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HyperFunction and SuperHyperFunction in Chemistry

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Abstract

Hyperstructures and their hierarchical extensions, the Superhyperstructures, furnish a flexible framework for modelling multilayered phenomena across a wide range of disciplines. Viewed through the lens of functions, these ideas manifest as *HyperFunctions* and *SuperHyperFunctions*, whose values belong to iterated powersets rather than to ordinary codomains. Although the structural and computational aspects of hyperstructures have been explored well beyond mathematics—including notable work in chemistry—the corresponding functional counterparts remain largely unexamined in that context. To address this gap, the present paper introduces several precise definitions of HyperFunctions and SuperHyperFunctions tailored to chemical systems and investigates their fundamental properties. These set-valued constructs capture nested reactivity patterns and multi-step pathways, thereby opening new avenues for describing complex chemical processes.

Keywords: Hyperfunction, Superhyperfunction, Hyperstructure, Superhyperstructure, Partition function, Reaction rate function, Dose-response function, Fitness function.

1| Introduction

This section fixes notation and recalls the basic notions used throughout the paper. Unless explicitly stated otherwise, all sets considered here are finite.

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1.1| Hyperfunctions and n -Superhyperfunctions

Hyperstructures[1, 2, 3, 4] and their iterated, hierarchical counterparts, n -superhyperstructures[5, 6], serve as general formalisms for modeling multilayered phenomena across diverse domains. Representative instances include the SuperHyperGraph[7, 8, 9, 10] and the SuperHyperAlgebra[11, 12, 13, 14], each realizing a superhyperstructure within a specific mathematical context. These frameworks have also been actively explored in chemistry and chemical-reaction theory, where their ability to encode nested interactions is particularly advantageous[4, 15, 16, 17, 18, 19]. At the level of functions, the notions of *hyperfunction* and *n -superhyperfunction* generalize classical single-valued maps to set-valued and, respectively, iterated set-valued outputs[20, 21]. These ideas have seen active development in recent years across multiple disciplines[22, 23, 24]. For convenience, the key definitions and statements required in this work are collected below.

Definition 1.1 (Universe). Let U be a nonempty finite set, called the *universe* (or *base set*). All subsequent constructions—powersets, hyperstructures, and their iterates—are built on U .

Definition 1.2 (Power set[25]). The *power set* of U is

$$\mathcal{P}(U) = \{A \mid A \subseteq U\}.$$

Definition 1.3 (Iterated powerset [26, 27, 28, 29]). For each integer $n \geq 1$, the n -fold iterated powerset of U is defined recursively by

$$\mathcal{P}^1(U) = \mathcal{P}(U), \quad \mathcal{P}^{n+1}(U) = \mathcal{P}(\mathcal{P}^n(U)).$$

If one wishes to exclude the empty set at every stage, replace $\mathcal{P}$ with

$$\mathcal{P}^*(X) = \mathcal{P}(X) \setminus \{\emptyset\}.$$

Remark 1.4. The iterated powerset construction organizes information in layers: elements of $\mathcal{P}(U)$ are *subsets* of a universe U (single-layer groupings); elements of $\mathcal{P}^2(U) = \mathcal{P}(\mathcal{P}(U))$ are *families of subsets* (collections of groupings); elements of $\mathcal{P}^3(U)$ are *families of families* (portfolios of alternative collections), and so on. In many practical settings, U is finite and one often uses the nonempty variant $\mathcal{P}^*(X) = \mathcal{P}(X) \setminus \{\emptyset\}$ at each level to exclude degenerate choices.

Example 1.5 (Trip planning: days, itineraries, and options). Let the universe of activities be

$$U_{\text{act}} = \{\text{Sensoji (Se)}, \text{teamLab (Te)}, \text{Tsukiji (Ts)}, \text{Onsen (On)}\}.$$

Single-day plans are subsets of activities, e.g.

$$D_1 = \{\text{Se}, \text{Ts}\}, \quad D_2 = \{\text{Te}, \text{On}\} \in \mathcal{P}(U_{\text{act}}).$$

A two-day itinerary is a *set of day plans*, e.g.

$$I_A = \{D_1, D_2\} \in \mathcal{P}^2(U_{\text{act}}).$$

Suppose we also consider an alternative itinerary

$$I_B = \{\{\text{Se}, \text{Te}\}, \{\text{Ts}, \text{On}\}\} \in \mathcal{P}^2(U_{\text{act}}).$$

A traveler’s shortlist of choices is then a *set of itineraries*

$$\mathcal{O} = \{I_A, I_B\} \in \mathcal{P}^3(U_{\text{act}}).$$

If empty days are disallowed, replace $\mathcal{P}$ by $\mathcal{P}^*$ at the appropriate level.

Example 1.6 (Role-based access control: privileges, roles, and policies). Let the universe of privileges be

$$U_{\text{priv}} = \{\text{read (r)}, \text{write (w)}, \text{deploy (d)}, \text{audit (a)}\}.$$

A *role* is a subset of privileges (an element of $\mathcal{P}(U_{\text{priv}})$):

$$R_{\text{dev}} = \{r, w\}, \quad R_{\text{ops}} = \{r, d\}, \quad R_{\text{audit}} = \{r, a\}.$$

A department policy bundles roles (an element of $\mathcal{P}^2(U_{\text{priv}})$):

$$B_{\text{Eng}} = \{R_{\text{dev}}, R_{\text{ops}}\}, \quad B_{\text{Risk}} = \{R_{\text{audit}}\}.$$

Corporate policy options across regions form a family of such bundles

$$\mathcal{C} = \{B_{\text{Eng}}, B_{\text{Risk}}\} \in \mathcal{P}^3(U_{\text{priv}}).$$

If a role must never be empty, use $\mathcal{P}^*$ in place of $\mathcal{P}$ at the role level.

Example 1.7 (Manufacturing: parts, modules, and product lines). Let the universe of parts be

$$U_{\text{parts}} = \{\text{frame (Fr)}, \text{battery (Ba)}, \text{screen (Sc)}, \text{SoC (So)}, \text{camera (Ca)}\}.$$

A *module/BOM slice* is a subset of parts (element of $\mathcal{P}(U_{\text{parts}})$):

$$M_{\text{core}} = \{\text{So}\}, \quad M_{\text{display}} = \{\text{Sc}\}, \quad M_{\text{power}} = \{\text{Ba}\}, \quad M_{\text{shell}} = \{\text{Fr}\}, \quad M_{\text{cam}} = \{\text{Ca}\}.$$

A product variant groups modules (element of $\mathcal{P}^2(U_{\text{parts}})$):

$$V_{\text{basic}} = \{M_{\text{core}}, M_{\text{display}}, M_{\text{power}}, M_{\text{shell}}\}, \quad V_{\text{pro}} = \{M_{\text{core}}, M_{\text{display}}, M_{\text{power}}, M_{\text{shell}}, M_{\text{cam}}\}.$$

A product line portfolio is a set of variants

$$\mathcal{L} = \{V_{\text{basic}}, V_{\text{pro}}\} \in \mathcal{P}^3(U_{\text{parts}}).$$

Requiring each module to be nonempty corresponds to using $\mathcal{P}^*$ at the module level.

Example 1.8 (Academic planning: courses, term schedules, and degree plans). Let the universe of courses be

$$U_{\text{crs}} = \{\text{Algebra (Alg)}, \text{Analysis (Ana)}, \text{CS (CS)}, \text{Physics (Phy)}, \text{Ethics (Eth)}\}.$$

A one-term schedule is a subset of courses:

$$S_{\text{Spring}} = \{\text{Alg}, \text{Ana}, \text{CS}\} \in \mathcal{P}(U_{\text{crs}}), \quad S_{\text{Fall}} = \{\text{Phy}, \text{Eth}\} \in \mathcal{P}(U_{\text{crs}}).$$

A degree plan is a set of term schedules:

$$D_{\text{Math}} = \{S_{\text{Spring}}, S_{\text{Fall}}\} \in \mathcal{P}^2(U_{\text{crs}}).$$

A catalog of admissible degree plans is then

$$\mathcal{A} = \{D_{\text{Math}}, D_{\text{CS}}\} \in \mathcal{P}^3(U_{\text{crs}}).$$

Excluding empty terms or empty degree plans is modeled by replacing $\mathcal{P}$ with $\mathcal{P}^*$ at the corresponding levels.

Definition 1.9 (Hyperoperation). (cf.[5]) A *hyperoperation* generalizes an ordinary binary operation by allowing the output to be a *set* of results rather than a single element. Precisely, for a set S , a map

$$\circ : S \times S \longrightarrow \mathcal{P}(S)$$

is a hyperoperation, where $\mathcal{P}(S)$ denotes the power set of S .

Definition 1.10 (Hyperfunction). [21, 20] A *hyperfunction* is a map whose domain is a classical set and whose codomain is its power set. Formally, for a set S ,

$$f : S \longrightarrow \mathcal{P}(S).$$

For each $x \in S$, the value $f(x) \subseteq S$ is a subset of S . Thus a single input may be associated with multiple outputs, in contrast to the single-valued case.

Example 1.11 (Ingredient pairing as a hyperfunction). Let the universe of ingredients be

$$S = \{\text{beef (B)}, \text{tomato (T)}, \text{basil (Ba)}, \text{parmesan (P)}\}.$$

A *pairing suggestion system* assigns to each ingredient a set of compatible ingredients. Define a hyperfunction $f : S \rightarrow \mathcal{P}(S)$ by

$$\begin{aligned} f(\text{B}) &= \{\text{T}, \text{Ba}\}, \\ f(\text{T}) &= \{\text{Ba}, \text{P}\}, \\ f(\text{Ba}) &= \{\text{T}, \text{P}\}, \\ f(\text{P}) &= \{\text{B}, \text{T}\}. \end{aligned}$$

Verification: since $|S| = 4$, $|\mathcal{P}(S)| = 2^4 = 16$. For each $x \in S$ we have $f(x) \subseteq S$, hence $f(x) \in \mathcal{P}(S)$ and f is a valid hyperfunction. This captures the real-world fact that a single ingredient can have multiple suitable partners.

Example 1.12 (Airport one-hop connectivity as a hyperfunction). Let S be a finite set of airports, e.g.

$$S = \{\text{HND}, \text{KIX}, \text{CTS}, \text{FUK}\}.$$

Define $f : S \rightarrow \mathcal{P}(S)$ where $f(a)$ is the set of airports reachable from a by a *direct* flight (within the current timetable):

$$f(\text{HND}) = \{\text{KIX}, \text{CTS}\}, \quad f(\text{KIX}) = \{\text{HND}, \text{FUK}\}, \quad f(\text{CTS}) = \{\text{HND}\}, \quad f(\text{FUK}) = \{\text{KIX}\}.$$

Each $f(a) \subseteq S$, so f is a hyperfunction. Practically, this aggregates multiple feasible next stops for a given origin.

Example 1.13 (Email triage labels as a hyperfunction). Let S be a set of *labels* used by a mail client:

$$S = \{\text{Work}, \text{Finance}, \text{Travel}, \text{Family}\}.$$

A rule engine maps a received message's *primary* label to a set of *additional* labels:

$$f(\text{Work}) = \{\text{Finance}\}, \quad f(\text{Finance}) = \{\text{Work}, \text{Travel}\}, \quad f(\text{Travel}) = \{\text{Finance}, \text{Family}\}, \quad f(\text{Family}) = \emptyset.$$

Again $f : S \rightarrow \mathcal{P}(S)$. The multi-valued output reflects that a single message may belong to several folders simultaneously.

