Bayesian LLM Finetuning for Statistical Inference

1 Introduction

Large language models (LLMs) have increasingly been employed in social science research. A common workflow involves three stages: (1) fine-tuning pre-trained LLMs on domain-specific datasets to improve performance on specialized tasks, (2) using the fine-tuned models to extract latent variables or classify text data, and (3) incorporating these outputs as outcomes or covariates in downstream statistical inference.

However, this approach ignores uncertainty quantification in the LLM output estimations, leading to invalid statistical inference. As shown in Appendix A, ignoring fine-tuning uncertainty creates bias in estimation and prediction as well as invalid inference. This is especially problematic because fine-tuning on small, domain-specific datasets, while necessary for task alignment, often produces overconfident predictions. The limited size of typical annotation datasets (often hundreds or thousands of examples) relative to the model's billions of parameters creates conditions where models memorize training patterns and become artificially overconfident about unseen cases.

In this research, we propose a framework that properly accounts for uncertainty from LLM fine-tuning in downstream statistical inference. Our approach jointly estimates LLM fine-tuning parameters and statistical model parameters within a Bayesian framework, rather than the conventional three-stage approach that treats LLM outputs as deterministic point estimates. Specifically, we obtain posterior distributions over fine-tuning parameters using tractable approximations, then propagate this uncertainty to statistical models, ensuring valid statistical inference. (We don't have a solution yet)

A key advantage of our approach is that it enables joint estimation of fine-tuning parameters specifically for the downstream statistical task. Traditional workflows treat fine-tuning and statistical analysis as separate stages, models are first fine-tuned on domain-specific classification or regression tasks, then the resulting features are used in entirely different downstream analyses. This separation ignores the potential mismatch between the fine-tuning objective and the research question. Our unified framework allows the fine-tuning process to be jointly optimized with the statistical model, enabling the LLM to learn representations that are specifically tailored to the downstream statistical task rather than just the intermediate labeling task. This joint estimation not only improves predictive performance but also ensures that the uncertainty quantification reflects the specific requirements of the statistical analysis, leading to more reliable statistical inference for the research question of interest.

2 Problem Setting

2.1 LLM Output with Uncertainty Quantification

We focus specifically on uncertainty arising from the fine-tuning stage rather than the pre-training uncertainty inherent in the base LLM. Pre-training uncertainty is essentially unidentifiable without access to the massive training corpus, while fine-tuning uncertainty is both tractable and often dominates when adapting to small domain datasets (Kong et al., 2020; Yang et al., 2023; Xiong et al., 2024). Unlike pre-training on vast unlabeled corpora, fine-tuning involves limited labeled data, and the immense capacity of LLMs can lead to overfitting and overconfident predictions on these small datasets (Kong et al., 2020; Lin et al., 2022).

Fine-tuning pre-trained LLMs often employs parameter-efficient methods like Low-Rank Adaptation (LoRA) (Hu et al., 2022). This overconfidence is particularly pronounced in parameter-efficient methods like LoRA when applied to domain-specific datasets with limited examples (Yang et al., 2023; Wang et al., 2024).

Standard LoRA fine-tuning proceeds as follows: the pre-trained weights of LLM, W_0, are adapted using low-rank decomposition $W = W_0 + BA$ where $B \in \mathbb{R}^{m\times r}$ and $A \in \mathbb{R}^{r\times n}$ with rank $r \ll \min(m, n)$. During fine-tuning, only the LoRA parameters $\theta_{LoRA} = [A, B]$ are optimized on a domain-specific dataset $D_{train} = \{(x_i, y_i)\}_{i=1}^N$ to obtain point estimates $\hat{A}, \hat{B}$. The fine-tuned model is then applied deterministically for feature extraction: $z_i = f_{LLM}(x_i; W_0 + \hat{B}\hat{A})$ where $D_{text} = \{x_i\}_{i=1}^n$ is raw text data and $z_i \in \mathbb{R}^d$.

