The AI Triplet: Computational, Conceptual, and Mathematical Representations in AI Education

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ABSTRACT
Expertise in AI requires integrating computational, conceptual, and mathematical knowledge and representations. We propose this triad as an "AI triplet," similar in spirit to the "chemistry triplet" that has influenced the past four decades of chemistry education. We describe a rationale for this triplet and how it maps onto topics commonly taught in AI courses, such as tree search and gradient descent. Also, similar to impacts of the chemistry triplet on chemistry education, we suggest an initial example of how considering the AI triplet may help pinpoint obstacles in AI education, i.e., how student learning might be scaffolded to approach expert-level flexibility in moving between the points of the triplet.

CCS CONCEPTS
• Computing methodologies → Philosophical/theoretical foundations of artificial intelligence; • Social and professional topics → Computing education.

KEYWORDS
AI, mental models, representations, cognition, student learning

1 INTRODUCTION
Experts in chemistry integrate knowledge about chemical phenomena at multiple levels: macroscopic, microscopic / submicroscopic, and symbolic [4, 7]. Macroscopic refers to observable properties of substances, e.g., water turning from liquid to solid at a particular temperature. Submicroscopic refers to properties at molecular and sub-molecular scales, e.g., the lattice shape formed by water molecules as they freeze, and the forces and geometry that cause this particular type of crystallization. And finally, symbolic refers to the mathematical, diagrammatic, and other notational formalisms of chemistry, e.g., the symbol H2O to indicate a water molecule, or the equation describing the energy change when ice melts:

\[ H_2O(s) \rightarrow H_2O(l) \quad \Delta H = 6.01 kJ/mol \]

This "chemistry triplet" of macroscopic, submicroscopic, and symbolic knowledge and representations—originally laid out in a scant three-page paper by Alex H. Johnstone in 1982—has been called "one of the most powerful and productive ideas in chemical education" [20, p. 179]. For example, it has been observed that:

"Trained chemists jump freely from level to level in a series of mental gymnastics. It is eventually very hard to separate these levels." [7, p. 377]

"[M]ost chemistry teaching is focused on the submicro–symbolic pair of the triplet and rarely helps students to build bridges to comfortably move between the three levels." [20, p. 181]

Many concrete proposals for improving chemistry education have flowed from these and similar observations [2, 3, 19].

We propose that expertise in AI similarly spans three levels of knowledge (and representations of that knowledge): computational, conceptual, and mathematical. In this paper:

1. We make the case for the proposed AI triplet of computational, conceptual, and mathematical knowledge and representations, including examples of how this triplet maps onto sample AI topics of tree search and gradient descent.
2. We describe how this framework is compatible with but different in scope from Marr's well-known "levels of analysis."
3. We suggest an example of how, like the chemistry triplet, the AI triplet can inform insights and practices in AI education, by discussing how student learning might be scaffolded to approach expert-level flexibility and robustness in moving between the points of the triplet.

We leave as open questions for other researchers and educators the extent to which this triplet, or variations thereof, might apply in areas of computer science besides AI.

A final disclaimer: We do not claim that our AI triplet represents some inviolable truth about AI, nor that it is the only way to carve up such a triplet. Rather, this paper provides a starting point for peeling apart common ideas that infuse AI expertise and AI education.

The original chemistry triplet proposed by Johnstone in 1982 has elicited much discussion, including refinements and re-imagineings [20]. It has also spurred many educational research studies in chemistry that have generated valuable knowledge about teaching and student learning. We hope that this AI triplet does the same.

2 THE PROPOSED AI TRIPLET
Chemistry is an empirical science, and the chemistry triplet specifies three different levels at which chemical phenomena can be analyzed. At the macroscopic level, properties like temperature and viscosity are observed through human senses and/or at human-interpretable scales. These properties emerge from, or are generated by, the interactions of molecules at the submicroscopic level, which in turn emerge from yet lower levels of atomic or subatomic interactions [12]. Thus, chemistry follows the blueprint of complex systems in which macro-level phenomena emerge from phenomena at the submicroscopic level.

