DEEP LEARNING IMPROVES PARAMETER ESTIMATION IN REINFORCEMENT LEARNING MODELS

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ABSTRACT

Cognitive modeling in psychology and neuroscience provides a formal approach to formulate and test hypotheses of cognitive processes. Such models rely on cognitive parameters that are intended to represent interpretable and identifiable psychological constructs. However, accurately and reliably estimating model parameters remains challenging due to common issues such as limited data, measurement noise, experimental constraints, and model complexity, hindering the interpretability and identifiability of cognitive parameters. Given the recent success of advanced optimization methods in deep learning, we investigate whether a deep learning pipeline that integrates neural networks and modern optimization techniques can improve parameter estimation in reinforcement learning (RL) models. We compare this approach with the Nelder-Mead method (`fminsearch`), the de facto optimization approach in cognitive modeling, by fitting RL models to *ten* diverse value-based decision-making datasets collected from both humans and animals. Surprisingly, while both approaches achieve comparable predictive performance, they produce distinct parameter estimates, indicating fitting performance alone is insufficient in identifying these parameters. We thus systematically evaluate the reliability of parameters estimated by each approach and find that parameters estimated via the deep learning pipeline consistently demonstrate smaller gaps between training and test performance (better generalizability), increased resistance to parameter perturbations (enhanced robustness), improved recovery of ground-truth parameters in low-data regimes (stronger identifiability), and greater consistency across repeated measurements from the same individuals (better test-retest reliability). Our findings advocate for the deep learning pipeline and systematic evaluation of cognitive parameters to better link these parameters to psychological constructs and neural mechanisms.

Keywords Computational Modeling · Parameter Estimation · Reinforcement Learning · Deep Learning

1 Introduction

In neuroscience and psychology, cognitive models are widely used to investigate the mental processes underlying human and animal behavior. These models formalize how organisms learn from experience, make decisions, and adapt to their environment. One of the most successful modeling frameworks is reinforcement learning (RL), which describes how agents make decisions by learning value functions based on rewards and task-related feedback (Rescorla and Wagner, 1972; Sutton and Barto, 1998). Previous research has identified neural substrates underlying RL computations (Lee et al., 2012; Niv, 2009; Schultz et al., 1997), providing evidence for the biological implementation of RL mechanisms.

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These RL models typically employ a small number of free parameters to characterize hypothesized cognitive processes. These parameters are not merely tunable quantities to produce model predictions, but are hypothesized to represent interpretable, identifiable psychological constructs (Wilson and Collins, 2019) such as learning rates for value updating, inverse temperatures for choice stochasticity, and choice perseveration for inertia. Accurately and reliably estimating these parameters is thus essential for interpreting the models and linking them to psychological traits and neural mechanisms (Browning et al., 2015; Huys et al., 2021; Suthaharan et al., 2021). In practice, however, obtaining reliable estimates is often challenging due to constraints common in human and animal experiments, including limited data, inherent stochasticity of behavior, non-convex loss landscapes in models' parameter space, and the low diagnostic power of task designs to precisely isolate specific cognitive mechanisms from observed behavior. The optimization methods for identifying parameter combinations that best predict subjects' behavior thus play a critical role in addressing these difficulties in parameter estimation.

A widely used parameter estimation technique in cognitive modeling is the Nelder–Mead simplex method (Nelder and Mead, 1965), which is the default optimization algorithm in MATLAB's `fminsearch` (The MathWorks, Inc., 2024) and SciPy's `fmin` (Virtanen et al., 2020) functions. Its off-the-shelf availability has led to widespread adoption across nearly every subfield of cognitive modeling (for representative applications, see Akam et al., 2015; Busemeyer and Myung, 1987; Busemeyer and Diederich, 2010; Dowman et al., 2016; Forstmann et al., 2011; Gershman, 2018; Li et al., 2023; Pouget et al., 2011; Shinn et al., 2020; Wilson et al., 2019; Yechiam and Busemeyer, 2005). In contrast, while modern optimization methods widely used in deep learning have achieved great success on estimating parameters in deep neural networks, they remain underutilized in cognitive modeling (cf. Binz et al., 2024; Giallanza et al., 2024). Furthermore, although different optimization methods have been compared in terms of model fitting performance in cognitive modeling (e.g., (Acerbi and Ma, 2017)), less is known about the reliability of the parameter estimates produced by these methods.

In this study, we propose a deep learning pipeline that integrates neural networks and modern optimization techniques to estimate RL model parameters. We then compare this pipeline with the Nelder–Mead method in estimating parameters across ten behavioral datasets involving humans and animals performing bandit tasks with different action spaces, reward structures, and time horizons. We find that, surprisingly, although both optimization methods achieve similar predictive performance on held-out data, they often yield different distributions of estimated parameters across subjects in most tasks. This suggests that predictive performance alone cannot sufficiently justify the estimated parameters — distinct estimates but with similar losses undermine the interpretability of these parameters.

We systematically evaluate the parameters estimated by both optimization methods along three key dimensions: generalizability, robustness, and identifiability. The deep learning pipeline yields a smaller generalization gap, more robust parameter estimates, and superior parameter recovery when data are limited. Additionally, it achieves higher test-retest reliability in a dataset with repeated measurements from the same subject. Our results demonstrate that different optimization methods can result in RL parameter estimates converging on different minima, thereby affecting their generalizability, robustness, and identifiability. Furthermore, our findings indicate that the modern deep learning pipeline provides a promising approach for parameter estimation in cognitive modeling.

2 Results

2.1 Datasets and models

To systematically compare different optimization methods in parameter estimation, we analyze ten diverse decision-making datasets: (1) a 2-armed horizon task in humans designed to study exploration behaviors under varying horizons and uncertainty (`Wilson2014`) (Wilson et al., 2014); (2) a 3-armed horizon task in humans, an extension of the previous horizon task with varying horizons and information availability (`Dubois2022`) (Dubois and Hauser, 2022); (3) a 2-armed restless bandit task in mice, featuring drifting reward probabilities for binary rewards (`Chen2021`) (Chen et al., 2021); (4) a 4-armed restless bandit task in humans with continuously drifting rewards (`Bahrami2020`) (Bahrami and Navajas, 2020); (5) a 3-armed probabilistic reversal learning task in humans with binary rewards and dynamically changing reward probabilities (`Suthaharan2021`) (Suthaharan et al., 2021; Reed et al., 2020); (6) a 3-armed probabilistic reversal learning task in mice (`Groman2018`) (Groman et al., 2018); (7, 8) a 2-armed bandit task in humans with continuous rewards sampled from a Gaussian distribution and a horizon of 10 trials (`Gershman2018` and `Schurr2024`) (Gershman, 2018; Schurr et al., 2024); (9) a 2-armed instrumental learning task in humans, where the two arms have different reward probabilities (`Dezfouli2019`) (Dezfouli et al., 2019); (10) the Iowa Gambling Task in humans (`Steingroever2015`) (Steingroever et al., 2015). These tasks encompass diverse experimental designs to investigate biological value-based decision-making across varying reward distributions, environmental volatility, and time horizons, providing a comprehensive benchmark for comparison (for details, see Methods "Datasets").