However, this approach ignores uncertainty in the fine-tuning parameters, particularly problematic when fine-tuning on small datasets. Bayesian fine-tuning (Yang et al., 2023; Wang et al.,

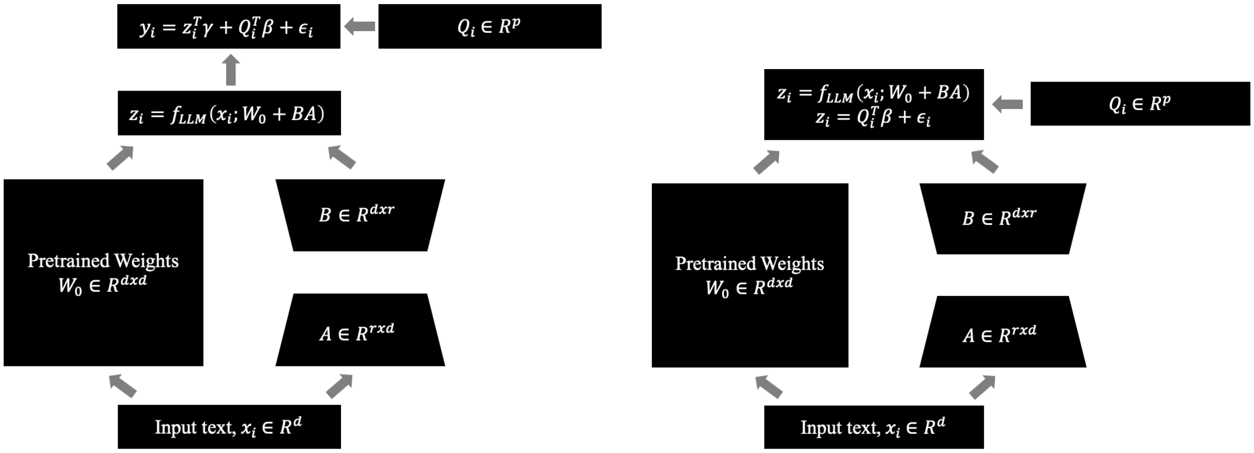
2024) addresses this by characterizing the full posterior distribution over parameters:

$$p(\theta_{LoRA}|D_{train}) \propto p(D_{train}|\theta_{LoRA}, W_0)p(\theta_{LoRA}) \tag{1}$$

where $p(D_{train}|\theta_{LoRA}, W_0)$ is the likelihood of the fine-tuning data and $p(\theta)$ is the prior over parameters. For feature extraction, instead of deterministic outputs z_i, we obtain posterior predictive distributions that integrate over parameter uncertainty:

$$p(z_i|x_i, D_{train}) = \int p(z_i|x_i, W_0 + \theta_{LoRA})p(\theta_{LoRA}|D_{train})d\theta_{LoRA} \tag{2}$$

This posterior predictive distribution properly reflects uncertainty from the fine-tuning process, providing calibrated feature representations that account for the limited size of domain-specific training data.


$y_i = z_i^T\gamma + Q_i^T\beta + \epsilon_i$
$Q_i \in R^p$
$z_i = f_{LLM}(x_i; W_0 + BA)$
Pretrained Weights
$W_0 \in R^{dxd}$
$B \in R^{dxr}$
$A \in R^{rxd}$
Input text, $x_i \in R^d$
$z_i = f_{LLM}(x_i; W_0 + BA)$
$z_i = Q_i^T\beta + \epsilon_i$
$Q_i \in R^p$
Pretrained Weights
$W_0 \in R^{dxd}$
$B \in R^{dxr}$
$A \in R^{rxd}$
Input text, $x_i \in R^d$

(a) Case A: LLM outputs as covariates

(b) Case B: LLM outputs as outcomes

Figure 1: Overview of the two cases of LLM uncertainty propagation in statistical inference

2.2 Case A: Inference with LLM Outputs Used as Covariates

We first consider the case where LLM outputs are used as covariates in downstream statistical models. When covariates are measured with error, this leads to attenuation bias—coefficient estimates are biased toward zero—if errors are independent of the input data and can result in underestimating the true effects of LLM-derived variables on outcomes of interest. However, this classical measurement error framework does not apply to fine-tuned LLMs, where prediction errors systematically depend on the training dataset used for fine-tuning. Fine-tuning on small, domain-specific datasets often creates overconfidence issues that lead to systematic prediction biases rather than independent measurement errors. The resulting measurement error violates the independence assumption, meaning bias can occur in either direction depending on how the limited training data relates to the broader application domain.