These two levels are the only parts of the chemistry triplet that might be said to "exist" in nature. The third level, symbolic, refers...
to the human-created trappings of scientific notation which are used to describe chemical phenomena at the other two levels, including chemical and mathematical symbols, equations, molecular diagrams, and so on [19].

Newell and Simon eloquently argued for viewing AI (and indeed, computer science more broadly) as an empirical science in which, "Each new program that is built is an experiment. It poses a question to nature, and its behavior offers clues to an answer" [16, p. 114]. More specifically, as Simon later wrote:

"An artificial system, like a natural one, produces empirical phenomena that can be studied by the methods of observation and experiment common to all science. It might be objected that a system designed deliberately to behave in a desired way can produce no surprise or new information. This objection shrugs off our enormous ignorance of natural law and of the effects produced by natural laws operating on complex systems. The world of artificial (and natural) objects is full of unanticipated consequences...." [18, p. 99]

The proposed AI triplet, described below and illustrated in Fig. 1, takes into careful consideration the empirical nature of the science of AI—particularly the ways in which empirical phenomena in artificial systems are generated, observed, and described.

In a nutshell, computational elements in AI (e.g., lines of code) generate "macro" level behaviors at the conceptual level that can be observed, studied, and used by people. Mathematics is often used within AI systems as part of what is computed, and mathematics is also used by people to describe the operations or performance of such systems. All three types of knowledge can be expressed using a multitude of representations. And, as with chemistry [7, p. 377], AI experts "jump freely from level to level in a series of mental gymnastics. It is eventually very hard to separate these levels."

2.1 Submicroscopic(CHEM) || Computational(AI)

If we draw an analogy between the complex natural systems of chemistry and the complex artificial systems of AI, then the low-level, causal elements in AI—i.e., the elements that make up the "submicroscopic" level of AI—are essentially lines of code: the pieces of formal computation that make up an artificial system or program. Just as submicroscopic interactions are what generate higher-level phenomena in chemistry, computation is what generates higher-level phenomena in AI.

We define the computational level of the AI triplet as having to do with the computation that takes place in an artificial system, e.g., as specified by its program.

Unlike chemistry, in which we are still working to understand submicroscopic processes, in AI, we know the exact rules that govern computation, and computations are directly observable. However, as noted in Simon’s quote above, the results of running a program are not always evident just from inspection of the code. Higher-level behaviors emerge from the interactions of lower-level elements, and as with all complex systems, the higher-level behaviors cannot often or easily be predicted, even with full knowledge of the starting conditions and the rules of the system. (The halting problem is an obvious example of this property.)

Moreover, just as the submicroscopic level in chemistry can be broken into molecular, then atomic, and then subatomic interactions, so too can the computational level in AI be broken into human-readable code, then assembly code, then machine code, and so on. And, just as the submicroscopic level in chemistry eventually devolves into quantum physics, so too does the computational level in AI eventually devolve into electrical engineering (and eventually also into quantum physics!), assuming computations are realized on a digital electronic computer. However, we still find it useful to describe these phenomena at the higher levels of molecules, for chemistry, and human-readable computations, for AI.

2.2 Macroscopic(CHEM) || Conceptual(AI)

In chemistry, the higher-level phenomena that emerge from low-level submicroscopic processes are easy to discern: they are the everyday, human-scale manifestations of matter that can be described quite casually by naive observers in terms of sensory impressions, or described more formally by chemistry experts in terms of properties like temperature and viscosity.

However, the higher-level phenomena emerging from low-level computations in an AI system are not so easy to discern. In a sense,
the “human-scale” manifestations of executing an AI program are artificial constructs that exist in some abstract, conceptual space. These constructs are often only partially built or accessed by the artificial system, and are also often only partially or vaguely represented in the mind of the human observing the system. However, the constructs themselves transcend both of these partial views.

