU): this provides a ready standardization of the input parameters to the model. Like any economic production function, the CD-HPF requires the optimization of an objective. The Cobb-Douglas Habitability Scores (CDHS) [3, 4] provides a quick insight into how balanced the planetary attributes of an exoplanet are, while also providing a perspective on the habitability potential.

The CD-HPF is calculated in a two-fold manner: by calculating the *interior*-CDHS using radius and density, and the exterior-CDHS, by using escape velocity and surface temperature; the final score is computed by calculating the mean of the interior and exterior scores. In the current work, we build up on [3] and [4] by posing the model as a multi-objective optimization problem based on Pareto optimality of the two scores within the model. In view of the 'production' of habitability scores, it should mean that reallocation of inputs to measuring interior score should not affect the exterior score. This also Our present work will provide yet better insights to the distribution of planetary factors, and how their trade-offs affect habitability. The Cobb-Douglas habitability scores are decomposed into two parts: the *interior* and the *surface* scores, denoted by $CDHS_i$ and $CDHS_s$, respectively. The inputs to the $CDHS_i$ are the radius and the density of a planet, and the inputs to the CDHS_s are the surface temperature and the escape velocity. The reason that these are computed separately is because in themselves, they can help us compare the different aspects of two exoplanets. For instance, the interior score could give us a quick insight into the physical constitution and serve as the basis for the comparison of the rocky

interior of different planets; and the surface score could provide us insights into the similarity of the surface of a planet of that of Earth, and consequently, into the similarities in temperature.

This paper presents the solution of the bi-objective optimization problem (Section 5) arising out of habitability score computation of exoplanets and dives deep in to the several layers of the problem. We draw an analogy from production economics (Sections 7 and 8), and solve the constrained approximation problem in production economics in Section 8. The correctness of our approach is verified by comparing with computations from past solution approaches [3, 4] (see Figure 4). We present HT-MOQPSO (novel multi-objective implementation of QPSO, described in Section 8). Section 3 provide strong essence and background of exploiting PSO as a viable alternative to the classical Newtonian ascent/descent methods in computing the optimal habitability score of exoplanets. A game theoretic interpretation of the components of the bi-objective framework is also presented in Section 6. The habitability score computation approach in section 5 is validated by PSO based clustering of exoplanet (section 10) thereby choosing a set of suitable candidates for habitable exoplanet. A possible colonization strategy and modeling to inhabit such potential candidates is discussed at length in section 11. To the best of our knowledge, such an exposition has not been previously presented in the literature.

2. Cobb-Douglas Habitability score (CDHS) and necessary background

Given the increasing rate of discovery of exoplanets (especially with the scheduled launch of the James Webb Space Telescope in 2019), it can be expected that the amount of data samples of exoplanets will reach the scale of a big-data problem (much like the the volume of samples collected by the SDSS³, which is terabytes in size). In this context, it is important to explore the current classification schemes and to devise methods which can automatically discover

³Sloan Digital Sky Survey

meaningful patterns in data and classify them. Since not one single parameter can suffice as the sole criteria for habitability, we explore methods which take into consideration multiple observable characteristics of exoplanets. For example, presence of water may increase the likelihood of an exoplanet to be potentially habitable [5]. If a planet resides in the HZ, it is considered to be potentially habitable since the atmospheric conditions in these zones are more likely to support life [6, 7]. However, in either case, the habitability cannot be affirmed until other parameters such as planet's orbital and physical properties are collectively considered.

We develop a method which does not require target class labels but finds an optimal convex combination of the observables. With 3875 confirmed and about 3000 unconfirmed discoveries⁴, the amount of accumulated data is rich and diverse. Consequently, the challenge in determining the potentially habitable candidates is manyfold and lies in the selection of principal parameters. The selection issue was first highlighted in [8] via formulation of the Planetary Habitability Index (PHI) and the Earth Similarity Index (ESI). The Biological Complexity Index (BCI) [5] was introduced to accommodate biological features. The following is a brief discussion on the mathematical representation of these indices.

Earth Similarity Index (ESI). ESI was designed to determine the exoplanet similarity to Earth [8], since we know that sustainability of life depends on Earth-similar conditions. ESI ranges from 0 to 1 depending on the increasing degree of similarity to Earth. A planetary body with an ESI over 0.8 is considered to be Earth-like. ESI is represented as:

$$ESI_x = \left(1 - \left|\frac{x - x_0}{x + x_0}\right|\right)^w,\tag{1}$$

with ESI_x being the ESI value of a planet for x property, x_0 the Earth's value for that property, and w the weighting component for adjusting the sensitivity of the

 $^{^4{\}rm Feb.}$ 2019, NASA Exoplanet Archive, https://exoplanet
archive.ipac.caltech.edu

scale. Four parameters: surface temperature T_s , density D, escape velocity V_e and radius R, are used to determine the total ESI, through calculating separately the interior ESI_i (from radius and density), and surface ESI_s (from escape velocity and surface temperature). Finally, the total ESI of a planet is calculated by taking the geometric mean of ESI_i and ESI_s . However, ESI in this form (1) only describes the similarity of a planet to the Earth. It does not determine habitability. For example, it is relatively high for the Moon – about 0.5.

Planetary Habitability Index (PHI). PHI is a metric for quantitative measurement of the ability of a planet to develop and sustain life, [8] represented as,

$$PHI = \left(S \cdot E \cdot C \cdot L\right)^{1/4},\tag{2}$$

where S is a substrate, E is available energy, C is appropriate chemistry and L stands for liquid medium. The PHI value of each parameter is divided by the maximum PHI to normalize the scale to between 0 to 1. However, the PHI parameters are difficult to measure, and may not represent other necessary properties for determining planet's present habitability. Safonova et al. [9] proposed to complement the PHI with the age of the planet (see their Eq. 6).

Biological Complexity Index (BCI). Another habitability index containing geophysical complexity G, temperature T and planetary age A was defined by the same group [5] as an extension of the PHI:

$$BCI = \left(S \cdot E \cdot T \cdot G \cdot A\right)^{1/5} \,. \tag{3}$$

This is again normalized to the maximum BCI value in the set to produce the scale from 0 to 1. Yet, Venus has BCI of zero and Enceladus has BCI of 0.17, while Gliese 581c has the highest BCI of any exoplanet, even higher than the Earth. However, this planet has more of a Venus-like environment being very close to its star. In addition, this index was mainly oriented at assessing the probability of finding a complex (evolved) life on a planetary body.

The standard conservative definition of a habitable planet is applied for planets residing in the classical HZ: a region where liquid water may exist on the surface [10, 11]. However, it is possible for a planet to be a good candidate for habitability even outside the classical HZ, or even without a host [12, 13, 14]. Also, our Moon is within the HZ but clearly is not potentially habitable for our kind of life. Though observational efforts focus on the search for Earth's twin (i.e. the planet with ESI = 1), it is quite possible that even with ESI close to 1, a planet is not potentially habitable. Recent 'best candidate' for a lifesupporting planet, Gliese 832c with ESI = 0.81 [15], was found more likely to be a super-Venus and is, probably, tidally locked with its star.

Cobb-Douglas Habitability Production Function (CD-HPF) and Cobb-Douglas Habitability Score (CDHS). The Cobb-Douglas (C-D) production function was originally proposed to model the growth of the American economy during the period of 1899-1922 and has been widely used in economics and in industries to obtain optimal input combinations subject to a budget constraint [16]. The C-D production function possesses a number of important properties including homogeneity, convexity of the isoquants (i.e. same output with many input combinations, and analogously, for indifference curves, same utility from various commodity combinations), and importantly, the satisfaction of the well-known Inada conditions for guaranteeing the stability of the growth path. We discuss some of these properties in further detail as part of our motivation behind using a specific structure for measuring Habitability Score.

The Cobb-Douglas Habitability score (we denote this as Y) comprises of two components: interior score $(CDHS_i)$ and surface score $(CDHS_s)$. These scores are estimated by maximizing the following input-output relationships,

$$Y_i = CDHS_i = R^{\alpha}.D^{\beta} \tag{4}$$

$$Y_s = CDHS_s = V_e^{\delta} . T_s^{\gamma} \tag{5}$$

where R, D, V_e and T_s are radius, density, escape velocity and temperature, respectively. $\alpha, \beta, \delta, \gamma$ are coefficients of elasticity and $0 < \alpha, \beta, \gamma, \delta < 1$. The above two equations are concave under constant returns to scale (CRS) [3], when $\alpha + \beta = 1$ and $\gamma + \delta = 1$, and also under decreasing returns to scale (DRS) [3], when $\alpha + \beta < 1$ and $\gamma + \delta < 1$. The final CDH score is calculated as the weighted linear combination of interior and surface score, where the weights w_i is the weight of the interior score, and w_s is the weight of the surface score.

$$Y = w_i \cdot Y_i + w_s \cdot Y_s \tag{6}$$

Here, $w_i, w_s \ge 0$ and $w_i + w_s = 1$. In [3], the final CDHS score of a planet is arrived at by estimating the interior and surface scores independently, which is done by finding the elasticities that maximize (4) and (5) under CRS and DRS. However, since $V_e = \sqrt{\frac{2GM}{R}}$, where G is the gravitational constant, the implication is that increasing interior score will not be possible without compromising on the surface score and vice versa. This paper attempts to bring out this tradeoff between Y_i and Y_s by setting up a penalized bi-objective maximization task that finds a non-dominated solution set (Pareto front) describing the interplay between the two components of the habitability score.