The standard downstream regression with LLM outputs as covariates perform $Y_i = z_i^T \gamma + Q_i^T \beta + \epsilon_i$, where $Q \in \mathbb{R}^{n \times p}$ is structured covariates, and $Y \in \mathbb{R}^n$ is an outcome variable. This approach considers z_i, LLM outputs, as deterministic data, thus ignoring uncertainty in the LoRA parameters θ_{LoRA} from fine-tuning and leading to invalid statistical inference.

We propose a unified Bayesian framework that addresses this by jointly modeling both the feature extraction and statistical modeling stages. Rather than treating z_i as observed covariates, we recognize that z_i are uncertain predictions from a fine-tuned LLM with parameter uncertainty. The joint model specifies:

$$\begin{aligned}
\text{Feature extraction:} \quad & p(z_i | x_i, \theta_{LoRA}, W_0) && (3) \\
\text{Downstream regression model:} \quad & Y_i | z_i, Q_i, \gamma, \beta \sim N(z_i^T \gamma + Q_i^T \beta, \sigma^2) && (4) \\
\text{LoRA parameter posterior:} \quad & p(\theta_{LoRA} | D_{train}) \propto p(D_{train} | \theta_{LoRA}, W_0) p(\theta_{LoRA}) && (5)
\end{aligned}$$

The joint inferential target:

$$\begin{aligned}
& p(\gamma, \beta, \sigma^2, \theta_{LoRA} | Y, Q, D_{train}) \propto && (6) \\
& \prod_i p(Y_i | z_i, Q_i, \gamma, \beta, \sigma^2) p(z_i | x_i, \theta_{LoRA}, W_0) p(\theta_{LoRA} | D_{train}) p(\gamma, \beta, \sigma^2)
\end{aligned}$$

This joint posterior properly accounts for uncertainty propagation from fine-tuning through to statistical inference, enabling valid statistical inferences that reflect the true uncertainty in LLM-derived measurements.

2.3 Case B: Inference with LLM outputs Used as Outcomes

We next consider the alternative case where LLM-generated measures serve as dependent variables in statistical models. Under classical assumptions, where measurement errors are independent of the regressors and mean-zero, errors in the dependent variable do not bias regression coefficients but do inflate the residual variance, leading to larger standard errors and reduced statistical power. However, this classical framework is often violated when LLMs are used as predictive instruments for outcomes. Fine-tuned LLMs, especially those trained on limited or domain-specific data, may exhibit systematic errors that correlate with the input variables or vary in structure across contexts. These violations can introduce endogeneity-like concerns, resulting in biased coefficient estimates and invalid inference. In particular, biased or structured prediction errors from LLMs may confound the relationship between covariates and outcomes, undermining the reliability of statistical conclusions drawn from such models.

The standard approach estimates $z_i = Q_i^T \beta + \epsilon_i$, where z_i represents the LLM-generated measure of interest and Q_i are explanatory variables. However, researchers observe $\hat{z}_i$ rather than the true construct z_i, where $\hat{z}_i$ contains measurement error from the fine-tuning process. This measurement error in the dependent variable contaminates all coefficient estimates β, and leads to inconsistent standard errors that invalidate hypothesis testing and confidence intervals.

Our unified Bayesian framework addresses this by jointly modeling the statistical relationship and the LLM measurement process. Rather than treating the observed LLM outputs $\hat{z}_i$ as the true dependent variable, our approach recognizes that we observe noisy measurements of an underlying latent construct z_i. The joint model specifies:

$$\text{Statistical relationship:} \quad z_i | Q_i, \beta, \sigma^2 \sim N(Q_i^T \beta, \sigma^2) \tag{7}$$

$$\text{LLM measurement process:} \quad \hat{z}_i | x_i, z_i, \theta_{LoRA} \sim p(\hat{z}_i | x_i, z_i, W_0 + \theta_{LoRA}) \tag{8}$$

$$\text{LoRA parameter posterior:} \quad p(\theta_{LoRA} | D_{train}) \propto p(D_{train} | \theta_{LoRA}, W_0) p(\theta_{LoRA}) \tag{9}$$