For example, consider a program that performs depth-first search over a tree. In many cases, the tree does not exist as an explicit entity in the program; it might be encoded implicitly as a starting node and a successor function. In addition, we (as human observers) do not have explicit access to the complete tree in our own mental representations. However, the complete tree can still be defined as an abstract but fully-specified conceptual construct. The complete tree “exists” in the same space that abstract mathematical objects might be said to “exist,” but partial views of the tree are in fact instantiated as concrete objects via the execution of a program.

We define the **conceptual level** of the AI triplet as having to do with the abstract conceptual constructs that are built and/or accessed by an artificial system.

In an interesting reversal, the levels associated with generating phenomena versus emergent phenomena are inverted in chemistry versus AI, with respect to whether we can fully or only partially observe each level. In the complex systems of chemistry, the submicroscopic level (which generates higher-level phenomena) is not directly observable by people, and we can often access only partial or indirect information about this level through our experiments, observations, and imagination. The macroscopic level (which encompasses the emergent phenomena in the complex system) is directly observable by people.

In contrast, in the complex systems of AI, the computational level (which generates higher-level phenomena) is directly observable by people. However, the conceptual level (which encompasses the emergent phenomena in the complex system) is not directly observable by people. And, as with the submicroscopic level in chemistry, we can often access only partial or indirect information about this level through our experiments, observations, and imagination.

### 2.3 Symbolic (Chem) || Mathematical (AI)

First of all, it is worth noting that the notion of “symbols” in chemistry is vastly different from what we mean by “symbols” in AI. For the remainder of this paper, we use the term “symbolic” as it is used in the context of the chemistry triplet, i.e., the use of signs by humans to convey ideas about a scientific topic [20].

In the chemistry triplet, the symbolic level refers to a wide variety of notation that includes chemical terminology and abbreviations, mathematical formulae and calculations, and diagrams, drawings, graphs, and other visualizations [20]. Some authors subdivide the symbolic level depending on whether notation is used to describe mathematical calculations versus non-mathematical concepts [14]. For example, acids and bases are often described using chemical formulae, which are not themselves directed to calculations, e.g., H\textsubscript{2}SO\textsubscript{4} and NaOH, while other notation is used to describe equations explicitly used for calculation, such as the equation relating pH to the concentration of H\textsuperscript{+} ions: \(pH = \log[H^+]\).

Other authors distinguish between notation that is visual and depictive versus other, non-depictive notation [6]. Depictive symbols can serve as iconic models of underlying concepts, i.e., as representations that enjoy some structural correspondence with what they represent [15]. For example, the chemical formula H\textsubscript{2}O describes the atomic contents of a water molecule, but the simple diagram \(H - O - H\) provides additional information about the structure of a water molecule, as reflected in the structure of the diagram itself. With respect to the chemistry triplet:

“The semi-symbolic, semi-iconic nature of many visual representations in chemistry gives them a hybrid status between signs and models... If we think of them as mere signs, then we may be inclined to classify them as belonging to the [symbolic] level; if we think of them as models with descriptive, explanatory, and predictive power we may prefer to think of them as part of the [submicro] level.” [20, p. 184–185]

All of these nuances regarding symbolic notation in the chemistry triplet can also be found in relation to symbolic notation in AI. There are many types of notation used in AI, most commonly including:

1. **Code (and pseudocode).**
2. **Visual diagrams of conceptual constructs such as trees, hyperplanes, neural networks, etc.**
3. **Mathematical notation such as equations, big O notation for algorithmic complexity, etc.**

Just as recent authors have parcelled out different types of chemistry notation to different levels of the chemistry triplet, instead of lumping them all together as Johnstone’s original proposal did [7], we see similar value in parceling out each type of AI notation.

