Generalization as Diffusion

Human function learning on graphs

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[1] Kondor, R. I., & Lafferty, J. (2002). Diffusion kernels on graphs and other discrete structures. In *Proceedings of the 19th International Conference on Machine Learning* (Vol. 2002, pp. 315–322).
[2] Stachenfeld, K. L., Botvinick, M., & Gershman, S. J. (2014). Design principles of the hippocampal cognitive map. In *Advances in Neural Information Processing Systems 27* (pp. 2528–2536).

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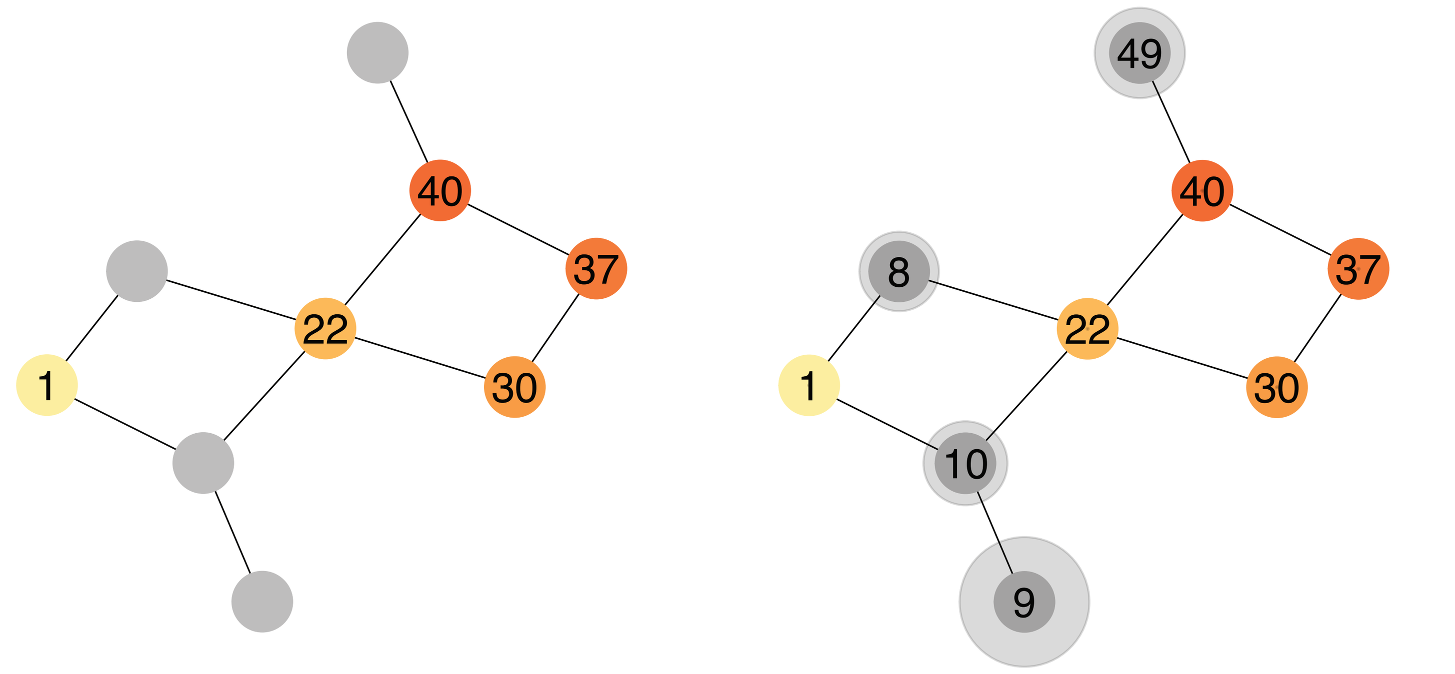
Introduction

