Computational-Statistical Tradeoffs at the Next-Token Prediction Barrier Autoregressive and Imitation Learning under Misspecification

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Abstract

Next-token prediction with the logarithmic loss is a cornerstone of autoregressive sequence modeling, but, in practice, suffers from $error\ amplification$, where errors in the model compound and generation quality degrades as sequence length H increases. From a theoretical perspective, this phenomenon should not appear in well-specified settings, and, indeed, a growing body of empirical work hypothesizes that misspecification, where the learner is not sufficiently expressive to represent the target distribution, may be the root cause. Under misspecification—where the goal is to learn as well as the best-in-class model up to a multiplicative approximation factor $C_{\rm apx} \geq 1$ —we confirm that $C_{\rm apx}$ indeed grows with H for next-token prediction, lending theoretical support to this empirical hypothesis. We then ask whether this mode of error amplification is avoidable algorithmically, computationally, or information-theoretically, and uncover inherent computational-statistical tradeoffs.

We show: (1) Information-theoretically, one can avoid error amplification and achieve $C_{\rm apx} = O(1)$. (2) Next-token prediction can be made robust to achieve $C_{\rm apx} = \widetilde{O}(H)$, representing moderate error amplification, but this is an inherent barrier: any next-token prediction-style objective must suffer $C_{\rm apx} = \Omega(H)$. (3) For the natural testbed of autoregressive linear models, no computationally efficient algorithm can achieve sub-polynomial approximation factor $C_{\rm apx} = e^{(\log H)^{1-\Omega(1)}}$; however, at least for binary token spaces, one can smoothly trade compute for statistical power and improve on $C_{\rm apx} = \Omega(H)$ in sub-exponential time. Our results have consequences in the more general setting of imitation learning, where the widely-used behavior cloning generalizes next-token prediction. 1

Keywords: Next-token prediction, imitation learning, language models, comp-stat tradeoffs

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References

- Jayadev Acharya, Ilias Diakonikolas, Chinmay Hegde, Jerry Zheng Li, and Ludwig Schmidt. Fast and near-optimal algorithms for approximating distributions by histograms. In *Symposium on Principles of Database Systems*, 2015.
- Jayadev Acharya, Ilias Diakonikolas, Jerry Li, and Ludwig Schmidt. Sample-optimal density estimation in nearly-linear time. In *Symposium on Discrete Algorithms*, 2017.
- Alekh Agarwal, Nan Jiang, and Sham M Kakade. Reinforcement learning: Theory and algorithms. https://rltheorybook.github.io/, 2019. Version: January 31, 2022.
- Michael Alekhnovich. More on average case vs approximation complexity. In *Symposium on Foundations of Computer Science*, 2003.
- Philip Amortila, Nan Jiang, and Csaba Szepesvári. The optimal approximation factors in misspecified off-policy value function estimation. In *International Conference on Machine Learning*, pages 768–790. PMLR, 2023.
- Benny Applebaum, David Cash, Chris Peikert, and Amit Sahai. Fast cryptographic primitives and circular-secure encryption based on hard learning problems. In *Advances in Cryptology*, 2009.
- Kushal Arora, Layla El Asri, Hareesh Bahuleyan, and Jackie Chi Kit Cheung. Why exposure bias matters: An imitation learning perspective of error accumulation in language generation. In *Findings of the Association for Computational Linguistics*, 2022.
- Gregor Bachmann and Vaishnavh Nagarajan. The pitfalls of next-token prediction. *arXiv:2403.06963*, 2024.
- Mayank Bansal, Alex Krizhevsky, and Abhijit Ogale. Chauffeurnet: Learning to drive by imitating the best and synthesizing the worst. *arXiv:1812.03079*, 2018.
- Yannick Baraud and Lucien Birgé. Rho-estimators revisited: General theory and applications. *The Annals of Statistics*, 2018.
- Yannick Baraud, Lucien Birgé, and Mathieu Sart. A new method for estimation and model selection: *ρ*-estimation. *Inventiones mathematicae*, 2017.
- Matt Barnes. World scale inverse reinforcement learning in Google Maps. https://research.google/blog/world-scale-inverse-reinforcement-learning-in-google-maps/, 2023. [Online; accessed 26-Oct-2024].
- Blair Bilodeau, Dylan J Foster, and Daniel M Roy. Minimax rates for conditional density estimation via empirical entropy. *Annals of Statistics*, 2023.
- Lucien Birgé. Model selection via testing: an alternative to (penalized) maximum likelihood estimators. In *Annales de l'IHP Probabilités et statistiques*, 2006.
- Adam Block, Dylan J Foster, Akshay Krishnamurthy, Max Simchowitz, and Cyril Zhang. Butterfly effects of SGD noise: Error amplification in behavior cloning and autoregression. *International Conference on Learning Representations*, 2024a.