3. Motivation

Considering the complexity of assessing the habitability of exoplanets, it's perhaps not wise to make definite conclusions about exoplanet habitability classes by label based classification approach alone. PHL data set contains six classes in the data set, of which the classes, non-habitable, mesoplanet and psychroplanet classes have non-negligible number of planets. The remaining three classes in the data are those of thermoplanet, hypopsychroplanet and hyper-thermoplanet. As a first step the data in the PHL-EC is preprocessed, described in detail by earlier work by Saha et. al [4]. Therefore, it is beyond reasonable doubt to explore different methods that can be proved mathematically justified by physical interpretations. However, unlike machine learning based classifiers investigated by Saha et. al and Basak et. al [4, 17] the current work proposes habitability assessment of newly discovered exoplanets via unsupervised (clustering) approaches. The proposed methods integrate com-



Figure 1: Observed behavior (scatter plot) of Interior and Surface habitability scores of some exoplanets: We expect the solutions to be non-dominating

putational methods to compute habitability scores and label-free grouping of Earth-like planets (unsupervised) for determining the degree of habitability of an exoplanet. This is a significant exercise as the uncertainty and challenges involved in finding and ascertaining habitable planets. We hope, the outcome of the proposed model agree with previous results and embellish the results further reported in Basak et. al [17] and thus, may be used as indicators while looking for new habitable worlds. Our principal contribution is to propose an integrated approach to habitability clustering of exoplanets. Clustering approach is novel as it doesn't use existing class labels as reported in catalogs and groups exoplanets to several clusters based on some geometric/spatial similarity using parameters (strictly excluding surface temperature and all parameters related to surface temperature in PHL-EC). This approach is thus, independent of any class labels and therefore free from possibly problematic ground truth and bias that might exist in the data set. We present Particle Swarm Based clustering (PSO) of exoplanets since the majority of the habitability score computation revolves around PSO [18].

3.1. Technical Motivation: Justifying the Optimization approach

As discussed in [3, 19], a Cobb-Douglas function models the response of an output variable on varying its inputs. The multiplicative input relationship allows inclusion of n number of such inputs, each with its respective elasticity. The function is concave when the sum of elasticities is not greater than one ensuring that an optimum exists for the function inside a feasible region defined by the constraints on elasticities. In the case of exoplanetary habitability, the proposed metric models as to how the habitability score Y changes on varying inputs on planetary parameters. This is achieved by allowing the coefficients of elasticity to be adjusted via an optimization algorithm.

The final CDHS (derived from (4) and (5)) defined in Equation (6), is equal to the convex combination of Y_i and Y_s . The weights w_i and w_s define the importance of the interior and surface scores in determining the final CDHS. The Cobb-Douglas Habitability production function can also be formally written as,

$$Y = R^{\alpha} . D^{\beta} . V_e^{\delta} . T_s^{\gamma} \tag{7}$$

CDHS is estimated by maximizing (7) subject to $\alpha + \beta + \delta + \gamma = 1$. CDHS can be calculated from both (6) and (7). In [3], for the ease of visualization in 3D space, CDHS is split into two components – (4) and (5) – and the final score is arrived by estimating these two components independently. Fig.2 shows the surface plot for the interior score and surface score along with their maximum values under CRS. A suitable value of w_i and w_s is manually set through hit and trial, and the final CDHS is estimated from (6). Based on the weights chosen, the final CDHS score can widely vary.

It is made clear in [3] that the sole motivation for splitting Y into two components is because the four decision variables $-\alpha,\beta,\gamma$ and δ – and Y cannot be represented visually. Can there be a more scientifically driven motivation to estimate Y_i and Y_s independently? This paper attempts to answer this question and serves as an extension to the ideas presented in [3].



Figure 2: Plots of interior CDHS_i for CRS [3] and surface CDHS_s have similar profile. 3.2. Our Contribution

This paper proposes a robust alternative to the methods proposed in [3] to quantify exoplanet habitability. A multi-objective framework is proposed to simultaneously establish both interior and surface score of an exoplanet. The solution sets which the proposed framework produces are explained with a game theoretic analysis.

Hypervolume Terminated Multi-Objective Quantum PSO, a novel mutiobjective algorithm, is also explored to estimate exoplanet habitability under a modified CRS constraint. Analogies from production economics are significantly highlighted to further strengthen the motivation for the proposed framework for exoplanet habitability estimation.

The cornerstone of the manuscript (underneath the deep technical novelty) is the integration of habitable candidates via clustering approach. We propose meta-heuristic based (PSO) clustering. This is because the spatial distribution of exoplanets is random, doesn't follow regular geometric patterns and therefore using spherical assumptions of distribution justifying K Means type method [20] can't be used. The clustering approach helps cross-validate habitability groups (Earth like planets) with CDHS to obtain a more reliable set of potentially habitable exoplanets. More specifically, our method finds planets similar to Earth in some spatial distributional sense using some distance measure. This approach finds and places some planets, apparently, in Earth's group while clustering other planets in different groups. The optimization approach finds validation if the planets with habitability score (CDHS) close to Earth (CDHS= 1) also belong to Earth's group by the clustering approach. We have shown this in section 10 and thus established the efficacy of the habitability score optimization approach proposed in the paper.

Finally, we offer a discussion and analytical model on tangible returns with marketable options to cater in relation to identifying habitable exoplanets. We discuss the economic viability of possible settlement of habitats in potentially habitable exoplanets. A colonization model is discussed in detail and analytical implications of optimal trade based on the time to reach nearer habitable planets are argued for. Section 11 provides ample justification for the colonization conjecture.

4. Representing the Single-objective problem in a bi-objective setting

Multi-objective optimization problems are challenging for various reasons. Saddle points are sometimes difficult to overcome. While some methods are globally good, they tend to suffer from oscillating local minima, especially when optimizing multiple objectives. Several variants of PSO or other meta-heuristics are employed to solve a variety of problems. Zhang et. al [21] proposed a method to handle additional control parameters by building a group teaching model for solving global optimization problems. Lai et. al [22] integrated diversitypreserving strategy and the probabilistic application of a local optimization procedure to solve the NP-hard 0/1 Knapsack problem. Their method uses a variant of Quantum Particle Swarm Optimization where a distanced-based diversity-preserving strategy was used to manage population over generations. Quadratic knapsack problem with conflict graphs is another interesting problem with diverse applications in Engineering. The method by Dahmani et. al [23] is inspired from the binary particle swarm optimization combined with a quick and efficient local search. THe vanilla PSO is bot designed to handle constraints in optimization problems. This could be tackled by imposing penalties or expanding search operator and directional information as proposed by Ang et. al [24]. Roshanzamir et. al designed a variant pf PSO where they managed to achieve balance between exploration and exploitation by assigning different tasks to different group of swarms[25].

Since the paper attempts to explore how the two components of the CDH score, surface score and interior score, interact when the decision variables are changed, we make use of a multi-objective variant of PSO known as Speed Constrained Multi-Objective Particle Swarm Optimization (SMPSO) [26]. While the basic idea of the multi-objective variant remains the same as that of the single objective-variant [27], SMPSO uses certain strategies to find a non-dominated solution set that simultaneously maximizes the two components of the CDH score. Constraints on the decision variables such as coefficients of elasticity of the planetary parameters are imposed by augmenting the objective functions with L1 penalty functions. The exoplanet catalog [28], hosted by the Planetary Habitability Laboratory at the University Of Puerto Rico at Arecibo, is the dataset that we use for conducting this experiment. To the best of our knowledge, this kind of interpretation of a typical single objective setting is not available in literature.

The problem of estimating CDHS score under CRS constraints in a biobjective optimization setup can be represented as:

$$\min_{\vec{x}} \vec{f}(\vec{x}) = [-Y_i, -Y_s] \tag{8}$$

subject to

$$\alpha + \beta = 1, \ \gamma + \delta = 1, \ 0 < \alpha, \beta, \gamma, \delta < 1 \tag{9}$$

where \vec{x} is a vector of decision variables $[\alpha, \beta, \delta, \gamma]$. Since our goal is to bring out the trade-off between the interior score and the surface score as implied by the relationship between a planet's escape velocity V_e and its radius R, it becomes necessary to bring out the relationship between the elasticity coefficients of V_e and R. In the appendix section in [3], the desired relationship between the elasticity coefficients has been derived successfully. This relationship is $V_e = \frac{\delta}{\alpha} \frac{W_R}{W_{V_e}} R$ where W_R and W_{V_e} are weights chosen to represent the importance of R and V_e respectively. This equation can be rearranged in the following way:

$$\delta = \alpha \frac{V_e}{R} C$$
 where, $C = \frac{W_{V_e}}{W_R}$ (10)

We use Equation (10) to bring out the dependence between Y_i and Y_s within the bi-objective optimization framework. To impose the DRS constraint, we simply replace equality constraints in (9) to the following inequality constraints:

$$\alpha + \beta < 1, \ \delta + \gamma < 1 \tag{11}$$

Since the goal is to bring out the trade-off between the surface score and the interior score, it is essential to use Equation (10) in the optimization task: instead of searching for δ , we derive δ using α and C. We add C, which is the ratio of importance of escape velocity to the importance of radius, to the list of decision variables so that the optimization algorithm looks for the best value of C that maximizes the surface score and the interior score while observing the CRS or DRS constraint (See Appendix B for constraint modeling using penalties).