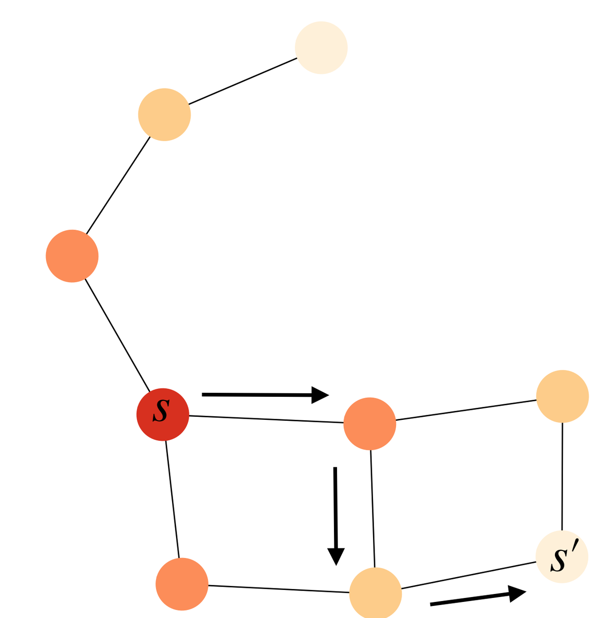
How do people learn functions and generalize in structured environments (e.g., social networks, subway maps, MDPs)?

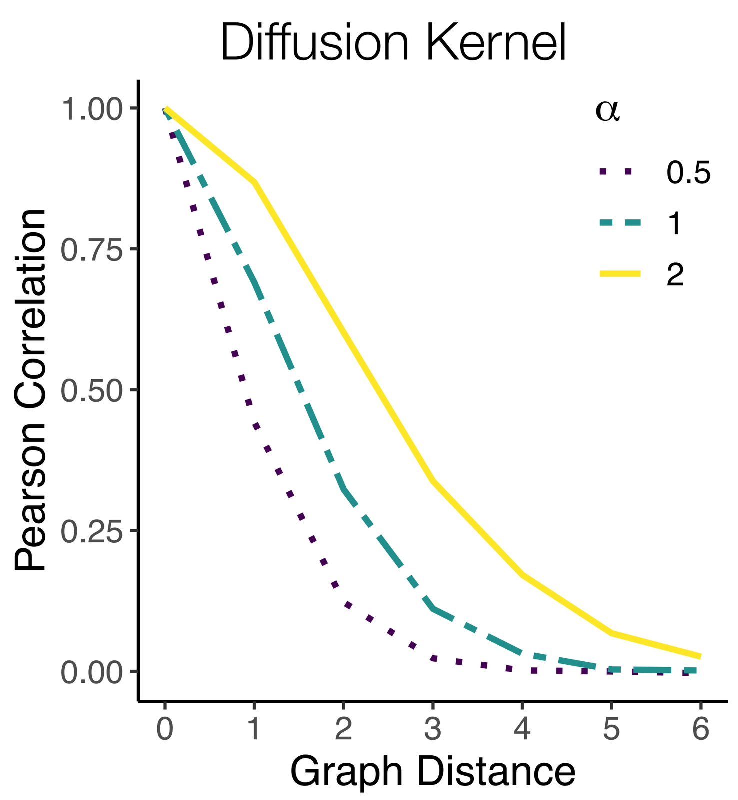


Observations Predictions (with uncertainty)

We propose the **diffusion kernel** [1] as model of human generalization in structured environments, by providing a similarity metric capturing the transition structure of a graph

