A Category-Theoretic Approach to Agent-based Modeling and Simulation

Kenneth A. Lloyd, Jr.
Watt Systems Technologies Inc.
Albuquerque, NM USA
kenneth.lloyd@wattsys.com

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Abstract

Category Theory represents a robust mathematical formalism for the study of systems, including system elements, coupling, structure, behavior and morphism[1]. These properties are also fundamental in the study and practice of Agent-Based Modeling and Simulation (ABMS).

The purpose of this presentation is to provide a very elementary, introductory overview of the application of a category-theoretic approach to ABMS. This approach is applied to a real-world biomedical problem domain involving emergent properties of inter-cellular interaction in Systemic Inflammatory Response Syndrome.

The objective is to raise awareness of the value of this approach and to demonstrate the representation of the universal properties of this methodology.

Keywords: category theory, agent-based modeling and simulation

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1 Introduction

> "Category theory has come to occupy a central position in contemporary mathematics and theoretical computer science, and is also applied to mathematical physics. Roughly, it is a general mathematical theory of structures and of systems of structures." – Stanford Encyclopedia of Philosophy [9]

This paper attempts to provide a broad overview of the possible application of Category Theory to Agent-based Modeling and Simulation. The objective is to show the powerful, conceptual capability of this mathematical approach in abstracting identifiable, universal background categories from the interaction between patterned models (theories) and patterned data. The purpose of a categorical approach is in forming better understandings of these elements at many levels, along with their coupling, structure, behavior, and morphism within system contexts, particularly when the elements represent agents.

Nothing of great value in life is free. Indeed there is a hefty price to be paid in understanding the world in Category-Theoretic terms. Unfortunately, the only way to reach the concepts of a categorical paradigm - the cost - is to learn some of the language of Category Theory[2], and practice the use of that language repeatedly. Once learned, however, the rewards are profound.

1.1 Category Theory

> "Much of mathematics consists in calculating in various abstract theories, specifically interpreting one abstract theory into another, interpreting an abstract theory into a background to obtain a concrete category of structures, and transforming these structures in and among these categories." – F. William Lawvere [7, pg. 10]

Category Theory represents a universal mathematical formalism that may be used to describe the relations between the elements, their coupling, structure, behavior and morphism from various objects in one domain to related objects in a another co-domain. It is emergent from the primitive, set-theoretic concepts that it now subsumes. Category Theory provides a more complete foundation for many areas of scientific discourse - including mathematics, physics, topology and logic [3]. In any modeling and simulation activity, this conceptual and descriptive capability is fundamental, precisely because it allows us to relate models with some measurable, real-world phenomenon. This description may be categorized in two ways: A *syntactic* compatibility of the operations (names, function signatures, and interfaces), and a *semantic* compatibility of the behavior given the algorithmic logic inherent in syntax. The *composition*[3] of the syntactic objects with semantic interaction functions provides the domain focus of the system under investigation.

> "…these [compatibilities] are both important, although most work published as "type theory" has concentrated on the first aspect [syntax], whereas the latter aspect comes under the heading of "semantics" or "model checking"." - Anthony JH Simons [15, pg. 56]

Specifically, in the context that follows, the formalism resides in a universal, Bayesian *background* domain, a category we shall call U that probabilistically relates the domain of agent-based models with a domain of associated data. This spatio-temporally extended background category simultaneously represents different perspectives, ordered (or conditioned) by the logically structured knowledge content of information objects in time. Another way of characterizing the two domains is: Which domain do we believe contains the most knowledge or contains the most information [18], at a certain places in time? Furthermore, to what extent can we believe in that belief?

For example, if we have a model we believe to be true *a priori*, and we are trying to predict data given certain parameters upon that model, the first categorical perspective is modeled by the *forward* functor, F, shown in Eq. 1.1, that relates the domain of model objects (theories), $\mathcal{M}$ to the the domain of expected, or predicted data values, $\mathcal{D}$.

$$F : \mathcal{M} \longrightarrow \mathcal{D} \tag{1.1}$$

In Category Theory, this descriptive representation of the forward relationship, F is referred to as a *functor*, which may be defined as the *structure preserving*[4] category of functional mappings, f, $\exists f \in F$ that relate model theory objects to data objects. The term *context* is that domain in which those objects are conceptualized, which may represent categories at different levels of abstraction.

The question arises: How did we come to believe in the model?