(1) **Code and pseudocode** are of course an essential part of AI notation. These not only describe phenomena at the computational level of the AI triplet, but code in fact defines computations. (It’s a bit like what would happen if, after writing down a chemical equation, the marks we made on paper actually got converted into molecules and interacted with each other!) Because code is so intimately tied to the phenomena of computation, we suggest that this type of notation should reside at the computational level of the AI triplet.

(2) **Visual diagrams** in AI often describe phenomena at the conceptual level of the AI triplet. For example, we often draw downward-fanning trees to illustrate principles of tree search. These diagrams are often iconic, i.e., they exhibit some structural correspondence with the conceptual constructs that they represent. And, just as iconic visual representations in chemistry can usefully be deemed to reside at the submicroscopic level of the chemistry triplet, we argue that iconic visual representations in AI should reside at the conceptual level of the AI triplet.

(3) **Mathematical notation and ideas** are used extensively in AI, and we argue that mathematics embodies a distinct, third type of knowledge and representation that is an essential part of AI expertise. We see two primarily roles for mathematics in AI.

First, artificial systems might themselves perform mathematical calculations during their operation, e.g., a program for doing gradient descent will contain some calculus-based implementation for computing the derivative of a multivariate function. We label this as an artificial system using mathematics.

Second, we (the human observers) frequently rely on mathematical notation for describing artificial systems. For instance, we might formally define a path \(P\) across a set of graph vertices \(V\) as:
Breadth-first search

```python
function breadth-first-search(problem)
    ... return end...
```

Gradient descent

```python
while True:
    ... weights_grad = evaluate_gradient(loss_fun, data, weights)
    ... weights += -step_size * weights_grad
```

### Computational

- **Numerical gradient**: approximate, slow, easy to write
- **Analytic gradient**: exact, fast, error-prone

### Mathematical

- Current W: \(W^*\)
- Gradient DW: \([-0.25, 0.6, 0, 0]\)

\(P = (q_1, q_2, \ldots, q_n) \in V \times V \times \ldots \times V\). Experts might readily parse this notation to understand that: (a) the path is an ordered sequence of individual items from \(V\); and (b) the path is thus an element in some \(n\)-dimensional space where each dimension is a copy of \(V\). We also often use mathematical notation and ideas to describe operational characteristics of artificial systems. For example, given a tree with branching factor \(b\) and depth \(d\), we can use some combinatorics and our knowledge of search algorithm behavior to mathematically infer that breadth first search will have a worst-case space complexity of \(O(b^d)\).

Regardless of whether mathematical ideas are used within an artificial system itself, or by human observers while describing such a system, these mathematical ideas and associated notation are distinct from both the computational level and the conceptual level of the AI triplet. Thus, we propose elevating mathematical representations to form the third leg of our proposed AI triplet:

We define the **mathematical level** of the AI triplet as having to do with the mathematical notation and ideas used to describe various aspects of an artificial system, including its internal procedures as well as externally observed characteristics.

As a final comment on notation, 2D/3D data plots are also a fairly ubiquitous notation in AI, and indeed in all empirical sciences. Interpreting such plots often requires both mathematical [9] and visuospatial [8] proficiency. Thus, we suggest that plots span both the conceptual and mathematical levels of the AI triplet.

3. **RELATIONSHIP TO MARR’S LEVELS**

Some readers may be thinking, “We already have an AI triplet! Isn’t this just a rehash of Marr’s three levels of analysis?” While both frameworks involve levels and the number three, we see them as orthogonal classifications, i.e., that are different in scope, and certainly not mutually exclusive.

3.1 **Marr’s Three Levels of Analysis**

Marr’s three levels refer to different lenses or levels of abstraction that can be applied to inspect and study an information processing system [13]. The levels often go by varying labels, but generally can be summarized as:

1. **Computational, functional, or behavioral level**: The outwardly observable behavior that a system produces, for example, in terms of input-output mappings.
2. **Representational or algorithmic level**: The internal information-manipulation procedures that a system uses to produce its outward behaviors.
3. **Implementational or hardware level**: The physical substrate on which the information processing system is run.