Definition 1.14 (SuperHyperOperations). [26] Let H be a nonempty set, and write $\mathcal{P}(H)$ for its power set. Define the iterated power sets recursively by

$$\mathcal{P}^0(H) = H, \quad \mathcal{P}^{k+1}(H) = \mathcal{P}(\mathcal{P}^k(H)) \quad (k \geq 0).$$

Write $\mathcal{P}_*^n(H)$ for the subset of $\mathcal{P}^n(H)$ consisting of all *nonempty* elements at the outermost level.

An (m, n) -SuperHyperOperation is an m -ary map

$$\circ^{(m,n)} : H^m \longrightarrow \mathcal{P}_*^n(H).$$

If the codomain excludes the empty set (i.e., $\mathcal{P}_*^n(H)$), we refer to the *classical-type* (m, n) -SuperHyperOperation; if the codomain is $\mathcal{P}^n(H)$ allowing the empty set, we obtain the *neutrosophic-type* variant. In both cases, these maps extend hyperoperations to higher levels through iterated power-set targets.

Definition 1.15 (n -Superhyperfunction). [21, 24, 20] For an integer $n \geq 2$ and $0 \leq r \leq n$, an n -superhyperfunction is a map

$$f : \mathcal{P}^r(S) \longrightarrow \mathcal{P}^n(S),$$

where $\mathcal{P}^k(S)$ denotes the k -fold iterated power set of a set S . Thus f sends subsets drawn from level r to objects at level n .

Definition 1.16 ((m, n) -Superhyperfunction). (cf.[30, 21]) Let S be a nonempty set and let $m, n \geq 1$. An (m, n) -superhyperfunction is a mapping

$$f : \mathcal{P}^m(S) \longrightarrow \mathcal{P}^n(S).$$

When $m = r \leq n$, this recovers the customary notion of an n -superhyperfunction $\mathcal{P}^r(S) \rightarrow \mathcal{P}^n(S)$.

Example 1.17 ($(m, n) = (1, 2)$ superhyperfunction for itinerary aggregation). Let the universe of activities be

$$S = \{\text{Sensoji (Se)}, \text{teamLab (Te)}, \text{Tsukiji (Ts)}, \text{Onsen (On)}\}.$$

Elements of $\mathcal{P}(S)$ are *day plans*. Elements of $\mathcal{P}^2(S) = \mathcal{P}(\mathcal{P}(S))$ are *itineraries* (sets of day plans). Define $g : \mathcal{P}^1(S) \rightarrow \mathcal{P}^2(S)$ by sending a chosen day plan to a family of two-day itineraries containing it. For

$$D_1 = \{\text{Se}, \text{Ts}\} \in \mathcal{P}(S), \quad D_2 = \{\text{Te}, \text{On}\} \in \mathcal{P}(S), \quad D_3 = \{\text{Te}\} \in \mathcal{P}(S),$$

set

$$I_A = \{D_1, D_2\} \in \mathcal{P}^2(S), \quad I_B = \{D_1, D_3\} \in \mathcal{P}^2(S),$$

and define

$$g(D_1) = \{I_A, I_B\} \in \mathcal{P}^2(S).$$

Membership check (explicit):

$$D_i \subseteq S \Rightarrow D_i \in \mathcal{P}(S); \quad \{D_1, D_2\} \subseteq \mathcal{P}(S) \Rightarrow I_A \in \mathcal{P}^2(S);$$

similarly $I_B \in \mathcal{P}^2(S)$, hence $\{I_A, I_B\} \subseteq \mathcal{P}^2(S)$ and $g(D_1) \in \mathcal{P}^2(S)$. Thus $g : \mathcal{P}^1(S) \rightarrow \mathcal{P}^2(S)$ is a valid $(1, 2)$ -superhyperfunction.

Example 1.18 ($(m, n) = (1, 2)$ superhyperfunction for role $\rightarrow$ policy bundles). Let the privilege universe be

$$S = \{\text{read (r), write (w), deploy (d), audit (a)}\}.$$

A *role* is a subset of privileges: $R_{\text{dev}} = \{r, w\}$, $R_{\text{ops}} = \{r, d\}$, $R_{\text{audit}} = \{r, a\}$ in $\mathcal{P}(S)$. An *access policy* is a set of roles, i.e. an element of $\mathcal{P}^2(S)$:

$$B_{\text{Eng}} = \{R_{\text{dev}}, R_{\text{ops}}\}, \quad B_{\text{Risk}} = \{R_{\text{audit}}\}.$$

Define $h : \mathcal{P}^1(S) \rightarrow \mathcal{P}^2(S)$ by

$$h(R_{\text{dev}}) = \{B_{\text{Eng}}, B_{\text{Risk}}\}, \quad h(R_{\text{ops}}) = \{B_{\text{Eng}}\}.$$

Then h is a $(1, 2)$ -superhyperfunction mapping a role (level 1) to a family of admissible policies (level 2).

Example 1.19 ($(m, n) = (2, 3)$ superhyperfunction for regional policy portfolios). Continue with the previous S . Elements of $\mathcal{P}^2(S)$ are policies (sets of roles). Elements of $\mathcal{P}^3(S)$ are *policy portfolios* (sets of policies). Consider the input

$$X = \{R_{\text{dev}}, R_{\text{ops}}\} \in \mathcal{P}^2(S).$$

Define two region-specific policies

$$B_{\text{JP}} = \{R_{\text{dev}}, R_{\text{ops}}\} \in \mathcal{P}^2(S), \quad B_{\text{US}} = \{R_{\text{dev}}, R_{\text{ops}}, R_{\text{audit}}\} \in \mathcal{P}^2(S),$$

and set the portfolio

$$\Pi = \{B_{\text{JP}}, B_{\text{US}}\} \in \mathcal{P}^3(S).$$

Define $H : \mathcal{P}^2(S) \rightarrow \mathcal{P}^3(S)$ by $H(X) = \Pi$. Since $\Pi \subseteq \mathcal{P}^2(S)$, indeed $\Pi \in \mathcal{P}^3(S)$, so H is a valid $(2, 3)$ -superhyperfunction mapping a set of roles (level 2) to a portfolio of regional policies (level 3).

Remark 1.20 (Cardinalities). If $|S| = s$, then $|\mathcal{P}(S)| = 2^s$ and, inductively, $|\mathcal{P}^2(S)| = 2^{2^s}$, $|\mathcal{P}^3(S)| = 2^{2^{2^s}}$, etc. The growth reflects the combinatorial explosion of feasible alternatives captured by superhyperfunctions.

2| Result: Partition Function

Functions have been extensively developed in the field of Chemistry as well [31, 32, 33, 34, 35, 36]. In this paper, we define the *HyperFunction* and *SuperHyperFunction* for several such functions. We begin with the Partition Function.

2.1| Partition Function

A thermodynamic system is a well-defined collection of matter or radiation enclosed by boundaries, exchanging heat and work with surroundings (cf.[37, 38, 39]). The partition function maps the inverse temperature to the sum of Boltzmann factors across all microstates, revealing thermodynamic properties (cf.[40, 41, 42]).

Definition 2.1 (Microstate of a Thermodynamic System). (cf.[43, 44]) Let a thermodynamic system consist of N classical particles confined to a region $V \subseteq \mathbb{R}^3$. Denote by

$$\Gamma = \underbrace{V \times \mathbb{R}^3 \times \cdots \times V \times \mathbb{R}^3}_{N \text{ times}}$$

the $6N$ -dimensional *phase space*, whose coordinates are $(q_1, p_1, \dots, q_N, p_N)$, where $q_i \in V$ is the position and $p_i \in \mathbb{R}^3$ the momentum of the i th particle. A *microstate* of the system is any point

$$\omega = (q_1, p_1, \dots, q_N, p_N) \in \Gamma,$$

i.e. a complete specification of all particle positions and momenta.

Definition 2.2 (Partition function). (cf.[45, 46]) Let Ω be the finite set of microstates of a thermodynamic system, and let

$$E : \Omega \longrightarrow \mathbb{R}$$

assign to each state $s \in \Omega$ its energy $E(s)$. For inverse temperature $\beta > 0$, the *partition function* is the map

$$Z : \mathbb{R}_{>0} \longrightarrow \mathbb{R}_{>0}, \quad \beta \longmapsto Z(\beta) = \sum_{s \in \Omega} e^{-\beta E(s)}.$$

2.2| Partition HyperFunction

A Partition HyperFunction maps each microstate of a thermodynamic system to a set containing its Boltzmann factor, thereby extending the classical partition function into a hyperfunction framework.

Definition 2.3 (Partition HyperFunction). Let Ω be a finite set of microstates of a thermodynamic system, and let

$$E : \Omega \longrightarrow \mathbb{R}$$

assign to each state $s \in \Omega$ its energy $E(s)$. Fix an inverse temperature $\beta > 0$. The *Partition HyperFunction* at β is the mapping

$$Z_{\mathcal{H}}^{\beta} : \Omega \longrightarrow \mathcal{P}(\mathbb{R}_{>0}), \quad s \longmapsto \{e^{-\beta E(s)}\}.$$

Here $\mathcal{P}(\mathbb{R}_{>0})$ denotes the power set of the positive reals.

Example 2.4 (Two-level atom as a Partition HyperFunction). Let the microstate set be $\Omega = \{g, e\}$ (ground/excited), with energies

$$E(g) = 0, \quad E(e) = \Delta > 0.$$

Fix an inverse temperature $\beta > 0$. The Partition HyperFunction at β is

$$Z_{\mathcal{H}}^{\beta} : \Omega \longrightarrow \mathcal{P}(\mathbb{R}_{>0}), \quad s \longmapsto \{e^{-\beta E(s)}\}.$$

Concretely,

$$Z_{\mathcal{H}}^{\beta}(\mathbf{g}) = \{1\}, \quad Z_{\mathcal{H}}^{\beta}(\mathbf{e}) = \{e^{-\beta\Delta}\}.$$

Verification (with numbers): if $\Delta = 2$ and $\beta = 1$, then

$$Z_{\mathcal{H}}^1(\mathbf{g}) = \{1\}, \quad Z_{\mathcal{H}}^1(\mathbf{e}) = \{e^{-2}\} \approx \{0.1353\}.$$

Recovering the classical partition function:

$$Z(\beta) = \sum_{s \in \Omega} e^{-\beta E(s)} = \sum_{s \in \Omega} \left(\bigcup Z_{\mathcal{H}}^{\beta}(s) \right) = 1 + e^{-\beta\Delta}.$$

Thus $Z_{\mathcal{H}}^{\beta}$ encodes each Boltzmann factor as a singleton, whose union-and-sum yields the usual $Z(\beta)$.

Example 2.5 (Three-conformer molecule as a Partition HyperFunction). Let $\Omega = \{A_1, A_2, B\}$ represent two microstates of conformer A and one of conformer B , with

$$E(A_1) = E(A_2) = 0.5, \quad E(B) = 1.2.$$

For $\beta = 1$,

$$Z_{\mathcal{H}}^1(A_1) = \{e^{-0.5}\} \approx \{0.6065\}, \quad Z_{\mathcal{H}}^1(A_2) = \{e^{-0.5}\} \approx \{0.6065\}, \quad Z_{\mathcal{H}}^1(B) = \{e^{-1.2}\} \approx \{0.3010\}.$$

Hence

$$Z(1) = \sum_{s \in \Omega} e^{-E(s)} = \sum_{s \in \Omega} \left(\bigcup Z_{\mathcal{H}}^1(s) \right) \approx 0.6065 + 0.6065 + 0.3010 = 1.5140.$$

Each image $Z_{\mathcal{H}}^1(s) \subset \mathbb{R}_{>0}$, so $Z_{\mathcal{H}}^1 : \Omega \rightarrow \mathcal{P}(\mathbb{R}_{>0})$ is a valid HyperFunction.