We adopt the simplest and most widely used formulation of the RL model, in which the action value Q_t for the chosen action A_t at trial t is updated as follows:

$$Q_t(A_t) = Q_{t-1}(A_t) + \alpha \left(r_t - Q_{t-1}(A_t)\right), \tag{1}$$

where r_t is the reward at trial t, and α denotes the learning rate specifying how quickly the values are updated.

For action selection, we use a Softmax policy:

$$\Pr(A_t) = \frac{e^{\beta Q_t(A_t) + \kappa \delta(A_t, A_{t-1})}}{\sum_{A'} e^{\beta Q_t(A') + \kappa \delta(A', A_{t-1})}}, \tag{2}$$

where β is the inverse temperature specifying the action determinism, κ is the choice perseverance parameter reflecting an inertia tendency, and $\delta(A_t, A_{t-1})$ equals 1 if $A_t = A_{t-1}$ and 0 otherwise.

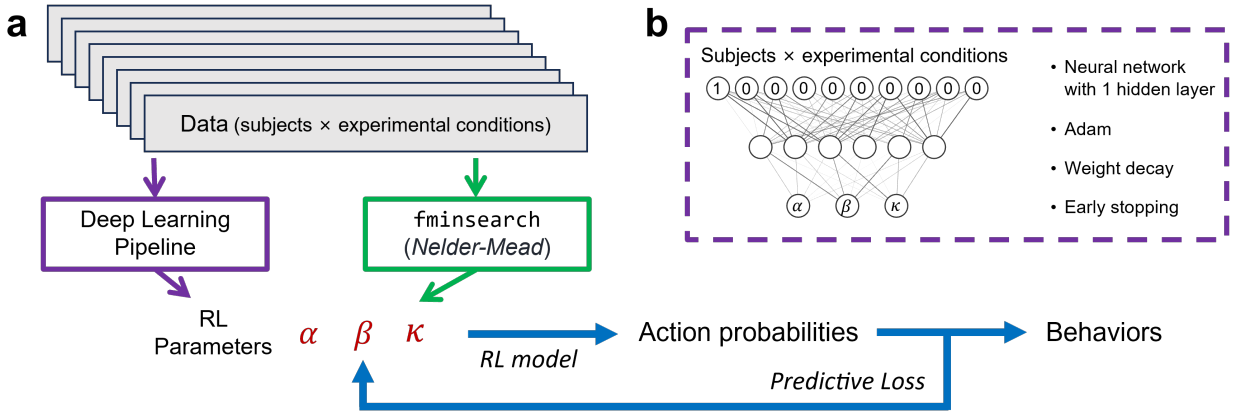

Figure 1: **Comparison of the Nelder-Mead method and the deep learning pipeline. a**, Both approaches optimize parameters in reinforcement learning (RL) models for each subject and each experimental condition to predict their choice behavior. **b**, The deep learning pipeline incorporates a neural network with one hidden layer, the AdamW optimizer (Adam with decoupled weight decay), and early stopping to estimate RL parameters.

2.2 Two optimization methods produce distinct parameter estimates

We apply the Nelder–Mead method and a deep learning pipeline to fit RL models to behavioral data by adjusting a set of RL parameters (α, β, κ) for each subject and experimental condition, aiming to minimize the cross-entropy between the models' predictions and subjects' choices (Fig. 1a). The Nelder–Mead method directly optimizes the RL parameters. In contrast, our deep learning pipeline (Fig. 1b) uses a neural network with one hidden layer, which takes one-hot embeddings of each subject and experimental condition as input and outputs the corresponding RL parameters (see Methods "Neural network model" for details). The network parameters are optimized by the gradient-based optimizer AdamW (Kingma and Ba, 2017) to minimize the cross-entropy between the models' predictions and subjects' choices. To improve generalization, we further incorporate weight-decay regularization (Krogh and Hertz, 1991; Loshchilov and Hutter, 2019) and early stopping (Amari et al., 1997; Finnoff et al., 1993). The fitting performance of both optimization methods is evaluated using cross-validation: the parameters are optimized on training data, and the performance is evaluated on held-out test data (see Methods "Model fitting" for details).

We find that the Nelder–Mead and deep learning pipeline performed similarly on held-out test data across ten datasets (Fig. 2a). No significant difference in average performance is observed across ten datasets (Fig. 2b, Wilcoxon signed-rank test: $W = 12.0, p = .131$, Cohen's $d = 0.031$), indicating that both methods performed similarly across diverse datasets.

To determine whether the two methods yield similar parameter estimates, we analyze the marginal distributions of estimated parameters across subjects and experimental conditions in ten datasets. Surprisingly, the two methods produce distinct parameter distributions (Fig. 3) despite achieving similar predictive performance on test data. While the distributions of κ largely overlap between the two methods, those of α and β differ significantly in some datasets. For instance, the deep learning pipeline tends to produce less extreme estimates (i.e., those on the boundary; e.g., see α

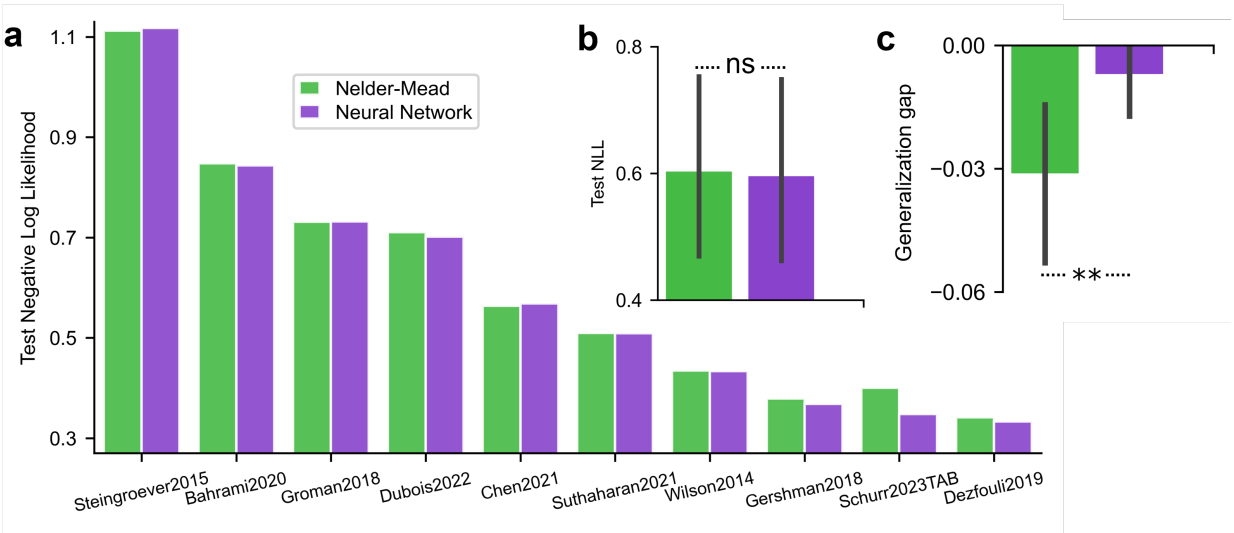

Figure 2: **Comparison of the Nelder–Mead and the deep learning pipeline across ten decision-making datasets. a**, Predictive performance of RL models optimized using both methods. The deep learning pipeline achieves a negative log-likelihood (lower is better) comparable to that of the Nelder–Mead method on held-out test data. **b**, Predictive performance averaged across all datasets. Both methods achieve comparable negative log-likelihoods on held-out test data. **c**, The generalization gap, defined as the difference in negative log-likelihood between training and testing, averaged across all datasets. The Nelder–Mead method exhibits a larger generalization gap, indicating potential overfitting on the training data. Error bars in **b,c** represent 95% confidence interval across ten datasets. `ns`: not significant. $**$: $p < 0.01$.