The joint inferential target:

$$
\begin{aligned}
&p(\beta, \sigma^2, Z, \theta_{LoRA} | \hat{Z}, Q, x_i, D_{train}) \propto \\
&\prod_i p(z_i | Q_i, \beta, \sigma^2) p(\hat{z}_i | x_i, z_i, \theta_{LoRA}) p(\theta_{LoRA} | D_{train}) p(\beta, \sigma^2)
\end{aligned} \tag{10}
$$

where z_i are treated as latent variables to be estimated jointly with the regression parameters β and LoRA parameters θ_{LoRA}. This approach enables valid inference about the factors driving the latent construct while properly accounting for both the uncertainty in measuring z_i from text and the parameter uncertainty from fine-tuning.

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A Inference Issues of Ignoring Fine-Tuning Uncertainty

The LLM output uncertainty comes from two sources: (i) baseline uncertainty, reflecting errors inherent in the pre-trained model $f_{LLM}(x_i; W_0)$, and (ii) fine-tuning uncertainty, reflecting the variability induced by adapting to a small domain-specific dataset.

Let the latent construct of interest (e.g., sentiment, topic proportion, policy position) be denoted by z_i. When we apply a pre-trained LLM with parameters W_0 to text x_i, we obtain an approximation $z_i^{(0)} = f_{LLM}(x_i; W_0) = z_i + u_i^{(0)}$, where $u_i^{(0)}$ represents baseline error from the pre-trained model. After fine-tuning with LoRA on a small domain dataset D_{train}, we obtain $\tilde{z}_i = f_{LLM}(x_i; W_0 + \theta_{LoRA}) = z_i^{(0)} + u_i^{(ft)} = z_i + u_i^{(0)} + u_i^{(ft)}$, where $u_i^{(ft)}$ captures fine-tuning uncertainty.

In principle, both $u_i^{(0)}$ and $u_i^{(ft)}$ contribute to measurement error. However, in this work, we focus on $u_i^{(ft)}$ and consider $u_i^{(0)}$ as absorbed into the latent construct z_i. The motivation is twofold: (i) baseline error from pretraining is essentially unidentifiable without access to the massive training corpus, and (ii) fine-tuning error is tractable and often dominates uncertainty when adapting to small domain datasets. By specifying priors on the LoRA parameters, θ_{LoRA}, and conditioning on the domain-specific dataset D_{train}, its posterior distribution can be approximated, making this error both estimable and consequential for downstream inference.

With this simplification, we write the observed LLM-derived surrogate as $\tilde{z}_i = z_i + u_i$, where $u_i \equiv u_i^{(ft)}$ denotes the fine-tuning error. Importantly, u_i may be correlated with the latent construct z_i, the structured covariates Q_i, and even the regression error ϵ_i.

For example, suppose z_i is the true stance of a political text, and the fine-tuned LLM was trained on a small, imbalanced dataset with mostly liberal examples. Then the fine-tuned model tends to systematically "over-predict" liberal stance, especially for borderline cases. In this case, the fine-tuning error u_i is larger (and systematically biased) when z_i is conservative, $\text{Cov}(u_i, z_i) \neq 0$. Similarly, if a structured covariate Q_i captures demographic attributes (e.g., age or region) that affect writing style, fine-tuning errors may be larger for certain groups, leading to $\text{Cov}(u_i, Q_i) \neq 0$. Finally, if the same unobserved factors affect both the downstream regression and misclassification by the LLM, then $\text{Cov}(u_i, \epsilon_i) \neq 0$.

A.1 Case A: Inference with LLM Outputs Used as Covariates

We now examine the statistical consequences of ignoring this uncertainty in downstream regression analysis. Consider the true model follows:

$$Y_i = z_i^T \gamma + Q_i^T \beta + \epsilon_i, \quad E[\epsilon_i | z_i, Q_i] = 0 \tag{11}$$

where z_i represents the latent construct of interest extracted from text x_i, Q_i denotes covariates, and Y_i is the outcome variable. In practice, researchers observe the noisy LLM output $\tilde{z}_i = z_i + u_i$ and estimate the model using $\tilde{z}_i$ in place of the unobserved true values z_i, ignoring the uncertainty in the fine-tuning process.