Theorem 2.6. *The map $Z_{\mathcal{H}}^{\beta}$ is indeed a Hyperfunction, since its codomain is a powerset.*

Proof: By construction, $Z_{\mathcal{H}}^{\beta}$ has domain Ω (a classical set) and codomain $\mathcal{P}(\mathbb{R}_{>0})$, so it satisfies the definition of a Hyperfunction. Moreover, for each $s \in \Omega$, $Z_{\mathcal{H}}^{\beta}(s)$ is a (nonempty) subset of $\mathbb{R}_{>0}$, as required. $\square$

Theorem 2.7. *Let*

$$Z : \mathbb{R}_{>0} \longrightarrow \mathbb{R}_{>0}, \quad \beta \longmapsto \sum_{s \in \Omega} e^{-\beta E(s)}$$

be the classical partition function. Then Z can be recovered from the Partition HyperFunction by

$$Z(\beta) = \sum_{s \in \Omega} \left(\bigcup Z_{\mathcal{H}}^{\beta}(s) \right),$$

i.e. by summing the singleton subsets produced by $Z_{\mathcal{H}}^{\beta}$. Hence $Z_{\mathcal{H}}^{\beta}$ truly generalizes Z as a Hyperfunction.

Proof: For each $s \in \Omega$, by definition

$$\bigcup Z_{\mathcal{H}}^{\beta}(s) = \{e^{-\beta E(s)}\},$$

so

$$\sum_{s \in \Omega} \left(\bigcup Z_{\mathcal{H}}^{\beta}(s) \right) = \sum_{s \in \Omega} e^{-\beta E(s)} = Z(\beta).$$

This shows that the classical partition function Z arises from the Hyperfunction $Z_{\mathcal{H}}^{\beta}$ by summation over its image-sets. $\square$

2.3| Partition SuperHyperFunction

Partition SuperHyperFunction further generalizes this idea by mapping aggregated collections of microstates to nested powersets of Boltzmann factors, enabling multi-level representation and analysis of thermodynamic properties.

Definition 2.8 (Partition (m, n) -SuperHyperFunction). Let Ω be a finite set of microstates, and let

$$E : \Omega \longrightarrow \mathbb{R}$$

assign to each $s \in \Omega$ its energy $E(s)$. Fix $\beta > 0$. For any integers $m, n \geq 0$, define the map

$$Z_{SH}^{(m,n),\beta} : \mathcal{P}_m(\Omega) \longrightarrow \mathcal{P}_n(\mathbb{R}_{>0})$$

recursively as follows:

(i) If $m = 0$, then $\mathcal{P}_0(\Omega) = \Omega$, and for each $s \in \Omega$,

$$Z_{SH}^{(0,n),\beta}(s) = \underbrace{\{\{\dots\{e^{-\beta E(s)}\}\dots\}\}}_{n \text{ nested braces}} \in \mathcal{P}_n(\mathbb{R}_{>0}).$$

(ii) If $m > 0$, then $\mathcal{P}_m(\Omega) = \mathcal{P}(\mathcal{P}_{m-1}(\Omega))$, and for each $X \subseteq \mathcal{P}_{m-1}(\Omega)$,

$$Z_{SH}^{(m,n),\beta}(X) = \{Z_{SH}^{(m-1,n),\beta}(Y) \mid Y \in X\} \subseteq \mathcal{P}_n(\mathbb{R}_{>0}).$$

Example 2.9 ($(m, n) = (1, 2)$ Partition SuperHyperFunction: coarse-grained ensembles). Let $\Omega = \{s_1, s_2, s_3\}$ be microstates with energies

$$E(s_1) = 0, \quad E(s_2) = 1, \quad E(s_3) = 2.$$

Fix $\beta = 1$. By the recursive definition, for any $X \in \mathcal{P}^1(\Omega) = \mathcal{P}(\Omega)$,

$$Z_{SH}^{(1,2),1}(X) = \{Z_{SH}^{(0,2),1}(s) \mid s \in X\} \in \mathcal{P}^2(\mathbb{R}_{>0}),$$

where $Z_{SH}^{(0,2),1}(s) = \{\{e^{-E(s)}\}\} \in \mathcal{P}^2(\mathbb{R}_{>0})$ is a doubly nested singleton.

Take $X = \{s_2, s_3\}$. Then

$$\begin{aligned} Z_{SH}^{(0,2),1}(s_2) &= \{\{e^{-1}\}\} \approx \{0.3679\}, \\ Z_{SH}^{(0,2),1}(s_3) &= \{\{e^{-2}\}\} \approx \{0.1353\}, \end{aligned}$$

and hence

$$Z_{SH}^{(1,2),1}(\{s_2, s_3\}) = \left\{ \{\{e^{-1}\}\}, \{\{e^{-2}\}\} \right\} \in \mathcal{P}^2(\mathbb{R}_{>0}).$$

Membership check: each inner $\{e^{-E(s)}\} \subset \mathbb{R}_{>0}$, so $\{\{e^{-E(s)}\}\} \in \mathcal{P}^2(\mathbb{R}_{>0})$; collecting these for $s \in X$ yields an element of $\mathcal{P}(\mathcal{P}^2(\mathbb{R}_{>0})) = \mathcal{P}^3(\mathbb{R}_{>0})$ if one more outer aggregation is applied. Here, by definition, we aggregate exactly once over $s \in X$, giving an object in $\mathcal{P}^2(\mathbb{R}_{>0})$, as required.

Example 2.10 ($(m, n) = (2, 3)$ Partition SuperHyperFunction: portfolios of ensembles). Continue with the same Ω and $\beta = 1$. Let

$$Y_1 = \{s_1, s_2\}, \quad Y_2 = \{s_2, s_3\}, \quad X = \{Y_1, Y_2\} \in \mathcal{P}^2(\Omega).$$

By recursion,

$$Z_{SH}^{(2,3),1}(X) = \{ Z_{SH}^{(1,3),1}(Y) \mid Y \in X \} \in \mathcal{P}^3(\mathbb{R}_{>0}),$$

with

$$Z_{SH}^{(1,3),1}(Y) = \{ Z_{SH}^{(0,3),1}(s) \mid s \in Y \}, \quad Z_{SH}^{(0,3),1}(s) = \{ \{ e^{-E(s)} \} \}.$$

Therefore,

$$\begin{aligned} Z_{SH}^{(1,3),1}(Y_1) &= \left\{ \{ \{ e^0 \} \}, \{ \{ e^{-1} \} \} \right\} = \left\{ \{ \{ 1 \} \}, \{ \{ e^{-1} \} \} \right\}, \\ Z_{SH}^{(1,3),1}(Y_2) &= \left\{ \{ \{ e^{-1} \} \}, \{ \{ e^{-2} \} \} \right\}. \end{aligned}$$

Finally,

$$Z_{SH}^{(2,3),1}(X) = \left\{ Z_{SH}^{(1,3),1}(Y_1), Z_{SH}^{(1,3),1}(Y_2) \right\} \in \mathcal{P}^3(\mathbb{R}_{>0}),$$

which is a *set of (sets of) nested singletons of Boltzmann factors*, i.e. a portfolio of ensemble-level contributions consistent with the (2, 3) codomain.

Theorem 2.11. *When $(m, n) = (0, 0)$, the map*

$$Z_{SH}^{(0,0),\beta} : \Omega \rightarrow \mathbb{R}_{>0}, \quad s \mapsto e^{-\beta E(s)}$$

is exactly the classical Boltzmann-factor function. Moreover,

$$Z(\beta) = \sum_{s \in \Omega} Z_{SH}^{(0,0),\beta}(s) = \sum_{s \in \Omega} e^{-\beta E(s)},$$

so the usual partition function arises by summation over this (0, 0)-superhyperfunction.

Proof: Since $\mathcal{P}_0(\Omega) = \Omega$ and $\mathcal{P}_0(\mathbb{R}_{>0}) = \mathbb{R}_{>0}$, by definition $Z_{SH}^{(0,0),\beta}(s) = e^{-\beta E(s)}$. Summing these values over all $s \in \Omega$ reproduces $Z(\beta) = \sum_s e^{-\beta E(s)}$, the classical partition function. $\square$

Theorem 2.12. *When $(m, n) = (0, 1)$, the map*

$$Z_{SH}^{(0,1),\beta} : \Omega \rightarrow \mathcal{P}(\mathbb{R}_{>0}), \quad s \mapsto \{ e^{-\beta E(s)} \}$$

coincides with the Partition HyperFunction $Z_{\mathcal{H}}^\beta$.

Proof: Here $\mathcal{P}_0(\Omega) = \Omega$ and $\mathcal{P}_1(\mathbb{R}_{>0}) = \mathcal{P}(\mathbb{R}_{>0})$. By the $m = 0$ rule,

$$Z_{SH}^{(0,1),\beta}(s) = \{ e^{-\beta E(s)} \},$$

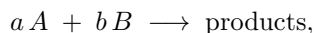
which is exactly the definition of the Partition HyperFunction $Z_{\mathcal{H}}^\beta : \Omega \rightarrow \mathcal{P}(\mathbb{R}_{>0})$, $s \mapsto \{ e^{-\beta E(s)} \}$. $\square$

3| Result: Reaction rate Function

3.1| Reaction rate Function

Chemical reactions are processes where substances, through making and breaking chemical bonds, transform into different substances, accompanied by energy changes (cf.[47, 16, 18, 48, 49]). The reaction rate function gives reaction velocity as rate constant multiplied by reactant concentrations raised to their stoichiometric powers (cf.[50, 51, 52, 53]).

Definition 3.1 (Reaction rate function). (cf.[54, 55, 56, 57]) Consider the elementary chemical reaction



where $a, b \in \mathbb{N}$ and the concentrations $[A], [B]$ lie in $\mathbb{R}_{\geq 0}$. The *reaction rate function* is

$$v : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \longrightarrow \mathbb{R}_{\geq 0}, \quad ([A], [B]) \longmapsto v([A], [B]) = k [A]^a [B]^b,$$

where $k > 0$ is the rate constant.

Example 3.2 (Bimolecular reaction, first order in each reactant). Consider $A + B \rightarrow \text{products}$ with $a = b = 1$, $k = 0.50 \text{ M}^{-1} \text{ s}^{-1}$, $[A] = 0.10 \text{ M}$, $[B] = 0.25 \text{ M}$. Then

$$v = k[A][B] = 0.50 \times 0.10 \times 0.25 = 0.0125 \text{ M s}^{-1}.$$

Calculation detail: $0.10 \times 0.25 = 0.025$, and $0.50 \times 0.025 = 0.0125$.

Example 3.3 (Termolecular rate law: $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$). A common kinetic model uses $v = k[\text{NO}]^2[\text{O}_2]$. Take $k = 4.0 \text{ M}^{-2} \text{ s}^{-1}$, $[\text{NO}] = 0.020 \text{ M}$, $[\text{O}_2] = 0.010 \text{ M}$. Then

$$v = 4.0 \times (0.020)^2 \times 0.010 = 4.0 \times 0.0004 \times 0.010 = 4.0 \times 0.000004 = 1.6 \times 10^{-5} \text{ M s}^{-1}.$$

3.2| Reaction rate HyperFunction

A Reaction rate HyperFunction maps each pair of reactant concentrations to a set containing its calculated reaction rate value.