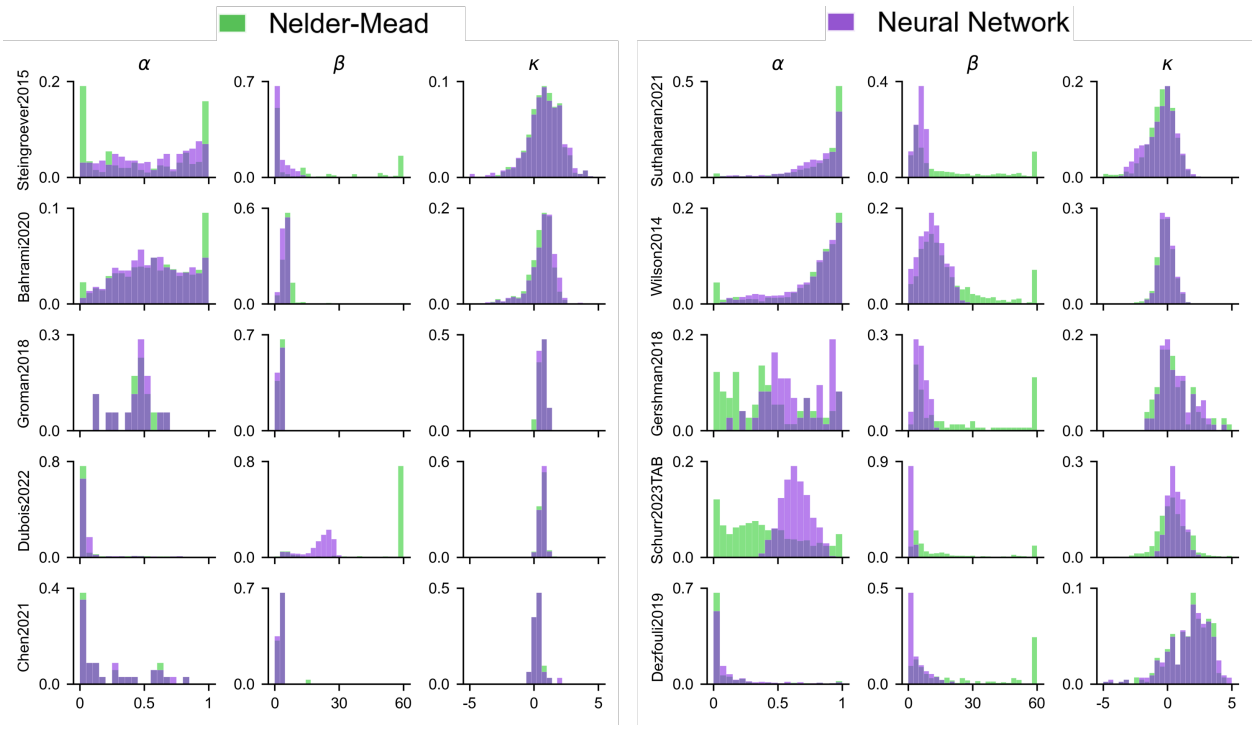

Figure 3: **Marginal distributions of RL parameters estimated by the Nelder–Mead and deep learning pipeline.** Each panel depicts the distribution of a single parameter (α, β, κ) across all subjects and experimental conditions within a dataset. The two methods produce distinct parameter distributions across ten datasets.

in `Steingroever2015` and β in `Dubois2022`). This finding that the two methods often find parameter estimates in different regions of the parameter space raises concerns about the reliability of the interpretation of the individual parameters. Without further metrics to discriminate among these different estimates, scientific conclusions tied to a single estimate could be ambiguous and misleading.

2.3 Deep learning pipeline shows better generalizability

Given that the two methods produce different parameter estimates, we examine how these estimates differ in their properties beyond predictive performance. We first assess potential overfitting by comparing the generalization gap (Keskar et al., 2017) between the two methods, defined as the difference in negative log-likelihood between the training and test sets. A negative generalization gap indicates potential overfitting on the training data. The deep learning pipeline exhibits a smaller generalization gap than the Nelder–Mead method (Fig. 2c, Wilcoxon signed-rank test: $W = 0.0, p = .002$, Cohen's $d = -0.956$), suggesting that it may produce better parameter estimates with reduced overfitting, thereby improving generalization.

2.4 Deep learning pipeline shows enhanced robustness

Next, we use expected sharpness (Neyshabur et al., 2017) to evaluate the robustness of each model to parameter perturbations around parameter estimates obtained by the two optimization methods. This metric quantifies the model's sensitivity to parameter perturbations, characterizing the flatness of the loss landscape around the identified minima. Such "wide flat minima" are associated with improved generalization (Hochreiter and Schmidhuber, 1997; Neyshabur et al., 2017; Xie et al., 2021).

We perturb the RL parameters estimated by both methods on each trial by adding the same independently and identically distributed (i.i.d.) zero-mean white Gaussian noise with varying levels of variance. We then compute the loss (negative log-likelihood) between subjects' behavior and the predictions of RL models using the perturbed parameters. The resulting loss increases are averaged across subjects and experimental conditions for each dataset (Fig. 4a), and then averaged across datasets (Fig. 4b). Across all datasets, we observe that loss increases (indicating decreased performance) with greater noise magnitude. Notably, the loss increases more slowly for the deep learning pipeline than for the Nelder–Mead method (Wilcoxon signed-rank test: $W = 49.0, p < .001$), indicating greater overall robustness. These findings suggest that parameters estimated by the deep learning pipeline are more robust, less sensitive to parameter noise, and correspond to flatter minima.