For example, let us use Marr’s levels to analyze a sorting program. The computational level is analogous to the program’s main function header: the program takes as input a list having some particular data type, and returns as output a sorted version of the list.

The representational level is analogous to the function body, including all of the intermediate data structures, operations, etc., that are carried out to produce the input-output behavior. Note that
for a given function (like sorting), there are many different algorithms that can produce the same input-output mappings (though of course other behavioral properties like running time may differ).

Finally, the implementational level refers to the actual physical machine that our sorting program is running on.

### 3.2 Relationship Between Frameworks

Marr’s levels essentially carve up an information processing system into horizontal slices. At the top level, you have the input-output behavior. This rests on the middle level of representations and algorithms. And this middle level rests on the bottom layer of physical implementation.

Our AI triplet, in contrast, carves up an information processing system into vertical slices. Really any one of Marr’s three levels can be seen in any corner of our AI triplet, and vice versa.

For example, keeping strictly to Marr’s level 1, the input-output behavior of a sorting program can be viewed in terms of:

1. (AI triplet level 1) Its computational definition, i.e., input arguments and parameters and return values.
2. (AI triplet level 2) Its conceptual meaning, i.e., “sorting order” can be evaluated with respect to a given concrete list, but it also exists as a theoretical abstraction that relates to sequences of elements and relations between them.
3. (AI triplet level 3) Any relevant mathematical formalisms. For instance, we can describe requirements on input list elements in mathematical terms: reflexivity ($\forall a \in S \mid a = a$), transitivity ($\forall a, b, c \in S \mid a \leq b \land b \leq c \Rightarrow a \leq c$), etc.

Similar examples obtain for Marr’s level 2, e.g., we can describe specific sorting algorithms in terms of their computational, conceptual, and mathematical aspects. And likewise for Marr’s level 3.

To summarize: Marr’s framework is about different levels of abstraction at which we can describe and analyze a given information processing system. The AI triplet is about different kinds of knowledge and representations that we can bring to bear to describe one or more levels of abstraction in a given system.

### 4 DISCUSSION: TWO INITIAL INSIGHTS FROM THE AI TRIPLET

Next, we provide two examples of the kinds of insights that can be generated by considering AI expertise and education in the context of the AI triplet.

#### 4.1 Helping Students Reach the Middle of the Triplet

We return to two of the core observations about chemistry expertise and learning that have emerged from the chemistry triplet:

“Trained chemists jump freely from level to level in a series of mental gymnastics. It is eventually very hard to separate these levels.” [7, p. 377]

“[M]ost chemistry teaching is focused on the submicro–symbolic pair of the triplet and rarely helps students to build bridges to comfortably move between the three levels.” [20, p. 181]

When students are learning formal chemistry, they encounter many new concepts and representations of those concepts that are very different from what they have previously experienced in their daily lives, e.g., the notion of pure substances, viewing all matter as made of particles, imagining particles that are somehow both particulate and wave-like, etc. [19]. The point is often made with the chemistry triplet that all three “points” of the triangle are new to most novice learners, and so introducing two or three forms of knowledge simultaneously can be overwhelming. Instead, a better approach may be:

“Offering sufficient scaffolding to support students in gradually learning to operate within and across the domains in the way experts can. So, for example, there will need to be times in teaching when the focus is on subsets of the macroscopic concepts, and how these are formally represented; and there will need to be times when the focus is on aspects of the sub-microscopic models, and the different ways these are formally represented. There will also be times when it is vital to shift between the macroscopic and submicroscopic domains to build up the explanations of the subject.... However, ventures into the triangle should be about relating previously taught material, and should be modelled carefully by the teacher before students are asked to lead expeditions there; and such explorations should initially be undertaken with carefully structured support.” [19]

While undergraduate students taking AI courses generally come in with prior knowledge about programming and mathematics, it is certainly the case that teaching about any particular AI topic often introduces new knowledge and representations at all three levels of the AI triplet, as shown in Figure 2.