If we have data, but the model is unknown or uncertain, the *inverse* problem relates the domain of observed data values, $\mathcal{D}$, to the domain of possible model theories, $\mathcal{M}$, that might explain that data. This relationship is represented by:

$$F' : \mathcal{D} \longrightarrow \mathcal{M} \tag{1.2}$$

Some readers will immediately recognize the above cycle of categorical perspectives from Inverse Theory. For those unfamiliar with the concepts of Inverse Theory, an accessible introduction may be found in Scales, Smith and Treitel [14], upon which the following example is based. We propose that categorical Inverse Theory is the means of *resolution analysis* for categories of both linear and non-linear inverse problems [10]. The concepts and methods of resolution analysis as compared with numerical analysis will be explored in more detail in Section 1.2.2.

We will make extensive use of the fact that categories may have categories as their constituent objects.

The method outlined is a Category-Theoretic application of Inverse Theory that follows Tarantola [17] which defines a scientific study of a physically embodied system, $\mathfrak{G}$. We extend categorically $G : \mathcal{G} \rightarrow \mathfrak{G}$, consisting of the following steps:

1. Define a parameter space (a form of data domain), χ, which we extend $X : \chi \rightarrow \mathbb{R}$ that will describe the system and its elements.
2. Forward modeling, F, which we extend functorally as $F : \mathcal{D} \rightarrow \mathcal{M}$.

3. Inverse modeling, F', which we extend functorally as $F' : \mathcal{M} \to \mathcal{D}$.

   To which we add,

4. Categorization $U : G \to \mathcal{C}$, with U being a Bayesian background category, and $\mathcal{C}$ being a probabilistic, conceptual domain.

The parameter space describes the system elements parameters, including the n-polynomial shape of functional elements, in the following case a uni-variant function, f:

$$y = f(x) = \sum_{i=0}^{n} w_i x^i \tag{1.3}$$

We now temporarily recast our knowledge from the categorical perspective into simple, functional, algebraic objects (non-categorical) terms, and as such define the forward problem as a system of equations[5]:

$$\mathbf{d} = m + \epsilon \tag{1.4}$$

where,
$\mathbf{d}$ represents data as a type-valued collection in the *range* of $\mathcal{D}$,
m represents a potential model, as a specific algorithm analogous to a functional program, and
ϵ represents error, being either a theoretical error (also known as a modeling or experimental error), or a random (noise) error within the data. Thus, ϵ is part of our functor, F, above.

We may elect to parameterize the functions to understand their range of $f \in F$ of m, explicitly with some parameter, x. The careful reader will recognize that the model object, m in the domain $\mathcal{M}$, is now, itself, a co-domain category of of all functions $f \in m$, and x is now a type-value in a parameter space (a categorical domain), χ.

$$m = f(x),\ \exists x \in \chi \tag{1.5}$$

And therefore by substitution:

$$\mathbf{d} = f(x) + \epsilon \tag{1.6}$$

Notice that as $f(x) \to 0$, then the relationship to any data is consistently caused by error! In reality, this system of data, models and errors is most often probabilistic, and each may be characterized by a probability from their associated probability densities, ρ.

1. ρ_{data}
2. ρ_{model}
3. ρ_{error}

Analyzing the contribution of error components in Eq. 1.12, we might start with an assumption given a variation on $\mathbf{d}$, such that $\mathbf{d} = (d_1, d_2, \ldots d_n)$ provided d is *iid*[6].

$$\epsilon_{data} = N(a, \sigma^2) \tag{1.7}$$

where,
σ^2 is the variance of the data, and
a may be considered an estimate of the the mean of $\mathbf{d}$, *iff* $f(a) = N(\mu, \beta^2)$ in Eq. 1.8.

$$\frac{n\bar{d}/\sigma^2 + \mu/\beta^2}{n/\sigma^2 + 1/\beta^2} \tag{1.8}$$

where,
β^2, the the variance of model, is evenly distributed around the mean, μ. If that is the case, then $\bar{\mathbf{d}} = a$, and the information that causes variance in the data is noise.

$$\frac{1}{n/\sigma^2 + 1/\beta^2} \tag{1.9}$$

The importance of the variance, β^2, is that as $\beta \to 0$ it indicates the existence of stronger prior information that might be used to strengthen posterior information.