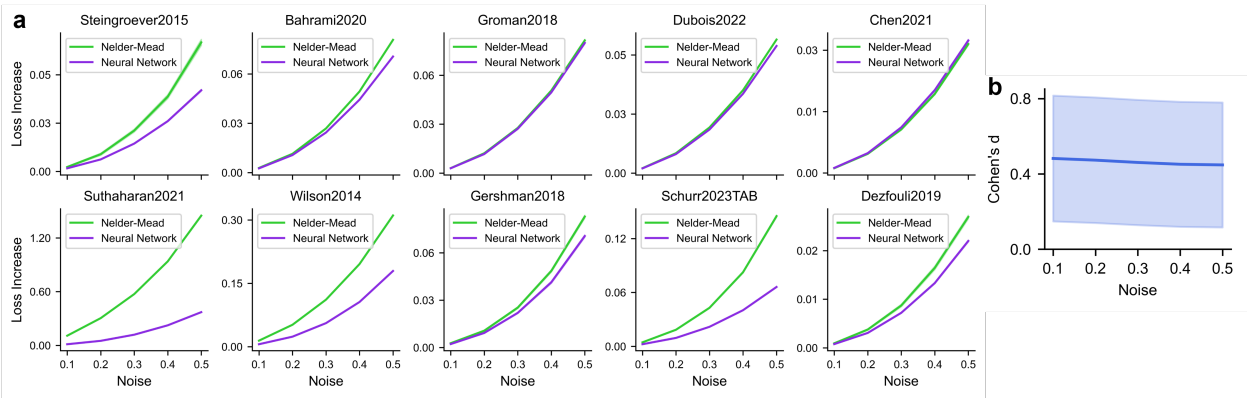

Figure 4: **Model robustness under parameter perturbations at varying noise levels. a,** Parameters estimated by the deep learning pipeline exhibit smaller increases in loss in response to injected white Gaussian noise, compared to the Nelder–Mead method, meaning lower expected sharpness and greater robustness to perturbation. The shaded area (mostly invisible) represents the 95% confidence interval across 10,000 simulations. **b,** Effect size of the difference in loss increase between the Nelder–Mead method and the neural network, in which the Nelder–Mead method shows a greater loss increase across ten datasets. The shaded area denotes the 95% confidence interval across ten datasets.

2.5 Deep learning pipeline shows better identifiability

Having shown that the deep learning pipeline yields RL parameters with greater generalizability and robustness, we now examine another crucial criterion for meaningful interpretation — identifiability, defined as the ability to reliably

recover ground-truth parameters from simulated data (Wilson and Collins, 2019). To this end, we generate simulated datasets from the model using fixed, known parameter values, and then re-estimate those parameters by fitting the same model structure to the data, treating those RL parameters as free parameters in both optimization methods. If the estimated parameters match the ground-truth values used to generate the data, the model is considered highly identifiable. Conversely, if the ground-truth parameters cannot be reliably recovered, the estimates derived from empirical data may lack interpretability with respect to underlying cognitive processes. Although identifiability is largely shaped by the task, data, and model, the optimization method also plays a critical role. For example, some methods may locate the global minimum of the loss landscape more efficiently, thereby enhancing identifiability. To compare the identifiability of the two methods, we select four tasks representing a range of task structures (Fig. 5).

We simulate varying amounts of data from RL models using 125 parameter combinations (five values spanning a plausible range for each parameter) and assess recovery performance using the correlation and mean absolute error between estimated and ground-truth parameters (see Methods "Parameter recovery"). Recovery performance improves for both methods as the number of trials per subject increases, reaching similar levels with sufficient data (3200 trials). However, residual errors between estimated and ground-truth parameters remain in some tasks even with sufficient trials (e.g., Fig. 5b, 2-armed instrumental learning, third row), suggesting that identifiability may be fundamentally constrained by the task and model structure.

Notably, the deep learning pipeline outperforms the Nelder–Mead method in most tasks when trial counts per subject are limited (a range comparable to typical sample sizes in psychological experiments, as indicated by red and blue bars in Fig. 5). This result is surprising given the common belief that deep learning methods require a large amount of data to be effective. These results suggest that the deep learning pipeline is well-suited for typical dataset sizes, as it more accurately recovers ground-truth parameters.

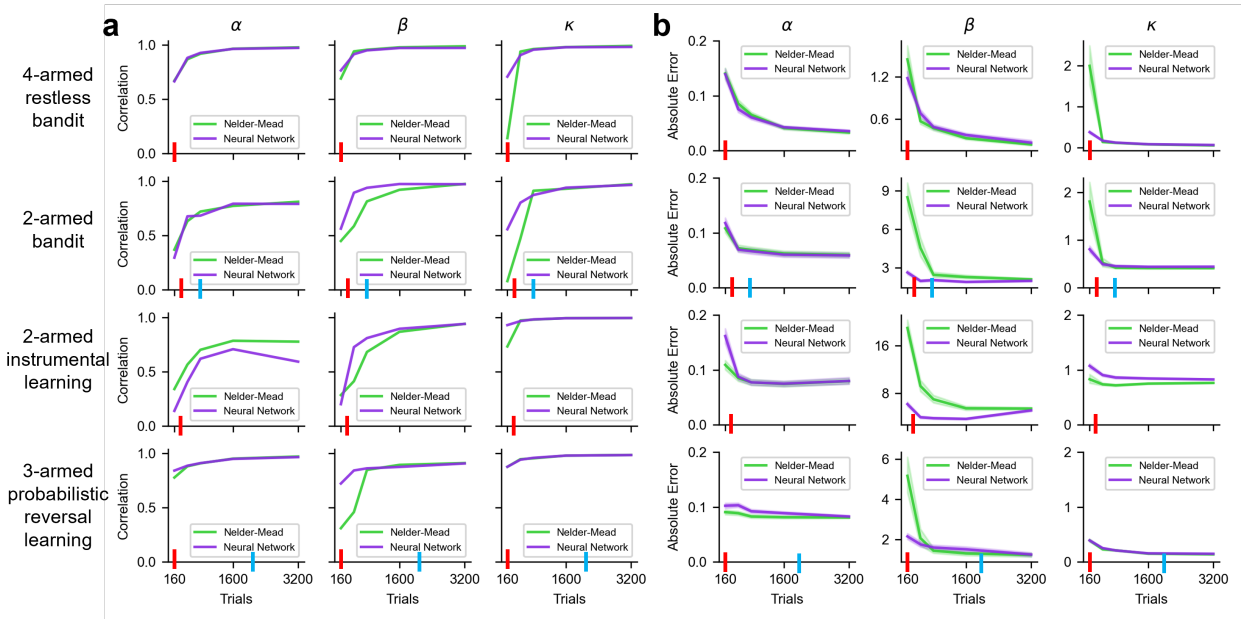

Figure 5: **Parameter recovery using the Nelder–Mead and deep learning pipeline across varying amounts of simulated data from an RL model.** The deep learning pipeline achieves higher or comparable **(a)** correlations with ground-truth parameters and **(b)** lower or comparable absolute errors across most tasks. The shaded area (barely visible) denotes the 95% confidence interval across all parameter combinations. Red and blue ticks on the x-axis indicate the average number of trials per subject in our datasets: 4-armed restless bandit (red - `Bahrami2020`); 2-armed bandit (red - `Gershman2018`, `Schurr2023TAB`; blue - `Wilson2014`); 2-armed instrumental learning (red - `Dezfouli2019`); and 3-armed probabilistic reversal learning (red - `Suthaharan2021`; blue - `Groman2018`).

2.6 Deep learning pipeline improves test-retest reliability

In previous sections, we showed that the deep learning pipeline demonstrates better generalizability, robustness, and identifiability in estimating RL parameters. But how do these properties translate into more direct and intuitive

connections to psychology and cognitive science? One such metric is test-retest reliability, a core concept in psychology, which assesses the consistency of scores for the same subjects tested under similar conditions at different time points. A high test-retest reliability of parameter estimates is favored by computational phenotyping (Patzelt et al., 2018) in predicting clinical outcomes and treatment development.