- Adam Block, Ali Jadbabaie, Daniel Pfrommer, Max Simchowitz, and Russ Tedrake. Provable guarantees for generative behavior cloning: Bridging low-level stability and high-level behavior. *Advances in Neural Information Processing Systems*, 2024b.
- Avrim Blum, Adam Kalai, and Hal Wasserman. Noise-tolerant learning, the parity problem, and the statistical query model. *Journal of the ACM*, 2003.
- Olivier Bousquet, Daniel Kane, and Shay Moran. The optimal approximation factor in density estimation. In *Conference on Learning Theory*, 2019.
- Mark Braverman, Xinyi Chen, Sham Kakade, Karthik Narasimhan, Cyril Zhang, and Yi Zhang. Calibration, entropy rates, and memory in language models. In *International Conference on Machine Learning*, 2020.
- Sébastien Bubeck. Convex optimization: Algorithms and complexity. *Foundations and Trends*® *in Machine Learning*, 2015.
- Ching-An Cheng and Byron Boots. Convergence of value aggregation for imitation learning. In *International Conference on Artificial Intelligence and Statistics*, 2018.
- Ching-An Cheng, Xinyan Yan, Evangelos Theodorou, and Byron Boots. Accelerating imitation learning with predictive models. In *International Conference on Artificial Intelligence and Statistics*, 2019.
- Ching-An Cheng, Andrey Kolobov, and Alekh Agarwal. Policy improvement via imitation of multiple oracles. *Advances in Neural Information Processing Systems*, 2020.
- Cheng Chi, Siyuan Feng, Yilun Du, Zhenjia Xu, Eric Cousineau, Benjamin Burchfiel, and Shuran Song. Diffusion policy: Visuomotor policy learning via action diffusion. *arXiv*:2303.04137, 2023.
- Sanjiban Choudhury, Mohak Bhardwaj, Sankalp Arora, Ashish Kapoor, Gireeja Ranade, Sebastian Scherer, and Debadeepta Dey. Data-driven planning via imitation learning. *The International Journal of Robotics Research*, 2018.
- Pim De Haan, Dinesh Jayaraman, and Sergey Levine. Causal confusion in imitation learning. *Advances in Neural Information Processing Systems*, 2019.
- Luc Devroye and Gábor Lugosi. *Combinatorial methods in density estimation*. Springer Science & Business Media, 2001.
- Ilias Diakonikolas. Learning structured distributions. Handbook of Big Data, 2016.
- Ilias Diakonikolas, Daniel Kane, Pasin Manurangsi, and Lisheng Ren. Hardness of learning a single neuron with adversarial label noise. In *International Conference on Artificial Intelligence and Statistics*, 2022a.
- Ilias Diakonikolas, Vasilis Kontonis, Christos Tzamos, and Nikos Zarifis. Learning a single neuron with adversarial label noise via gradient descent. In *Conference on Learning Theory*, 2022b.
- John Duchi, Shai Shalev-Shwartz, Yoram Singer, and Tushar Chandra. Efficient projections onto the 11-ball for learning in high dimensions. In *International Conference on Machine learning*, 2008.