Moreover, as AI education is beginning to percolate down to younger students, the need for sufficient scaffolding will only increase. For example, a recent cognitive-interview-based study of eight middle and high school students found that students faced challenges in multiple distinct areas that correspond to facets of the AI triplet [5], for instance:

- **Mathematical:** “Even in cases where students demonstrated competency with the necessary mathematical skills, they often struggled to identify connections and/or make use of those skills until explicitly prompted.... Once introduced, however, students generally recognized the method and were able to apply it to the problem.” [5, p. 15530]

- **Conceptual:** “Students found difficulty with the abstract representations characteristic in AI problems. Across all interviews, students needed explicit scaffolding in understanding how to interpret and construct a search tree.... Thus, even after the interviewer scaffolding enabled students to construct a search tree from the slider puzzle, students struggled to make use of the search tree representation to consider the depth and breadth of a problem space (both for the search trees they constructed and for pre-constructed exemplars). able to build a tree from a node to branches to new nodes, yet only one student was able to recognize the salience of tree abstractions such as branching factor and tree depth (albeit using colloquial language) to estimate the relative complexity of a problem.” [5, p. 15530]
• Conceptual/Computational: “A challenge for all students interviewed, even those with advanced mathematical skills, was recognizing how a problem in the world could be made amenable to the computational power of AI. That is to say, students needed support in conceiving a problem space in a way that would enable an AI system to solve it. Thus while some students in the study volunteered ways a computer program might be able to implement an AI solution once identified, the initial step of reconceiving a problem as an AI problem was elusive: the broad strategies AI systems leverage to make predictions or to find a solution from an array of possibilities were unknown to students and thus unavailable resources in their mental models of the problem space.” [5, p. 1553]  

Thus, one potentially fruitful direction of study for AI education lies in evaluating how students are able to approach individual versus combined aspects of the AI triplet, and strategies for scaffoldings for helping students build up competence along individual aspects before explicitly guiding them to think across multiple levels.

Another observation arising from the chemistry triplet is that, for experts, representations of a particular topic are often ambiguous, in that they can be interpreted in terms of multiple levels of the triplet. This ambiguity can be challenging for students to parse:

“e.g., at a particular moment, the teacher might be talking about molecules, but the student may be interpreting the signsifier as representing samples of substances.” [19]

However, what is challenging for students is actually an important affordance for experts:

“the affordance of this ambiguity is the potential for these symbols to allow us to shift between the macroscopic and submicroscopic levels... An equation for a chemical reaction...can act as a bridge between the two levels by simultaneously representing both the macroscopic and submicroscopic, and aiding us in shifting between these levels in our explanations.” [19]

Anecdotally, while AI educational practices often present multiple and/or ambiguous representations to students, there is little focused and explicit instruction about these ambiguities and strategies students can use to learn to jump between or build bridges between levels. For instance, again anecdotally, many standard AI exam problems (like those posted to publicly available course websites) present as either “code” problems or “math” problems or “conceptual” problems, without necessarily evaluating students on the ability to bridge multiple levels. In contrast, many in-depth homework assignments or projects do require students to both conceptually describe and implement a particular AI idea. It is worth more purposefully exploring how these kinds of bridging activities can be designed, used, and evaluated in AI education.

5 CONCLUSION

A recent analysis proposed a framework for AI literacy in the context of HCl that spans 17 competencies (such as recognizing AI, decision making, sensors, etc.) and 15 design considerations (such as explainability, social interaction, etc.) [11]. The proposed AI triplet is very compatible with such taxonomies and with other existing AI resources like textbooks, as it offers a way to more explicitly carve up each individual competency or topic into computational, conceptual, and mathematical slices.

ACKNOWLEDGMENTS

Acknowledgments omitted for blind review.

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