Article

Interpretable Deep Knowledge Tracing via Theory-Grounded Embeddings: Toward Individualized Learning Trajectories

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Abstract

This study introduces iDKT, an interpretable-by-design Transformer model that utilizes *Representational Grounding* to align deep latent representations with educational constructs, leveraging the high accuracy of deep knowledge tracing models while addressing their inherent lack of interpretability. We introduce a formal validation framework to verify the alignment of iDKT's internal representations and, using Bayesian Knowledge Tracing as a reference, evaluate the model across multiple educational datasets. Results demonstrate that iDKT maintains state-of-the-art predictive performance while yielding additional interpretable insights at a significantly higher granularity than those provided by the reference model. Specifically, iDKT identifies student-level initial knowledge and learning velocities, providing mastery estimates that are more sensitive to the nuances of individual behavioral patterns than those produced by standard BKT. These individualized insights enable precise diagnostic placement and dynamic pacing, allowing adaptive learning environments to tailor instruction to each student's unique learning profile with enhanced precision. This work offers both a robust methodology for evaluating the interpretability of Transformer-based models and a practical tool for improving educational effectiveness through data-driven personalization.

Keywords: deep knowledge tracing; transformer; interpretability; Bayesian Knowledge Tracing; educational data analysis; personalized learning

1. Introduction

Knowledge Tracing [1] is a fundamental task in the fields of Artificial Intelligence in Education, Intelligent Tutoring Systems and Massive Open Online Courses. Its primary objective is to model a student's dynamic knowledge state over time based on their history of interactions with learning materials, enabling systems to predict future performance and provide personalized instruction. As educational environments become increasingly diverse and digital, the ability to accurately track and interpret student mastery has become a critical requirement for scalable, effective education.

Historically, the field has been dominated by two distinct paradigms. The first, exemplified by Bayesian Knowledge Tracing and its variants [2], relies on probabilistic graphical models that explicitly represent knowledge states. BKT models are intrinsically interpretable, being based on parameters such as initial knowledge, learning rate, or slipping and guessing probabilities that map directly to pedagogical constructs, allowing educators

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to understand how they work and trust their decisions. However, this interpretability comes at the cost of a simplicity that often limits its predictive power, making them struggle to capture the complex, non-linear dependencies often present in educational datasets.

The second paradigm emerged with the advent of Deep Knowledge Tracing (DKT) [3], which uses different variants of deep learning techniques from the initial Recurrent Neural Networks to current Transformers [4] to model student interactions. These models have achieved state-of-the-art predictive performance, significantly outperforming classical approaches by leveraging the high capacity of deep learning models that allows them to learn complex patterns [5]. Yet, this predictive power has come at a significant cost: interpretability. Deep learning models are notoriously opaque "black boxes," where the learned representations are distributed across high-dimensional latent spaces that bear no direct correspondence to constructs with a clear semantic meaning. This lack of transparency creates a trust gap for practitioners, who cannot easily discern why a model predicts a student has failed or succeeded, nor can derive actionable pedagogical insights from the model's internal state [6].

Current efforts to bridge this gap typically rely on post-hoc explainability methods, such as weights visualization or perturbation analysis [7,8]. While valuable for debugging, these techniques often provide only a superficial view of the model's decision-making process and do not guarantee that the learned representations align with meaningful constructs. Moreover, their application and interpretation require technical deep learning expertise, limiting their accessibility to practitioners without this specialized knowledge.

To address these limitations, we propose a shift towards interpretability-by-design, inspired by the emerging paradigm of Theory-Guided Data Science (TGDS) [9]. In TGDS, maintaining consistency with theoretical postulates is an architectural constraint rather than an afterthought. By integrating extensive domain knowledge, TGDS-based models can be constrained to learn representations that are both theoretically plausible and highly predictive. While this approach has been applied mostly to science—and specifically to physics [10]—we adapt it here to the educational domain.

Standard TGDS implementations typically rely on auxiliary loss functions to incorporate formal knowledge expressed as rules, algebraic constraints, or differential equations [11]. We propose a novel approach called *Representational Grounding* that, in contrast, utilizes auxiliary losses operating on projections of the Transformer's embeddings. This mechanism enables the model to learn representations that are consistent with semantically meaningful constructs.

The major contributions of this work are as follows:

- Proposal of Representational Grounding, a novel method that overcomes the black-box nature of Transformers by providing interpretability-by-design.
- Introduction of a formal validation framework to quantify interpretability via representational alignment, enabling a systematic characterization of the trade-off between reference fidelity and predictive performance.
- Application of Representational Grounding to the development of iDKT, a new type of knowledge tracing models that leverage the high accuracy inherent in deep learning while achieving pedagogical interpretability.
- Empirical demonstration of iDKT benefits by showing how it captures granular, student-specific insights—such as individualized initial knowledge and learning rates—that are beyond the capabilities of simpler models such as BKT.

The remainder of this paper is structured as follows. Section 2 reviews related work on knowledge tracing, deep learning interpretability, and theory-guided data science. Section 3 describes the proposed iDKT architecture and the *Representational Grounding* framework. Sections 4 and 5 detail the individualized embedding mechanism and the multi-objective loss system, respectively. Section 6 presents the results of the experimental validation, interpretability results, and the analysis of individualization granularity. Finally, Section 7 concludes the paper.

2. Related Work

2.1. Deep Knowledge Tracing Interpretability

Knowledge Tracing [1]—the task of modeling the evolution of student knowledge states through interactions with learning materials—was traditionally dominated by *Bayesian Knowledge Tracing* and *Factor Analysis Models*. While these classical approaches are intrinsically interpretable, they often lack the predictive capacity to capture the complex, non-linear dynamics inherent in student behavior. The inception of *Deep Knowledge Tracing* addressed these limitations by applying *Recurrent Neural Networks*, specifically *Long Short-Term Memory* architectures, to capture temporal dependencies in large-scale interaction data [3]. Following this pioneering work, numerous variants have emerged exploring alternative architectures—including memory-augmented networks, graph-based methods, and Transformer-based approaches—while increasingly investigating how to incorporate auxiliary knowledge sources to enhance performance prediction [5].

This auxiliary information can be analyzed through the lens of *Informed Machine Learning* [9,11], a paradigm that aims to enhance purely data-driven models by integrating prior knowledge—such as scientific laws, logical constraints, or pedagogical theories—directly into the machine learning process, thereby improving interpretability and generalizability in scenarios with sparse or noisy data. Zanellati et al. [12] reviewed Knowledge Tracing (KT) models, classifying their knowledge sources according to the Informed Machine Learning (IML) taxonomy proposed by Von Rueden et al. [11]. The sources in KT generally fall into three categories: domain knowledge, student behavior, and pedagogical theories, being primarily represented through algebraic equations, knowledge graphs, probabilistic relations, and embeddings or attention mechanisms. They are usually integrated into the training dataset, the functional form of the model, or the learning algorithm (e.g. the loss function). Despite these advances, significant questions remains open, particularly regarding how the integration of diverse prior knowledge impacts model interpretability, which specific psychological or pedagogical theories are most relevant to KT improvement, and what representational forms best facilitate this integration [12].