In many real-world problems, the Pareto front cannot be calculated for a variety of reasons. Instead, most existing algorithms estimate an approximation set [29] of objective vectors that is not necessarily equal to the "true" Pareto front of the problem. The paper proposes an experimental setup that uses exoplanetary data from the aforementioned catalog to find solution sets that minimize the negative of the interior and surface scores while observing the CRS constraint.

5. CDHS Results

The PHL catalog contains observed and estimated stellar and planetary parameters of 3415 confirmed exoplanets. However, estimates for surface temperature is available for only 1586 planets. To conduct our experiments, we drop the planets for which the estimates of surface temperature are not available. We performed our experiments using data from 664 rocky planets out of which the results from TRAPPIST-1 planetary system are emphasized.

Under DRS, an increase in input does not lead to an equivalent increase in output. In fact, the proportion of the increase in the output is less than the increase in the input. However, CRS conditions will ensure that our model for habitability estimation generates outcomes that change in the same proportion as the changes in all inputs. Because of this characteristic and the fact that CRS constraint subsumes several functional structures and properties within itself, CRS is preferred over DRS to model exoplanetary habitability.

5.1. Results Obtained Under CRS Constraints

It can be observed from the Pareto front graphs of two of the TRAPPIST-1 planets illustrated in figure 3 that there is a clear trade-off between the interior and surface scores. The series of (Y_i, Y_s) values in the objective space invites the following question: which among the points in the solution set should be chosen to calculate the final CDHS of an exoplanet? To answer this, we need to recall that the CDHS is a linear combination of the interior and surface scores. The definition of CDHS is equivalent to that of a line segment between two given points which means that CDHS is a real number that lies between Y_i and Y_s and the choice of weights w_i and w_s will determine the proximity of CDHS to Y_i and Y_s . For a given weight pair (w_i, w_s) , the most ideal (Y_i, Y_s) from the Pareto front will be the one for which CDHS is maximum. Let us set $w_i = 1.0$ and $w_s = 0.0$, and take $Y_i = 0.885$ and $Y_s = 0.97$ from the solution set detailed in table 1. The CDHS value for this selection is 0.885 but for the given selection of weight pairs, the most ideal solution from the Pareto front is $Y_i = 0.898$ and $Y_s = 0.958$.

The trade-off between these two components implies cooperation rather than competition which means that a decrease in one component of the score is compensated by the increase in the other component of the score and hence, maintaining a consistent final score. The different *CDHS* values for different choices of weight pairs are close to each other since $|Y_i - Y_s|$ is a really small



Figure 3: Pareto front for TRAPPIST-1 b and e under CRS. The computed habitability scores using our approach when compared with previous approaches [3][4], we observe that the scores match closely for more than 664 rocky exoplanets.

value. This is not observed in earlier computations where a fixed weight pair worked for the desired habitability score. This is not the case here and therefore, the weight selection and the optimization approach yields habitability scores of planets (believed to be in the same league as Earth) close enough to 1, which is the Earth's habitability score! This is a robust approach compared to earlier gradient ascent/descent based approaches [3, 4]. Moreover, a simple choice of the coefficients will yield a range of values of habitability for each planet. The range is within acceptable limits (i.e. in terms of proximity to Earth's habitability score, for the TRAPPIST-1 system of planets in particular). Instead of a fixed number for the habitability score, we obtain an acceptable range. This is a marked departure from the earlier approaches.

5.2. Comparison With Past Approaches

We compare our results with the ones in [3] and [4] for more than 600 rocky planets. To calculate CDHS using our approach, we will assign an arbitrary weight pair of $w_i = 0.5$ and $w_s = 0.5$ and pick (Y_i, Y_s) from the solution set that leads to the largest CDHS value. The observed distribution of divergence in figure 4 provides a strong validation that the results obtained from the proposed

α	β	γ	δ	C	Y_i	Y_s	Y
0.571	0.429	0.197	0.803	1.722	0.885	0.97	0.9615
0.575	0.425	0.194	0.806	1.717	0.886	0.969	0.9607
0.583	0.417	0.187	0.813	1.708	0.89	0.966	0.9583
0.585	0.415	0.185	0.815	1.706	0.891	0.965	0.9576
0.587	0.413	0.183	0.817	1.704	0.892	0.964	0.9568
0.59	0.41	0.18	0.82	1.702	0.893	0.963	0.9560
0.602	0.398	0.168	0.832	1.692	0.898	0.958	.952

Table 1: Solution set for TRAPPIST-1 b under CRS. Note, the CDHS is close to 1, implying potential habitability



Figure 4: Distribution of absolute differences between the habitability scores under CRS and the scores from [3] & [4])

multi-objective model do not deviate much from the calculated CDHS in [3] and [4].

6. Game Theoretic Interpretation

In cooperative games, the participants or the players cooperate to achieve a common goal and there is no conflict of interests. Now, we define a twoplayer game in which the participants – interior score and surface score – play to achieve a common goal of maximizing the final CDHS score. $N = \{I, S\}$ are participants of the game and let $S \subseteq N$ be a coalition that forms among the participants N. There are 2^n , where n = number of participants, coalitions that are possible. The coalitions can be represented as powerset of (N) = $\{\{\emptyset\}, \{I\}, \{S\}, \{I, S\}\}$. We quantify the benefit of a coalition through a characteristic function $v: 2^n \to \mathbb{R}$. For our game model, we define the characteristic function as: $v(\emptyset) = 0, v(\{I\}) = 0, v(\{S\}) = 0, v(\{I,S\}) = maxE(u(x_i, y_j))$ where $u(x_i, y_j)$ is a payoff function, $x_i \in S_i, y_j \in S_s$ and S_i and S_s are strategy sets for players I and S respectively. The value of the coalition is the maximum possible expectation of the payoff function. As the CDHS of an exoplanet depends on both interior and surface scores, coalitions of only one participant have no benefits: this means that the game is essential [30]. Let us assume that players I and S are playing to maximize CDHS of the planet TRAPPIST-1 b under CRS constraint. Let S_i , strategy for I, be a set of all Y_i values from table 1 and S_s , strategy for S, be a set of all Y_s values from table 1, For this game, we define the following payoff function:

$$u(x_{i}, y_{j}) = \begin{cases} 0.1 * x_{i} + 0.9 * y_{j}, & \text{if } (x_{i}, y_{j}) \in D\\ 0, & otherwise \end{cases}$$
(12)

Here, $D = \{(x_i, y_j) | x_i \in S_i, y_j \in S_s \text{ and } i = j\}$. The payoff function $u(x_i, y_j)$ is CDHS with weights w_i and w_s set to 0.1 and 0.9 respectively for pairs of scores (x_i, y_j) from Table 1. We assume that both players get an equal payoff for their contribution to the final CDHS. In this game, a player might

either choose a pure strategy or a mixed strategy to maximize payoff. These strategies are chosen according to some probability distribution.

A vector $X = [P(x_1), ..., P(x_n)]$ is mixed strategy for player I and $Y = [P(y_1), ..., P(y_n)]$ is mixed strategy for player S, where $P(x_i) \ge 0$, $\sum_{i=1}^n P(x_i) = 1$, $P(y_j) \ge 0$, and $\sum_{j=1}^m P(Y_j) = 1$. A pure strategy is a special case of mixed strategy. X represents a pure strategy if $P(x_i) = 1$ and $P(x_j) = 0 \forall j \neq i$.

Now, given mixed strategies X and Y, the expected payoff of the game is $E(X,Y) = \sum_{i=1}^{n} \sum_{j=1}^{m} u(x_i, y_j) P(x_i) P(y_j)$. There exist points (X^*, Y^*) for which E(X,Y) is maximum. We can now define the optimization problem as: $\max_{P(x),P(y)} E(X,Y)$ subject to $\sum_{i=1}^{n} P(x_i) = 1$, $\sum_{j=1}^{m} P(y_j) = 1$ and, $0 \leq P(x_i), P(y_j) \leq 1$. We plug in the required values in E(X,Y) and we get the equation: $E(X,Y) = P(x_1)P(y_1)0.9615 + P(x_2)P(y_2)0.9607 + \dots$. Since there is no pair (x_i, y_j) , such that $i \neq j$, for which $u(x_i, y_j) > 0$, the players I and S should cooperate and choose their strategies x_i and y_j so that i = j to maximize the payoff. Because of this, we make $P(x_i) = P(y_j)$, where i = j.