We analyze a unique dataset, `Schurr2023TAB` (Schurr et al., 2024), in which subjects performed a two-armed bandit task over 12 consecutive weeks, allowing us to measure correlations across repeated assessments for the same individuals. Following the exclusion criteria and methodology from the original study (Schurr et al., 2024), we compute the intra-class correlation (ICC) of the RL model parameters, a widely used measure of test-retest reliability.

To further control for differences in fitting performance between the two methods, we select a subset of subjects (41 out of 90) for whom the negative log-likelihood (NLL) differed by less than 0.02 (Fig. 6a; NLL quantile: Q1 = -0.006, Q3 = 0.012). These results remain consistent when applying different threshold values.

Despite controlling for fitting performance, the two methods produce distinct parameter distributions (Fig. 6b). The deep learning pipeline also demonstrates greater robustness to parameter perturbations (Fig. 6c). Crucially, the deep learning pipeline yields significantly higher ICC values for the estimated RL parameters (Fig. 6d): β: $t(40) = 3.25, p = .002$, Cohen's $d = 0.52$; κ: $t(40) = 5.10, p < .001$, Cohen's $d = 0.97$. The only exception is α, which shows no significant difference ($t(40) = 0.71, p = .481$, Cohen's $d = 0.06$), indicating stronger test-retest reliability overall. These findings suggest that the deep learning pipeline extracts more consistent parameter estimates across repeated measurements from the same individuals.

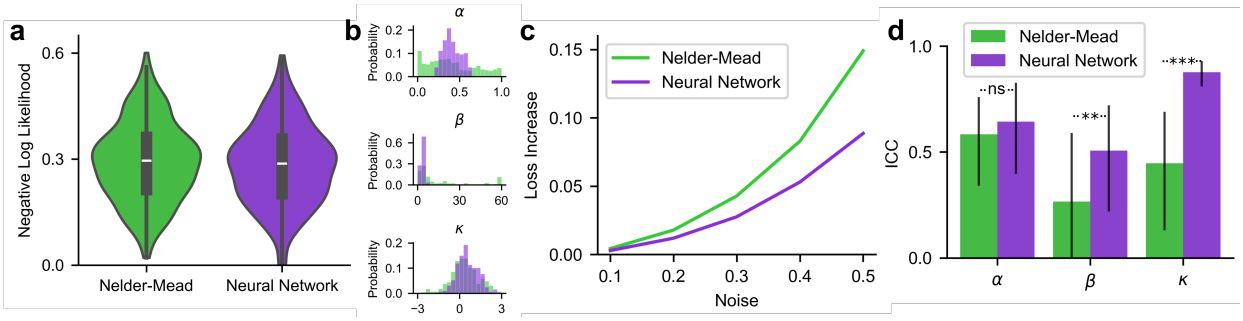

Figure 6: **Comparison of the Nelder–Mead method and the deep learning pipeline on the `Schurr2023TAB` dataset with multiple measurements from the same subjects.** A subset of subjects was selected to control for fitting performance (see main text). **a**, Both methods show similar distributions of fitting performance. **b**, The two methods yield distinct parameter distributions. **c**, The deep learning pipeline exhibits greater robustness to parameter perturbations. The shaded area (mostly not visible) represents the 95% confidence interval across 10,000 simulations. **d**, The deep learning pipeline achieves higher ICC values for the estimated parameters across eight weekly measurements from the same subjects, compared to the Nelder–Mead method. Error bars represent 95% confidence intervals across subjects. Significance levels are denoted as follows: ns = not significant, * $p < .05$, ** $p < .01$, *** $p < .001$.

3 Discussion

In cognitive modeling, parameters are not merely tunable quantities that yield good predictions; they are intended to represent interpretable psychological constructs. Therefore, accurate and reliable parameter estimation is crucial for interpreting cognitive strategies and linking them to neural data. In this work, we proposed a deep learning pipeline for parameter estimation and systematically evaluated its properties against traditional optimization methods in fitting RL models, using ten value-based decision-making datasets. Our evaluation focuses on several key dimensions: fitting performance, generalizability, robustness, identifiability, and test-retest reliability.

While both the de facto Nelder–Mead method (`fminsearch`) and our deep learning pipeline achieve comparable performance on held-out test data, they produce notably different parameter distributions. Since cognitive parameters are assumed to index distinct psychological constructs, these discrepancies carry important scientific implications. They suggest that identical behavior may be interpreted differently due to the fitting method used, potentially affecting conclusions about cognitive mechanisms or individual differences.

Moreover, the deep learning pipeline exhibits a smaller generalization gap, reduced sensitivity to parameter noise, and superior parameter recovery in low-data settings. Most notably, it substantially improves test-retest reliability, a

key determinant of replicability in cognitive research. Our contribution lies not only in demonstrating that the deep learning pipeline can outperform canonical methods but also in highlighting that the choice of optimization algorithm can meaningfully affect estimated cognitive parameters across diverse datasets, even when predictive performance is similar. To our knowledge, this is the first systematic evaluation of how different optimization methods influence parameter estimation across multiple metrics and datasets in cognitive modeling.

Generalizability refers to a model's ability to perform well on unseen, held-out data, ideally under novel conditions. Greater generalization suggests that a model has captured deeper mechanisms that more effectively summarize behavioral patterns. In our study, both methods achieve similar test performance across the ten datasets, indicating no significant advantage in out-of-sample predictive accuracy for the deep learning pipeline. This may reflect the simplicity of the RL model used. However, the deep learning pipeline exhibits a smaller generalization gap—the performance difference between training and test data—indicating stronger generalizability in a weaker sense. We anticipate that its advantages in predictive performance will become more pronounced when applied to complex cognitive models and high-dimensional tasks, given the established strength of deep neural networks in such settings.

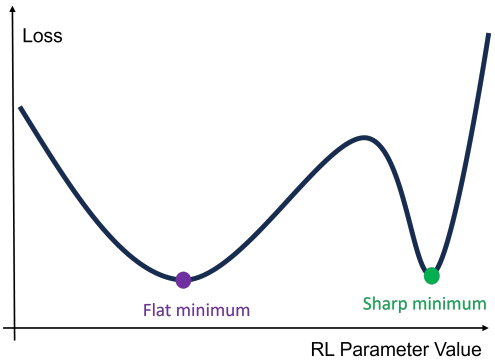

Figure 7: **Illustration of parameter flatness and sharpness.** In a non-convex loss landscape, different parameter estimates may produce similar losses. flatter minima, where loss remains stabler under small parameter perturbations, are generally considered better solutions and are often associated with stronger generalizability.