The lack of interpretability in Deep Knowledge Tracing (DKT) remains a primary barrier to its deployment in educational settings, where stakeholders require models that are both accurate and pedagogically sound. Numerous approaches have been proposed to bridge this gap, which are generally categorized into post-hoc and ante-hoc modalities [6]. Post-hoc methods attempt to derive explanations after a model has been trained, typically employing techniques such as *Layer-wise Relevance Propagation* (LRP), *Causal Inference*, *Attention Visualization*, *Local Interpretable Model-Agnostic Explanations* (LIME), *Deep SHapley Additive Explanations* (DeepSHAP), or *Causal Explanations*.

In contrast, ante-hoc interpretability refers to models that are either inherently transparent—like the traditional Bayesian Knowledge Tracing (BKT) and Factor Analysis models (FAM)— or incorporate model-intrinsic interpretability. The latter adds specific modules within the architecture to achieve transparency, effectively resembling an interpretable model from the outside. According to [6], one type of these modules are the attention heads charcateristics of Transformer architectures. Notable models in this category include SAKT [13], the first self-attentive model for KT; SAINT [14], that proposed a cross-attention architecture; and AKT [15], a cross-attention model that incorporates principles from Item Response Theory (IRT).

While providing valuable insights, these methods often fail to ensure that learned representations align with valid educational constructs; furthermore, they still require significant technical expertise, which limits their utility for real-world pedagogical diagnostics.

In this paper, we propose a novel interpretable-by-design model called iDKT, based on a *Grounded Embeddings* approach that addresses these limitations. It incorporates prior knowledge from intrinsically interpretable models (such as BKT) directly into the embedding layers of a Transformer architecture. By utilizing a multi-objective learning algorithm with specialized loss functions, we guide the model toward learning latent representations that are formally anchored to pedagogically valid constructs. This allows iDKT to achieve state-of-the-art predictive performance while maintaining a level of transparency that is actionable for educators and stakeholders.

2.2. Probing Methods

Linear classifier probes [16] have emerged as a robust framework for investigating the information encoded in the intermediate layers of neural networks. Originally introduced to analyze representations in deep vision and language models, probing involves training a simple diagnostic classifier to predict a specific property or construct—such as a student's latent mastery state—from a frozen embedding. The fundamental intuition is that if a construct can be accurately predicted by a simple model, it must be explicitly encoded and accessible within the deep model's representational space. This methodology is particularly relevant in the context of recent surveys on Large Language Models (LLMs) and foundation models, where understanding the internal mechanics and *representation engineering* has become a central research frontier [17,18].

The state-of-the-art in probing emphasizes the importance of utilizing low-capacity models, typically linear or logistic regressions, to ensure that the probe is merely extracting existing information rather than learning the task itself through its own parameters. This distinction is critical in our context, where we seek to verify that the deep model has internalized valid constructs of pedagogical theories as part of its internal reasoning process. Recent advances have expanded this methodology to include *structural probes*, which evaluate whether relational properties between concepts are preserved within the latent manifold. A significant challenge in interpreting probe results is the potential for false positives, where a probe achieves high accuracy by exploiting statistical artifacts rather than meaningful structure. To address this, current research highlights the necessity of methodological rigor through the use of *selectivity* metrics and *control tasks* . By comparing the probe's performance on the target construct against its performance on randomized or nonsensical data, researchers can quantify the extent to which the deep model genuinely represents the theory [19,20].

Drawing upon these validation protocols, we demonstrate the theoretical anchoring of iDKT's internal representations and provide a quantitative measure of its interpretability by evaluating the degree of alignment with educational constructs.

2.3. Individualized Bayesian Knowledge Tracing

Bayesian Knowledge Tracing (BKT) [1] models student mastery as a latent variable $L_t \in \{0,1\}$ that transitions based on learning opportunities. BKT is governed by four parameters that map directly to latent and observed behavior:

- $P(L_0)$: Initial Mastery — the probability that the student already knows the skill before the first interaction.
- T: Transit probability — the probability of learning a skill after an interaction.

- G: Guess probability — the probability of a student getting the correct answer despite not having mastered the skill.
- S: Slip probability — the probability of a student making a mistake despite having mastered the skill.

The model updates the knowledge state after each observation r_t (correct or incorrect) using the following recurrence relation:

$$P(L_t|r_t) = \begin{cases} \frac{P(L_t)(1-S)}{P(L_t)(1-S)+(1-P(L_t))G} & \text{if } r_t = 1 \\ \frac{P(L_t)S}{P(L_t)S+(1-P(L_t))(1-G)} & \text{if } r_t = 0 \end{cases} \tag{1}$$

The model calculates the mastery probability for the subsequent learning opportunity by applying the transition update:

$$P(L_{t+1}) = P(L_t|r_t) + (1 - P(L_t|r_t))T \tag{2}$$

A fundamental limitation of standard BKT is the assumption of per-skill, population-level parameters, where the same parameter values are assigned to all students for a given knowledge component. Individualized BKT (iBKT) models attempt to address this by incorporating student-specific parameters. According to the taxonomy proposed by Yudelson et al. [21], individualization typically targets three primary aspects: (i) student-specific prior knowledge ($P(L_0)$), (ii) student-specific learning rates (T), or (iii) student-specific performance (guess G and slip S). While individualizing performance parameters is less common due to the assumption that they are item-dependent, empirical evidence consistently demonstrates that individualizing prior knowledge and learning rates significantly improves predictive performance compared to population-level models. However, these classical individualized approaches face substantial challenges, including the cold-start problem for new students, parameter sparsity when training separate parameters for every student-skill pair, and a significant increase in computational complexity.

Our proposed iDKT model automates this individualization process by leveraging the high-capacity representational power of Transformers to learn student-specific parameters within a theoretically-grounded latent space. Specifically, iDKT uses *Grounded Embeddings* representations, where individualized parameters such as proficiency (l_c) and learning velocity (t_c) are decomposed into a population-level base (derived from a static BKT reference) and a student-specific deviation. These deviations are learned by the Transformer from the student's interaction history, allowing the model to generalize across skills and students without requiring explicit, per-individual parameter fitting. By anchoring these representations through specialized multi-objective loss functions—which penalize deviations from the reference BKT parameters—iDKT maintains the diagnostic granularity of individualized models while overcoming the technical hurdles of data sparsity and scalability inherent in classical iBKT implementations.

3. iDKT Model

We propose an Interpretable Deep Knowledge Tracing (iDKT) model with a Transformer-based architecture designed to bridge the gap between the high predictive capacity of deep learning and the intrinsic interpretability of simpler models such as Bayesian Knowledge Tracing (BKT). Unlike standard black-box models, iDKT utilizes a novel mechanism called Representational Grounding to anchor its latent representations to the conceptual space of a interpretable model choosen as reference.

The core architecture of iDKT, as illustrated in Figure 1, extends the standard Transformer framework [4] by incorporating specialized components for Representational

Grounding, primarily integrated within the embedding layers and the multi-objective loss pipeline.

