TIC-TAC: A Framework for Improved Covariance Estimation in Deep Heteroscedastic Regression

Megh Shukla [1] **Mathieu Salzmann** [1] **Alexandre Alahi** [1]

Deep heteroscedastic regression involves jointly optimizing the mean and covariance of the predicted distribution using the negative log-likelihood. However, recent works show that this may result in sub-optimal convergence due to the challenges associated with covariance estimation. While the literature addresses this by proposing alternate formulations to mitigate the impact of the predicted covariance, we focus on improving the predicted covariance itself. We study two questions: (1) Does the predicted covariance truly capture the randomness of the predicted mean? (2) In the absence of supervision, how can we quantify the accuracy of covariance estimation? We address (1) with a *Taylor Induced Covariance (TIC)*, which captures the randomness of the predicted mean by incorporating its gradient and curvature through the second order Taylor polynomial. Furthermore, we tackle (2) by introducing a *Task Agnostic Correlations (TAC)* metric, which combines the notion of correlations and absolute error to evaluate the covariance. We evaluate TIC-TAC across multiple experiments spanning synthetic and real-world datasets. Our results show that not only does TIC accurately learn the covariance, it additionally facilitates the optimal convergence of the negative log-likelihood. Our code is available at `https://github.com/vita-epfl/TIC-TAC`.

Impact in transportation research: Vehicular and pedestrian trajectory prediction is a key problem statement in transportation research. The goal is to model the complex interactions between various agents to accurately predict the motion in subsequent time frames. Estimating these trajectories is typically done through deep regression, which leverages neural networks to extract complex interactions implicitly from the observations. Our work addresses the machine learning aspect of this problem, with a direct potential impact on trajectory prediction.

[1]École Polytechnique Fédérale de Lausanne (EPFL).
Correspondence to: Megh Shukla <megh.shukla@epfl.ch>.

Full paper available in the *Proceedings of the 41^{st} International Conference on Machine Learning*, Vienna, Austria. PMLR 235, 2024.