In our study, robustness is measured by expected sharpness—the sensitivity of the loss function to parameter perturbations. Despite different parameter estimates yielding similar losses, we found that the solutions identified by the deep learning pipeline exhibit lower sharpness (i.e., greater flatness). Although such flatness is rarely evaluated in cognitive models (but see Frank, 2014), the connection between "wide flat minima" and improved generalization is well established in the machine learning literature (Fig. 7) (Hochreiter and Schmidhuber, 1997; Dinh et al., 2017; Hoffer et al., 2017; Neyshabur, 2017; Xie et al., 2021). Intuitively, when the loss function is highly sensitive to parameter perturbations at sharp minima, stochastic gradient-based optimizers (such as AdamW, which we used) are more likely to "escape" these regions due to noisy updates. Such optimizers act as entropy maximizers, favoring solutions with broader support in parameter space (Chaudhari et al., 2019). They have been theoretically shown to prefer flat over sharp minima, leading to more generalizable solutions in deep neural networks (Xie et al., 2021). In addition, other components of the deep learning pipeline, such as overparameterization and regularization techniques (e.g., weight decay and early stopping), may introduce implicit biases that further promote generalization. Our expected sharpness metric is closely related to the trace of the Hessian (or the Fisher information; see below) and connects to the PAC-Bayesian framework for bounding generalization error in neural networks (Bjorck et al., 2021; Dziugaite and Roy, 2017; Fukumizu et al., 2019; Gubri et al., 2024; Xie et al., 2021). In summary, the deep learning pipeline we employed enhances the robustness and reliability of parameter estimation in cognitive models.

The parameter recovery test provides a measure of model identifiability by examining whether ground-truth parameters can be accurately recovered from simulated data generated using those parameters. High identifiability indicates that the estimated values faithfully represent the underlying cognitive mechanisms. We demonstrated that the deep learning pipeline achieves superior parameter recovery across four widely used decision-making tasks, particularly in the low-data regime typical of human behavioral experiments. Parameter identifiability is closely related to the Fisher information, which underlies the theoretical consistency of maximum likelihood estimation. Taken together, the findings on flatness and identifiability suggest that the deep learning pipeline more reliably identifies flat minima that both generalize better and align more closely with ground-truth parameters compared to the Nelder–Mead method.

Finally, as a concrete application, we show that the deep learning pipeline significantly improves test-retest reliability, which measures the consistency of parameter estimates across repeated measurements. Prior research has reported that

the test-retest reliability of RL parameters is generally poor to modest (Schaaf et al., 2024; Schurr et al., 2024). Owing to the improved generalizability, robustness, and identifiability of the deep learning pipeline, the observed increase in test-retest reliability suggests that the estimated parameters are more stable over time, providing more accurate characterizations of the underlying cognitive processes. This improvement enhances longitudinal cognitive research, including cognitive phenotyping in studies of individual differences in personality, development, and psychiatry (Huys et al., 2021; Montague et al., 2012; Patzelt et al., 2018).

At first glance, identifiability and robustness may appear to be contradictory: the former requires high sensitivity of the likelihood function to changes in parameters (i.e., higher Fisher information), while the latter favors low sensitivity (i.e., a smaller negative Hessian) in the parameter space. However, as shown in the Methods ("Relations between identifiability, robustness, Hessian, and Fisher information"), identifiability and robustness are in fact complementary properties. A well-designed computational model can balance both, where higher Fisher information ensures identifiability, while a bounded Hessian ensures robustness.

In conclusion, our study systematically highlights an important and underappreciated factor in cognitive modeling: the choice of optimization algorithm can significantly shape parameter estimates, even when predictive performance is similar. Compared to the commonly used Nelder–Mead method, the deep learning pipeline—leveraging modern optimization techniques—produces more generalizable, robust, identifiable, and reliable parameter estimates, positioning it as a promising and scalable tool for cognitive modeling.

4 Method

4.1 Datasets

The ten datasets include several types of decision-making tasks performed by both humans and animals, featuring different levels of uncertainty, various reward structures, and horizon lengths.

The two-armed horizon task (Wilson et al., 2014) involves two options (arms), where the value difference between the two arms is sampled from 4, 8, 12, 20, and 30, and rewards are sampled from a normal distribution. The task includes a forced-choice phase in the first four trials, which facilitates the control of the uncertainty level regarding the value of each option. In the free-choice phase, the horizon is set to either 1 or 6, allowing researchers to study how decision-making changes with the amount of available information in the future. This dataset includes data from multiple labs and experiments (Wilson et al., 2014; Feng et al., 2021; Somerville et al., 2017; Waltz et al., 2020; Sadeghiyeh et al., 2020; Zajkowski et al., 2017) with n_{subjects} = 609 and n_{trials} = 754,890.

A three-armed version of this horizon task is presented in (Dubois and Hauser, 2022). This version increases task complexity by introducing a third arm, requiring more strategic considerations when choosing the best option. This dataset includes n_{subjects} = 1,012 and n_{trials} = 173,120.

The two-armed restless bandit task in mice (Chen et al., 2021) uses binary rewards. In this task, the reward probability for each arm changes gradually over time, requiring the mice to continuously adapt their choices based on these shifting probabilities. This dataset includes n_{subjects} = 32 and n_{trials} = 70,778.

The four-armed restless bandit task in humans (Bahrami and Navajas, 2020) features continuously evolving arm values ranging from 0 to 100, which follow an Ornstein–Uhlenbeck process toward 50. The initial values are sampled from a normal distribution, and rewards are drawn based on the arm's current value. Thus, the task incorporates both reward stochasticity and environmental volatility due to the fluctuating arm values. This dataset includes n_{subjects} = 965 and n_{trials} = 139,816.

The three-armed probabilistic reversal learning task in humans (Suthaharan et al., 2021) requires subjects to choose between three arms, each associated with different reward probabilities. In the first two blocks, probabilities are set to [0.9, 0.5, 0.1], and in later blocks, they shift to [0.8, 0.5, 0.2]. After ten consecutive selections of the best option, the reward probabilities are reversed, allowing researchers to examine how individuals respond to changing reward contingencies. This dataset includes n_{subjects} = 1,012 and n_{trials} = 173,120.

The three-armed probabilistic reversal learning task was also conducted in mice (Groman et al., 2018), with reward probabilities of [0.8, 0.5, 0.2], enabling cross-species comparisons of decision-making strategies. This dataset includes n_{subjects} = 17 and n_{trials} = 38,475.

The two-armed bandit task in humans (Gershman, 2018) has a horizon length of 10, with mean reward values sampled from a normal distribution. In experimental condition 1, the mean reward for one arm is fixed at 0, while the other arm's mean reward varies. In experimental condition 2, both arms have varying mean reward values, allowing researchers to examine how subjects balance exploration and exploitation. This dataset includes n_{subjects} = 89 and n_{trials} = 17,800.

Schurr et al. (2024) also tested Experimental Condition 2 of the two-armed bandit task to assess test-retest reliability. In this study, subjects engaged in a two-armed bandit task over 12 consecutive weeks. The dataset comprises 90 subjects and 78,820 trials. Participant exclusion criteria were consistent with those reported in the original paper.

The two-armed instrumental learning task in humans (Dezfouli et al., 2019) involves binary rewards, where the probability of obtaining a reward from one arm is higher than from the other. For the arm with the higher reward probability, the reward probabilities are [0.25, 0.125, 0.08]. For the arm with the lower reward probability, the reward probability is 0.05. The duration of each experimental condition is fixed, allowing the analysis of learning behavior over a defined period, particularly how subjects adapt to consistent reward probabilities. This dataset includes n_{subjects} = 101 and n_{trials} = 132,251.