We find that E(X,Y) is maximum when $P(x_1) = P(y_1) = 1$ and $P(x_i) = P(y_j) = 0 \forall i \neq 1, j \neq 1$. This means that max(E(X,Y)) = 0.9615 and the optimal strategy for maximizing payoff is a pure strategy where I plays x_1 and S plays y_1 all the time. One important thing to note is that we set weights w_i and w_s to 0.1 and 0.9 respectively and the values of x_i and y_j are interior scores and surface scores from table 1. If we change the weights w_i and w_s , the expected payoff function will change and players I and S will start playing a different strategy to maximize the expected value of payoff (final CDHS). This explains the trade-off between the interior and surface scores; when one score decreases, it is compensated by an increase in the other score. The ideal (Y_i, Y_s) for the CDHS calculation is determined by the choice of (w_i, w_s) . No matter what w_i and w_s is set to, the observed trade-off between Y_i and Y_s makes sure that a consistent CDHS is maintained.

When player I chooses a strategy x_1 , the best strategy for S to play is y_1 , and if S were to choose y_1 , the best strategy for I to play is x_1 . We can generalize this fact by saying that when player I chooses strategy x_i , the best strategy for S to play is y_j and if S chooses y_j , the best strategy for I to play is x_i and i = j. Hence, all points $(x_i, y_j) \forall i = j$ are pure strategies Nash Equilibria.

7. A Production Economics Argument for the PSO approach

Perfect competition is a market structure where several firms coexist, each apparently using a CRS production function such that no one has an advantage in this market from producing more at a lower cost than the rest. That would be feasible only with IRS (increasing returns to scale), and one or two firms will dominate the entire market instead of a large number of homogeneous firms. Perfect competition implies the presence of a large number of firms driving a stable market equilibrium. It is well known in related disciplines that perfect competition implies the complete absence of inter-firm competition because each is a small entity in view of the market size, such that individual firms have little control or influence over price formation and the aggregate quantity sold in the market. CRS in the usage of economics is integral to the presence of perfectly competitive markets by ensuring equi-proportionate returns to factor inputs. Conversely, DRS implies that the use of inputs generate less than proportionate increase in the output. Therefore, to the extent that firms optimize on profit or cost, these should resist the expansion of production beyond the point where output grows less than proportionately to the use of inputs. In industries, where DRS is the dominant production relation, it is expected that sustenance of production would be questionable beyond a reasonable point in time, simply because the factor returns cannot be paid up from the profit earned. Yet, in some case, particularly, public sector operations in many countries, DRS seems to be prevalent owing to various commitments (such as, job creation for the less privileged) of the government, albeit not as a technological strategy. Since the concept of the *CDH* score is borrowed from production economics, we deem it necessary to interpret the objective in the light of economics and therefore, we explore the bi-objective framework under CRS constraints rather than the DRS constraints. It is easy to understand that non-adherence to CRS would lead to either DRS or IRS in operation, of which DRS is sub-optimal and may be ignored given the much wider coverage available under CRS technology. Therefore, the model under this particular CRS constraint provides an adequate motivation to explore the bi-objective optimization framework where the players, the interior and surface scores are in perfect competition with each other and ensures a Pareto front. We observe this for all the simulations offered subsequently. For example, a multi-objective optimization framework in economics which is more of a theoretical curiosity [31] is often not entertained, typically because the point which optimizes all objective functions may be infeasible in view of the available data and may exist only as a utopia. The dominant approach has been to consider one, or a related set of objective functions as the core optimization problem. In contrast to this, in the current work, we entertain a bi-objective production function and successfully obtain converging Pareto fronts. This should not only serve as a strong motivation behind what we conceptualize but should also serve as possible direction for many other applications in related disciplines.

8. Motivation for Q-PSO: An Analogy From Production Economics

We embark on an important corollary of our investigation by drawing an analogy from production relations widely used in economics. Indeed, the approach to the production relations commonly adopted in industries can be a natural influence for modeling habitability in exoplanets. The structure follows a direct application of the well known CD production function offering a wide array of general formulations. So we investigate if there is an ϵ difference between the DRS and the CRS production functions (in our case CD-Habitability Score) if optimized separately. Note that the proposed production relations determine the output elasticity of factors as estimates and if the output responds less than proportionately to increases in inputs, the relation is of DRS nature and the production cannot be sustained beyond a critical level of (negative) profit consequent to that. In the case of CRS, the production can continue infinitely. In other words, if we write $\alpha + \beta = 1$ as $\alpha + \beta - \epsilon < 1$ where $\epsilon > 0$ but is infinitesimally small, then can we use Q-PSO [32] to solve the modified optimization problem under modified CRS constraints and discover that the optimal solution obtained under original CRS is insignificantly different from modified CRS (an approximation of the DRS constraints). As we discussed in section 5, DRS is less preferred since it could amount to leakage and eventual shut down of production as the production is less than proportionate to inputs. However, if a firm, experiencing a downturn, seeks a change of fortunes within their budgetary constraints, can they inflict an ϵ change and still hope to sustain itself? We note that ϵ must facilitate this movement via some variable input, say technology, which in many cases, functions as a black box at an initial phase. Alternatively for DRS to approach CRS, it is possible that an existing parameter is aggravated by epsilon as an infinitesimal change, replicating a productivity surge owing to unaccounted for external factors. Thus, if we raise β , viz, by a factor ϵ , it helps to approach the limit. It could also be owing to the adoption of a policy, such as the minimum wage or efficiency wage. If that helps labor to behave more productively than before, then a situation of DRS may approach CRS in the limit. For capital, it could be the influence of innovations in investment plans or use of a better technology or super-CEO that raises its productivity. We took the second approach (i.e., modified DRS \rightarrow CRS) as the ideal test case for our method, HT-MOQPSO: a novel implementation of Quantum PSO with hypervolume based termination criteria.

We expect the difference in optimal values between the two constraint settings to be minimized by Q-PSO. In other words, we ask if the optimal value of y (production) under modified DRS (\rightarrow CRS) will be agonizingly close to the optimal production (equivalent CDHS) guaranteed under original CRS. The answer is yes, as observed by the experimental results (see table 3) performed on CDHS (analogous to the production function in Economics). We adopt a twophase approach to address the above questions. First, we attempt to solve the bi-objective problem using Q-PSO. Next, we solve the modified DRS problem (with an ϵ jump i.e. rewriting the DRS constraint, $\alpha + \beta < 1$ as $\alpha + \beta + \epsilon = 1$) and check for similarity in solution front with the original CRS. We used Hausdorff distance metric for comparison between the solution fronts and inspect random samples manually for proximity check. We have also solved the modified optimization problem by two ways. First, we fix the ϵ to a very small number and compare the two solution fronts. Additionally, we let ϵ to be defined as a small constraint in the optimization framework so that we obtain different values of it (via the solution process of the constrained MOO problem) while maintaining proximity in the solution fronts. This outcome fortifies what is known in production Economics as "scale efficiency". We observe that the ϵ -jump is handled quite efficiently by HT-MOQPSO. Details are demonstrated via Hausdorff distance (please see Table 3).

8.1. Hypervolume Terminated Multi-Objective Quantum PSO (HT-MOQPSO)

Algorithm 1: HT-MOQPSO pseudocode				
1 initialize Swarm()				
2 initialize LeadersArchive()				
$\mathbf{s} \mathbf{i} = 0$				
4 while not terminationCriteria() do				
5 update ParticlePosition()				
6 perturb constraints()				
7 evaluate Swarm()				
8 update LeadersArchive()				
9 update LocalBest()				
10 calculate HyperVolume()				
11 i++				
12 end				
13 return LeadersArchive				

Unlike classical PSO, quantum PSO [32], as the name suggests, draws inspiration from the principles of quantum mechanics. In the standard PSO system, the trajectory of a particle is determined by its position \vec{x} and its velocity vector \vec{v} . This model of exploration of search space is based on Newtonian mechanics but this is not the case in PSO with **quantum behaved particles**. In quantum mechanics, **Heisenberg's uncertainty principle** states that position \vec{x} and velocity \vec{v} cannot be determined simultaneously and hence the concept of particle trajectory becomes meaningless in quantum PSO. Because of this reason, the algorithm for QPSO is drastically different from the standard PSO. In this paper, we present a novel implementation of multi-objective variant of QPSO [32] written using modules offered in *jmetalpy* python framework.