Definition 3.4 (Reaction rate HyperFunction). Consider the elementary chemical reaction



where $a, b \in \mathbb{N}$ and the concentrations $[A], [B]$ lie in $\mathbb{R}_{\geq 0}$. Let $k > 0$ be the rate constant. The *reaction rate HyperFunction* is the map

$$v_{\mathcal{H}} : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \longrightarrow \mathcal{P}(\mathbb{R}_{\geq 0}), \quad ([A], [B]) \longmapsto \{k [A]^a [B]^b\}.$$

Example 3.5 (Catalyst on/off uncertainty produces a set of possible rates). Suppose $A + B \rightarrow \text{P}$ with $a = b = 1$. If a catalyst valve might be *off* or *on*, the rate constant is

$$k_{\text{off}} = 0.10 \text{ M}^{-1} \text{ s}^{-1}, \quad k_{\text{on}} = 0.60 \text{ M}^{-1} \text{ s}^{-1}.$$

For $[A] = 0.20 \text{ M}$, $[B] = 0.30 \text{ M}$,

$$\begin{aligned} v_{\text{off}} &= k_{\text{off}}[A][B] = 0.10 \times 0.20 \times 0.30 = 0.006 \text{ M s}^{-1}, \\ v_{\text{on}} &= k_{\text{on}}[A][B] = 0.60 \times 0.20 \times 0.30 = 0.036 \text{ M s}^{-1}. \end{aligned}$$

Thus

$$v_{\mathcal{H}}([A], [B]) = \{v_{\text{off}}, v_{\text{on}}\} = \{0.006, 0.036\} \subset \mathbb{R}_{\geq 0},$$

which is a valid HyperFunction output (a subset of $\mathbb{R}_{\geq 0}$).

Theorem 3.6. *The map $v_{\mathcal{H}}$ is a Hyperfunction.*

Proof: By definition a Hyperfunction is any map whose domain is a classical set and whose codomain is a powerset. Here the domain is $\mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0}$ and the codomain is $\mathcal{P}(\mathbb{R}_{\geq 0})$. Since for each $([A], [B])$, $v_{\mathcal{H}}([A], [B])$ is a (singleton) subset of $\mathbb{R}_{\geq 0}$, $v_{\mathcal{H}}$ satisfies the definition of a Hyperfunction. $\square$

Theorem 3.7. *Let*

$$v : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \longrightarrow \mathbb{R}_{\geq 0}, \quad ([A], [B]) \mapsto k [A]^a [B]^b$$

be the classical reaction rate function. Then for all $[A], [B]$,

$$v([A], [B]) = \bigcup v_{\mathcal{H}}([A], [B]),$$

so v is recovered by taking the union over the image-sets of the Hyperfunction $v_{\mathcal{H}}$.

Proof: By definition of $v_{\mathcal{H}}$,

$$v_{\mathcal{H}}([A], [B]) = \{k [A]^a [B]^b\},$$

hence

$$\bigcup v_{\mathcal{H}}([A], [B]) = k [A]^a [B]^b = v([A], [B]).$$

This shows that the classical reaction rate function v is obtained from $v_{\mathcal{H}}$ by union, demonstrating that $v_{\mathcal{H}}$ indeed generalizes v as a Hyperfunction. $\square$

3.3| Reaction rate SuperHyperFunction

A Reaction rate SuperHyperFunction generalizes this by mapping aggregated concentration sets to nested powersets of possible reaction rate values.

Definition 3.8 (Reaction rate (m, n) -SuperHyperFunction). Let

$$D = \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0}, \quad v([A], [B]) = k [A]^a [B]^b,$$

with $a, b \in \mathbb{N}$ and $k > 0$. For integers $m, n \geq 0$, define

$$v_{SH}^{(m, n)} : \mathcal{P}_m(D) \longrightarrow \mathcal{P}_n(\mathbb{R}_{\geq 0})$$

recursively by:

(i) If $m = 0$, then $\mathcal{P}_0(D) = D$. For $x = ([A], [B]) \in D$,

$$v_{SH}^{(0, n)}(x) = \underbrace{\{\{\dots \{k [A]^a [B]^b\} \dots\}\}}_{n \text{ nested braces}} \in \mathcal{P}_n(\mathbb{R}_{\geq 0}).$$

(ii) If $m > 0$, then $\mathcal{P}_m(D) = \mathcal{P}(\mathcal{P}_{m-1}(D))$. For any $X \subseteq \mathcal{P}_{m-1}(D)$,

$$v_{SH}^{(m, n)}(X) = \{v_{SH}^{(m-1, n)}(Y) \mid Y \in X\} \subseteq \mathcal{P}_n(\mathbb{R}_{\geq 0}).$$

Example 3.9 $((m, n) = (1, 2))$: a set of operating points $\rightarrow$ a set of nested singletons). Let $a = b = 1$ and $k = 0.50 \text{ M}^{-1} \text{ s}^{-1}$. Consider two operating points

$$x_1 = (0.10, 0.20), \quad x_2 = (0.30, 0.10) \in D,$$

representing $([A], [B])$ in M. Compute

$$\begin{aligned} v(x_1) &= 0.50 \times 0.10 \times 0.20 = 0.010, \\ v(x_2) &= 0.50 \times 0.30 \times 0.10 = 0.015. \end{aligned}$$

By the $(m, n) = (1, 2)$ rule,

$$v_{SH}^{(1,2)}(\{x_1, x_2\}) = \left\{ \underbrace{\{0.010\}}_{\in \mathcal{P}(\mathbb{R}_{\geq 0})}, \underbrace{\{0.015\}}_{\in \mathcal{P}(\mathbb{R}_{\geq 0})} \right\} \in \mathcal{P}^2(\mathbb{R}_{\geq 0}).$$

Membership check: each $\{v(x_i)\} \subset \mathbb{R}_{\geq 0}$ lies in $\mathcal{P}(\mathbb{R}_{\geq 0})$; collecting them yields an element of $\mathcal{P}(\mathcal{P}(\mathbb{R}_{\geq 0})) = \mathcal{P}^2(\mathbb{R}_{\geq 0})$.

Example 3.10 ($(m, n) = (2, 3)$: batches of operating sets $\rightarrow$ portfolios of nested outputs). Let $a = 2$, $b = 1$, $k = 4.0 \text{ M}^{-2} \text{ s}^{-1}$. Define three points

$$x_1 = (0.020, 0.010), \quad x_2 = (0.015, 0.020), \quad x_3 = (0.025, 0.008).$$

Compute the scalar rates

$$\begin{aligned} v(x_1) &= 4.0 \times (0.020)^2 \times 0.010 = 4.0 \times 0.0004 \times 0.010 = 1.6 \times 10^{-5}, \\ v(x_2) &= 4.0 \times (0.015)^2 \times 0.020 = 4.0 \times 0.000225 \times 0.020 = 1.8 \times 10^{-5}, \\ v(x_3) &= 4.0 \times (0.025)^2 \times 0.008 = 4.0 \times 0.000625 \times 0.008 = 2.0 \times 10^{-5}. \end{aligned}$$

Form two *batches* (level $m = 2$ inputs)

$$Y_1 = \{x_1, x_2\}, \quad Y_2 = \{x_3\}, \quad X = \{Y_1, Y_2\} \in \mathcal{P}^2(D).$$

By recursion,

$$\begin{aligned} v_{SH}^{(0,3)}(x_i) &= \{\{\{v(x_i)\}\}\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}), \\ v_{SH}^{(1,3)}(Y_j) &= \{v_{SH}^{(0,3)}(x) \mid x \in Y_j\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}), \\ v_{SH}^{(2,3)}(X) &= \{v_{SH}^{(1,3)}(Y) \mid Y \in X\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}). \end{aligned}$$

Hence explicitly,

$$\begin{aligned} v_{SH}^{(1,3)}(Y_1) &= \left\{ \{\{\{1.6 \times 10^{-5}\}\}\}, \{\{\{1.8 \times 10^{-5}\}\}\} \right\}, \\ v_{SH}^{(1,3)}(Y_2) &= \left\{ \{\{\{2.0 \times 10^{-5}\}\}\} \right\}, \end{aligned}$$

and

$$v_{SH}^{(2,3)}(X) = \left\{ v_{SH}^{(1,3)}(Y_1), v_{SH}^{(1,3)}(Y_2) \right\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}),$$

which is a portfolio (set) of batch-level nested outputs, consistent with the $(2, 3)$ codomain.

Theorem 3.11. When $(m, n) = (0, 0)$, the map

$$v_{SH}^{(0,0)} : D \rightarrow \mathbb{R}_{\geq 0}, \quad ([A], [B]) \mapsto k [A]^a [B]^b$$

coincides with the classical reaction rate function v .

Proof: Since $\mathcal{P}_0(D) = D$ and $\mathcal{P}_0(\mathbb{R}_{\geq 0}) = \mathbb{R}_{\geq 0}$, by definition

$$v_{SH}^{(0,0)}([A], [B]) = k [A]^a [B]^b = v([A], [B]),$$

so $v_{SH}^{(0,0)} \equiv v$. □

Theorem 3.12. *When $(m, n) = (0, 1)$, the map*

$$v_{SH}^{(0,1)} : D \rightarrow \mathcal{P}(\mathbb{R}_{\geq 0}), \quad ([A], [B]) \mapsto \{k [A]^a [B]^b\}$$

coincides with the Reaction rate HyperFunction $v_{\mathcal{H}} : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \rightarrow \mathcal{P}(\mathbb{R}_{\geq 0})$.

Proof: Here $\mathcal{P}_1(\mathbb{R}_{\geq 0}) = \mathcal{P}(\mathbb{R}_{\geq 0})$. By the $m = 0$, $n = 1$ rule,

$$v_{SH}^{(0,1)}([A], [B]) = \{k [A]^a [B]^b\} = v_{\mathcal{H}}([A], [B]),$$

so $v_{SH}^{(0,1)} \equiv v_{\mathcal{H}}$. □

4| Result: Dose–response Function

4.1| Dose–response Function

Drug dose is the specific quantity of medication administered at one time to achieve desired therapeutic effect safely and effectively (cf.[58, 59]). The Hill dose–response function transforms drug dose into continuous biological effect bounded between minimal and maximal response levels (cf.[60, 61, 62]).

Definition 4.1 (Dose–response function). (cf.[63, 64, 65]) Let $D \in \mathbb{R}_{\geq 0}$ denote the dose of a drug or toxin. Fix parameters $E_{\min}, E_{\max} \geq 0$, the Hill coefficient $h > 0$, and the half-maximal concentration $EC_{50} > 0$. The *Hill dose–response function* is

$$f : \mathbb{R}_{\geq 0} \longrightarrow [E_{\min}, E_{\max}], \quad D \longmapsto f(D) = E_{\min} + (E_{\max} - E_{\min}) \frac{D^h}{EC_{50}^h + D^h}.$$

Example 4.2 (Analgesic dose–response (Hill model)). Fix parameters $E_{\min} = 0$, $E_{\max} = 100$ (percent effect), Hill coefficient $h = 2$, and $EC_{50} = 50$ mg. The Hill function is

$$f(D) = 100 \cdot \frac{D^2}{50^2 + D^2}.$$

Explicit evaluations:

$$\begin{aligned} f(25) &= 100 \cdot \frac{25^2}{50^2 + 25^2} = 100 \cdot \frac{625}{2500 + 625} = 100 \cdot \frac{625}{3125} = 100 \cdot 0.2 = 20, \\ f(50) &= 100 \cdot \frac{50^2}{50^2 + 50^2} = 100 \cdot \frac{2500}{5000} = 50, \\ f(100) &= 100 \cdot \frac{100^2}{50^2 + 100^2} = 100 \cdot \frac{10000}{2500 + 10000} = 100 \cdot \frac{10000}{12500} = 100 \cdot 0.8 = 80. \end{aligned}$$

Interpretation: 25, 50, 100 mg yield approximately 20%, 50%, and 80% of maximal analgesic effect.