Finally, the Iowa Gambling Task (Steingroever et al., 2015) presents subjects with four decks of cards, each associated with different reward and punishment structures. This task assesses decision-making under risk, as subjects must learn which decks are more beneficial in the long term based on experienced rewards and penalties. This dataset includes data from multiple labs and experiments, with n_{subjects} = 577 and n_{trials} = 62,525.

4.2 Neural network model

The neural network we used in the deep learning pipeline consists of a single hidden layer with no activation functions and is defined as follows:

$$[\alpha, \beta, \kappa] = \mathbf{W}_2(\mathbf{W}_1\mathbf{e}_{\text{sub}} + \mathbf{b}_2) + \mathbf{b}_1 \tag{3}$$

where $\mathbf{e}_{\text{sub}} \in \mathbb{R}^{n\times n}$ is a one-hot embedding for each subject per experimental condition, with n representing the total number of subjects multiplied by the number of experimental conditions in a given task. The weight matrix $\mathbf{W}_1 \in \mathbb{R}^{h\times n}$ maps the one-hot embedding to a hidden representation, while $\mathbf{b}_1 \in \mathbb{R}^h$ is the corresponding bias term. The second weight matrix $\mathbf{W}_2 \in \mathbb{R}^{3\times h}$ maps the hidden representation to the RL parameters, with bias term $\mathbf{b}_2 \in \mathbb{R}^3$. While this two-layer linear network is equivalent to a single-layer network in its representational power, they have substantially different training dynamics (Saxe et al., 2013). The output RL parameters α, β, κ are then fed in the RL models.

In PyTorch implementation, the entire RL recurrent computation and neural network feedforward computation are both embedded within the computational graph, enabling gradients to be computed via backpropagation through time.

4.3 Model fitting

The optimization objective is the negative log-likelihood of the observed choice data:

$$\mathcal{L} = -\sum_{t=1}^{T}\sum_{i=1}^{n}\Big[c_t^{(i)}\log\big(p_t^{(i)}\big) + \big(1 - c_t^{(i)}\big)\log\Big(1 - p_t^{(i)}\Big)\Big]. \tag{4}$$

Here, $c_t^{(i)}$ denotes the actual choice of subjects i on trial t and $p_t^{(i)}$ denotes the model's prediction probability for the subjects' choices (Eq. 2).

To mitigate overfitting and ensure a fair comparison between both optimization methods, we implemented a rigorous cross-validation protocol. For the Nelder–Mead method, we employed five-fold cross-validation, allocating 80% of the data for training and 20% for testing. For the deep learning pipeline, we adopted a nested cross-validation approach (Ji-An et al., 2023). Specifically, 70% of the data was designated for training, 12.5% for validation (used for early stopping and hyperparameter tuning), and 17.5% for testing. The outer loop comprised eight folds, while the inner loop included five folds.

Given the variability in datasets, experimental designs, and trial counts, we tailored the cross-validation data splits accordingly. For datasets comprising multiple short blocks with identical trial counts (Gershman, 2018; Schurr et al., 2024), we partition data into different blocks. For datasets with multiple short blocks of varying trial counts (each block containing fewer than 40 trials) (Wilson et al., 2014; Dubois and Hauser, 2022), we divided the data into non-overlapping 40-trial segments. When necessary, we added padding to maintain structural uniformity; padded trials were excluded from loss computation. For datasets with relatively few blocks and fewer than 200 trials per block (Bahrami and Navajas, 2020; Suthaharan et al., 2021; Reed et al., 2020; Steingroever et al., 2015), we split the data into non-overlapping trial sets by applying different masks for training, validation, and testing (Hans et al., 2024). For datasets with few blocks but more than 200 trials (Chen et al., 2021; Groman et al., 2018), we divided each session into non-overlapping blocks of 100 trials and add padding when necessary.

For the Nelder–Mead optimization method, parameter fitting for each subject within a given experimental condition underwent 64 independent initializations. For RL parameter estimation, we uniformly sampled four initial points: $\alpha \in [0, 1]$, $\beta \in [0, 60]$, and $\kappa \in [-5, 5]$.

To enhance the robustness of the deep learning pipeline, we augmented the training data by adding Gaussian noise $N(0, 0.01)$ to continuous rewards. Early stopping was applied when validation performance did not improve after 50 training epochs, ensuring that only models with superior validation loss were retained. This strategy has effectively prevented overfitting. Hyperparameters were optimized over the following search space: learning rate from {0.01, 0.02, 0.03}, weight decay from {0.01, 0.1, 0.2}, dropout from {0, 0.1}, and hidden layer sizes h from {50, 100}. The AdamW optimizer with default hyperparameters was used for training. Constraints were enforced on RL parameter estimation, ensuring $\alpha \in [0, 1]$ and $\beta \geq 0$.

The best model was selected based on the lowest negative log-likelihood on the test data, averaged across all folds. For the RL parameters, we averaged them over cross-validation folds. In the Nelder–Mead method, we used all five folds. In the deep learning pipeline, we use five selected folds (outer j and inner fold 0, where $j = 0, 1, 2, 3, 4$). Our results remained consistent for other fold selection protocols.

4.4 Estimating parameter robustness

We assessed parameter robustness by perturbing model parameters and measuring the resulting change in the loss function. Specifically, we added white Gaussian noise at each trial to the fitted parameters $\hat{\theta} \in \{\hat{\alpha}, \hat{\beta}_t, \hat{\kappa}_t\}$ estimated by each optimization method. The noise was independently sampled from a zero-mean Gaussian distribution, with variance scaled by the average parameter:

$$\tilde{\theta}_t = \hat{\theta} + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2 \mu_{\hat{\theta}}^2). \tag{5}$$

μ_θ is the parameter averaged over all subjects and both optimization methods, which ensures a fair comparison. The noise variance coefficient σ^2 was selected from $\{0.1, 0.2, 0.3, 0.4, 0.5\}$. For each predefined σ and optimization method, we generated 10,000 perturbed parameter sets. Each set was used to simulate model predictions, and the corresponding loss was computed as the negative log-likelihood between perturbed model output probabilities and observed behavioral data. We defined robustness (expected sharpness) as the average increase in loss, quantified by the difference between the perturbed and original losses.

4.5 Parameter recovery

For each task, we selected simulated parameters within the most plausible range to perform the parameter recovery test (Wilson and Collins, 2019). This range was approximately defined using the interquartile range (second-to-third quartile) of parameter distributions obtained from our two methods. For tasks where subjects exhibited highly concentrated parameter distributions, we slightly expanded the range. This resulted in the following parameter ranges for each task: $\alpha \in [0.3, 0.9]$, $\beta \in [4, 10]$, and $\kappa \in [0, 1.5]$ for the four-armed restless bandit task (Bahrami and Navajas, 2020); $\alpha \in [0.3, 0.8]$, $\beta \in [4, 15]$, and $\kappa \in [-0.5, 1.5]$ for the two-armed bandit task (Gershman, 2018; Schurr et al., 2024); $\alpha \in [0.05, 0.35]$, $\beta \in [1, 20]$, and $\kappa \in [0, 3]$ for the two-armed instrumental learning task (Dezfouli et al., 2019); and $\alpha \in [0.4, 0.9]$, $\beta \in [4, 12]$, and $\kappa \in [-1.5, 0.5]$ for the three-armed probabilistic reversal learning task (Suthaharan et al., 2021; Reed et al., 2020; Groman et al., 2018).