The classical PSO suffers from local convergence but QPSO addresses this flaw as it is globally convergent [33]. In PSO with quantum behaved particles, the quantum state of each particle is denoted by a wave function $\Psi(x,t)$ instead of its position and velocity vector. Ψ is a function of space and time and gives a complex number. What is physically meaningful is the squared of the magnitude of the wave function $|\Psi|^2$, which offers a probabilistic measure of finding a particle at a particular point in an n-dimensional space. At any point in time t, the wave function $\Psi(x,t)$ in a system is such that $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$. Now, the position update of a particle x_i in the j^{th} dimension is governed by the following equations:

$$x_{ij(t)} = p + \chi_j . L. ln(\frac{1}{u}), \text{ if } k > 0.5$$
 (13)

$$x_{ij(t)} = p - \chi_j . L. ln(\frac{1}{u}), \text{ otherwise}$$
 (14)

 χ_j is a constriction factor calculated for the j^{th} decision variable that ensures that the swarm does not explode [34]. χ_j is the difference of upper and lower bound imposed on the j^{th} decision variable multiplied by 10^{-3} . p, L, u, ϕ_1, ϕ_2 and k are usual terms defined in [32]. Here, the only configurable parameter is gwhich is used to compute the value of L and it is set to 0.95 in our experiments. Our implementation of multi-objective QPSO remains the same as the algorithm described in [26]. However, particles do not have a velocity component associated with them and hence, there is no step for velocity computation. The position of the swarm is updated according to equations 13 and 14. We introduce via HT-MOQPSO, a hyper-volume [35] based termination criteria described by the boolean expression: $k \ge \text{maxIteration OR}$ ($k \ge 0.02 * \text{maxIteration AND}$ $hv(k) - hv(k-1) < \tau$). Here k is the current iteration, hv(k) is the hypervolume of the solution at the k^{th} iteration and $\tau > 0$. The idea is to terminate the algorithm when the change in hypervolume from the previous iteration is less than a very small positive real number τ which is set to 10^{-8} . Algorithm 1 is the pseudocode for the proposed HT-MOQPSO.

8.2. Complexity Analysis

The complexity analysis of HT-MOQPSO is provided in this section. If M is the number of objectives, N is the number of decision variables, S is the swarm size, L is the size of the archive and F is the sum of complexities of objective functions, then the basic operations and their worst case are as follows:

- Archive initialization : O(LN)
- Swarm initialization : O(SN)
- Swarm Evaluation : O(FS)
- Procedure to check the domination status of any two solutions: O(M)
- Crowding distance computation: O(ML)
- Local best particle initialization : O(S)
- Global best particle initialization: O(S(L + ML)) = O(SML)
- Position update: O(S(N+M))
- Local best particle update : O(SM)
- Leaders archive update: O(S(L + ML)) = O(SML)
- Hyper volume calculation : $O(L^{N-2}logL)$

Functions	SMPSO	HT-MOQPSO	NSGAII
Kursawe	295.76	296.87	297.27
Fonseca-Flemming	23.75	24.33	24.33
ZDT1	14.04	23.85	23.99
ZDT2	7.52	22.63	22.32
ZDT3	16.98	27.51	28.13
Viennet 2	790.47	790.55	790.24

Table 2: Hypervolume quality measure on the benchmark functions

Therefore, the total complexity of HT-MOQPSO becomes $O(SN) + O(FS) + O(S) + O(SML) + \eta \cdot (O(S(N+M)) + O(SF) + O(SM) + O(SML) + O(L^{N-2}logL))$ where η is the total number of iterations.

8.3. Benchmark Results

To test the performance of HT-MOQPSO, we selected 6 multi-objective optimization benchmark functions for comparison with SMPSO and NSGA-II [36]. The benchmark functions are Kursawe [37], Fonseca-Flemming [38], ZDT1 [39], ZDT2 [39], ZDT3 [39] and Viennet 2 [40]. For fairness in comparison, we apply the hypervolume based termination criteria for all three algorithms under test and set the population size of all three algorithms to 100.

Table 2 documents the performance of the three multi-objective algorithms on the selected benchmark functions. We compute hypervolume for the solution sets found by the algorithms to measure the quality of the sets. Hypervolume calculates the region in the objective space dominated by the solution set bounded above by a reference point. We set this reference point to (5,5) for all the benchmark functions and compute the hypervolume. The greater the hypervolume, the better the quality of the solution set. It is apparent from Table 2 that the performance of the three is identical for Kurasawe, Fonseca-Flemming and Viennet2. However HT-MOQPSO and NSGAII outperform SMPSO on benchmark functions ZDT1, ZDT2 and ZDT3.

Planets	$\begin{array}{c} \text{Hausdorff Distance} \\ \text{(fixed } \epsilon \end{array}) \end{array}$	$\begin{array}{c} \text{Hausdorff Distance} \\ (\text{variable } \epsilon) \end{array}$
TRAPPIST-1 b	0.2361	0.1591
TRAPPIST-1 c	0.0076	0.0265
TRAPPIST-1 d	0.0032	0.0546
TRAPPIST-1 e	0.0404	0.0032
TRAPPIST-1 f	0.0197	0.1172
TRAPPIST-1 g	0.1636	0.0407
TRAPPIST-1 h	0.0138	0.0111

8.4. Results Under Modified DRS (the ϵ -Correction)

Table 3: Hausdorff distance between solutions obtained under modified CRS (ϵ - perturbed) and the original CRS constraint: introduction of "production economics scale efficiency" bridges the gap between CRS and DRS further.

The solution set obtained under the modified DRS constraint is compared with the solution set obtained under the original CRS constraint. As mentioned, we run two optimizations under the modified CRS constraint. In the first run, we fix ϵ to 10^{-8} and in the second run, we make ϵ a decision variable which is estimated by the optimization algorithm. For the purpose of comparison, we need to calculate a distance measure between two solution sets A and Bin the bi-objective space. We have chosen Hausdorff Distance to quantify how close the solution sets obtained under the modified CRS constraint are to the ones obtained under the original CRS constraint. Table 3 depicts the Hausdorff distance measured for the planets in the TRAPPIST-1 system. It can be observed that the distance measurement ranges from 0.003 to 0.16 for optimization results where ϵ is varied by the algorithm. For fixed ϵ values, the Hausdorff distance varied from 0.003 to 0.2361. These distances are very small due to the fact that the solutions obtained under the new modified DRS constraint is insignificantly different from the solutions under CRS constraint. This justifies our claim that the leakage caused due to DRS constraints (output being lesser to proportionate inputs) can be bridged by introducing the " ϵ -perturbation". This " ϵ -perturbation" or " ϵ -jump from DRS to CRS" is handled very well by HT-MOQPSO, especially in the case of scale-efficient production (ϵ is varied and not fixed). We attribute this to the quantum states of the particles in the swarm and the corresponding jumps between these states.

	Hypervolume				Purity	У
Planets	SMPSO	NSGAII	HT-MOQPSO	SMPSO	NSGAII	HT-MOQPSO
TRAPP-1 b	1.3357	1.4615	1.4868	0.0	0.0	1.0
TRAPP-1 c	1.3892	1.4143	1.4135	0.0	1.0	0.5058
TRAPP-1 d	0.8681	0.9137	0.9132	0.0	1.0	0.0
TRAPP-1 e	0.8059	0.8318	0.8316	0.0	0.0869	0.9393
TRAPP-1 f	0.7828	0.8288	0.8289	0.0	0.1379	0.8181
TRAPP-1 g	1.0123	1.2223	1.2248	0.0	0.8	0.9444
TRAPP-1 h	0.5412	0.5524	0.5390	0.25	1.0	0.1764

9. Quality measurement on CDHS production functions

Table 4: Performance metrics of HT-MOQPSO, SMPSO and NSGAII for computing habitability under CRS constraint

We compared the performance of HT-MOQPSO against that of SMPSO and NSGA-II for estimating the two components of the Cobb-Douglas Habitability Score. As mentioned earlier, hypervolume measures the region in the objective space dominated by a solution set. In our problem, since the goal is to optimize two objective functions, the objective space is two dimensional and hence, hypervolume is a measure of the **area** dominated by a solution set. We measure hypervolume with respect to a reference point (0,0). Another quality measure that we have used is purity [41], which measures the portion of rank one solutions of an algorithm that makes up the rank one solutions of the union of rank one solutions of all the algorithms under comparison. Rank one solutions of a solution set is the subset of the solution set which is non-dominated within the solution set. Purity is a number that lies between [0, 1]. When the purity measure of an algorithm is 1, it implies that all solutions in the rank one set of the algorithm contain solutions that are non-dominated by any other solutions of other algorithms in comparison. When the purity measure is 0, it implies that all solutions in the rank one solution set of an algorithm are dominated by some solutions belonging to another algorithm. For both of these performance metrics, the higher the measure the better the quality of the result is. It is observed from Table 4 that hypervolume values are comparable for all three algorithms. However, SMPSO performs poorly in terms of purity while NSGAII and HT-MOQPSO have purity measurement ranging from 0.1 to 1.0.