To analyze the bias introduced by this substitution, we employ the residual maker $M_Q = I - Q(Q'Q)^{-1}Q'$ to partial out the covariates. Let $\dot{z} = M_Q \tilde{z}$, $z^* = M_Q z$, $\dot{u} = M_Q u$, and $\dot{\epsilon} = M_Q \epsilon$ denote the variables after partialling out Q. The OLS estimator for γ becomes:

$$\hat{\gamma} = (\dot{z}'\dot{z})^{-1}\dot{z}'\dot{Y} \tag{12}$$

where $\dot{Y} = \gamma z^* + \dot{\epsilon}$ represents the true model after transformation.

Substituting the relationship $\dot{z} = z^* + \dot{u}$ into the OLS formula yields:

$$\hat{\gamma} = \frac{(z^* + \dot{u})'(\gamma z^* + \dot{\epsilon})}{(z^* + \dot{u})'(z^* + \dot{u})} \tag{13}$$

The numerator expands to $\gamma(z^*)'z^* + (z^*)'\dot{\epsilon} + \gamma \dot{u}'z^* + \dot{u}'\dot{\epsilon}$, while the denominator becomes $(z^*)'z^* + 2(z^*)'\dot{u} + \dot{u}'\dot{u}$. Taking probability limits and applying the exogeneity assumption $\text{Cov}(z^*, \dot{\epsilon}) = 0$, we obtain:

$$\text{plim } \hat{\gamma} = \gamma \cdot \frac{\text{Var}(z^*) + \text{Cov}(z^*, \dot{u})}{\text{Var}(z^*) + \text{Var}(\dot{u}) + 2\text{Cov}(z^*, \dot{u})} + \frac{\text{Cov}(\dot{u}, \dot{\epsilon})}{\text{Var}(\dot{z})} \tag{A1}$$

This result reveals several important deviations from classical measurement error, with consequences for both estimation and inference.

Biased coefficient estimates: The classical measurement error assumes $u \perp (z, Q, \epsilon)$

with $E[u] = 0$, yielding the attenuation bias:

$$\text{plim } \hat{\gamma} = \gamma \cdot \frac{\text{Var}(z^*)}{\text{Var}(z^*) + \text{Var}(\dot{u})} \in (0, 1) \cdot \gamma \quad \text{(attenuation)} \tag{A2}$$

However, this classical case rarely applies to fine-tuned LLMs due to two key violations. Structured measurement error occurs when $\text{Cov}(z^*, \dot{u}) \neq 0$—arising from overconfident patterns learned from small training datasets—causing the bias in equation (A1) to be either upward or downward. Endogeneity-type correlation emerges when LLM errors correlate with the regression error ($\text{Cov}(\dot{u}, \dot{\epsilon}) \neq 0$), where the second term in equation (A1) introduces additional bias that compounds the measurement error problem.

Invalid standard errors and confidence intervals: Standard OLS procedures treat $\dot{z}$ as fixed regressors and construct confidence intervals around the pseudo-true limit in equation (A1) rather than the true parameter γ. This creates two distinct problems: (1) confidence intervals center around the biased probability limit from equation (A1) rather than the true parameter γ, leading to systematic mis-coverage; and (2) variance underestimation, where the variance calculations omit first-stage uncertainty from LLM fine-tuning.

Biased point predictions: Plug-in predictions $\hat{Y}_i = \hat{\gamma}\tilde{z}_i + Q_i'\hat{\beta}$ suffer from two sources of bias: coefficient bias, where predictions inherit the bias in $\hat{\gamma}$ from equation (A1), and input bias, where the systematic distortion in $\tilde{z}_i$ (using noisy LLM outputs instead of true values) further distorts predictions. The combined effect yields systematically biased mean predictions, with the direction (upward or downward bias) depending on the sign of the bias in equation (A1).