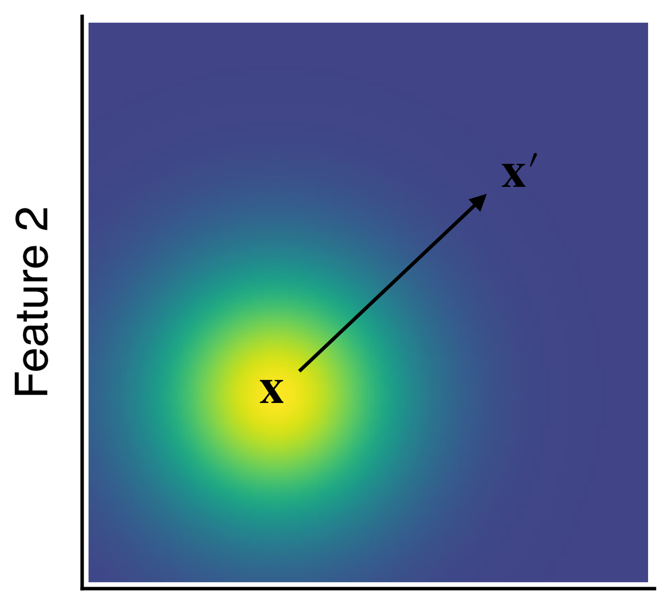
$$k_{DF}(s, s') = \exp(\alpha L)$$

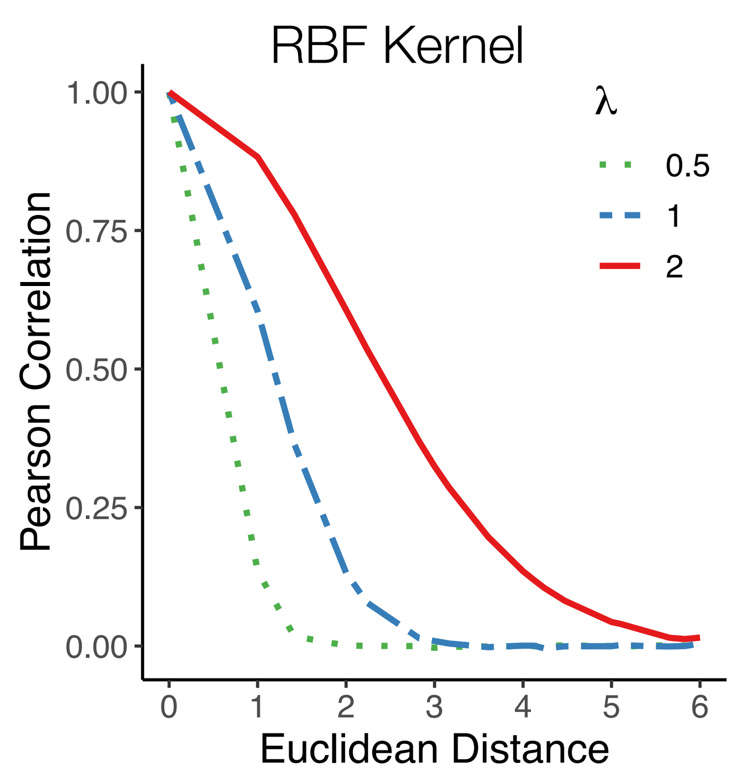




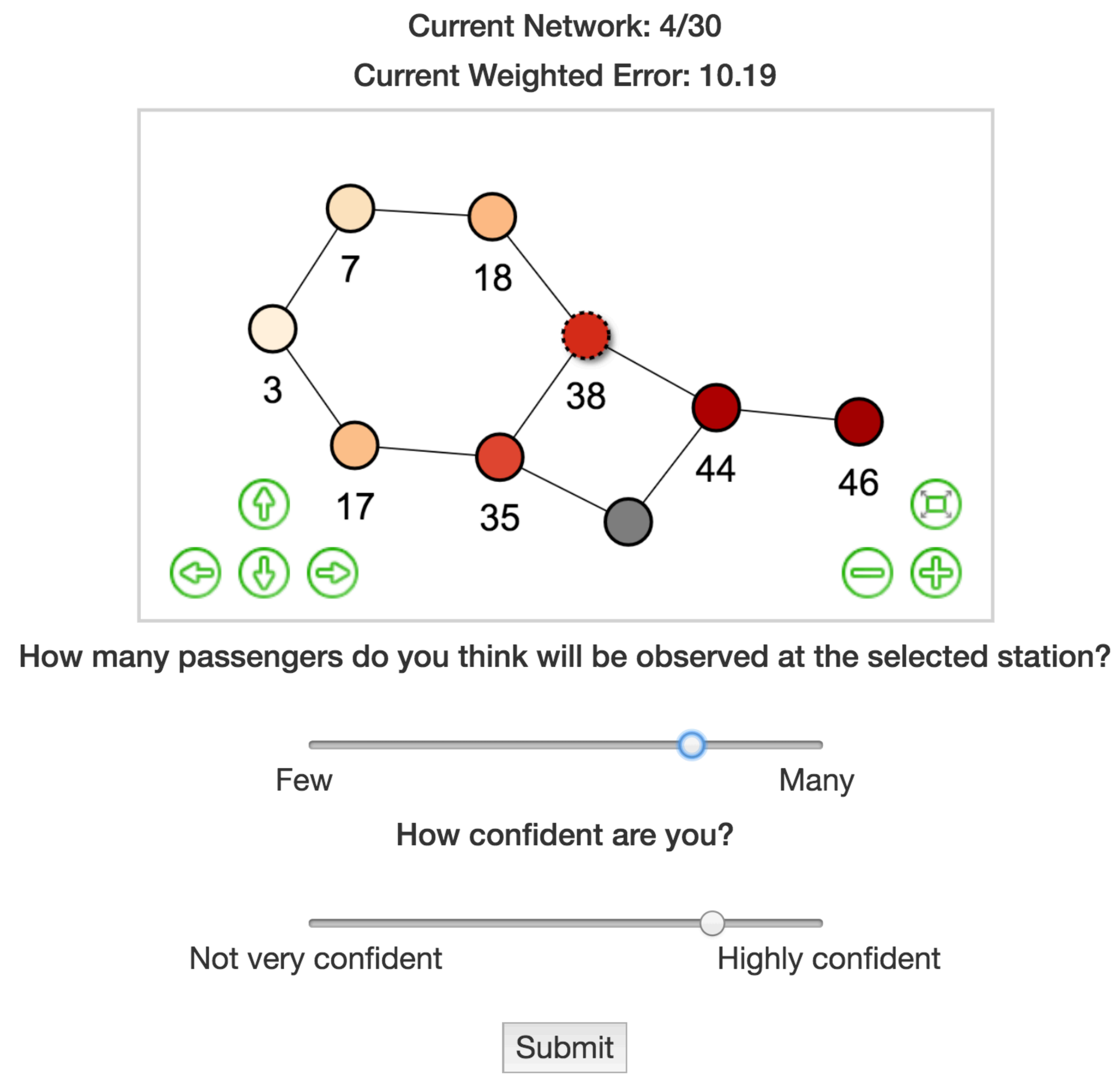
In the case of a lattice graph, the diffusion kernel is equivalent to an RBF kernel, thus extending existing theories of function learning from continuous to structured environments