1. **Input Data**: This stage handles the ingestion of student interactions (concepts, questions, and binary responses $r \in \{0, 1\}$). Crucially, it also loads values from the BKT reference model, including performance predictions (p_{BKT}) and per-skill parameters such as initial mastery (l_0) and learning transition rates (T), which serve as grounding targets for the model.
2. **Embeddings**: Task and history information are projected into a continuous embedding space. We then apply the individualization transformations described in Section 4 where base embeddings are augmented by student-specific parameters: a Proficiency Offset (lc) and a Rate Augmentation (tc). This produces the Transition Gap (individualized task representation x') and the Transition Gain (individualized interaction history y'), effectively defining the difficulty of a task relative to the student's baseline proficiency.
3. **Transformer Core**: The model employs a dual-encoder architecture followed by a cross-attention decoder. One encoder processing the individualized interaction history ($y'_{1:t-1}$) to capture global student behavior, while a task encoder processes the current individualized task (x'_t). The decoder uses multi-head cross-attention to synthesize these streams into a latent Proficiency Context, representing the student's current specialized knowledge state for the target task.
4. **Output Stage**: The latent Proficiency Context is passed through a multi-layer perceptron (MLP) that maps the deep representations to the final output space. The final output is the iDKT prediction (p_{iDKT}), representing the probability that the student will respond correctly to the current task.
5. **Loss Functions (Grounding Pipeline)**: During training, the architecture is supervised not only by the prediction loss (L_{sup}) against ground truth outcomes but also by an alignment pipeline. This includes the Alignment Loss (L_{ref}) which penalizes deviations from the BKT prediction, and Parameter Losses (L_{init}, L_{rate}) that ground the model's internal proficiency and rate parameters to their BKT-derived theoretical counterparts.

4. Embeddings

In standard educational datasets, such as ASSISTments 2009, ASSISTments 2015, Algebra 2005, and others [22], student interactions are recorded at the level of specific questions or tasks, each of which is associated with one or more underlying concepts or knowledge components. This structure reflects the fact that proficiency in a concept (e.g., the Pythagorean Theorem) is acquired through interactions with a diverse range of tasks. While all tasks involving a concept share the same semantic core, they differ in their specific manifestations—most notably in their intrinsic difficulty or complexity. Therefore, an effective representation must capture both the shared identity of the concept and the unique deviation of the specific task.

In Transformer-based models [4] we can operationalize this principle representing the tasks as embedding vectors:

$$x' = c + u \cdot d \quad \text{(Task)} \tag{3}$$

In this formulation, c acts as the *Concept Anchor*, a vector representing the invariant semantic identity of the concept while the vector d represents the learnable *Question Variation Axis*, defining the specific direction of the "transition gap". The scalar u serves as the *Relational Magnitude*, representing the question's specific relative difficulty compared to

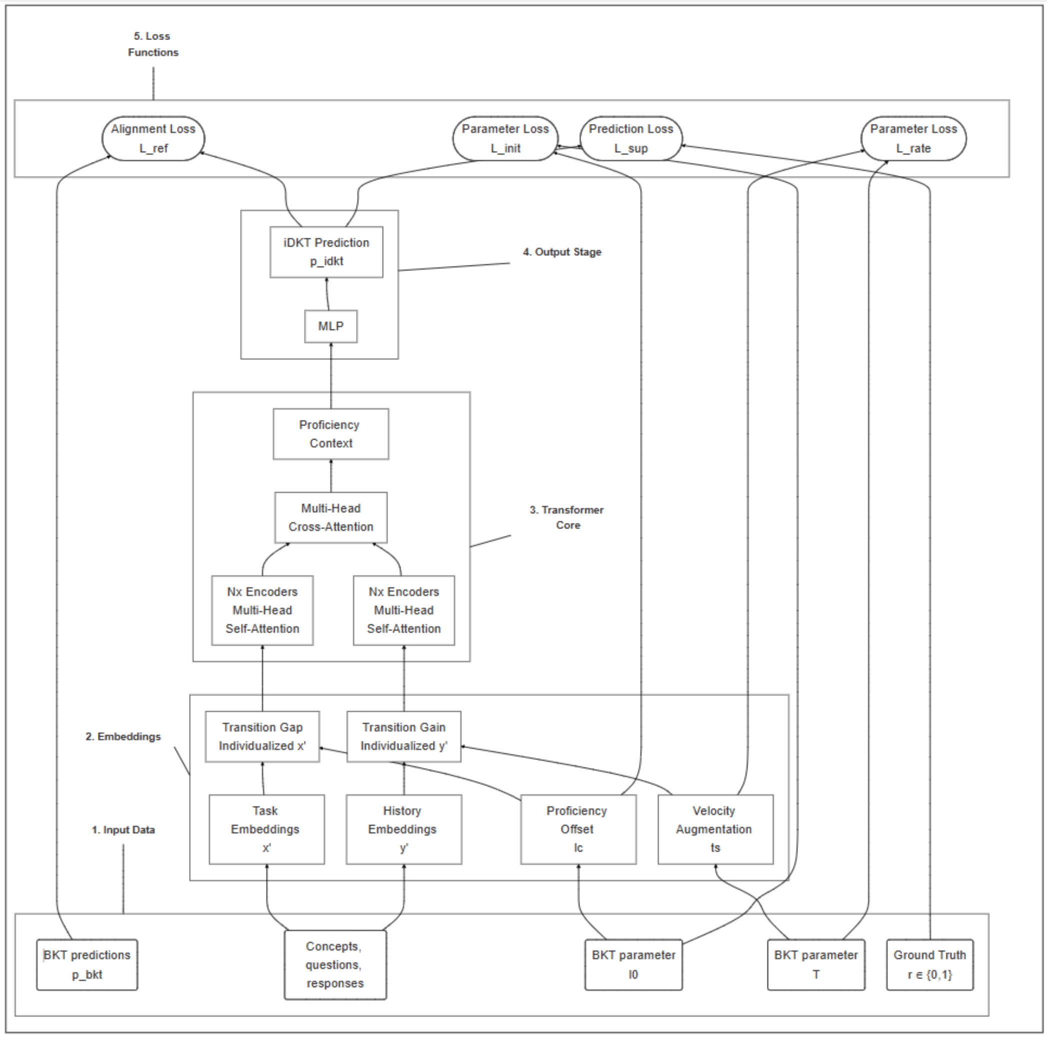

Figure 1. The iDKT Architecture. The diagram illustrates the five functional stages: (1) Input Data ingestion including BKT targets, (2) Individualized Embeddings, (3) the Transformer Core, (4) the MLP-based Output, and (5) the Loss Functions for representational grounding.

other questions involving the same concept. Consequently, rather than encode arbitrary embeddings for every question, we encode the vector sum of two distinct components with clear semantic meaning: a base *concept identity* and a *difficulty shift*.