4.2 | Dose-response HyperFunction

Dose-response HyperFunction maps each drug dose to a set of possible effect values, capturing parameter uncertainty, patient variability, and regimes.

Definition 4.3 (Dose-response HyperFunction). Let

$$f : \mathbb{R}_{\geq 0} \longrightarrow [E_{\min}, E_{\max}], \quad f(D) = E_{\min} + (E_{\max} - E_{\min}) \frac{D^h}{\text{EC}_{50}^h + D^h},$$

be the Hill dose-response function with parameters $E_{\min}, E_{\max} \geq 0$, $h > 0$, and $\text{EC}_{50} > 0$. The *Dose-response HyperFunction* is

$$f_{\mathcal{H}} : \mathbb{R}_{\geq 0} \longrightarrow \mathcal{P}([E_{\min}, E_{\max}]), \quad D \longmapsto \{f(D)\}.$$

Example 4.4 (Dose-response HyperFunction: interpatient variability (pharmacogenomics)). Keep $E_{\min} = 0$, $E_{\max} = 100$, $h = 2$. Suppose population variability induces two plausible half-maximal doses $\text{EC}_{50} \in \{40, 70\}$ mg (e.g., ultrarapid vs. poor metabolizers). Define the HyperFunction

$$f_{\mathcal{H}} : \mathbb{R}_{\geq 0} \longrightarrow \mathcal{P}([0, 100]), \quad D \longmapsto \{f_{40}(D), f_{70}(D)\},$$

where $f_x(D) = 100 \cdot \frac{D^2}{x^2 + D^2}$. For a fixed prescription $D = 50$ mg,

$$\begin{aligned} f_{40}(50) &= 100 \cdot \frac{50^2}{40^2 + 50^2} = 100 \cdot \frac{2500}{1600 + 2500} = 100 \cdot \frac{2500}{4100} \approx 60.98, \\ f_{70}(50) &= 100 \cdot \frac{50^2}{70^2 + 50^2} = 100 \cdot \frac{2500}{4900 + 2500} = 100 \cdot \frac{2500}{7400} \approx 33.78. \end{aligned}$$

Hence $f_{\mathcal{H}}(50) = \{60.98, 33.78\} \subset [0, 100]$, capturing heterogeneous patient responses to the same dose.

Theorem 4.5. *The map $f_{\mathcal{H}}$ is a Hyperfunction.*

Proof: By definition, a Hyperfunction is any map whose domain is an ordinary set and whose codomain is a powerset. Here the domain is $\mathbb{R}_{\geq 0}$ and the codomain is $\mathcal{P}([E_{\min}, E_{\max}])$. For each $D \geq 0$, $f_{\mathcal{H}}(D) = \{f(D)\}$ is a singleton subset of $[E_{\min}, E_{\max}]$. Thus $f_{\mathcal{H}}$ satisfies the requirements of a Hyperfunction. $\square$

Theorem 4.6. *The classical dose-response function f is recovered by union over the HyperFunction $f_{\mathcal{H}}$:*

$$\forall D \geq 0, \quad f(D) = \bigcup f_{\mathcal{H}}(D).$$

Hence $f_{\mathcal{H}}$ generalizes f .

Proof: By definition of $f_{\mathcal{H}}$,

$$f_{\mathcal{H}}(D) = \{f(D)\},$$

so

$$\bigcup f_{\mathcal{H}}(D) = f(D).$$

Therefore the classical function f arises from the HyperFunction $f_{\mathcal{H}}$ by taking the union of its image-sets. $\square$

4.3| Dose–response SuperHyperFunction

Dose–response SuperHyperFunction maps aggregated dose sets to nested powersets of effects, enabling multi-level analysis across titration menus, clinics, and cohorts.

Definition 4.7 (Dose–response (m, n) -SuperHyperFunction). Let

$$D = \mathbb{R}_{\geq 0}, \quad f(D) = E_{\min} + (E_{\max} - E_{\min}) \frac{D^h}{\text{EC}_{50}^h + D^h},$$

with parameters $E_{\min}, E_{\max} \geq 0$, Hill coefficient $h > 0$, and half-maximal concentration $\text{EC}_{50} > 0$. For integers $m, n \geq 0$, define the (m, n) -SuperHyperFunction

$$f_{SH}^{(m,n)} : \mathcal{P}_m(D) \longrightarrow \mathcal{P}_n([E_{\min}, E_{\max}])$$

recursively by:

(i) If $m = 0$, then $\mathcal{P}_0(D) = D$, and for each $D \in \mathbb{R}_{\geq 0}$,

$$f_{SH}^{(0,n)}(D) = \underbrace{\{\{\cdots \{f(D)\} \cdots\}\}}_{n \text{ nested braces}} \in \mathcal{P}_n([E_{\min}, E_{\max}]).$$

(ii) If $m > 0$, then $\mathcal{P}_m(D) = \mathcal{P}(\mathcal{P}_{m-1}(D))$, and for any $X \subseteq \mathcal{P}_{m-1}(D)$,

$$f_{SH}^{(m,n)}(X) = \{ f_{SH}^{(m-1,n)}(x) \mid x \in X \} \subseteq \mathcal{P}_n([E_{\min}, E_{\max}]).$$

Example 4.8 ($(m, n) = (1, 2)$ Dose–response SuperHyperFunction: titration menus $\rightarrow$ nested response sets). Let $D = \mathbb{R}_{\geq 0}$ (dose space) and retain the first example’s parameters $E_{\min} = 0$, $E_{\max} = 100$, $h = 2$, $\text{EC}_{50} = 50$ mg. A clinic offers two titration options $X = \{25, 100\} \subset D$. Define

$$f_{SH}^{(1,2)} : \mathcal{P}(D) \longrightarrow \mathcal{P}^2([0, 100]), \quad f_{SH}^{(1,2)}(X) = \{ \{f(25)\}, \{f(100)\} \}.$$

Using the calculated values $f(25) = 20$ and $f(100) = 80$,

$$f_{SH}^{(1,2)}(\{25, 100\}) = \{ \{20\}, \{80\} \} \in \mathcal{P}^2([0, 100]).$$

This encodes, at nesting level $n = 2$, the menu of dose options and their respective effects.

Example 4.9 ($(m, n) = (2, 3)$ Dose–response SuperHyperFunction: multi-center portfolios). Two hospitals use different titration sets: $X_1 = \{25, 50\}$, $X_2 = \{50, 100\} \subset D$. Form the portfolio $X = \{X_1, X_2\} \in \mathcal{P}^2(D)$. Define recursively

$$\begin{aligned} f_{SH}^{(0,3)}(d) &= \{ \{ \{ f(d) \} \} \} \in \mathcal{P}^3([0, 100]), \\ f_{SH}^{(1,3)}(Y) &= \{ f_{SH}^{(0,3)}(d) \mid d \in Y \}, \\ f_{SH}^{(2,3)}(X) &= \{ f_{SH}^{(1,3)}(Y) \mid Y \in X \}. \end{aligned}$$

Using $f(25) = 20$, $f(50) = 50$, $f(100) = 80$,

$$\begin{aligned} f_{SH}^{(1,3)}(X_1) &= \{ \{ \{20\} \}, \{ \{50\} \} \}, \\ f_{SH}^{(1,3)}(X_2) &= \{ \{ \{50\} \}, \{ \{80\} \} \}, \\ f_{SH}^{(2,3)}(X) &= \{ f_{SH}^{(1,3)}(X_1), f_{SH}^{(1,3)}(X_2) \} \in \mathcal{P}^3([0, 100]). \end{aligned}$$

This represents a portfolio (across centers) of dose menus and their nested effect sets.

Theorem 4.10. For $(m, n) = (0, 0)$, the superhyperfunction $f_{SH}^{(0,0)} : D \rightarrow \mathbb{R}_{\geq 0}$ satisfies

$$f_{SH}^{(0,0)}(D) = f(D),$$

and hence coincides with the classical dose-response function f .

Proof: Since $\mathcal{P}_0(D) = D$ and $\mathcal{P}_0([E_{\min}, E_{\max}]) = [E_{\min}, E_{\max}]$, by definition

$$f_{SH}^{(0,0)}(D) = f(D).$$

Therefore $f_{SH}^{(0,0)} \equiv f$. □

Theorem 4.11. For $(m, n) = (0, 1)$, the superhyperfunction $f_{SH}^{(0,1)} : D \rightarrow \mathcal{P}([E_{\min}, E_{\max}])$ satisfies

$$f_{SH}^{(0,1)}(D) = \{f(D)\},$$

and hence coincides with the dose-response HyperFunction $f_{\mathcal{H}}$.

Proof: Here $\mathcal{P}_1([E_{\min}, E_{\max}]) = \mathcal{P}([E_{\min}, E_{\max}])$, and by the $m = 0, n = 1$ case,

$$f_{SH}^{(0,1)}(D) = \{f(D)\} = f_{\mathcal{H}}(D).$$

Thus $f_{SH}^{(0,1)} \equiv f_{\mathcal{H}}$. □

5| Result: Fitness Function

5.1| Fitness Function

The fitness function assigns each genotype the expected number of viable offspring that genotype produces over its lifetime (cf.[66, 67, 68, 69]).

Definition 5.1 (Fitness function). (cf.[70, 71, 72]) Let G be the set of all genotypes in a population. Define the *fitness function*

$$w : G \rightarrow \mathbb{R}_{\geq 0}, \quad g \mapsto w(g) = \mathbb{E}[\text{number of offspring of an individual with genotype } g].$$

Example 5.2 (Classical fitness function from survival and fecundity). Let $G = \{g_A, g_B, g_C\}$ be three genotypes in a laboratory *Drosophila* population. Model the expected viable offspring count as

$$w(g) = s(g) \times F(g),$$

where $s(g) \in [0, 1]$ is the probability of surviving to reproduction and $F(g) \geq 0$ is the expected number of offspring conditional on survival. Take

$$\begin{aligned} s(g_A) = 0.75, \quad F(g_A) = 4.00 &\implies w(g_A) = 0.75 \times 4.00 = 3.00, \\ s(g_B) = 0.60, \quad F(g_B) = 5.50 &\implies w(g_B) = 0.60 \times 5.50 = 3.30, \\ s(g_C) = 0.90, \quad F(g_C) = 2.50 &\implies w(g_C) = 0.90 \times 2.50 = 2.25. \end{aligned}$$

Thus the classical fitness function $w : G \rightarrow \mathbb{R}_{\geq 0}$ yields $w(g_A) = 3.00$, $w(g_B) = 3.30$, $w(g_C) = 2.25$.

5.2| Fitness HyperFunction

Fitness HyperFunction maps each genotype to a set of possible fitness values under varying environments, capturing uncertainty, heterogeneity, and regime-dependent reproductive success.