10. PSO based clustering of Exoplanets: Cross validating habitable candidates identified by CDHS

Data clustering is an unsupervised learning algorithm which involves grouping similar data points into non-overlapping subsets. Clustering algorithms have immense application in the fields of machine learning, data analysis and pattern recognition. Data points in the same cluster should have similar properties, while the data points in different cluster should have dissimilar properties. Clustering helps us find the relationship between the data points by seeing what clusters they fall into. Success of any clustering method depends on choosing an optimal set of parameters/attributes. The selection of appropriate attributes is very crucial for any analysis. We plot the distribution of attributes of habitable and non-habitable exoplanets and try to find a pattern in their distribution. We have made use of Hausdorff distance metric to find the distance between the distribution of attributes of habitable and non-habitable planets. Hausdorff distance between two distribution A and B is defined as following,

$$d_H(A,B) = \max_{\forall a \in A} \min_{\forall b \in B} | a - b |$$
(15)

For every point a in A, we find the distance of the nearest point in B , store this in a set, and then find the maximum of all these distances. Some of the selected parameters selected for input to the PSO clustering algorithm 5 are

 $^{^{5}}$ The PSO clustering suite has implemented several clustering algorithms, K Means being one of those. main.py needs to be run where KMeans was not used but has as default in the

period, escape velocity, gravity, mass etc.

Each iteration of swarm updates the velocity of the particle towards its pbest and gbest values. The minimization function is quantization error which is a metric of error introduced by moving each point from its original position to its associated quantum point. In clustering, we often measure this error as the root-mean-square error of each point(moved to the centroid of its cluster). When a particle finds a location that is better than the previous locations, it updates this location as the new current best for the particle i. The aim is to find the global best among all the current best solutions until the objective no longer improves or after a certain number of iterations. Here x_i and v_i are position vector and velocity vector respectively. The new velocity is found by the velocity update as explained earlier.

Here f(x) is a function to be minimized which is also called as the fitness function, where x is an n-dimensional array. Algorithm 2 outlines the approach to minimizing f(x) using PSO and Algorithm 3 assigns cluster label. A set of particles are randomly initialized with a position and a velocity. The position of the particle corresponds to its associated solution. Here each particle has cluster centroids which is the solution and *pbest* score calculated using the fitness function. The *pbest* position that corresponds to the minimum fitness is selected to be the *gbest* position of the swarm.

The algorithm finds 7 clusters, out of which cluster 4 is where Earth belongs (see Fig. 5). Cluster 4 also contains several other exoplanets which include prominently, among others, Trappist 1-e, Proxima Cen-b etc. More importantly, the CDHS computed by the proposed method of the planets belonging to cluster 4 are close to 1 (Note, CDHS_Earth=1). Clusters 3 and 5 are the next closest to Earth's cluster and contain some of the following planets whose CDHS are also close to Earth. Clusters 1, 2, 7 for example contain planets whose CDHS are far away from that of the Earth.

suite. Assigning hybrid ==false will disable automatic choice of KMeans

Algorithm 2: Algorithm for PSO						
iı	nput : An n-dimensional array of data x					
0	output : An array of cluster labels					
1 fe	1 for $j \leftarrow 1$ to max_iterations do					
2	for each particle $i \leftarrow 1$ to $n_particles$ do					
3	$u_{\rm p}, u_{\rm g} pprox U(0, 1)$					
4	$v_{i} \leftarrow w.v_{i} + \lambda_{g}u_{g}(gbest - p_{i}) + \lambda_{p}u_{p}(pbest_{i} - p_{i})$					
5	$p_{\rm i} \leftarrow p_{\rm i} + v_{\rm i}$					
6	if $f(p_i < f(pbest_i)$ then					
7	$pbest_{i} \leftarrow p_{i}$					
8	end					
9	end					
10	for each particle $i \leftarrow 1$ to $n_particles$ do					
11	$\mathbf{if} \ f(pbest_i) < f(gbest) \ \mathbf{then}$					
12	$gbest \leftarrow pbest_{i}$					
13	end					
14	end					
15 end						
16 <i>C</i>	16 $cluster \leftarrow g(x, gbest)$					
17 re	17 return cluster					

Algori	thm 3: Algorithm for clustering		
i	nput : An n-dimensional array of data x and gbest		
	centroids		
C	• An array of cluster labels		
1 f	$\mathbf{or} \ each \ gbest_centroids \ c \ \mathbf{do}$		
2	for each data x do		
3	for each param $i \leftarrow 1$ to n_params do		
4	$d \leftarrow d + (x_{\mathrm{i}} - c_{\mathrm{i}})^2$		
5	end		
6	distance.append(d)		
7	end		
8	$global_distance.append(distance)$		
9 e	and		
10 g	$lobal_distance \leftarrow transpose(global_distance)$		
11 C	$luster \leftarrow argmin(global_distance)$		
12 r	12 return cluster		



Figure 5: Earth belongs to cluster 4, and so do a number of planets including Trappist 1-e, Proxima Cen-b and others whose CDHS is close to that of Earth. The clustering approach is independent of CDHS scores, rather based on physical attributes and a similarity measure, driven by PSO clustering algorithm

The concept of developing a clustering method based on evolving body of knowledge of exoplanets is appealing. What we propose and implement here is a method of inference based on the fusion of two orthogonal approaches. CDHS symbolizes Earth similarity and PSO based clustering searches for habitable candidates without computing any sort of Earth similarity score. Table 5 demonstrates results of the clustering algorithm which didn't use CDHS while assigning planets to different clusters or groups. Thus, the clustering approach is independent of the habitability score computation method and stands as a validation technique for the CDHS approach. For example, let us consider a couple of samples from Table 5. GJ 176 b belongs to cluster 1 by virtue of the algorithmic assignment (algorithms 2 and 3) and it's easy to see from the scores computed that its CDHS is 2.78. Thus, over-reliance on a particular

Planets	cluster number	CDHS
GJ 176 b	cluster 1	2.78
Kepler-163 b	cluster 2	1.89
Kepler-171 b	cluster 3	2.02
Kepler-186 f	cluster 4	2.00
Kepler-290 b	cluster 3	264.7
Kepler-292 d	cluster 3	2.24
Kepler-1393 b	cluster 1	2.98
Proxima Cen-b	cluster4	1.01
Kepler-20 c	cluster 3	2.4
Kepler-59 b	cluster 2	263.4
Kepler 61 b	cluster 2	2.01
Trapp 1-c	cluster 3	1.24
Trapp 1- d	cluster 5	0.96
Trapp 1-e	cluster 4	1.17
Trapp 1-f	cluster 5	1.02
Trapp 1-g	cluster 4	1.09
GJ 667 C b	cluster 7	3.88

Table 5: CDHS of a representative sample of planets from PHL-EC and their corresponding cluster association: Earth belongs to Cluster 4 by automatic selection via Algorithm 2 and Algorithm 3

Earth-similarity score (CDHS) is successfully avoided. We now have a method which testifies for the efficacy of such scoring methods. PSO based clustering described in this section offers us that flexibility.

From table 5, we observe that Proxima Cen b belongs to Earth's cluster and also possess favorable habitability score. If such a planet is not too far away from the Earth, we could build a model for interstellar migration using the time to travel to such a planet (if possible) as one of the key parameters. Next section deliberates on colonization opportunities on such set of discovered and potentially habitable exoplanets found by our analysis.

11. Exoplanets and Inter-stellar Trade: Some Conjectures

This section deals with two issues concerning the 'space dimension' of international trade. First and foremost, in order to justify the inclusion of these issues in the current context one might invoke the applications of standard economic principles that underlie many of the path-breaking scientific projects and explorations that have changed the global order over generations. It is well-known that in the recent times scientific discoveries and innovations like those in the sphere of information technology have completely revolutionized the patterns of economic transactions between agents. In the process, scientific discoveries and the economic outcomes associated with these have become complementary to each other leading to more prosperity as also vulnerabilities of different orders. In addition to the quality and academic merits associated with exploring scientific ideas, such as that in the present context of identifying habitable exoplanets and assigning scores to these, sheer market forces behind public budgetary allocations and private initiatives warrant that tangible returns are explored alongside. We offer a brief overview of what such tangible returns with marketable options cater in relation to identifying habitable exoplanets. Earlier Krugman (2010) in a rare extension of the traditional theory of international trade to interstellar transactions argued that the recent progress in the technology of space travel as well as the prospects of the use of space for energy production and colonization make the critic's assertions about limited use of economics as a pragmatic tool, doubtful. The discovery of a habitable exoplanet shall require all the fundamental theorems and laws of economics to be re-established with the same importance as the rules and conditions of astrophysics, for example. The discovery and plans to explore an exoplanet cannot be too different from arriving at the 'new world' in 1492. Once the habitability score is obtained, it is ideal to focus on the marginalist analysis commonly used in economics and compare gains from interstellar trade with that of the cost involved. This is expected to cover many dimensions, such as resources, technology, time and entrepreneurship, etc., where risk, uncertainty and discount

factors among different agents play crucial roles. We will assume a model of colonization to begin with, where the main thrust shall be on expanding the resource base for earth as potential gains from trade. This shall predominantly interact with models of interplanetary negotiations, spillover and distribution.