In a similar way, we can operationalize the interactions between questions and students as embedding vectors:

$$y' = e + u \cdot (f + d) \quad \text{(Interaction History)} \tag{4}$$

Here e represents the *Interaction Base*, which is a combined representation of concept c and the binary outcome r (correct/incorrect), while f represents the *Interaction Variation Axis*, which is similar to the Question Variation Axis (d_c) but is specific to the interaction between a question and a student. The inclusion of d_c in the interaction shift ensures that the difficulty vectors are consistent across both questions (x') and interactions (y').

Extending this rationale, we can enrich the x' embeddings by integrating additional components with explicit semantic significance. Specifically, by adopting Bayesian Knowledge Tracing (BKT) as a reference model, we can incorporate vectors corresponding to its core theoretical parameters—Initial Knowledge (L_0) and Learning Rate (T)—thereby grounding the deep representation in established pedagogical constructs.

To get individualized values for these parameters, we decompose them into population-level bases and student-specific deviations:

$$l_c = L_0 + k_s \cdot d_k \quad \text{(Personalized Initial Knowledge)} \tag{5}$$

$$t_c = T + v_s \cdot d_v \quad \text{(Personalized Learning Rate)} \tag{6}$$

where l_c is the personalized initial knowledge for concept, t_c is the personalized learning rate for concept, L_0 and T are the population-level base embeddings, d_k and d_v are the learnable variation axes vectors (similar to the difficulty axis d), and k_s and v_s are the scalar student-specific deviations learned for each individual.

We include these vectors to get the final input embedding for the encoder and decoder components of the Transformer:

$$x' = (c + u \cdot d) - l_c \quad \text{(Individualized Task)} \tag{7}$$

$$y' = (e + u \cdot (f + d)) + t_c \quad \text{(Individualized Interaction History)} \tag{8}$$

where c represents the concept embedding, u the question-specific difficulty shift, d the task variation axis, e the interaction base, f the interaction variation axis, l_c the personalized initial knowledge, and t_c the personalized learning rate.

The rationale for using difference for the individualized task (x') and sum for the interaction history (y') is due to their distinct semantic roles:

- x' represents the *Transition Gap*: $\textit{Difficulty} - \textit{Proficiency}$. Under this relational logic, objective task difficulty is offset by prior proficiency, ensuring that task demands are defined relative to the subject's baseline. This formulation captures the difference between the task requirements and the current state, representing the residual gap after accounting for latent proficiency.
- y' represents the *Transition Gain*: $\textit{Interaction} + \textit{Rate}$. The history encoder accumulates evidence from interactions, applying a consistent relational logic where the signal value is augmented by latent rate, ensuring that interaction outcomes are defined relative to the subject's pace. Under this formulation, the total value encompasses not

only the interaction outcome but also the rate of progress through the state trajectory, as this incremental gain serves as a robust indicator of future performance. This approach, therefore, captures latent progression by augmenting observed outcomes with transition rate, thereby reflecting individualized acquisition rates.

5. Loss Functions

The model is trained using a multi-objective loss function designed to ensure that the high-capacity Transformer remains aligned with pedagogical principles through Representational Grounding. The total loss $\mathcal{L}_{total}$ is defined as a weighted sum of different loss components described in detail below.

$$\mathcal{L}_{total} = L_{sup} + \lambda_{ref} L_{ref} + \lambda_{init} L_{init} + \lambda_{rate} L_{rate} + L_{reg} \tag{9}$$

5.1. Supervised Alignment (L_{sup})

The primary objective L_{sup} uses standard Binary Cross-Entropy (BCE) between the iDKT performance predictions $\hat{y}_t$ and the observed ground truth outcomes $r_t \in \{0,1\}$. This loss ensures predictive accuracy by minimizing the deviance from observed student behavior:

$$L_{sup} = -\frac{1}{N} \sum_{t=1}^{N} [r_t \log(\hat{y}_t) + (1 - r_t) \log(1 - \hat{y}_t)] \tag{10}$$

5.2. Representational Grounding

The grounding losses ($L_{ref}, L_{init}, L_{rate}$) use Mean Squared Error (MSE) to anchor deep representations to BKT-derived values. Specifically, L_{ref} forces behavioral predictions to stay close to the theoretical baseline, while L_{init} and L_{rate} ground the individualized parameters l_c and t_c in meaningful educational starting points and acquisition paces, respectively. Instead of arbitrary latent weights, the model's internal states are projected through a sigmoid activation $\sigma(\cdot)$ and compared directly to the reference values:

$$L_{ref} = \text{MSE}(\hat{y}, p_{BKT}) \tag{11}$$

$$L_{init} = \text{MSE}(\sigma(\bar{l}_c), L0_{BKT}) \tag{12}$$

$$L_{rate} = \text{MSE}(\sigma(\bar{t}_c), T_{BKT}) \tag{13}$$

where $\bar{l}_c$ and $\bar{t}_c$ are the average across the feature dimension of the individualized embeddings for proficiency and rate, respectively. This formulation forces the deep representation to be not only predictive but also semantically consistent with the reference constructs.

5.3. Inductive Bias Regularization (L_{reg})

While the grounding losses anchor the global position of the latent space to the BKT parameter estimations, L_{reg} ensures that student-level individualization is *parsimonious*. This loss acts directly on the individualization parameters (u_q, k_s, v_s) to ensure that the model only deviates from the theoretical prior when functionally necessary. We apply distinct L_2 penalties to the scalar parameters governing variation:

$$L_{reg} = \lambda_{\text{u}} \sum_{q \in Q} u_q^2 + \lambda_{\text{k}} \sum_{s \in S} k_s^2 + \lambda_{\text{v}} \sum_{s \in S} v_s^2 \tag{14}$$

where u_q represents item difficulty, k_s is the student-specific knowledge gap, and v_s is the learning rate deviation. This formulation implements a *normal student prior*: the model assumes every subject adheres to the population-level parameters derived from the BKT

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reference unless their unique interaction history provides sufficient signal to justify the regularization cost.

6. Results and Discussion

6.1. Research Questions

The experimental validation of iDKT is guided by the following research questions:

1. **Interpretability Validation (RQ1)**: Is it possible to rigorously validate that a iDKT model, whose representations are grounded in a reference model, actually yields interpretable constructs?
2. **Trade-Off between Predictive Performance and Interpretability (RQ2)**: To what extent can deep knowledge tracing models be constrained for interpretability alignment without significantly degrading predictive performance?
3. **Improvement of Pedagogical Diagnostics (RQ3)**: How can the Transformer's ability to capture longitudinal context be utilized to improve or complement pedagogical diagnostics?

6.2. Experimental Setup

We implemented the iDKT model in `PyTorch` and used the benchmark library `PYKT` [22] to leverage standardized data preprocessing, dataset splitting and benchmarking of baseline models. For training, we used standard 5-fold cross-validation with an 80/20 train/test split. The model was trained using the Adam optimizer with a learning rate of $1e-4$, a batch size of 64, and a dropout rate of 0.2 to prevent overfitting. The maximum number of epochs was set to 200, with an early stopping mechanism (patience=10) to terminate training if validation performance plateaued.