Within these ranges, we uniformly sampled five values for each parameter. This sampling effectively decouples correlations between the ground-truth parameters. Using these 125 parameter combinations, we simulated data for 1, 3, 5, 10, and 20 sequence, with each sequence consisting of 160 trials. This resulted in datasets containing 160, 480, 800, 1,600, and 3,200 trials per parameter set.

For the four-armed restless bandit task and the three-armed probabilistic reversal learning task, each sequence contained a single block of 160 trials. In the three-armed probabilistic reversal learning task, we used reward probabilities of [0.8, 0.5, 0.2]. In the two-armed bandit task, each sequence consisted of eight blocks of 20 trials, and we used experimental condition 2 from (Gershman, 2018). In the two-armed instrumental learning task, each sequence consisted of two blocks of 80 trials, and we used reward probabilities of [0.125, 0.05], corresponding to the condition in which one arm had a higher reward probability. These choices were made to align with the original task designs.

We then estimated the parameters from the simulated data using both optimization methods across different data sizes, following the same model fitting and selection procedure described in Methods Model fitting. Due to the computational cost of model recovery and the fact that we had 125 distinct parameter combinations, we performed the recovery procedure once for each combination. While this introduces some stochasticity at the level of individual simulations, the large number of combinations provides a robust basis for assessing overall trends in recovery performance.

4.6 Parameter test-retest reliability

To assess the test-retest reliability of RL parameters over multiple measurements, we computed non-parametric bootstrapped intraclass correlations, ICC(2,1), using 1,000 samples, following methods from (Enkavi et al., 2019; Vallat, 2018). For each RL parameter, we used the mean of the posterior distribution as a point estimate and calculated the ICC based on the data of 90 participants with 12 sessions each. However, ICC cannot be computed when data is missing. To address this, we included all participants but restricted the analysis to the maximal number of sessions with complete data, using eight weekly measurements from the same subjects.

4.7 Relations between identifiability, robustness, Hessian, and Fisher information

In this section, we examine the mathematical relationship between robustness (expected sharpness) and identifiability measured in this paper and well-known properties like Fisher information and the Hessian.

Below we consider a statistical model with one parameter θ (the generalization to more parameters is direct). The data X is generated by the model where the parameter takes $\theta = \theta^*$ ($X \sim \theta^*$). The log-likelihood function (equivalent to the negative loss) is defined as

$$\ell(\theta; X) = \log p(X \mid \theta). \tag{6}$$

When θ is a local minimum, ℓ can be locally expanded to the second-order approximation:

$$\ell(\theta + \Delta\theta; X) \approx \ell(\theta; X) + \nabla_\theta \ell(\theta; X)\Delta\theta + \frac{1}{2}\nabla_\theta^2 \ell(\theta; X)\Delta\theta^2 = \ell(\theta; X) + \frac{1}{2}\nabla_\theta^2 \ell(\theta; X)\Delta\theta^2, \tag{7}$$

where the term $\nabla_\theta \ell(\theta; X)$ vanishes. The expected sharpness is then given by:

$$\mathbb{E}_{\Delta\theta}\, \mathbb{E}_{X\sim\theta^*}[\ell(\theta + \Delta\theta; X) - \ell(\theta; X)] \approx \frac{1}{2}\, \mathbb{E}_{X\sim\theta^*}[\nabla_\theta^2 \ell(\theta; X)]\, \mathbb{E}_{\Delta\theta}[\Delta\theta^2] = \frac{1}{2}\, \mathbb{E}_{X\sim\theta^*}\, \mathbf{H}(\theta; X)\, \mathbb{E}_{\Delta\theta}[\Delta\theta^2], \tag{8}$$

where $\mathbf{H}$ is the Hessian matrix which captures the local curvature. When $\Delta\theta \to 0$, the equation between expected sharpness and expected Hessian becomes exact.

When $\theta = \theta^*$, the Fisher information matrix, defined as

$$\mathbf{I}(\theta^*) = \mathbb{E}_{X\sim\theta^*}\left[\nabla \ell(\theta^*; X)\right]^2. \tag{9}$$

is equal to the negative expected Hessian (under standard regularity conditions):

$$\mathbf{I}(\theta^*) = -\mathbb{E}_{X\sim\theta^*}\left[\nabla^2 \ell(\theta^*; X)\right] = -\,\mathbb{E}_{X\sim\theta^*}\, \mathbf{H}(\theta^*; X). \tag{10}$$

The Fisher information matrix measures the amount of information that the data X carries about the unknown ground-truth parameter θ^*. Thus, it directly reflects the identifiability of the ground-truth parameters, as shown in the fact that the maximum likelihood estimator converges in distribution to a normal distribution:

$$\sqrt{N}(\hat{\theta}_{\text{MLE}} - \theta^*) \xrightarrow{d} \mathcal{N}(0, \mathbf{I}(\theta^*)^{-1}). \tag{11}$$

In practice, both the Fisher information matrix and the Hessian are estimated empirically:

$$\hat{F}(\theta^*) = \frac{1}{N}\sum_{i=1}^{N}(\nabla_{\theta^*}\ell(\theta^*; x_i))^2. \tag{12}$$

$$\hat{H}(\theta) = \frac{1}{N}\sum_{i=1}^{N}\nabla_\theta^2 \ell(\theta; x_i). \tag{13}$$

Specifically, these concepts measure distinct aspects of model parameters. The Fisher information for identifiability is always calculated at the ground truth parameters: if $\hat{\mathbf{I}}(\theta_1^*; \{x_1, ..., x_n\} \sim \theta_1^*) > \hat{\mathbf{I}}(\theta_2^*; \{y_1, ..., y_n\} \sim \theta_2^*)$, then θ_1^* has higher identifiability. On the other hand, if $-\hat{\mathbf{H}}(\theta_1^*; \{x_1, ..., x_n\} \sim \theta_1^*) < -\hat{\mathbf{H}}(\theta_2; \{x_1, ..., x_n\} \sim \theta_1^*)$, then then θ_1^* has lower expected sharpness (higher robustness) than θ_2. Notice that θ_2 is referring to a local minimum of the data generated by the ground-truth parameter θ_1^*. Therefore, θ_1^* can have both high identifiability and high robustness.

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Author contributions

Hua-Dong Xiong, Conceptualization, Formal analysis, Data curation, Investigation, Methodology, Project administration, Software, Visualization, Writing – original draft, Writing – review and editing, Conceived the work; Li Ji-An, Conceptualization, Methodology, Project administration, Writing – original draft, Writing – review and editing, Conceived the work; Marcelo G. Mattar, Supervision, Writing – review and editing; Robert C. Wilson, Resources, Supervision, Funding acquisition, Writing – review and editing.

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