$$k_{RBF}(\mathbf{x}, \mathbf{x}) = \frac{||\mathbf{x} - \mathbf{x}||^2}{2\lambda^2}$$





Subway Prediction Task

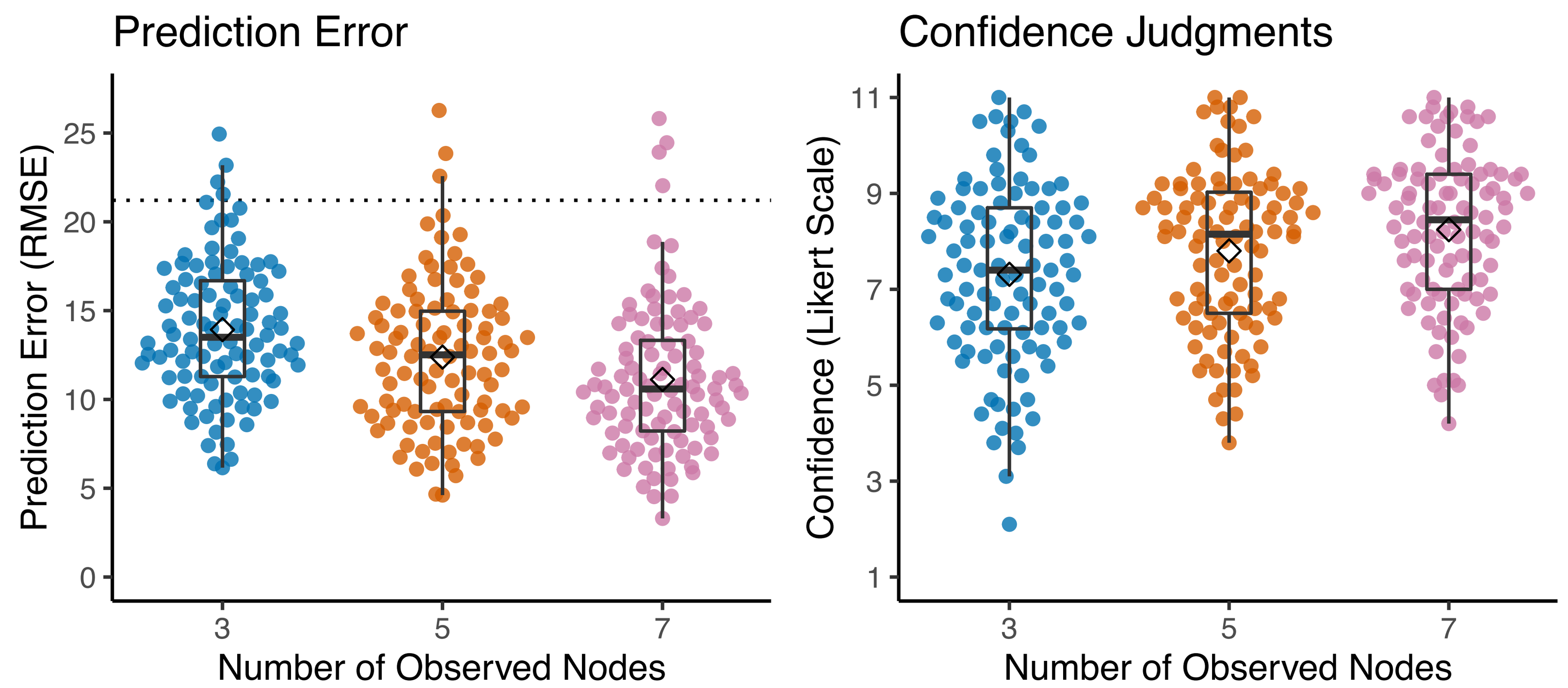


Methods

- 100 participants performed 30 rounds of a graph prediction task
- Each graph displayed 3, 5, or 7 observed nodes, with participants asked to predict the value of a randomly selected target node along with a confidence judgment
- Graphs were generated by taking 3x3 lattice graphs and randomly pruning 1/6th of the edges
- Participants saw 10 fully revealed graphs before starting the task and were incentivized based on performance

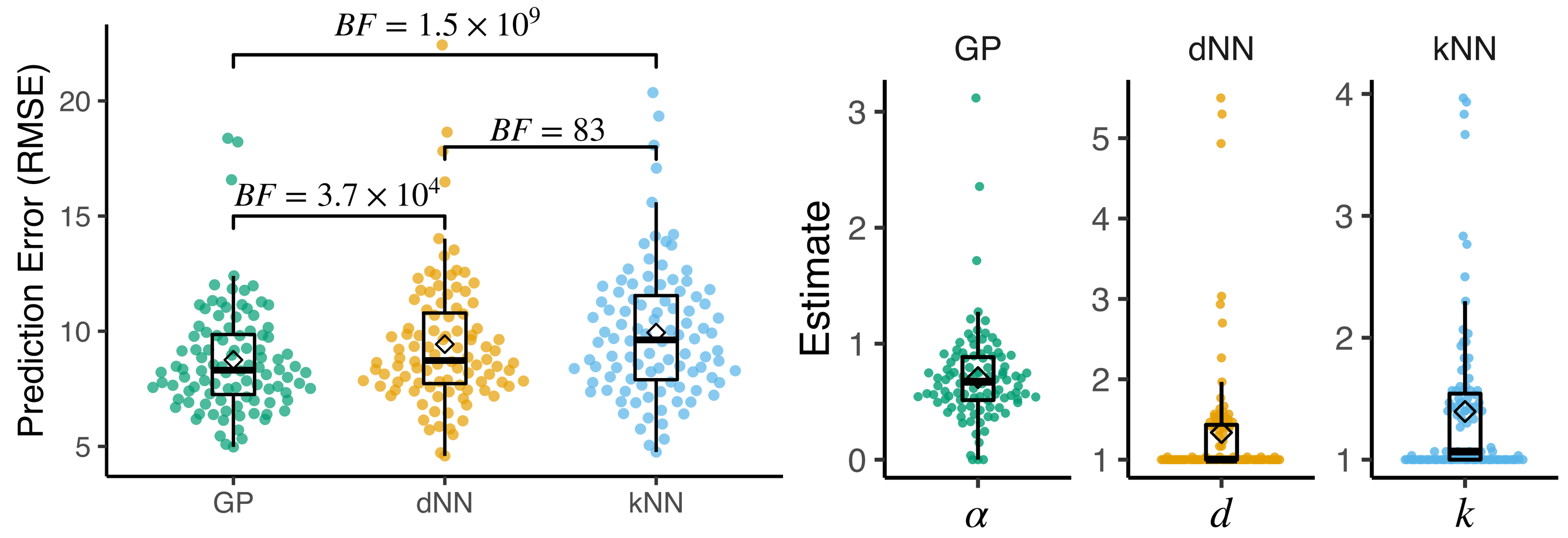
Behavioral Results

Prediction error decreased (left) and confidence increased (right) with more observed nodes