The Transformer architecture was configured with an embedding dimension d_{model} of 256, 8 attention heads, and 4 encoder/decoder blocks. The feed-forward dimension d_{ff} was set to 512. Regularization penalties for individualization parameters (L_2 on u_q, k_s, v_s) were all set to $1e-5$. For reproducibility, all experiments were seeded (seed=42) and executed on NVIDIA A100 GPU infrastructure. Predictive performance was evaluated using Area Under the ROC Curve (AUC) and Accuracy (ACC), while interpretability was assessed using the metrics defined in Section 6.5.

6.3. Datasets

We did the evaluation of iDKT with these 5 widely used datasets:

• ASSISTments2009: A dataset consisting of math exercises, collected from the free online tutoring ASSISTments platform in 2009-2010. It is one of the most widely used and has been the standard benchmark for many years [23].

• ASSISTments2015: This dataset was collected from the ASSISTments platform in the year of 2015. It has the largest number of students among the other ASSISTments datasets [23].

• Algebra2005: A dataset from the KDD Cup 2010 EDM Challenge containing questions from the Carnegie Learning Algebra system deployed 2005-2006 [24].

• Bridge2006: A dataset from the KDD Cup 2010 EDM Challenge with the Carnegie Learning Bridge to Algebra system, deployed 2006-2007 [25].

• NIPS34: A dataset collected from the Eedi platform [26] containing answers to multiple-choice diagnostic math questions for the Tasks 3 & 4 at the NeurIPS 2020 Education Challenge.

6.4. Predictive Performance

To evaluate the predictive performance of the iDKT model, we used the Area Under the Curve (AUC) and the Classification Accuracy (ACC) of the models on the test set with the 5 datasets described in Section 6.3. The results are shown in the Table 1.

Table 1. Predictive Performance of the iDKT model across 5 datasets.

Model	AS2009_S	AS2015	Algebra2005	Bridge2006	NIPS34
iDKT	0.8255	0.7252	0.9281	0.8092	0.7987

When comparing these results with state-of-the-art DKT models reported in [22], we observe that iDKT achieves the best predictive performance on the AS2009 and Algebra2005 datasets and ranks second on the Bridge2006 and NIPS34 datasets, surpassed only by the AKT model.

6.5. Interpretability Validation (RQ1)

To verify that iDKT's internal representations—specifically Personalized Initial Knowledge ($\mathbf{l}_c$) and Personalized Learning Rate ($\mathbf{t}_c$) as defined in Equations 5 and 6—faithfully represent the educational constructs postulated by the reference model, we employ two metrics widely utilized in psychometrics and educational measurement [27,28]:

1. *Convergent Validity (Latent Fidelity)*: This metric, denoted as I_1, is calculated as the Pearson correlation (r) between the projected latent factors (l_u, t_u) and the reference BKT parameters (L_0 and T). High alignment proves the model has successfully internalized the theoretical constructs.
   The metrics are expressed as:
   $$I_{1l} = \text{Corr}(l_u, L_0) \quad \text{and} \quad I_{1t} = \text{Corr}(t_u, T) \tag{15}$$
   where the projected latent factors are calculated via:
   $$l_u = \sigma(\bar{l}_c), \quad t_u = \sigma(\bar{t}_c) \tag{16}$$
   with $\bar{l}_c$ and $\bar{t}_c$ representing the mean across the feature dimension of the individualized embeddings.
2. *Predictor Equivalence (Behavioral Alignment)*: This metric, denoted as I_2, assesses the functional substitutability of iDKT parameters by executing a *cross-model simulation*. We "inject" the projected iDKT parameters (l_u and t_u) into the canonical BKT recurrence equations to generate *induced mastery trajectories*. This allows us to verify whether the learned factors preserve their causal roles. The metric is statistically quantified as the Pearson correlation coefficient between these induced trajectories and the theoretical reference trajectories generated by the original BKT model:
   $$I_2 = \text{Corr}\Big(P(L)_{ind}, P(L)_{ref}\Big) \tag{17}$$
   where $P(L)_{ind}$ and $P(L)_{ref}$ represent the sequences of mastery probabilities at each timestep for the induced and reference models, respectively.

Table 2 shows interpretability metrics for the unconstrained iDKT model ($\lambda_{ref} = 0$).

Upon enabling Representational Grounding ($\lambda_{ref} = 0.10$), we observe a significant restoration of semantic alignment, as detailed in Table 3.

Table 2. Interpretability Alignment Metrics for unconstrained iDKT ($\lambda_{ref} = 0$).

Dataset	I_1 **(Init.)**	**Int.**	I_1 **(Rate)**	**Int.**	I_2	**Int.**
AS2009	-0.1382	Poor	-0.0067	Negl.	0.1870	Poor
AS2015	-0.0392	Negl.	0.0908	Negl.	0.0975	Negl.
Algebra2005	-0.0602	Negl.	-0.0273	Negl.	0.0600	Negl.
Bridge2006	-0.0645	Negl.	0.0160	Negl.	0.0809	Negl.
NIPS34	0.2070	Poor	-0.0425	Negl.	0.1722	Poor

Table 3. Interpretability Alignment Metrics for grounded iDKT ($\lambda_{ref} = 0.1$).

Dataset	I_1 **(Init.)**	**Int.**	I_1 **(Rate)**	**Int.**	I_2	**Int.**
AS2009_S	0.5409	Good	0.3131	Fair	0.6250	Excell.
AS2015	0.9217	Excell.	0.8801	Excell.	0.1749	Poor
Algebra2005	0.5444	Good	0.3310	Fair	0.0661	Negl.
Bridge2006	0.4561	Fair	0.6422	Good	0.0859	Negl.

The results presented in Tables 2 and 3 reveal a notable divergence between *Convergent Validity* (I_1) and *Predictor Equivalence* (I_2). Although I_1 attains high levels across most datasets even with relatively low λ_{ref} grounding weights, I_2 remains consistently low.

High I_1 scores demonstrate that iDKT successfully internalizes the *semantic identity* of the theoretical constructs (Initial Knowledge and Learning Rate). However, I_2 measures functional substitutability within a comparatively constrained reference model that is unable to capture the intricate behavioral patterns identified by iDKT. As a high-capacity Transformer, iDKT captures complex, long-range dependencies and context-aware dynamics that exceed the modeling capability of classical BKT. This discrepancy provides empirical evidence that iDKT does not merely mimic the reference model, but rather maps its core pedagogical constructs onto a more sophisticated and predictive architecture.

6.6. Accuracy–Interpretability Trade-Off (RQ2)

Prediction performance and interpretability are considered as two opposing goals. Our approach to explore such trade-off is based in building a Pareto frontier, which is constructed by gradually increasing the grounding weight λ_{ref} defined in Equation **??** and plotting the resulting values of performance and interpretability.

We measure interpretability using the *Composite Alignment* $\bar{I}$ metric, defined as the arithmetic mean of the individual alignment components I_1 and I_2 defined in Equations 15 and 17:

$$I = \frac{1}{3}(I_{1l} + I_{1t} + I_2) \tag{18}$$

Tables 4 and 6 summarize the performance and alignment results for the ASSISTments 2009 and 2015 datasets across a systematic sweep of the grounding weight λ_{ref} (Equation **??**).