Definition 5.3 (Fitness HyperFunction). Let G be the finite set of all genotypes in a population, and let

$$w : G \longrightarrow \mathbb{R}_{\geq 0}, \quad g \longmapsto w(g) = \mathbb{E}[\text{number of offspring of an individual with genotype } g].$$

The *Fitness HyperFunction* is the map

$$w_{\mathcal{H}} : G \longrightarrow \mathcal{P}(\mathbb{R}_{\geq 0}), \quad g \longmapsto \{w(g)\}.$$

Example 5.4 (Fitness HyperFunction captures environmental regimes). Suppose fitness depends on two field environments: nutrient-rich (R) and nutrient-poor (P). For each genotype g , define two regime-specific expectations

$$w_{\text{R}}(g) = s_{\text{R}}(g) F_{\text{R}}(g), \quad w_{\text{P}}(g) = s_{\text{P}}(g) F_{\text{P}}(g),$$

and set the *Fitness HyperFunction*

$$w_{\mathcal{H}}(g) = \{w_{\text{R}}(g), w_{\text{P}}(g)\} \in \mathcal{P}(\mathbb{R}_{\geq 0}).$$

Take concrete values:

$$\begin{aligned} s_{\text{R}}(g_A) = 0.80, \quad F_{\text{R}}(g_A) = 4.00 &\Rightarrow w_{\text{R}}(g_A) = 3.20, & s_{\text{P}}(g_A) = 0.50, \quad F_{\text{P}}(g_A) = 3.00 &\Rightarrow w_{\text{P}}(g_A) = 1.50, \\ s_{\text{R}}(g_B) = 0.70, \quad F_{\text{R}}(g_B) = 5.00 &\Rightarrow w_{\text{R}}(g_B) = 3.50, & s_{\text{P}}(g_B) = 0.60, \quad F_{\text{P}}(g_B) = 3.50 &\Rightarrow w_{\text{P}}(g_B) = 2.10. \end{aligned}$$

Hence

$$w_{\mathcal{H}}(g_A) = \{3.20, 1.50\}, \quad w_{\mathcal{H}}(g_B) = \{3.50, 2.10\}.$$

Each hypervalue is a subset of $\mathbb{R}_{\geq 0}$, so $w_{\mathcal{H}} : G \rightarrow \mathcal{P}(\mathbb{R}_{\geq 0})$ is a valid HyperFunction.

Theorem 5.5. *The map $w_{\mathcal{H}}$ is a Hyperfunction.*

Proof: By definition, a Hyperfunction is any mapping whose domain is a classical set and whose codomain is a powerset. Here the domain is G and the codomain is $\mathcal{P}(\mathbb{R}_{\geq 0})$. For each $g \in G$, $w_{\mathcal{H}}(g) = \{w(g)\}$ is a singleton subset of $\mathbb{R}_{\geq 0}$. Therefore $w_{\mathcal{H}}$ satisfies the definition of a Hyperfunction. $\square$

Theorem 5.6. *The classical fitness function w is recovered by taking the union over the image-sets of $w_{\mathcal{H}}$:*

$$\forall g \in G, \quad w(g) = \bigcup w_{\mathcal{H}}(g).$$

Hence $w_{\mathcal{H}}$ generalizes w .

Proof: For any $g \in G$,

$$w_{\mathcal{H}}(g) = \{w(g)\},$$

so

$$\bigcup w_{\mathcal{H}}(g) = w(g).$$

This shows that the classical fitness function w arises from the Hyperfunction $w_{\mathcal{H}}$ by union, confirming that $w_{\mathcal{H}}$ indeed generalizes w . $\square$

5.3| Fitness SuperHyperFunction

Fitness SuperHyperFunction maps aggregated genotype sets to nested powersets of fitness values, enabling multilevel analysis across diverse cohorts, subpopulations, breeding programs, regimes.

Definition 5.7 (Fitness (m, n) -SuperHyperFunction). Let G be a finite set of genotypes, and let

$$w : G \longrightarrow \mathbb{R}_{\geq 0}, \quad g \longmapsto w(g) = \mathbb{E}[\text{number of offspring of an individual with genotype } g].$$

For integers $m, n \geq 0$, define the (m, n) -SuperHyperFunction

$$w_{SH}^{(m,n)} : \mathbb{P}_m(G) \longrightarrow \mathbb{P}_n(\mathbb{R}_{\geq 0})$$

recursively by:

(i) If $m = 0$, then $\mathbb{P}_0(G) = G$, and for each $g \in G$,

$$w_{SH}^{(0,n)}(g) = \underbrace{\{\{\cdots \{w(g)\} \cdots\}\}}_{n \text{ nested braces}} \in \mathbb{P}_n(\mathbb{R}_{\geq 0}).$$

(ii) If $m > 0$, then $\mathbb{P}_m(G) = \mathbb{P}(\mathbb{P}_{m-1}(G))$, and for any $X \subseteq \mathbb{P}_{m-1}(G)$,

$$w_{SH}^{(m,n)}(X) = \{w_{SH}^{(m-1,n)}(Y) \mid Y \in X\} \subseteq \mathbb{P}_n(\mathbb{R}_{\geq 0}).$$

Example 5.8 $((m, n) = (1, 2))$ Fitness SuperHyperFunction: cohort of genotypes $\rightarrow$ nested fitness sets). Let $G = \{g_A, g_B, g_C\}$ and use the classical expectations from the first example:

$$w(g_A) = 3.00, \quad w(g_B) = 3.30, \quad w(g_C) = 2.25.$$

An input at level $m = 1$ is a *set of genotypes* $X \in \mathcal{P}(G)$; the $(1, 2)$ -SuperHyperFunction returns a level- $n = 2$ object:

$$w_{SH}^{(1,2)}(X) = \{\{w(g)\} \mid g \in X\} \in \mathcal{P}^2(\mathbb{R}_{\geq 0}).$$

For the cohort $X = \{g_A, g_B, g_C\}$,

$$w_{SH}^{(1,2)}(\{g_A, g_B, g_C\}) = \{\{3.00\}, \{3.30\}, \{2.25\}\} \in \mathcal{P}^2(\mathbb{R}_{\geq 0}).$$

Membership check: each $\{w(g)\} \subset \mathbb{R}_{\geq 0}$ lies in $\mathcal{P}(\mathbb{R}_{\geq 0})$; collecting them yields an element of $\mathcal{P}(\mathcal{P}(\mathbb{R}_{\geq 0})) = \mathcal{P}^2(\mathbb{R}_{\geq 0})$.

Example 5.9 $((m, n) = (2, 3))$ Fitness SuperHyperFunction: subpopulations and program portfolios). Consider two subpopulations using different genotype sets:

$$Y_1 = \{g_A, g_B\}, \quad Y_2 = \{g_B, g_C\} \in \mathcal{P}(G),$$

and a *portfolio* of breeding programs $X = \{Y_1, Y_2\} \in \mathcal{P}^2(G)$ (level $m = 2$ input). Define recursively

$$\begin{aligned} w_{SH}^{(0,3)}(g) &= \{\{\{w(g)\}\}\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}), \\ w_{SH}^{(1,3)}(Y) &= \{w_{SH}^{(0,3)}(g) \mid g \in Y\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}), \\ w_{SH}^{(2,3)}(X) &= \{w_{SH}^{(1,3)}(Y) \mid Y \in X\} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}). \end{aligned}$$

Using $w(g_A) = 3.00$, $w(g_B) = 3.30$, $w(g_C) = 2.25$, we get

$$\begin{aligned}
w_{\mathcal{SH}}^{(1,3)}(Y_1) &= \{ \{ \{3.00\} \}, \{ \{3.30\} \} \}, \\
w_{\mathcal{SH}}^{(1,3)}(Y_2) &= \{ \{ \{3.30\} \}, \{ \{2.25\} \} \}, \\
w_{\mathcal{SH}}^{(2,3)}(X) &= \{ w_{\mathcal{SH}}^{(1,3)}(Y_1), w_{\mathcal{SH}}^{(1,3)}(Y_2) \} \in \mathcal{P}^3(\mathbb{R}_{\geq 0}),
\end{aligned}$$

which is a set of (sets of) nested singletons of fitness values, aligned with the $(2, 3)$ codomain.

Theorem 5.10. *When $(m, n) = (0, 0)$, the map*

$$w_{\mathcal{SH}}^{(0,0)} : G \rightarrow \mathbb{R}_{\geq 0}, \quad g \mapsto w(g)$$

coincides with the classical fitness function w .

Proof: Since $\mathbb{P}_0(G) = G$ and $\mathbb{P}_0(\mathbb{R}_{\geq 0}) = \mathbb{R}_{\geq 0}$, by definition

$$w_{\mathcal{SH}}^{(0,0)}(g) = w(g)$$

for all $g \in G$. Hence $w_{\mathcal{SH}}^{(0,0)} \equiv w$. □

Theorem 5.11. *When $(m, n) = (0, 1)$, the map*

$$w_{\mathcal{SH}}^{(0,1)} : G \rightarrow \mathbb{P}(\mathbb{R}_{\geq 0}), \quad g \mapsto \{w(g)\}$$

coincides with the Fitness HyperFunction $w_{\mathcal{H}}$.

Proof: Here $\mathbb{P}_1(\mathbb{R}_{\geq 0}) = \mathbb{P}(\mathbb{R}_{\geq 0})$. By the $m = 0, n = 1$ case,

$$w_{\mathcal{SH}}^{(0,1)}(g) = \{w(g)\} = w_{\mathcal{H}}(g),$$

so $w_{\mathcal{SH}}^{(0,1)} \equiv w_{\mathcal{H}}$. □

6| Conclusion

To address this gap, the present paper introduced precise definitions of HyperFunctions and SuperHyperFunctions tailored to chemical systems and examined their fundamental properties. For future work, we plan to investigate further extensions of these concepts using Fuzzy Sets[73, 74, 75], Intuitionistic Fuzzy Sets[76], Neutrosophic Sets (including QuadriPartitioned Neutrosophic Sets)[77, 78, 79, 80], Hesitant Fuzzy Sets[81, 82, 83], Meta Sets[84, 85, 86], Picture Fuzzy Sets[87, 88, 89], q-rung orthopair fuzzy sets[90, 91], Spherical Fuzzy sets[92, 93, 94], HyperFuzzy Sets[95, 96], and Plithogenic Sets[97, 98]. It is also expected that future research will advance in exploring the chemical applications of the function concepts presented in this paper, the chemical applications of fuzzy sets and their extensions, as well as studies employing computational experiments.

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Data Availability

This manuscript presents purely conceptual work without empirical data. Scholars interested in these ideas are invited to undertake experimental or case-study research to substantiate and extend the proposed frameworks.

Ethical Approval

This paper involves no human or animal subjects and thus did not require ethics committee review or approval.

Use of Generative AI and AI-Assisted Tools

We use generative AI and AI-assisted tools for tasks such as English grammar checking, and We do not employ them in any way that violates ethical standards.

Conflicts of Interest

The authors declare that there are no competing interests concerning the content or publication of this article.

Disclaimer

The theoretical models and propositions herein have not yet been subjected to practical validation. Readers should independently verify all citations and be aware that inadvertent inaccuracies may remain. The opinions expressed are those of the authors and do not necessarily represent the views of affiliated organizations.