ROHATGI BLOCK HUANG KRISHNAMURTHY FOSTER

- Dylan J Foster and Alexander Rakhlin. Foundations of reinforcement learning and interactive decision making. *arXiv*:2312.16730, 2023.
- Dylan J Foster, Sham M Kakade, Jian Qian, and Alexander Rakhlin. The statistical complexity of interactive decision making. *arXiv*:2112.13487, 2021.
- Dylan J Foster, Adam Block, and Dipendra Misra. Is behavior cloning all you need? understanding horizon in imitation learning. *Advances in Neural Information Processing Systems*, 2024a.
- Dylan J Foster, Yanjun Han, Jian Qian, and Alexander Rakhlin. Online estimation via offline estimation: An information-theoretic framework. *arXiv*:2404.10122, 2024b.
- Aravind Gollakota, Parikshit Gopalan, Adam Klivans, and Konstantinos Stavropoulos. Agnostically learning single-index models using omnipredictors. *Advances in Neural Information Processing Systems*, 2024.
- Noah Golowich, Ankur Moitra, and Dhruv Rohatgi. Exploration is harder than prediction: Cryptographically separating reinforcement learning from supervised learning. *arXiv:2404.03774*, 2024a.
- Noah Golowich, Ankur Moitra, and Dhruv Rohatgi. Exploring and learning in sparse linear mdps without computationally intractable oracles. In *Symposium on Theory of Computing*, 2024b.
- Saurabh Gupta, James Davidson, Sergey Levine, Rahul Sukthankar, and Jitendra Malik. Cognitive mapping and planning for visual navigation. In *Conference on Computer Vision and Pattern Recognition*, 2017.
- Yanjun Han, Jiantao Jiao, and Tsachy Weissman. Minimax estimation of discrete distributions under 11 loss. *IEEE Transactions on Information Theory*, 2015.
- Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. Distilling the knowledge in a neural network. *arXiv:1503.02531*, 2015.
- Jonathan Ho and Stefano Ermon. Generative adversarial imitation learning. *Advances in Neural Information Processing Systems*, 2016.
- Ari Holtzman, Jan Buys, Li Du, Maxwell Forbes, and Yejin Choi. The curious case of neural text degeneration. *arXiv:1904.09751*, 2019.
- Liyiming Ke, Sanjiban Choudhury, Matt Barnes, Wen Sun, Gilwoo Lee, and Siddhartha Srinivasa. Imitation learning as f-divergence minimization. In *Algorithmic Foundations of Robotics*, 2021.
- Michael Kearns, Yishay Mansour, Dana Ron, Ronitt Rubinfeld, Robert E Schapire, and Linda Sellie. On the learnability of discrete distributions. In *Symposium on Theory of Computing*, 1994.
- Michael Kelly, Chelsea Sidrane, Katherine Driggs-Campbell, and Mykel J Kochenderfer. Hg-dagger: Interactive imitation learning with human experts. In *International Conference on Robotics and Automation*, 2019.
- Beomjoon Kim, Amir-massoud Farahmand, Joelle Pineau, and Doina Precup. Learning from limited demonstrations. *Advances in Neural Information Processing Systems*, 2013.

- Michael Laskey, Jonathan Lee, Roy Fox, Anca Dragan, and Ken Goldberg. Dart: Noise injection for robust imitation learning. In *Conference on Robot Learning*, 2017.
- Lucien Le Cam. Maximum likelihood: an introduction. *International Statistical Review/Revue Internationale de Statistique*, 1990.
- Yann LeCun. Do large language models need sensory grounding for meaning and understanding. In *Workshop on Philosophy of Deep Learning*, 2023.
- Matthieu Lerasle. Lecture notes: Selected topics on robust statistical learning theory. *arXiv:1908.10761*, 2019.
- David Lopez-Paz, Léon Bottou, Bernhard Schölkopf, and Vladimir Vapnik. Unifying distillation and privileged information. *arXiv:1511.03643*, 2015.
- Tyler Ga Wei Lum, Martin Matak, Viktor Makoviychuk, Ankur Handa, Arthur Allshire, Tucker Hermans, Nathan D Ratliff, and Karl Van Wyk. Dextrah-g: Pixels-to-action dexterous arm-hand grasping with geometric fabrics. *arXiv*:2407.02274, 2024.
- Nishant A Mehta. Fast rates with high probability in exp-concave statistical learning. *International Conference on Artificial Intelligence and Statistics*, 2017.
- Elchanan Mossel and Sébastien Roch. Learning nonsingular phylogenies and hidden markov models. In *Symposium on Theory of Computing*, 2005.
- Wenlong Mou, Ashwin Pananjady, and Martin J Wainwright. Optimal oracle inequalities for projected fixed-point equations, with applications to policy evaluation. *Mathematics of Operations Research*, 48(4):2308–2336, 2023.
- Daniel Pfrommer, Thomas Zhang, Stephen Tu, and Nikolai Matni. Tasil: Taylor series imitation learning. *Advances in Neural Information Processing Systems*, 2022.
- Krzysztof Pietrzak. Cryptography from learning parity with noise. In *International Conference on Current Trends in Theory and Practice of Computer Science*, 2012.
- Yury Polyanskiy and Yihong Wu. *Information theory: From coding to learning*. Cambridge University Press, 2024.
- Dean A Pomerleau. Alvinn: An autonomous land vehicle in a neural network. *Advances in Neural Information Processing Systems*, 1988.
- Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. *OpenAI blog*, 2019.
- Nived Rajaraman, Lin Yang, Jiantao Jiao, and Kannan Ramchandran. Toward the fundamental limits of imitation learning. *Advances in Neural Information Processing Systems*, 2020.
- Nived Rajaraman, Yanjun Han, Lin Yang, Jingbo Liu, Jiantao Jiao, and Kannan Ramchandran. On the value of interaction and function approximation in imitation learning. *Advances in Neural Information Processing Systems*, 2021a.