Figures 5 and 7 illustrate the resulting Pareto frontiers. We observe that theoretical guidance serves as a powerful regularizer, although the *Saturation Point* (the weight at which interpretability is maximized) varies by dataset complexity. For the problem-level *ASSISTments 2009*, synergy is achieved at $\lambda = 0.10$ and saturation at $\lambda = 0.30$. Conversely, the concept-level *ASSISTments 2015* reaches saturation faster at $\lambda = 0.10$, retaining 99.9% of accuracy. Beyond these points, we observe a *grounding collapse* in both datasets, where the model fails to reconcile excessive constraints with behavioral evidence.

6.7. Improvement of Pedagogical Diagnostics (RQ3)

In the following sections, we analyze how the architectural design of iDKT can be leveraged to improve pedagogical diagnostics

Table 4. Pareto Sweep results for ASSISTments 2015.

λ_{ref}	Performance (AUC)	Interpretability (I)	Interpretation
0.0 (Baseline)	0.7248	-0.0012	Black Box
0.1 (Saturation Point)	0.7245	0.6673	99.9% AUC Retained
0.2	0.7181	0.6453	High-Fidelity Diagnostic
0.3	0.7112	0.6095	Latent Degradation
0.4	0.7047	0.6377	Latent Degradation
0.5	0.6975	0.5691	Theory-Dominant
0.6	0.6918	0.5337	Latent Degradation
0.7	0.6874	0.5331	Latent Degradation
0.8	0.6830	0.4828	Grounding Collapse
1.0	0.6763	0.4828	Grounding Collapse

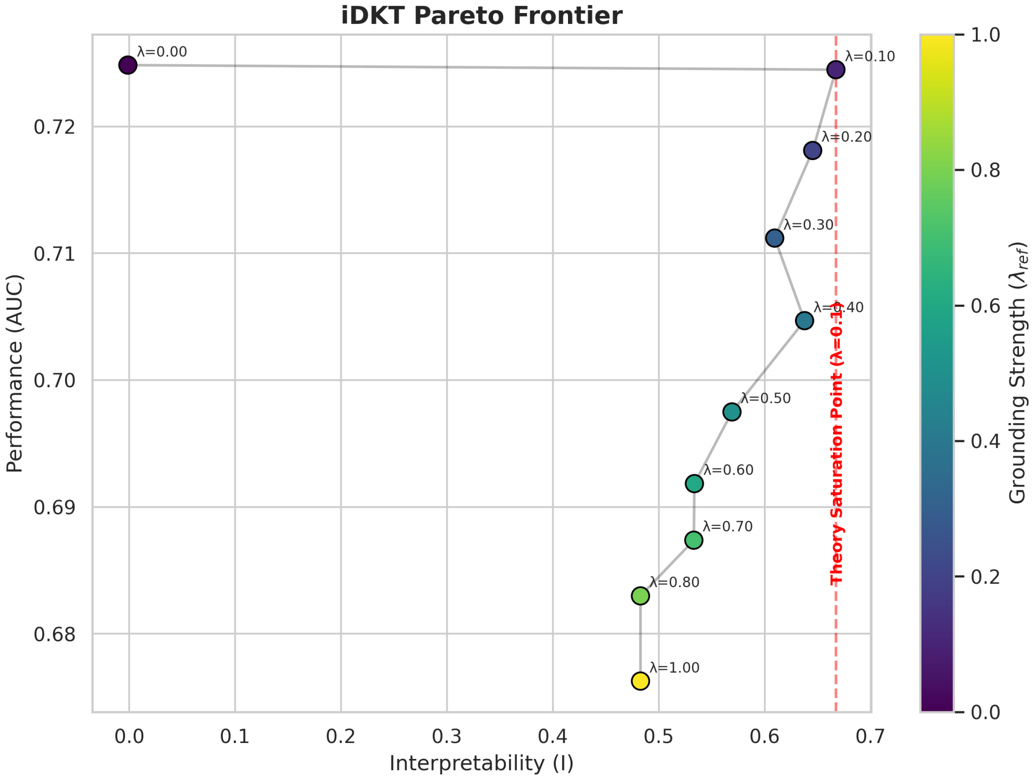

Table 5. iDKT Pareto Frontier for ASSISTments 2015. The trajectory illustrates a saturation of theoretical alignment at $\lambda \approx 0.2$, followed by a drift at higher weights where performance is traded without gaining interpretability.

Table 6. Pareto Sweep results for ASSISTments 2009.

λ_{ref}	Performance (AUC)	Interpretability (I)	Interpretation
0.0 (Baseline)	0.8207	0.0293	Unconstrained Black Box
0.1 (Synergy Spot)	0.8255	0.3846	Accuracy-Interpretability Synergy
0.2	0.8110	0.4270	Theory-Balanced Inductive Bias
0.3 (Saturation Point)	0.7963	0.4790	Theoretical Saturation (Max Int.)
0.4	0.7824	0.2740	Non-monotonicity
0.5	0.7760	0.4125	Grounding Degradation
0.6	0.7692	0.3587	Grounding Degradation
0.7	0.7629	0.2781	Grounding Degradation
0.8	0.7552	0.0708	Grounding Collapse
1.0	0.7501	0.0714	Grounding Collapse