References

- [1] Amiri, G. R., Mousarezaei, R., & Rahnama, S. (2025). Soft hyperstructures and their applications. *New mathematics and natural computation*, 21(02), 577-595. <https://doi.org/10.1142/S1793005725500267>
- [2] Oguz, G., & Davvaz B. (2021). Soft topological hyperstructure. *Journal of intelligent & fuzzy systems: Applications in engineering and technology*, 40(5), 8755-8764. <https://doi.org/10.3233/JIFS-200242>
- [3] Vougiouklis, T. (2020). Fundamental relations in hv-structures. The 'judging from the results' proof. *Journal of algebraic hyperstructures and logical algebras*, 1(1), 21-36. <https://doi.org/10.29252/hatef.jahla.1.1.2>
- [4] Al Tahan, M., & Davvaz, B. (2018). Weak chemical hyperstructures associated to electrochemical cells. *Iranian journal of mathematical chemistry*, 9(1), 65-75. <https://doi.org/10.22052/ijmc.2017.88790.1294>
- [5] Smarandache, F. (2024). Foundation of superhyperstructure & neutrosophic superhyperstructure (review paper). *Neutrosophic sets and systems*, 63, 367-381. <chrome-extension://efaidnbmnnnibpcajpcgclcfndmkaj/https://fs.unm.edu/NSS/SuperHyperStructure.pdf>
- [6] Das, A. K., Das, R., Das, S., Debnath, B. K., Granados, C., Shil, B., & Das, R. (2025). A comprehensive study of neutrosophic superhyper bci-semigroups and their algebraic significance. *Transactions on fuzzy sets and systems*, 4(2), 80-101. <https://doi.org/10.71602/tfss.2025.1198050>
- [7] Villegas, S. M. B., Fritas, W. M., Villegas, C. R. B., Rivera, M. Y. F. F., Rivera, R. E., Puma, L. D. B., & Fernández, D. M. M. (2025). Using plithogenic n-superhypergraphs to assess the degree of relationship between information skills and digital competencies. *Neutrosophic sets and systems*, 84, 513-524. <https://doi.org/10.5281/zenodo.15641273>
- [8] Ghods, M., Rostami, Z., & Smarandache, F. (2022). Introduction to neutrosophic restricted superhypergraphs and neutrosophic restricted superhypertrees and several of their properties. *Neutrosophic sets and systems*, 50(1), 480-487. <https://www.researchgate.net/publication/362188894>
- [9] Huang, M., & Li, F. (2025). Optimizing AI-driven digital resources in vocational english learning using plithogenic n-superhypergraph structures for adaptive content recommendation. *Neutrosophic sets and systems*, 88(1), 283-295. <https://B2n.ir/tr7255>

- [10] Hamidi, M., Smarandache, F., & Davneshvar, E. (2022). Spectrum of superhypergraphs via flows. *Journal of mathematics*, 2022(1). <https://doi.org/10.1155/2022/9158912>
- [11] Kargin, A., & Şahin, M. (2023). Superhyper groups and neutro-superhyper groups. In *neutrosophic superhyperalgebra and new types of topologies* (pp. 25-42). University of New Mexico. <https://B2n.ir/bk5781>
- [12] Jahanpanah, S., & Daneshpayeh, R. (2024). An outspread on valued logic superhyperalgebras. *Facta universitatis, series: Mathematics and informatics*, 39(3), 427-437. <https://doi.org/10.22190/FUMI230707029J>
- [13] Smarandache, F., Şahin, M., Bakbak, D., Uluçay, V., & Kargin, A. (2022). History of superhyperalgebra and neutrosophic superhyperalgebra (revisited again). In *Neutrosophic algebraic structures and their applications* (pp. 10-15). Infinite Study. <https://www.researchgate.net/publication/365789500>
- [14] Smarandache, F. (2022). Extension of hyperalgebra to superhyperalgebra and neutrosophic superhyperalgebra (revisited). *International conference on computers communications and control* (pp. 427-432). Springer international publishing. https://doi.org/10.1007/978-3-031-16684-6_36
- [15] Al-Tahan, M., & Davvaz, B. (2022). Chemical hyperstructures for elements with four oxidation states. *Iranian journal of mathematical chemistry*, 13(2), 85-97. <https://doi.org/10.22052/ijmc.2022.246174.1615>
- [16] Ostadhadi-Dehkordi, S., Abdizadeh, S., & Hamrazzadeh, F. (2024). A hyperstructural approach to chemical reactions as mathematical Models. *Afrika matematika*, 35(1), 15. <https://doi.org/10.1007/s13370-023-01152-7>
- [17] Davvaz, B., Dehghan Nezhad, A., & Benvidi, A. (2012). Chemical hyperalgebra: Dismutation reactions. *Match-communications in mathematical and computer chemistry*, 67(1), 55-63. <https://www.researchgate.net/publication/267150018>
- [18] Chun, K. M. (2014). Chemical hyperstructures of chemical reactions for iron and indium. *Journal of the chungcheong mathematical society*, 27(2), 319-319. <https://doi.org/10.14403/jcms.2014.27.2.319>
- [19] Agusfrianto, F. A., Andromeda, S., & Hariri, M. (2024). Hyperstructures in chemical hyperstructures of redox reactions with three and four oxidation states. *JTAM (Jurnal Teori dan Aplikasi Matematika)*, 8(1), 50-57. <https://doi.org/10.31764/jtam.v8i1.17011>
- [20] Smarandache, F. (2022). The superhyperfunction and the neutrosophic superhyperfunction (Revisited again) (Vol. 3). Infinite Study. <https://B2n.ir/ns6697>
- [21] Smarandache, F. (2023). Superhyperfunction, superhyperstructure, neutrosophic superhyperfunction and neutrosophic superhyperstructure: Current understanding and future directions. Infinite Study. <https://doi.org/10.61356/j.nswa.2023.115>
- [22] Huang, M., & Li, F. (2025). Modeling cross-cultural competence in vocational education internationalization using neutrosophic superhyperfunctions and big data driven cultural clusters. *Neutrosophic sets and systems*, 88(1), 262-373. <https://doi.org/10.5281/zenodo.15786743>
- [23] Xie, Y. (2025). A neutrosophic superhyper number framework for accurate statistical evaluation of financial performance in high-tech enterprises. *Neutrosophic sets and systems*, 88(1), 905-918. <https://B2n.ir/du6647>
- [24] Jdid, M., Smarandache, F., & Fujita, T. (2025). A linear mathematical model of the vocational training problem in a company using neutrosophic logic, hyperfunctions, and superhyperfunction. *Neutrosophic sets and systems*, 87, 1-11. <https://www.researchgate.net/publication/392238093>
- [25] Jech, T. (2003). *Set theory: The third millennium edition, revised and expanded*. Springer. <https://doi.org/10.1017/S1079898600003358>
- [26] Smarandache, F. (2024). Foundation of superhyperstructure & neutrosophic superhyperstructure. *Neutrosophic sets and systems*, 63, 367-381. <chrome-extension://efaidnbmnnnnibpcajpcgclefindmkaj/https://fs.unm.edu/NSS/SuperHyperStructure.pdf>
- [27] Rahmati, M., & Hamidi, M. (2023). Extension of g-algebras to superhyper g-algebras. *Neutrosophic sets and systems*, 55, 557-567. <https://doi.org/10.5281/zenodo.7879543>
- [28] Al-Odhari, A. (2025). Neutrosophic power-set and neutrosophic hyper-structure of neutrosophic set of three types. *Annals of pure and applied mathematics*, 31(2), 125-146. <http://dx.doi.org/10.22457/apam.v31n2a05964>
- [29] Al-Odhari, A. (2025). A brief comparative study on hyperstructure, super hyperstructure, and n-super superhyperstructure. *Neutrosophic knowledge*, 6, 39-49. <https://doi.org/10.5281/zenodo.15107294>
- [30] Fujita, T., Jdid, M., & Smarandache, F. (2025). Hyperfunctions and superhyperfunctions in linear programming: Foundations and applications. *international journal of neutrosophic science*, 26(4), 65-76. <https://doi.org/10.54216/IJNS.260408>
- [31] Rychlewski, J. (2013). *Explicitly correlated wave functions in chemistry and physics: Theory and applications* (Vol. 13). Springer Science & Business Media. <https://doi.org/10.1007/978-94-017-0313-0>
- [32] Hwang, J. T., Dougherty, E. P., Rabitz, S., & Rabitz, H. (1978). The green's function method of sensitivity analysis in chemical kinetics. *The journal of chemical physics*, 69(11), 5180-5191. <https://doi.org/10.1063/1.436465>
- [33] Csanak, G., Taylor, H. S., & Yaris, R. (1971). Green's function technique in atomic and molecular physics. In *Advances in atomic and molecular physics* (pp. 287-361). Academic Press. [https://doi.org/10.1016/S0065-2199\(08\)60363-2](https://doi.org/10.1016/S0065-2199(08)60363-2)
- [34] Pernot, P., & Savin, A. (2018). Probabilistic performance estimators for computational chemistry methods: The empirical cumulative distribution function of absolute errors. *The journal of chemical physics*, 148(24), 241707-241707. <https://doi.org/10.1063/1.5016248>

- [35] Crichton, R. R. (2012). *Biological inorganic chemistry: A new introduction to molecular structure and function*. Elsevier. <https://B2n.ir/hm4017>
- [36] Kolb, H. C., Finn, M. G., & Sharpless, K. B. (2001). Click chemistry: Diverse chemical function from a few good reactions. *Angewandte chemie international edition*, 40(11), 2004-2021. [https://doi.org/10.1002/1521-3773\(20010601\)40:11%3C2004::AID-ANIE2004%3E3.0.CO;2-5](https://doi.org/10.1002/1521-3773(20010601)40:11%3C2004::AID-ANIE2004%3E3.0.CO;2-5)
- [37] Haddad, W. M., Chellaboina, V., & Nersesov, S. G. (2009). *Thermodynamics: A dynamical systems approach*. Princeton University Press. <https://B2n.ir/pn7366>
- [38] Anderson, G. M. (2005). *Thermodynamics of natural systems*. Cambridge University Press. <https://B2n.ir/hm3462>
- [39] Hill, T. L. (1962). Thermodynamics of small systems. *The journal of chemical physics*, 36(12), 3182-3197. <https://doi.org/10.1063/1.1732447>
- [40] Vidler, M., & Tennyson, J. (2000). Accurate partition function and thermodynamic data for water. *The journal of chemical physics*, 113(21), 9766-9771. <https://doi.org/10.1063/1.1321769>
- [41] Hartmann, A. K. (2005). Calculation of partition functions by measuring component distributions. *Physical review letters*, 94(5), 050601. <https://doi.org/10.1103/PhysRevLett.94.050601>
- [42] Grosh, J., Jhon, M. S., Ree, T., & Eyring, H. (1967). On an improved partition function of significant structure theory. *Proceedings of the national academy of sciences*, 57(6), 1566-1572. <https://doi.org/10.1073/pnas.57.6.1566>
- [43] Ganesh, N. (2017). A thermodynamic treatment of intelligent systems. 2017 IEEE International conference on rebooting computing (ICRC) (pp. 1-4). IEEE. <https://doi.org/10.1109/ICRC.2017.8123676>
- [44] Enderle, J. S. (2020). Toward a thermodynamics of meaning. <https://doi.org/10.48550/arXiv.2009.11963>
- [45] Elstner, M., Cui, Q., & Gruden, M. (2024). State sum (partition function) for noninteracting systems. In *Introduction to statistical thermodynamics: A molecular perspective* (pp. 293-315). Springer International Publishing. https://doi.org/10.1007/978-3-031-54994-6_11
- [46] Palma, C. A., Björk, J., Klappenberger, F., Arras, E., Kühne, D., Stafström, S., & Barth, J. V. (2015). Visualization and thermodynamic encoding of single-molecule partition function projections. *Nature communications*, 6(1). <https://doi.org/10.1038/ncomms7210>
- [47] Agusfianto, F. A., Al Tahan, M., & Mahatma, Y. (2023). An introduction to neutrohyperstructures on some chemical reactions. In *NeutroGeometry, neutroalgebra, and superhyperalgebra in today's world* (pp. 81-96). IGI Global. <https://doi.org/10.4018/978-1-6684-4740-6.ch004>
- [48] Eyring, H. (1935). The activated complex in chemical reactions. *The Journal of chemical physics*, 3(2), 107-115. <https://doi.org/10.1063/1.1749604>
- [49] Tavakoli, M., Shmakov, A., Ceccarelli, F., & Baldi, P. (2022). Rxn hypergraph: A hypergraph attention model for chemical reaction representation. <https://doi.org/10.48550/arXiv.2201.01196>
- [50] Pollak, E., & Talkner, P. (2005). Reaction rate theory: What it was, where is it today, and where is it going?. *Chaos: An interdisciplinary journal of nonlinear science*, 15(2). <https://doi.org/10.1063/1.1858782>
- [51] Hänggi, P., Talkner, P., & Borkovec, M. (1990). Reaction-rate theory: Fifty years after Kramers. *Reviews of modern physics*, 62(2), 251-341. <https://doi.org/10.1103/RevModPhys.62.251>
- [52] Hammond, G. S. (1955). A correlation of reaction rates. *Journal of the American chemical society*, 77(2), 334-338. <https://doi.org/10.1021/ja01607a027>
- [53] Connors, K. A. (1990). *Chemical kinetics: The study of reaction rates in solution*. Wiley-VCH Verlag GmbH. https://books.google.com/books/about/Chemical_Kinetics.html?id=nHux3YED1HsC
- [54] Levenspiel, O. (1998). *Chemical reaction engineering*. John Wiley & Sons. <https://B2n.ir/hq7538>
- [55] Yu, P. Y., & Craciun, G. (2018). Mathematical analysis of chemical reaction systems. *Israel journal of chemistry*, 58(6-7), 733-741. <https://doi.org/10.1002/ijch.201800003>
- [56] Zhang, Y., Xu, A., Zhang, G., & Zhu, C. (2015). Study on the influence of chemical reaction rate on detonation characteristics. *Advances in condensed matter physics*, 4(3), 85-92. <http://dx.doi.org/10.12677/cmp.2015.43010>