We may analyze data distributions to see if there is extant prior information in $\mathbf{d}$

$$p(\mathbf{d}|m) = \mathtt{exp}\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(d_i - m)^2\right] \tag{1.10}$$

The answers to the inverse problem are always a probability distribution

$$p(m|d) = \frac{p(d|m)p(m)}{p(d)} \tag{1.11}$$

Bayes Theorem

Returning to our categorical perspectives of Eqs. 1.1 and 1.2, it is important to note that these functors (F *and* F') are not often isomorphic - meaning the functorial path that takes you from the model to the data is probably not the same path that takes you from the data back to model. This is referred to as inverse scattering caused by the interaction of probabilities. In other words, the conceptualization in Eq. 1.6 is over-simplified, incomplete and ultimately misleading. Eq. 1.12 is a more correct statement, representing the relationships at equilibrium, and at various distances from (thermodynamic) equilibrium.

$$\mathbf{d} \rightleftarrows f(x) + \epsilon \tag{1.12}$$

The subtlety emerges from a third, more universal perspective on the system of forward and inverse functors[7]. This universal background category is a generative, abstract system of functions of

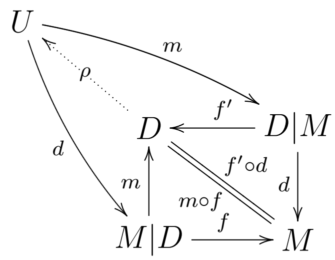

Fig. 1: Background Categorical System

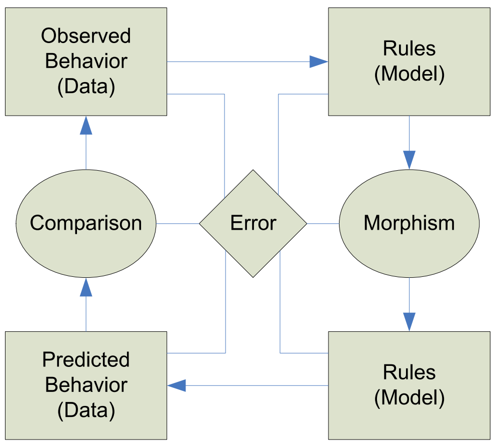

Fig. 2: Forward Cycle

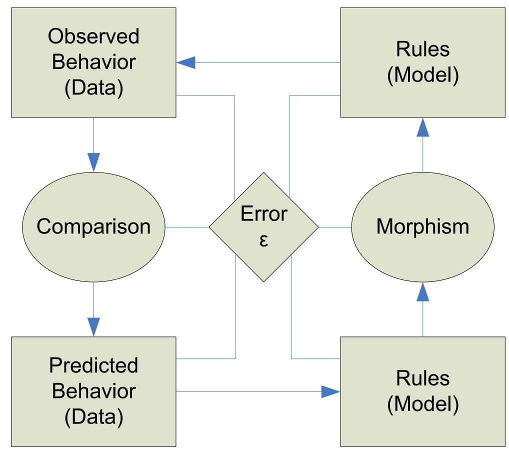

Fig. 3: Inverse Cycle

models, m, and data values, d, from errors (more correctly, their probabilities, p derived from a probability density, ρ), collectively categorized, U, that may be described and applied to a system of agent-based models and their data shown in Fig. 1.1.

> "In mathematics, category theory deals in an abstract way with mathematical structures and relationships between them: it abstracts from sets and functions respectively to objects linked in diagrams by morphisms or arrows." – Wikipedia

In Section 1.3, we shall apply this abstraction to the mathematical structures and relationships of agents within a system context, in order to better understand and describe the behavior and morphism of agent objects.

1.2 Agents and Agent-based Models

Category Theory is also a representational form of computer software concepts[8] representing abstract mathematics. These concepts have a close and coherent relationship with certain functional programming languages such as Haskell or ML. But it also has interesting structural relations to LISP, Logo and Church's Lambda Calculus - even Swarm's Objective-C.

These relationships form the mathematical basis of computer science [13]. The purpose of these notes is to provide a context for understanding the paradigm of Category Theory and its ultimate relationship to Agent Based Modeling and Simulation (ABMS) through various functional programming activities - programming as descriptive of the behavior of agents. Furthermore, categories provide the classification mechanism for Types and Type Theory, taxonomies, and ontologies.

> "[An] agent based model is a class of computational models for simulating the actions and interactions of autonomous agents (both individual or collective entities such as organizations or groups) with a view to assessing their effects on the system as a whole."
> – Wikipedia [1]

Compare the conceptualization of agent-based models from the quotation above to the characterization by Dr. Gary An below:

> "Therefore, ABMs are not "mathematical models" per se, being able to be subjected to formal analysis and "solved." Rather, the use of ABM falls into the category of "simulation science," in which computational analogs of real world systems are produced and used in a fashion similar to traditional experimental preparations." – Gary An, MD [2]

In agent-based modeling, there are two important distinctions made in these perspectives that an agent-based modeler must be aware of.