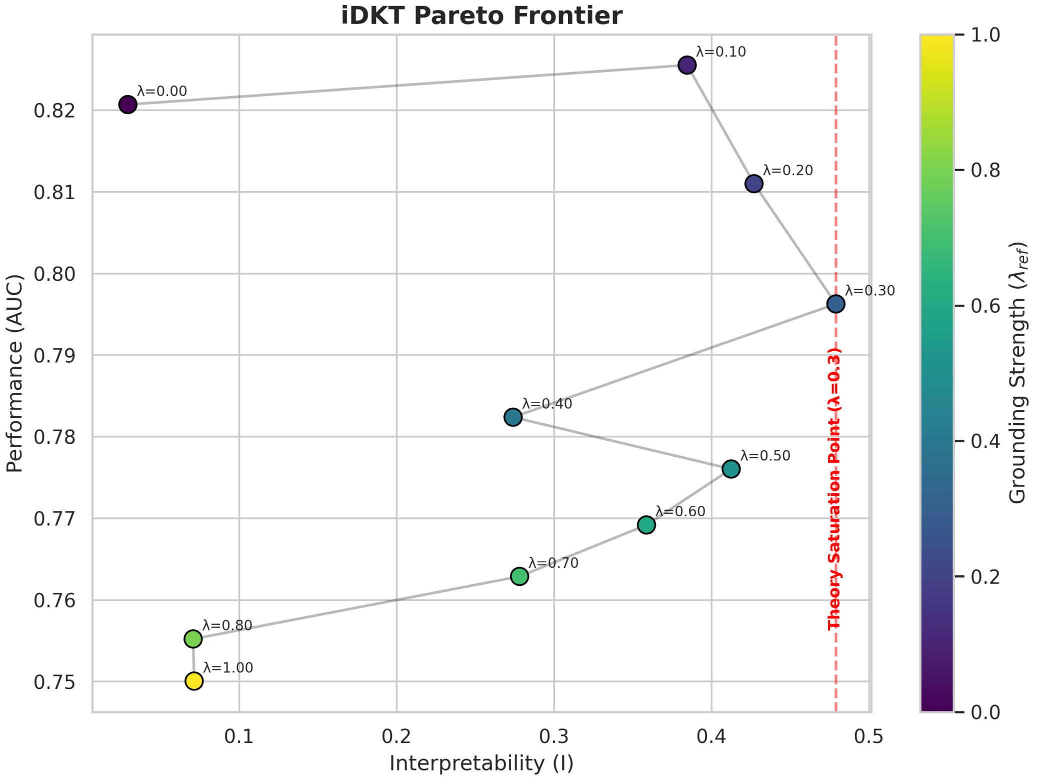

Table 7. iDKT Pareto Frontier for ASSISTments 2009. The curve displays a *synergy point* where performance peaks at $\lambda = 0.1$, followed by a *grounding collapse* as excessive constraints over-regularize the latent space.

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6.7.1. Contextualization

The capability of iDKT to leverage longitudinal context is illustrated in Figure 2, which contrasts its mastery estimations with the BKT baseline for a high-proficiency learner. While BKT leads to excessive volatility—where isolated failures are interpreted as significant knowledge drops—iDKT maintains a stable and resilient diagnostic trajectory.

The core of this advantage lies in the self-attention mechanism, which enables iDKT to encode longitudinal context by dynamically weighting the entire interaction history. Instead of relying solely on the most recent state, iDKT evaluates each interaction in the context of the student's established behavioral patterns. In the scenario shown in Figure 2, the model maintains a high mastery estimation despite sporadic failures because the attention weights remain anchored to the student's longitudinal progression. This capacity to distinguish between temporary behavioral noise (e.g., slips) and genuine changes in knowledge state represents a fundamental improvement over classical baselines, supporting robust and individualized diagnostics.

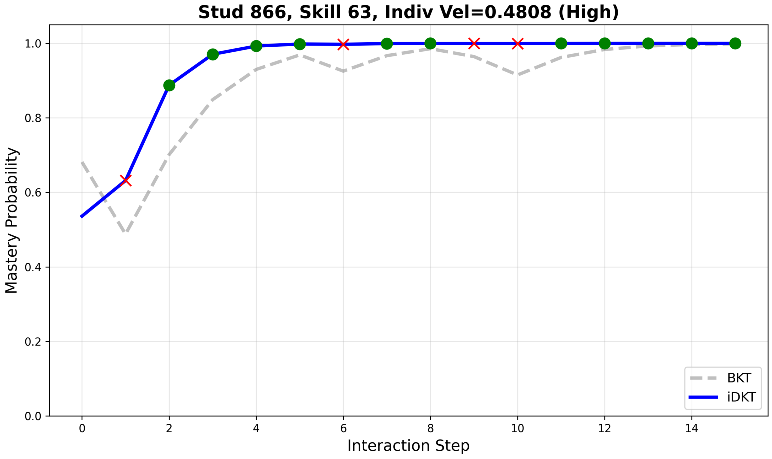

Figure 2. Comparison of two mastery trajectories estimated by iDKT and BKT illustrating how iDKT can be more stable and resilient against behavioral noise.

6.7.2. Individualization

The primary value of iDKT lies in its ability to transform population-level theoretical averages into high-granular contextual diagnostics. While standard BKT assumes that every student shares a fixed initial mastery (L_0) and learning rate (T) for a given skill, iDKT decomposes these into individualized profiles.

To statistically quantify this granularity, we analyze the *delta distribution* ($\Delta = t_s - T$), representing the student-specific deviation from the theoretical learning rate across all skills. In both ASSISTments datasets, we observe a significant non-zero standard deviation ($\sigma \approx 0.019$ for AS2009 and $\sigma \approx 0.039$ for AS2015). This represents a substantial increase in diagnostic resolution compared to the BKT baseline, where $\sigma = 0$. The right-skewed tail in the distributions identifies a sub-population of fast learners whose true acquisition pace is systematically underestimated by classical models.

Figure **??** visualizes the delta distributions for both datasets. The width of the curves quantifies the pedagogical information that is lost when using population-level averages. This variance allows the system to distinguish between students who are faster than suggested by theoretical priors and those who require additional practice to reach mastery.

6.7.3. High-Granularity Trajectory Analysis

To provide definitive visual evidence for RQ3, we generated a Mastery Alignment Mosaic (Figure 3) displaying individualized trajectories for three learning archetypes (Fast, Median, Slow) across 15 skills. For rigorous validation, we utilized the “Set S Isolation” strategy, restricting the analysis to students with continuous interaction histories (≤ 200 steps) and recalibrating the BKT reference exclusively on this population.

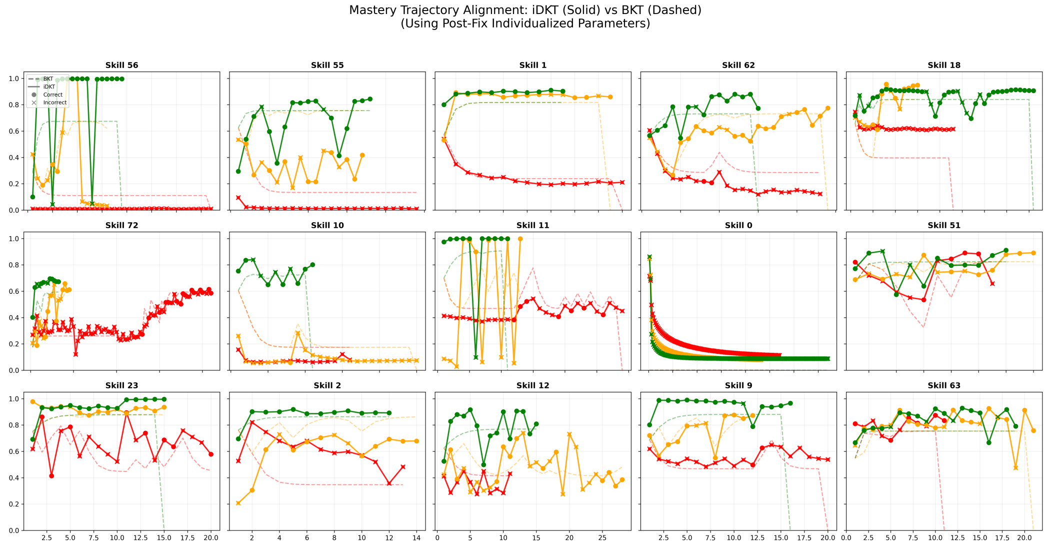

Figure 3. Mastery Trajectory Alignment Mosaic for AS2009_S. Solid lines represent iDKT individualized mastery, while dashed lines show the BKT baseline. Markers indicate observed student performance (Circle: Correct, X: Incorrect). Trajectories are selected from students with > 10 interactions per skill.