11.1. The Model

Assume that the fixed cost of sending a carrier to the exoplanet is c and the cost of research and development building up to the point of engaging in a voyage is M. These are large fixed costs to be borne by the public or private agency which wishes to use the outcome of identifying habitable exoplanets and choosing one or more to send the voyages to. Let the interest rate prevailing on earth be r, which is the opportunity cost of investing billions of dollars in this project. On the same note, we will disregard any other interest calculation either by observers external to earth, or if at all, by anybody aboard the carrier (also see Krugman, 2010 in this regard as to why the estimate has relevance only in view of the observer-cum-investor on earth rather than other entities). Indeed, the discounted future stream of earnings following the investment is analogous to investing in a long-run bond or over indefinite future, which for the sake of obtaining closed-form solutions is considered as 2N years, where it takes N years to visit the exoplanet in question. We further assume that the carrier is equipped with instruments that can identify and extract commodities or resources considered of value over a long horizon, to the investor and if exchangeable, then of value to potential buyers in future. The model applies a pure colonial extraction mode, whereby, the voyage procures these items for a per unit extraction cost of $p_E > 0$. Once delivered back to earth on return the per unit price of these items is $\hat{p}_E > 0$. The decision problem here is how much to quantity to extract, i.e., the optimal quantity, \hat{q}_E . From this rather simple specification, the voyage must deliver back an amount which ensures that the total revenue earned from selling these items is greater than the total cost:

$$\hat{p}_E \hat{q}_E > (c + M + \hat{q}_E p_E) * (1 + r)^{2N}$$
(16)

which solves for,

$$\hat{q_E} \ge \frac{(c+M)*(1+r)^{2N}}{\hat{p_E} - p_E(1+r)^{2N}} \equiv \tilde{q_E}$$
(17)

Obviously, a change in fixed costs should raise the optimal quantity to be extracted at a fixed rate. However, if the time to reach the exoplanet increases, the optimal quantity extracted rises, and for even longer spells the optimal quantity may fall. These are directly observable from equations (27) and (28) below.

$$\frac{\delta \tilde{q_E}}{\delta N} = 2 \frac{\ln (1+r)(c+M)(1+r)^{2N} \hat{p_E}}{(-\hat{p_E} + p_E(1+r)^{2N})^2}$$
(18)

And,

$$\frac{\delta^2 \tilde{q_E}}{\delta N^2} = -4 \frac{\ln(1+r)^2 (c+M) \hat{p_E} [(1+r)^{2N} \hat{p_E} + (1+r)^{4N} p_E]}{(-\hat{p_E} + p_E (1+r)^{2N})^3}$$
(19)

Equation (28) suggests that

 $\delta^2 \tilde{q_E^{\circ}} < 0, \, \text{iff} \, \, (-\hat{p_E} + p_E (1+r)^{2N})^3 > 0$

In other words, with passage of time if the discounted return from selling the interstellar commodities on earth falls below the price of extracting the same, the quantity extracted would fall. Although we do not model preference in this framework, but this might be an outcome of preference shifting away from the commodity in question over time. This is a source of uncertainty manifested in the form of lower discounted price of the commodity. Thus, the relation between the optimal quantity extracted and the time taken to complete the round-trip journey from the exoplanet in question might display an inverted u-shape over longer time horizon. Indeed, by assuming the rate of interest to be 2% annually, the fixed cost of the voyage (c=\$100 bn), the cost of research and development spread over several years (M=\$75 bn), the price of per unit of the commodity on earth as \$20,000 and extraction cost at \$10,000 per unit, then the relation appears as in Figure 6 below.

Further, in figure 7, we explore the trajectory of what should be the optimal extraction strategy for the business investing in voyages to exoplanets in terms of an admissible range of years taken to complete the voyage and variations in the price of extraction of materials from the exoplanet. Not unexpectedly, as



Figure 6: Relation between number of years and optimal extraction



Figure 7: Relation between number of years, cos;t of extraction and optimal extraction

the number of years taken to complete the voyage increases along the horizontal axis (N), and the rate of extraction increases along the y-axis (), the optimal volume of extraction is the maximum attainable.

11.2. Scope of Interstellar Trade

Instead of the extraction model discussed above, if earth and the exoplanets are engaged in trade in the same fashion as countries engage in it, the above conditions would undergo suitable changes. Suppose the per unit price of the earth's commodity in the exoplanet is \tilde{p}_{E} (export price, f.o.b) and the quantity that gets traded from earth is q^T . Balance of trade with the exoplanet requires that:

$$\tilde{p_E} * q^T = \hat{p_E} * \tilde{q_E}$$
(20)

Where, is now the import (c.i.f) price of the commodity from exoplanet. It is natural to assume that if trade takes place instead of extraction, the quantity in question receivable from the exoplanet shall be less than and could be equal to . Since we apply the discount rate effective for a trade from earth, the interest rate assumed in the previous sub-section remains unchanged. From (29), the quantity trade by businesses on earth equals:

$$q^T = \frac{\hat{p_E} * \tilde{q_E}}{\tilde{p_E}} \tag{21}$$

Substituting from (26), equation (30) leads to:

$$q^{T} = \frac{\hat{p}_{E}(c+M)(1+r)^{2N}}{\tilde{p}_{E}\hat{p}_{E} - p_{E}(1+r)^{2N}}$$
(22)

Equation (31) suggests that a rise in N should affect the volume of trade following the condition of balanced trade, when the previously defined extraction cost in the exoplanet may now be treated as a collection (shipment) cost borne by the importer from earth. The volume of trade with the exoplanet is concave with the passage of time. The first and second order differentiation with respect to N are given in (32) and (33) respectively, such that, q_E is constant at a high value of N and that trade might cease if the discounted return from future value of the imports consumed on earth is lower than the exports shipped out in the present times.

$$\frac{\delta q_T}{\delta N} = 2 \frac{\ln(1+r)(c+M)(1+r)^{2N}\hat{p}_E^2}{\tilde{p}_E(-\hat{p}_E + p_E(1+r)^{2N})^2}$$
(23)

and

$$\frac{\delta^2 q_T}{\delta N^2} = 4 \frac{\ln(1+r)^2 (c+M) \hat{p}_E^2 [(1+r)^{2N} \tilde{p}_E + (1+r)^{4N} p_E]}{\tilde{p}_E (-\hat{p}_E + p_E (1+r)^{2N})^3}$$
(24)

Figure 8 treats the shipping cost in the exoplanet and the time travelled as variables in the same estimate of trade volume between earth and the exoplanet. Using the same numerical specifications (and assuming that the cost of shipping and the cost of extraction are same in the exoplanet) as applicable for the



Figure 8: Relation between number of years and optimal trade volume from earth

previous results, here we find that the quantity traded (vertical axis) undergoes cyclical fluctuations for different values of the extraction cost and the length of time involved.

Equation 33 and figures 6, 7 clearly indicate that the time, N, to reach any exoplanet is a key factor in determining volume of interstellar trade and possible migration. In any catalog, e.g. Exoplanets Data Explorer [42] there is a column 'Distance to star' in Stellar parameters. We, upon arranging it in increasing order, observe the nearby exoplanets. Proxima Cen b is one such with exoplanet which also happens to be potentially habitable by our computation in Sections 5 and 10 (Please see Table 5).

12. Conclusion

We illustrate the results of our proposed model using planetary inputs from the recently discovered group of seven Earth-like planets known as the TRAPPIST-1 system. Please note, the method was applied to all discovered and conformed Rocky exoplanets. Trappist system is used for illustration purpose. TRAPPIST-1 e (belongs to Earth Cluster as shown in section 10) has been established to be the most habitable candidate out of the seven [43]. The manuscript provides empirical evidence of the correctness of our approach by



Figure 9: Relation between number of years, collection cost and optimal trade volume from earth

comparing the computed habitability scores (see table 1 and fig 4) for the TRAPPIST-1 system with existing values in the literature. The solution sets obtained for planets under the TRAPPIST-1 system exhibit a clear trade-off between the interior and the surface scores. Through a game theoretical analysis, we find that this structural relationship between the two scores ensures that the weighted combination of the two results in a consistent CDHS value regardless of the weights chosen for the scores. A multi-objective optimization framework is proposed to solve the problem in order to gain structural information about the original optimization problem. We precisely accomplish this objective by gaining insight on the trade-off between interior and surface habitability sores. This is something not observed with single objective optimization approach [44]. There is no clear relationship between the surface and interior score which we would like to understand. It needs to be explored whether this trade-off is a catalyst for habitability or whether this is accidental. We say this because the trade-off is observed in the TRAPPIST-1 system, particularly in the planets which are considered potentially habitable (earth-like). Interior and Surface scores serve two different purposes in determining the habitability of exoplanets. In other words, one cannot be replaced by the other and the goal is to include both toward developing a reliable habitability indicator. Therefore, the bi-objective framework is justified and we gain rich insights from it! The strength of this proposed approach has been validated using machine learning algorithms such as KNN [3] and XGBoosted trees [4] by utilizing computed *CDHS* values and labeling corresponding exoplanets into appropriate classes. However, in past approaches, CDHS is computed by splitting it into two components – surface score and interior score – which are estimated independently. The sole reason for this split is due to the ease of visualization of these components against their input parameters. Because of the dependence between the planetary parameters that are used to estimate these components, it is speculated that there is an intrinsic relationship between the interior score and surface score. And hence, a new model for *CDHS* estimation is proposed that factors in the relationship between the two scores. A multi-objective optimization task is defined to search for coefficients of elasticity that simultaneously maximizes both interior and surface score. The result is a non-dominated solution set that is characterized by trade-offs between the two components of the score. This relationship between the interior (Y_i) and surface score (Y_s) implies cooperation between the two components. Since the final CDHS is a number that lies between Y_i and Y_s in which weights w_i and w_s determine the proximity of CDHSto Y_i and Y_s , the trade-off relationship implicates that a decrease in Y_i is compensated by an increase in Y_s and vice-versa. This allows a consistent CDHS to be maintained. We take a game theoretic approach and prove that the choice of weight pairs will decide what (Y_i, Y_s) from the Pareto front is ideal for CDHS calculation. The conclusion is that unlike [3] and [4], no matter what w_i and w_s are set to, the trade-off between Y_i and Y_s ensures a consistent CDHS. The result is a robust methodology for quantifying exoplaneteray habitability.