1.2.1 Functorial semantics

The first is the functorial aspect of agent-based models [7]. This is to say, we are not describing the functional behavior of one autonomous entity, but of the category of agents, being the totality of aspects of the agents, their structure, behavior, interaction, coupling and change (morphism), in time and space.

1.2.2 Resolution Analysis

The second, and perhaps most important distinction, is the difference between traditional, numerical analysis upon those aspects, and the *resolution analysis*[9] made possible by category-theoretic Inverse Theory.

In other words, in category-theoretic terms what does a range of solutions in one domain, along with their morphisms, tell us about the range of likely solutions in the co-domain? Moreover, what do these domains inform us about universal, background properties?

The category U, as has been mentioned earlier, is a category of knowledge consisting of a distribution of information objects, some of which are partially known, and some of which are unknown, a-priori. If nothing can be known from the prior information, then $\rho \to \infty$ and any parametric value will yield an equally probable result. But even that possibility may be tested against a normally distributed function, $\rho \mapsto u(0, 1)$. As $\rho \to 0$, a deterministic certainty exists for a particular value.

1.2.3 Selection of Agent-based Models from a Probability Density

Probability densities, ρ, have a characteristic shape generated by their probability density function. For the generalized Gaussian distribution shapes are generated by:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-/mu)^2}{2\sigma^2}} \tag{1.13}$$

where,
μ is the zero-centered mean, and
σ is the standard deviation.

When $\sigma^2 = 1$, the Gaussian shape is considered a normal distribution.

L is a frequentist likelihood function, that can be derived from the data and applied to the model by:

$$L(\mathbf{x}) = \rho_{data}(f(\mathbf{x}))$$

This may be applied to the probability distribution for each model by:

$$\sigma_{model}(\mathbf{x}) = \rho_{model}(\mathbf{x}) L(\mathbf{x})$$

1.3 Rationale for the Approach

ABMS seems to be a concrete, computational endeavor. Why would anyone propose an abstract, theoretical mathematical approach to ABMS? One might even ask: What does one have to do with the other?

Category Theory is a top-down approach from abstract concepts to concrete, real-world behavior. Agent based modeling and simulation is a bottom-up activity, from concrete phenomena exhibited by agents to their abstracted rules, called algorithms. It is precisely the resolution and refinement from the cycles of these two perspectives that allows us to abstract algorithms. Algorithms are a sequence of computational instructions (rules) that accurately represent the generative rules of agent behavior. The relationship between the algorithm and the observed behavior, while often closely coupled in non-interacting systems, becomes complex when (minimally) the number of

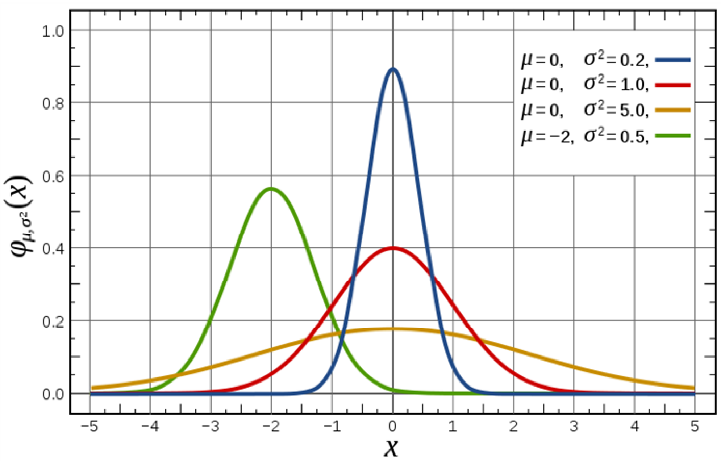

Fig. 4: Gaussian distributions

coupled, interacting elements reaches 3, the autonomous behavior is non-linear, and the system is not at thermodynamic or informational equilibrium.

The complex nature of non-linearity (more correctly, highly non-Gaussian problems) yields to Metropolis - Monte Carlo sampling methods from the probability density, ρ, under the assumption that a random function from the pdf, $\rho \in U(x^n)$, is aperiodic and irreducible. The result asymptotically approaches (converges upon) the solution[10], f as $n \to \infty$.

$$f(x)^{n+1} = U(x^n) : \mathcal{D} \to \mathcal{M} \Rightarrow \rho \tag{1.14}$$

where,
n is the number of sampled iterations.