Invalid prediction intervals: Standard prediction intervals ignore LLM uncertainty and use only the residual variance σ^2. However, the correct conditional predictive variance includes additional uncertainty terms. Starting from the true model $Y_i = \gamma z_i + Q_i'\beta + \epsilon_i$ and substituting $z_i = \tilde{z}_i - u_i$, we get $Y_i = \gamma\tilde{z}_i + Q_i'\beta - \gamma u_i + \epsilon_i$. The conditional variance becomes:

$$\text{Var}(Y_i|Q_i, \tilde{z}_i) = \sigma^2 + \gamma^2\text{Var}(u_i|x_i, D_{train}) + 2\gamma\text{Cov}(u_i, \epsilon_i|Q_i, \tilde{z}_i) \tag{A3}$$

where we use $\text{Var}(u_i|x_i, D_{train})$ because LLM measurement error depends on the text input and fine-tuning dataset rather than the covariates. The three components represent: the usual regression error variance (σ^2), additional uncertainty from LLM measurement error ($\gamma^2 \text{Var}(u_i|x_i, D_{train})$), and cross-correlation between measurement error and regression error ($2\gamma \text{Cov}(u_i, \epsilon_i)$). Omitting these components produces prediction intervals that are systematically too narrow, leading to overconfident predictions about future outcomes.

A.2 Case B: LLM Outputs Used as Outcomes

Consider next the case where LLM-derived measures serve as dependent variables. The latent structural relationship is:

$$z_i = Q_i'\beta + \epsilon_i, \quad E[\epsilon_i|Q_i] = 0 \tag{14}$$

where researchers observe $\hat{z}_i = z_i + u_i$ and estimate the model by regressing $\hat{z}_i$ on Q_i. The resulting OLS estimator satisfies:

$$\hat{\beta} = \beta + (Q'Q)^{-1}Q'u \tag{15}$$

which converges in probability to:

$$\text{plim } \hat{\beta} = \beta + (E[Q_iQ_i'])^{-1}E[Q_iu_i] \tag{B1}$$

Biased coefficient estimates. This expression reveals that coefficient bias depends entirely on whether fine-tuning errors correlate with the covariates. When $E[Q_iu_i] \neq 0$—for instance, when fine-tuning errors systematically depend on observable features correlated with Q_i—the estimator becomes biased according to equation (B1). For a single regressor, this simplifies to:

$$\text{plim } \hat{\beta} = \beta + \frac{\text{Cov}(Q, u)}{\text{Var}(Q)} \tag{B2}$$

Invalid standard errors and confidence intervals. Even when coefficient estimates remain unbiased ($E[Q_iu_i] = 0$), the regression errors become $\epsilon_i + u_i$ because we observe $\hat{z}_i = z_i + u_i$ instead of the true z_i, so the LLM measurement error u_i appears as additional noise in the residuals alongside the structural error ϵ_i. This creates two opposing effects on confidence intervals: the observed residual variance inflates to $\text{Var}(\epsilon_i + u_i) = \text{Var}(\epsilon_i) + \text{Var}(u_i) + 2\text{Cov}(\epsilon_i, u_i)$ (making intervals wider), while standard error calculations treat $\hat{z}_i$ as fixed data rather than estimates with uncertainty, omitting the additional variance component $\text{Var}(\hat{\beta}|\hat{z})$ that accounts for first-stage estimation (making intervals narrower). The net effect on coverage depends on whether $\text{Var}(u_i) + 2\text{Cov}(\epsilon_i, u_i)$ outweighs the ignored first-stage uncertainty, but likely results in invalid inference due to centering around the wrong target and incorrect variance estimation.

Biased predictions. When $\text{Cov}(Q_i, u_i) \neq 0$, the coefficient estimates are biased according to equation (B1), so predictions of the true latent construct are systematically biased: $E[\hat{z}_j|Q_j] - E[z_j|Q_j] = Q_j'(E[Q_iQ_i'])^{-1}E[Q_iu_i]$, where the magnitude and direction of bias depend on both the covariate values Q_j and the correlation structure between LLM errors and covariates.

Invalid prediction intervals. Standard procedures use the residual variance $\text{Var}(\epsilon_i + u_i) = \text{Var}(\epsilon_i) + \text{Var}(u_i) + 2\text{Cov}(\epsilon_i, u_i)$ rather than the true latent variance $\text{Var}(\epsilon_i)$, producing prediction intervals for the latent construct z_i that overestimate uncertainty when $\text{Cov}(\epsilon_i, u_i) = 0$ due to the additional measurement error variance $\text{Var}(u_i)$.