We combined clustering approach with habitability score computation to develop richer inference from the data of exoplanets. The planets which are identified as both having CDHS close to the Earth and belonging to the same cluster as Earth are probably the most likely candidates for habitable planets. This method can bolster our understanding of factors that affect habitability in the long run. The clustering approach is also free from any class labels that already exist in the catalog and are not beyond reasonable doubt, either due to bias or dependence of surface temperature. The clustering approach didn't consider surface temperature or related attributes in feature selection.

The manuscript develops a tool for planetary habitability prediction using bi-objective optimization method for habitability score computation combined with planetary features to generate a predictor. Unlike earlier work, the predictor is developed as a computational intelligence (CI) tool, departing significantly from label-based classification approach. We observe convergence between the outcome of two approaches, thus fortifying the belief of producing a more reliable set of habitable planets for further physical investigation.

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Appendix A. Convergence for hypervolume terminated QPSO (HT-MOQPSO)

We assume the quantum delta potential model of PSO where,

$$|\psi|^2 dx dy dx = Q dx dy dz \tag{A.1}$$

 $|\psi|^2$ is the probability density function satisfying

$$\int_{-\infty}^{+\infty} |\psi|^2 dx dy dx = \int_{-\infty}^{+\infty} Q dx dy dx = 1$$
 (A.2)

The state function, $\psi(x,t)$ is described by Schrödinger equation. Consider H as the Hamiltonian operator, for a single particle of mass m in a potential field V(x), given as

$$H = -\frac{h^2}{2m}\Delta^2 + V(x) \tag{A.3}$$

where h is the Planck's constant. Let us consider the time dependent and time independent Schrodinger equation to arrive at the variant describing the delta potential well of QPSO: $H\psi = i\hbar\frac{\partial\psi}{\partial t}$; time dependent variant and $H\psi = E\psi$; time independent variant where E = Energy eigen value and $V(x) = -\gamma\partial(x - p) = -\gamma\partial(y)$; y = x - p. p is the center of the attraction potential field. This is essential for stability and bound state of the potential. Using the above variants, we can write

$$[-\frac{h^2}{2m}\frac{d^2}{dy^2} - \gamma\partial(y)]\psi = E\psi$$
$$\implies \frac{d^2\psi}{dy^2} + \frac{2m}{h^2}\gamma\partial(y)\psi = -\frac{2m}{h^2}E\psi$$
$$\implies \frac{d^2\psi}{dy^2} + \frac{2m}{h^2}[\gamma\partial(y) + E]\psi = 0$$
$$\implies \frac{d^2\psi}{dy^2} - \beta^2\psi = 0; \text{where } \beta = \sqrt{\frac{-2mE}{h^2}}$$

Let $L = \frac{1}{\beta}$. The wave function (normalized) and the probability density function can be represented as $\psi(y) = \frac{1}{\sqrt{L}}e^{-|y|/L}$ and $Q(y) = \frac{1}{L}e^{-2|y|/L}$ respectively. The termination condition on the MOQPSO algorithm based on hypervolume is based on the assumption that successive iterative computation of the area including soluton set (pareto front) would converge i.e. the differences between the successive areas bounded by ϵ implying the swarm movement being restricted in an ϵ - neighborhood to guarantee convergence. Since, the probability density function is computed already. We arrive at the expression stating the difference in hypervolume. $||A_{i+1} - A_i|| = \int_{-\epsilon}^{+\epsilon} ||Q(A_{i+1}) - Q(A_i)|| dy \to \epsilon$. As $\epsilon \to 0$ when $i \to \infty$, HT-MOQPSO is guaranteed to converge asymptotically.

Appendix B. Modeling constraints using penalties

We represent all strict inequality and equality constraints as non-strict equality constraint as described by Ray and Liew [45]. We convert strict inequality constraint of the type g'(x) < 0 to a non-strict inequality constraint g(x) by introducing an error term ϵ such that $g(x) = g'(x) + \epsilon \leq 0$. By introducing a tolerance value τ , we convert equality constraint of the form h(x) = 0 to $g(x) = |h(x)| - \tau \leq 0$. For a solution p_i , let c_i denote the vector of constraint values. Then $c_{ik} = max(g_k(p_i), 0) \forall k = 1, 2, 3, ..., m$. When $c_{ik} = 0$, then solution p_i lies in the feasible region of the search space.

Applying this rule, constraints under CRS can be translated to

$$-\phi + \epsilon \le 0, \ \phi - 1 + \epsilon \le 0 \ \forall \phi \in \{\alpha, \beta, \delta, \gamma\}$$
(B.1)

$$|\alpha + \beta - 1| - \tau \le 0, \ |\delta + \gamma - 1| - \tau \le 0 \tag{B.2}$$

Under DRS, we replace (B.2) with $\alpha + \beta + \epsilon - 1 \leq 0$, $\delta + \gamma + \epsilon - 1 \leq 0$. We impose these constraints through the use of **penalty** methods. In penalty methods, we augment the objective functions with penalty functions that "penalizes" a candidate solution when it violates any of the constraints. In case of a minimization problem, penalty functions return a large positive value, when a candidate solution moves outside of the feasible region, that gets added to the base objective function. This, in turn, makes the objective function large and undesirable and hence, making the candidate solution weak. We define the following penalty functions:

$$\psi(x) = \begin{cases} 0, & \text{if } |x| - \tau \le 0, \\ k_1 \cdot |x|, & otherwise \end{cases}, \Omega(x) = \begin{cases} 0, & \text{if } x + \epsilon \le 0 \\ k_2 \cdot |x|, & otherwise \end{cases}$$

 k_1 and k_2 are penalty factors. Larger the penalty factors, the more severe the penalty is. Using functions ψ and Ω , we augment objective functions (4) and (5) under CRS condition as

$$PY_i = -Y_i + \psi(\alpha + \beta - 1) + \Omega(-\alpha) + \Omega(\alpha - 1) + \Omega(-\beta) + \Omega(\beta - 1)$$
 (B.3)

$$PY_s = -Y_s + \psi(\delta + \gamma - 1) + \Omega(-\delta) + \Omega(\delta - 1) + \Omega(-\gamma) + \Omega(\gamma - 1)$$
 (B.4)

Using these augmented objective functions, the constrained optimization task (8) subject to (9) is equivalent to the unconstrained optimization task: $\min_{\vec{x}} \vec{f}(\vec{x}) = [PY_i, PY_s]$. In our experiments, we set k1 and k2 to 10^{12} and make ϵ and τ equal to 10^{-8} .

Appendix C. Hyper-parameter tuning

Tuning and improvising parameters such as max and min velocity, learning factors such as cognitive and social factors, inertia weight etc. is not possible through the methods that the classes in *Jmetalpy* provides. Tuning of these parameters is really crucial for the algorithm to converge. With respect to the range of the functions that we are trying to optimize and the constraints that are imposed on the search space, the algorithm, with the default parameters provided by the library, did not yield desirable solutions. Most of the solutions in the solution set were outside of the feasible region of the search space. We suspected that *Vmax* was too large and *Vmin* was too small. And hence, some changes were made in *Jmetalpy's* source code to make parameter tuning possible. Initially, for j^{th} decision variable, $Vmax_j = \frac{upperbound_j-lowerbound_j}{2.0}$; $Vmin_j = -Vmax_j$, where $upperbound_j$ is the largest allowable value for the j^{th} decision variable and *lowerbound_j* is the smallest allowable value for the j^{th} decision variable. For our problem, these values where changed to $Vmax_j = \frac{upperbound_j - lowerbound_j}{1000.0}$ with $Vmin_j$ still set to $-Vmax_j$. Learning factors w, C_1 and C_2 are sampled from a uniform distribution with specified ranges i.e. $w \sim U(w_{min}, w_{max}), C_1 \sim U(C_{1min}, C_{1max}), \text{ and } C_2 \sim U(C_{2min}, C_{2max}).$ We set $w_{min} = w_{max} = 0.1, C_{1min} = 0.1, C_{1max} = 0.5, C_{2min} = 0.8$ and $C_{2max} = 1.5$. The swarm size is set to 100.