The qualitative analysis of these trajectories reveals three significant pedagogical insights:

1. **Dynamic Diagnostic Placement**: Even when BKT is forced to start at the population prior (L_0), iDKT starting points ($t = 1$) vary per student. This demonstrates that iDKT leverages cross-skill behavioral transfers to perform individualized placement before the first interaction with a new skill.
2. **Trajectory Crossovers**: We observe instances where students starting with lower initial mastery overtake peers due to a higher identified learning velocity (t_s). This confirms iDKT’s ability to model individualized acquisition rates beyond population-level curves.
3. **Diagnostic Resilience**: iDKT displays superior stability compared to BKT baselines. While isolated failures cause sharp drops in BKT dashed lines, iDKT solid lines for high-velocity learners remain stable, correctly identifying temporary slips vs. fundamental knowledge loss.

6.7.4. Confidence

Individualized student profiling offers new opportunities for pedagogical monitoring and adaptive intervention. A significant practical application is evaluating the reliability of predictions made by intrinsically interpretable models, such as BKT. By comparing BKT mastery estimations with those from iDKT, we can derive a measure of pedagogical confidence in the theoretical baseline.

This relationship is visualized in Figure 4, which displays the concordance between BKT and iDKT mastery predictions across the sub-population of the most frequent skills

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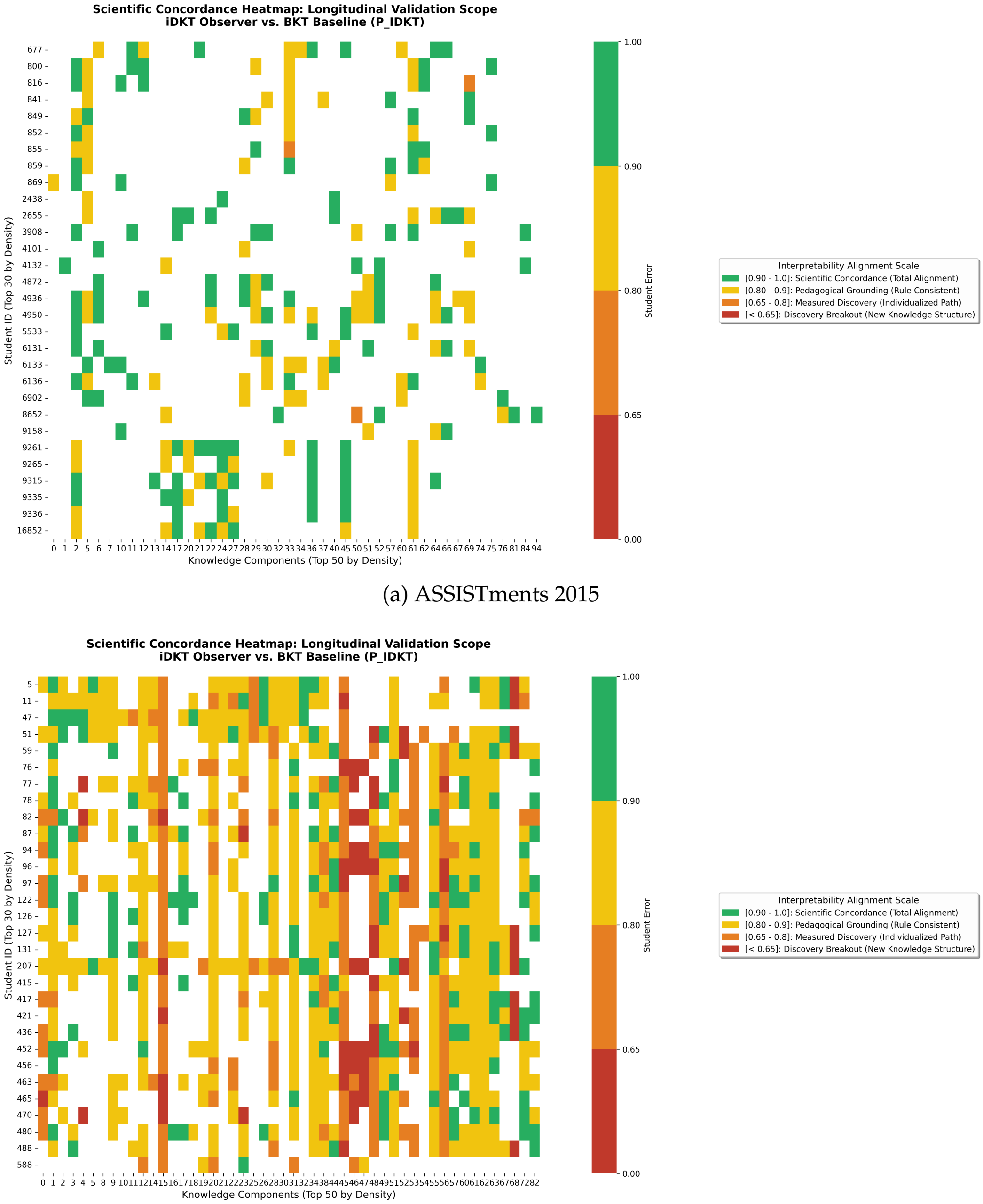
and students for both datasets. The ASSISTments 2015 results demonstrate high levels of agreement, whereas the ASSISTments 2009 data reveals more divergence, where iDKT uncovers individualized patterns beyond the theoretical prior. Such visualizations provide actionable pedagogical insights that complement traditional baseline diagnostics. This visualization framework provides robust support for personalized longitudinal tracking by identifying students or curricular content that deviate from theoretical expectations. These divergences serve as critical diagnostic indicators for cases that may warrant prioritized pedagogical intervention.



(a) ASSISTments 2015

(b) ASSISTments 2009

Figure 4. Heatmaps of per-skill prediction alignment.

7. Conclusions

This work has introduced iDKT, a Transformer-based Knowledge Tracing model that bridges the gap between the high predictive capacity of deep learning and the intrinsic in-

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terpretability of models such as BKT, which utilize constructs with clear semantic meanings. By utilizing Representational Grounding, we have demonstrated that it is possible to anchor deep latent representations to semantically meaningful constructs without sacrificing state-of-the-art performance.

Our experimental results successfully address the research questions. First, we proved that iDKT successfully internalizes the theoretical constructs of the reference model, achieving high convergent validity (I_1). Second, we formalized a methodology for measuring the trade-off between predictive performance and interpretability, enabling the identification of the "Interpretability Sweet Spot" where significant alignment is achieved with minimal loss in predictive AUC. Finally, we demonstrated that iDKT provides a high increase in diagnostic granularity compared to population-level baselines by identifying individualized learning velocities that enable truly adaptive pacing.

The primary contribution of this research is twofold: a robust methodology for evaluating the internal interpretability of Transformer-based models in education, and a practical architecture that transforms "black-box" predictors into interpretable tools for knowledge tracing. By grounding deep learning in established educational concepts, iDKT offers a path toward AI-driven personalization that is both highly accurate and pedagogically actionable, providing a foundation for next-generation intelligent tutoring systems.

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