> "The fact of the matter is that category theory is an intensely computational subject, as all its practitioners well know. Categories themselves are the models of an essentially algebraic theory and nearly all the derived concepts are finitary and algorithmic in nature." – John Gray [13, Forward pg. 7]

Much like the methods described by Tarantola , above 1.1:

1. Collect a large number of models from the posterior probability density.
2. Compare all models in the sample with the aim of recognizing structures repeated in a large number of realizations. Alternatively, identify realizations which contain structures of particular interest to the application from which the inverse problem originates.
3. Compute the fractions of all realizations that contain the considered structures. The fractional occurrence of a structure approximates the posterior probability that the structure is present (per construction of the sample).

In other words, Category Theory minimally represents a complementary path with models of agents in the systematic study of agent-based systems. At a more fundamental level, the importance of a Category-Theoretic approach is that it enables a more complete, universal understanding of agents as "relevant entities", as described below:

> "The conceptual clarity gained from a categorical understanding of some particular circumstance in mathematics enables one to see how a computation of relevant entities can be carried out for special cases. When the special case is itself very complex, as frequently is the case, then it is a tremendous advantage to know exactly what one is trying to do and in principle how to carry out the computation." – John Gray [13, Forward pg. 8]

2 Category Theory Applied to ABMS of SIRS

Systemic Inflammatory Response Syndrome (SIRS) is an emergent physiological response of the immune system that may lead to organ dysfunction, organ failure, and perhaps death. SIRS is often associated with the dynamics of infection, but not always.

The challenge in understanding SIRS is a categorical inverse problem. This is to say, in a living organism the model of the underlying phenomenon may only be inferred by existence and metrics of some number of other physiological phenomenon such as temperature, heart rate, respiration rate (tachypnea) and white blood cell count. Yet these have little direct relationship to the actual processes of intercellular cytokine communication from which SIRS emerges.

While omitting the specific details in this paper, we have applied a Category-Theoretic approach to a paper detailing the agent-based modeling and simulation of SIRS by Dr. Gary An[11] [2]. An describes the use of agent-based modeling and simulation of the cellular interaction model based upon cytokine communication, the term cytokine communication being a category of various signaling molecules, seen in generality in Fig. 5 [2]. It is precisely the myriad levels of agent abstraction from categories of intracellular processes, through categories of intercellular cytokine communication, categories of organ failure, to categories of agent-based models that might represent those phenomena that essential model theories can be formulated and tested.

> "Therefore, to accomplish this goal, a very abstract means of organ support is modeled in the form of "supplementary oxygen." This function increases the amount of "oxy" that is able to be diffused through the pulmonary epithelial barrier and therefore available as systemic oxygenation. This is the qualitative equivalent of increasing the fraction of inspired oxygen, and therefore alveolar oxygen, and therefore can increase the partial pressure of oxygen diffused in the blood. It is qualitative in so much as there is no attempt to reproduce the dynamics of gas exchange ..."

An's term "qualitative equivalent" describes the background category of all functional (process) objects characterized as agents that provide oxygen in support of organs.

Notice, too, that the expression of cytokines is emergent from categories of intracellular processes.

Agent-based Modeling and Simulation represents the universal background category of computation at myriad levels of abstraction, consisting of agents, algorithmic rules and interaction. From universal background categories, mathematical and algorithmic patterns may be applied abstractly to the *special cases* referred to by Gray in [13].

These special cases are categorical patterns, and enable abstraction such as those presented in An's paper to be further abstracted and applied to other diverse domains. For example, the concepts of cytokine communication has been applied to agent-based models and simulations for security in wireless computer networks [12].