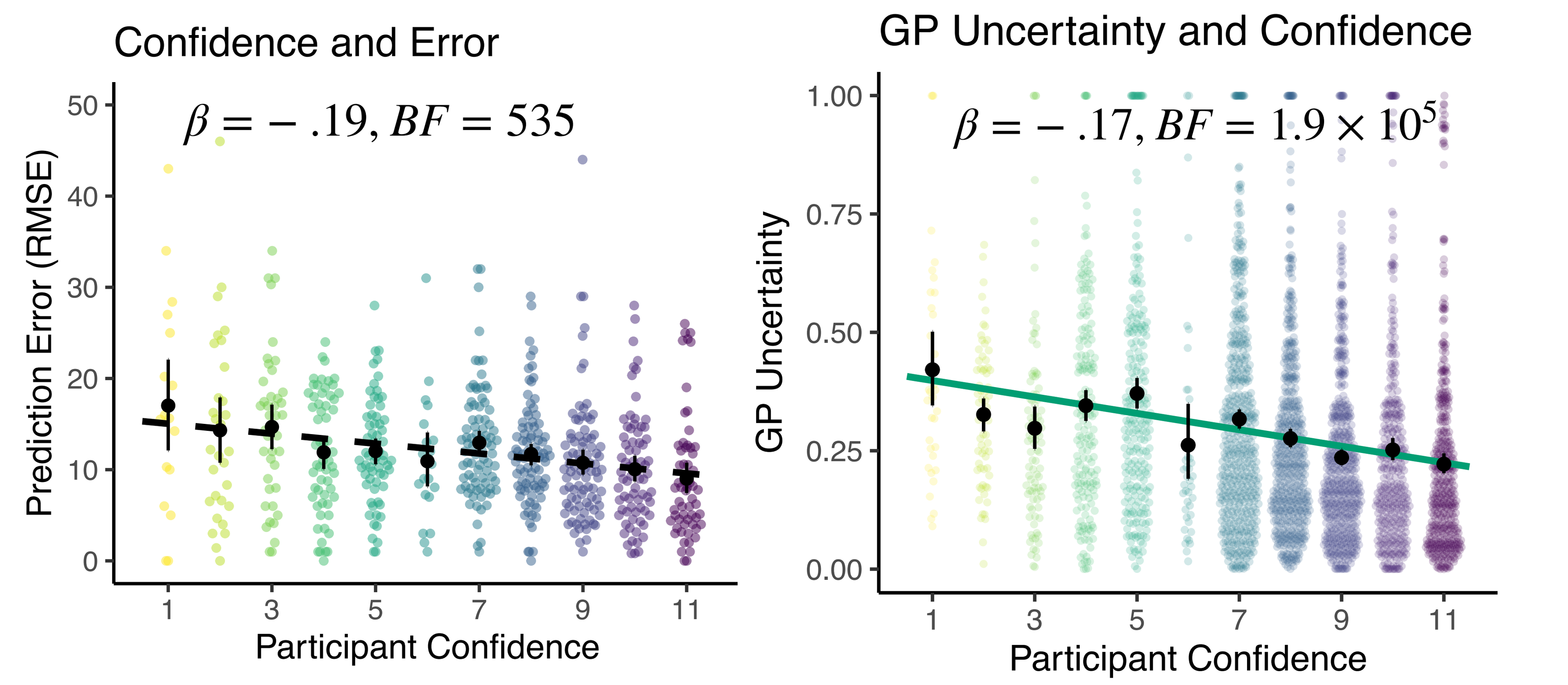


Modeling Results

We use leave-one-round-out cross validation and compare models using out-of-sample prediction error (RMSE)



- The Gaussian Process (GP) model uses the diffusion kernel to generalize based on the connectivity structure of the graph
- d-Nearest Neighbors (dNN) and k-Nearest Neighbors (kNN) are heuristics that make predictions by averaging observed nodes within distance *d* or the *k* nearest nodes
- Participant confidence judgments predicted error (left) while the GP uncertainty estimates predicted confidence judgments (right)



Conclusions and Future Directions

- Gaussian Process (GP) regression using a diffusion kernel captures human inferences and confidence judgments on graph structures
- Opens up a rich set of theoretical connections to theories of function learning and generalization
- e.g., The diffusion kernel has equivalencies [2] to the Successor Representation (SR) used in reinforcement learning
  - Two-way advantages: SR can be learned on the fly while GP makes predictions about uncertainty
- Ongoing work shows that GP uncertainty estimates are predictive of how people explore in a bandit task