- [57] Huang, C. H., & Li, B. Y. (2014). A non-linear inverse problem in estimating the reaction rate function for an annular-bed reactor. *International journal of chemical reactor engineering*, 12(1), 271-283. <https://doi.org/10.1515/ijcre-2013-0142>
- [58] Peper, A. (2009). Aspects of the relationship between drug dose and drug effect. *Dose-Response*, 7(2), 172-192. <https://doi.org/10.2203/dose-response.08-019.Peper>
- [59] Doogue, M. P., & Polasek, T. M. (2011). Drug dosing in renal disease. *The clinical biochemist reviews*, 32(2), 69-73. <https://pmc.ncbi.nlm.nih.gov/articles/PMC3100283/>
- [60] Schindler, M. (2022). Modeling synergistic effects by using general Hill-type response surfaces describing drug interactions. *Scientific reports*, 12(1), 10524. <https://doi.org/10.1038/s41598-022-13469-7>
- [61] Chow, C. C., Ong, K. M., Dougherty, E. J., & Simons Jr, S. S. (2011). Inferring mechanisms from dose-response curves. In *Methods in enzymology* (pp. 465-483). Academic Press. <https://doi.org/10.1016/B978-0-12-381270-4.00016-0>
- [62] Schindler, M. (2017). Theory of synergistic effects: Hill-type response surfaces as 'null-interaction' models for mixtures. *Theoretical biology and medical modelling*, 14(1), 15. <https://doi.org/10.1186/s12976-017-0060-y>
- [63] Guardabascio, B., & Ventura, M. (2014). Estimating the dose-response function through a generalized linear model approach. *The Stata Journal*, 14(1), 141-158. <https://doi.org/10.1177/1536867X1401400110>
- [64] Roman, H. A., Walsh, T. L., Coull, B. A., Dewailly, É., Guallar, E., Hattis, D., ... , & Rice, G. (2011). Evaluation of the cardiovascular effects of methylmercury exposures: current evidence supports development of a dose-response function for regulatory benefits analysis. *Environmental health perspectives*, 119(5), 607-614. <https://doi.org/10.1289/ehp.1003012>
- [65] Williams, M. S., Ebel, E. D., & Vose, D. (2011). Methodology for determining the appropriateness of a linear dose-response function. *Risk analysis: An international journal*, 31(3), 345-350. <https://doi.org/10.1111/j.1539-6924.2010.01518.x>
- [66] Srivastava, M., & Payne, J. L. (2022). On the incongruence of genotype-phenotype and fitness landscapes. *PLoS computational biology*, 18(9), e1010524. <https://doi.org/10.1371/journal.pcbi.1010524>
- [67] Wahl, L. M., & Campos, P. R. (2023). Evolutionary rescue on genotypic fitness landscapes. *Journal of the royal society interface*, 20(208), 20230424. <https://doi.org/10.1098/rsif.2023.0424>
- [68] Katsonis, P., & Lichtarge, O. (2014). A formal perturbation equation between genotype and phenotype determines the evolutionary action of protein-coding variations on fitness. *Genome research*, 24(12), 2050-2058. <https://doi.org/10.1101/gr.176214.114>
- [69] De Jong, G. (1994). The fitness of fitness concepts and the description of natural selection. *The quarterly review of biology*, 69(1), 3-29. <https://doi.org/10.1086/418431>
- [70] Almulla, H., & Gay, G. (2022). Learning how to search: generating effective test cases through adaptive fitness function selection. *Empirical software engineering*, 27(2), 38. <https://doi.org/10.1007/s10664-021-10048-8>
- [71] Wedge, D. C., & Kell, D. B. (2008). Rapid prediction of optimum population size in genetic programming using a novel genotype- fitness correlation. *Proceedings of the 10th annual conference on Genetic and evolutionary computation* (pp. 1315-1322). Association for computing machinery. <https://doi.org/10.1145/1389095.1389346>
- [72] Lande, R. (2007). Expected relative fitness and the adaptive topography of fluctuating selection. *Evolution*, 61(8), 1835-1846. <https://doi.org/10.1111/j.1558-5646.2007.00170.x>
- [73] Zadeh, L. A. (1965). Fuzzy sets. *Information and control*, 8(3), 338-353. [https://doi.org/10.1016/S0019-9958\(65\)90241-X](https://doi.org/10.1016/S0019-9958(65)90241-X)
- [74] Zimmermann, H. J. (2011). *Fuzzy set theory—and its applications*. Springer science & business media. <https://doi.org/10.1007/978-94-010-0646-0>
- [75] Rosenfeld, A. (1975). Fuzzy graphs. In *Fuzzy sets and their applications to cognitive and decision processes* (pp. 77-95). Academic press. <https://doi.org/10.1016/B978-0-12-775260-0.50008-6>
- [76] Akram, M., Davvaz, B., & Feng, F. (2013). Intuitionistic fuzzy soft K-algebras. *Mathematics in computer science*, 7(3), 353-365. <https://doi.org/10.1007/s11786-013-0158-5>
- [77] Wang, H., Smarandache, F., Zhang, Y., & Sunderraman, R. (2010). Single valued neutrosophic sets. *Infinite study*. <https://B2n.ir/sf7979>
- [78] Smarandache, F. (2016). Neutrosophic overset, neutrosophic underset, and neutrosophic offset. Similarly for neutrosophic over-/under-/off-logic, probability, and statistics. *Infinite Study*. <https://B2n.ir/jg5713>
- [79] Broumi, S., Talea, M., Bakali, A., & Smarandache, F. (2016). Single valued neutrosophic graphs. *Journal of New theory*, (10), 86-101. <https://dergipark.org.tr/en/pub/jnt/issue/34504/381241>

- [80] Balamurugan, M., Hakami, K. H., Ansari, M. A., Al-Masarwah, A., & Loganathan, K. (2024). Quadri-polar fuzzy fantastic ideals in bci-algebras: A tosis framework and application. *European journal of pure and applied mathematics*, 17(4), 3129-3155. <https://doi.org/10.29020/nybg.ejpam.v17i4.5429>
- [81] Torra, V., & Narukawa, Y. (2009). On hesitant fuzzy sets and decision. 2009 IEEE international conference on fuzzy systems (pp. 1378-1382). IEEE. <https://doi.org/10.1109/FUZZY.2009.5276884>
- [82] Xu, Z. (2014). *Hesitant fuzzy sets theory* (Vol. 314). Springer international publishing. <https://doi.org/10.1007/978-3-319-04711-9>
- [83] Torra, V. (2010). Hesitant fuzzy sets. *International journal of intelligent systems*, 25(6), 529-539. <https://doi.org/10.1002/int.20418>
- [84] Starosta, B., & Kosiński, W. (2009). Meta sets—another approach to fuzziness. In *Views on fuzzy sets and systems from different perspectives: Philosophy and Logic, criticisms and applications* (pp. 509-532). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-540-93802-6_25
- [85] Starosta, B. (2009). Fuzzy sets as metaset. *Proceeding of XI international PhD workshop (OWD 2009)* (pp. 11-15). Conference archives polish association for knowledge management. <https://B2n.ir/xd3798>
- [86] Iomiej Starosta, B. (2009). Application of meta sets to character recognition. *Foundations of intelligent systems* (pp. 602-611). Springer. <https://doi.org/10.1007/978-3-642-04125-9#page=616>
- [87] Khan, W. A., Arif, W., Nguyen, Q. H., Le, T. T., & Van Pham, H. (2024). Picture fuzzy directed hypergraphs with applications toward decision-making and managing hazardous chemicals. *IEEE Access*, 12, 87816-87827. <https://doi.org/10.1109/ACCESS.2024.3415120>
- [88] Das, S., Poulik, S., & Ghorai, G. (2024). Picture fuzzy ϕ -tolerance competition graphs with its application. *Journal of ambient intelligence and humanized computing*, 15(1), 547-559. <https://doi.org/10.1007/s12652-023-04704-8>
- [89] Cuong, B. C., & Kreinovich, V. (2013). Picture fuzzy sets—a new concept for computational intelligence problems. 2013 third world congress on information and communication technologies (WICT 2013) (pp. 1-6). IEEE. <https://doi.org/10.1109/WICT.2013.7113099>
- [90] Ali, J. (2023). Norm-based distance measure of q-rung orthopair fuzzy sets and its application in decision-making. *Computational and applied mathematics*, 42(4), 184. <https://doi.org/10.1007/s40314-023-02313-x>
- [91] Asif, M., Kattan, D. A., Pamučar, D., & Ali, G. (2021). q-rung orthopair fuzzy matroids with application to human trafficking. *Discrete dynamics in nature and society*, 2021(1), 8261118. <https://doi.org/10.1155/2021/8261118>
- [92] Akram, M., Saleem, D., & Al-Hawary, T. (2020). Spherical fuzzy graphs with application to decision-making. *Mathematical and computational applications*, 25(1). <https://doi.org/10.3390/mca25010008>
- [93] PA, F. P., John, S. J., & P, R. K. (2020). On spherical fuzzy soft expert sets. *American institute of physics conference proceedings* (pp. 030001). American institute of physics publishing limited liability company. <https://doi.org/10.1063/5.0017243>
- [94] Kutlu Gündoğdu, F., & Kahraman, C. (2019). Spherical fuzzy sets and spherical fuzzy TOPSIS method. *Journal of intelligent & fuzzy systems*, 36(1), 337-352. <https://doi.org/10.3233/JIFS-181401>
- [95] Jun, Y. B., Song, S. Z., & Kim, S. J. (2018). Length-fuzzy subalgebras in bck/bci-algebras. *Mathematics*, 6(1). <https://doi.org/10.3390/math6010011>
- [96] Tacha, N., Phayapsiang, P., & Iampan, A. (2022). Length and Mean Fuzzy UP-subalgebras of UP-algebras. *Caspian journal of mathematical sciences*, 11(1), 264-303. <https://doi.org/10.22080/cjms.2021.17121.1416>
- [97] Smarandache, F. (2018). Plithogenic set, an extension of crisp, fuzzy, intuitionistic fuzzy, and neutrosophic sets-revisited. *Infinite study*. <https://B2n.ir/uk4359>
- [98] Sultana, F., Gulistan, M., Ali, M., Yaqoob, N., Khan, M., Rashid, T., & Ahmed, T. (2023). A study of plithogenic graphs: Applications in spreading coronavirus disease (covid-19) globally. *Journal of ambient intelligence and humanized computing*, 14(10), 13139-13159. <https://doi.org/10.1007/s12652-022-03772-6>

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