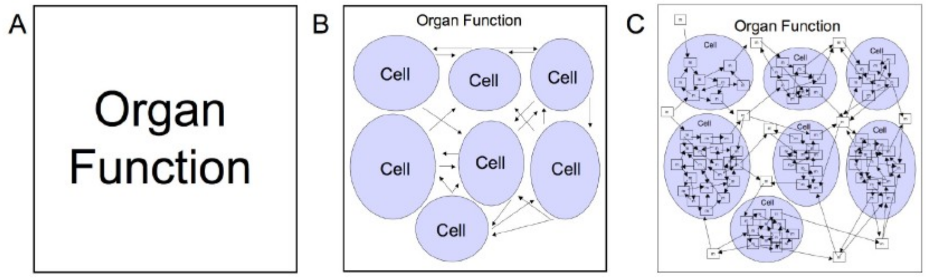

Fig. 5: Categories of Agent Functions

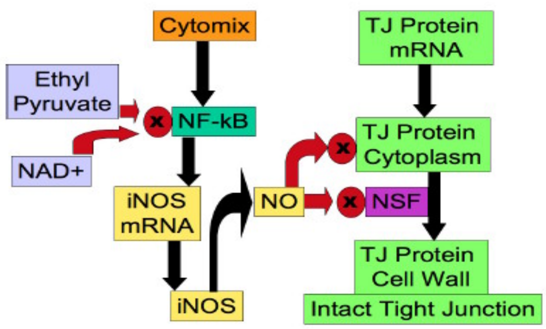

Fig. 6: Intercellular Processes in Fig. 5c (From An 2009)

3 Discussion

Agent-based modeling and simulations is a relatively recent technique of identifying patterns of emergent behavior in complex systems by the use of human or artificial intelligence. However, the

$$
\begin{tikzcd}
ABMS \arrow[drr, bend left, "m"] \arrow[ddr, bend right, "d"'] & & \\
& D \arrow[ul, dotted, "\rho"'] \arrow[dr, equal, "f'\circ d", "m\circ f"'] & D|M_{SIRS} \arrow[l, "f'"'] \arrow[d, "d"] \\
& M_{SIRS}|D \arrow[u, "m"] \arrow[r, "f"] & M_{SIRS}
\end{tikzcd}
$$

Fig. 7: Background Categorical System of ABMS of SIRS

$$
\begin{tikzcd}
SIRS \arrow[drr, bend left, "m"] \arrow[ddr, bend right, "d"'] & & \\
& D \arrow[ul, dotted, "\rho"'] \arrow[dr, equal, "f'\circ d", "m\circ f"'] & D|M_{cytokine} \arrow[l, "f'"'] \arrow[d, "d"] \\
& M_{cytokine}|D \arrow[u, "m"] \arrow[r, "f"] & M_{cytokine}
\end{tikzcd}
$$

Fig. 8: Background Categorical System of Cytokine Communication in SIRS

connections to a scientific formalism allowing "separating the demonstrably false from the probably true" have been weak.

> "...the interpretation of [agent-based] simulations tends to be ad hoc, often with little theoretical justification. Related to this is the fact that there currently exists no universal formalism for describing specific emergent properties in multi-agent systems in terms of agent properties even though significant work has been done to formalise emergence, both from a multi-agent systems perspective ... and from an information theoretic perspective ..." – Chen Chih-chun [5]

Chen proposes an information-theoretic formalism that may allow epistemological identification, that becomes more interesting when recast from Whitehead Processes into a Category-Theoretic understanding.

Using a Tarantola approach to model and hypothesis testing in a category-theoretic application of Inverse Theory, we propose the more robust formalism as described in this paper to computational Agent-based Modeling and Simulation.

Notes

[1]For example, Stanford Encyclopedia of Philosophy states: "[Category Theory] is a general mathematical theory of structures and of systems of structures."

[2]For various, computational viewpoints of Category Theory, see Fokkinga [6] or Stepanov & McJones [16]

[3]Composition is a monoidal category of binary arithmetic operations defined in Category Theory

[4]The term *structure preserving* is used as a general case as preserving the semantics and syntax of the functional interaction. When the functor perfectly preserves the structure, it is referred to as a *faithful* functor. Likewise, when a functor loses some of its structural information, it is referred to as a *forgetful* functor.

[5]Notice that in Eq. 1.4, the model domain (the theory) is on the right-hand side of the equation, the co-domain is on the left-hand side, and the functor (in this case =) solely represents an equality isomorphism, but categorically could represent any comparator

[6]The term *iid* refers to independent, identically distributed random variables.

[7]U represents the background category referenced by Lawvere in 1.1.

[8]See Stepanov & McJones [16] as put forward in Stepanov & McJones [16] for an interesting definition of a *concept*.

[9]The term resolution in inverse theory embraces the ability of an inversion method to reveal structures in the true model, using the given data. "In probabilistic, sample-based analysis of highly non-linear inverse problems, resolution analysis and uncertainty analysis are inseparable, and the combined investigation is simply termed resolution analysis." [10, pg. 23]

[10]" The term *asymptotically* means in this case that the set of points $x_1, \ldots, x_n$ visited in n successive steps by the algorithm Eq. 1.14 converges towards a sample of f as n goes to infinity." Mosegaard [11]

[11]Figures used with permission of author under Creative Commons License 3.0 US.

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