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- Nived Rajaraman, Yanjun Han, Lin F Yang, Kannan Ramchandran, and Jiantao Jiao. Provably breaking the quadratic error compounding barrier in imitation learning, optimally. *arXiv:2102.12948*, 2021b.
- Stéphane Ross and Drew Bagnell. Efficient reductions for imitation learning. In *International Conference on Artificial Intelligence and Statistics*, 2010.
- Stephane Ross and J Andrew Bagnell. Reinforcement and imitation learning via interactive no-regret learning. *arXiv*:1406.5979, 2014.
- Stéphane Ross, Geoffrey Gordon, and Drew Bagnell. A reduction of imitation learning and structured prediction to no-regret online learning. In *International Conference on Artificial Intelligence and Statistics*, 2011.
- Stéphane Ross, Narek Melik-Barkhudarov, Kumar Shaurya Shankar, Andreas Wendel, Debadeepta Dey, J Andrew Bagnell, and Martial Hebert. Learning monocular reactive uav control in cluttered natural environments. In *International Conference on Robotics and Automation*, 2013.
- Shai Shalev-Shwartz and Shai Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge University Press, 2014.
- Shai Shalev-Shwartz, Ohad Shamir, and Karthik Sridharan. Learning kernel-based halfspaces with the 0-1 loss. *SIAM Journal on Computing*, 2011.
- Claude E Shannon. Prediction and entropy of printed english. Bell System Technical Journal, 1951.
- Jonathan Spencer, Sanjiban Choudhury, Arun Venkatraman, Brian Ziebart, and J Andrew Bagnell. Feedback in imitation learning: The three regimes of covariate shift. *arXiv*:2102.02872, 2021.
- Wen Sun, Arun Venkatraman, Geoffrey J Gordon, Byron Boots, and J Andrew Bagnell. Deeply aggrevated: Differentiable imitation learning for sequential prediction. In *International Conference on Machine Learning*, 2017.
- Gokul Swamy, Sanjiban Choudhury, J Andrew Bagnell, and Steven Wu. Of moments and matching: A game-theoretic framework for closing the imitation gap. In *International Conference on Machine Learning*, 2021.
- Gemini Team. Gemini 1.5: Unlocking multimodal understanding across millions of tokens of context. *arXiv*:2403.05530, 2024.
- Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, Ďan Bikel, Lukas Blecher, Cristian Canton Ferrer, Moya Chen, Guillem Cucurull, David Esiobu, Jude Fernandes, Jeremy Fu, Wenyin Fu, Brian Fuller, Cynthia Gao, Naman Goswami, Vedanuj a nd Goyal, Anthony Hartshorn, Saghar Hosseini, Rui Hou, Hakan Inan, Marcin Kardas, Viktor Kerkez, Madian Khabsa, Isabel Kloumann, Artem Korenev, Punit Singh Koura, Marie-Anne Lachaux, Thibaut Lavril, Jenya Lee, Diana Liskovich, Yinghai Lu, Yuning Mao, Xavier Martinet, Todor Mihaylov, Pushkar Mishra, Igor Molybog, Yixin Nie, Andrew Poulton Jeremy Reizenstein, Rashi Rungta, Kalyan Saladi, Alan Schelten, Ruan Silva, Eric Michael Smith, Ranjan Subramanian, Xiaoqing Ellen Tan, Binh

- Tang, Ross Taylor, Adina Williams, Jian Xiang Kuan, Puxin Xu, Zheng Yan, Iliyan Zarov, Yuchen Zhang, Angela Fan, Melanie Kambadur, Sharan Narang, Aurelien Rodriguez, Robert Stojnic, Sergey Edunov and Thomas Scialom. Llama 2: Open foundation and fine-tuned chat models. *arXiv:2307.09288*, 2023.
- Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in Neural Information Processing Systems*, 2017.
- Martin J Wainwright. *High-dimensional statistics: A non-asymptotic viewpoint*. Cambridge University Press, 2019.
- Xinyan Yan, Byron Boots, and Ching-An Cheng. Explaining fast improvement in online imitation learning. In *Uncertainty in Artificial Intelligence*, 2021.
- Yuhong Yang and Andrew R Barron. An asymptotic property of model selection criteria. *IEEE Transactions on Information Theory*, 1998.
- Yu Yu and Jiang Zhang. Smoothing out binary linear codes and worst-case sub-exponential hardness for LPN. In *Advances in Cryptology*, 2021.
- Yu Yu, Jiang Zhang, Jian Weng, Chun Guo, and Xiangxue Li. Collision resistant hashing from sub-exponential learning parity with noise. In *International Conference on the Theory and Application of Cryptology and Information Security*, 2019.
- Tony Z Zhao, Vikash Kumar, Sergey Levine, and Chelsea Finn. Learning fine-grained bimanual manipulation with low-cost hardware. *arXiv*:2304.13705, 2023.
- Ziwen Zhuang, Zipeng Fu, Jianren Wang, Christopher Atkeson, Soeren Schwertfeger, Chelsea Finn, and Hang Zhao. Robot parkour learning. *arXiv:2309.05665*, 2023.