Can large language models assist choice modelling? Insights into prompting strategies and current models capabilities

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Abstract

Large Language Models (LLMs) are becoming widely used to support various workflows across different disciplines, yet their potential in discrete choice modelling remains relatively unexplored. This work examines the potential of LLMs as assistive agents in the specification and, where technically feasible, estimation of Multinomial Logit models. We implement a systematic experimental framework involving thirteen versions of six leading LLMs (ChatGPT, Claude, DeepSeek, Gemini, Gemma, and Llama) evaluated under five experimental configurations. These configurations vary along three dimensions: (i) modelling goal (suggesting vs. suggesting and estimating MNL models); (ii) prompting strategy (Zero-Shot vs. Chain-of-Thoughts (CoT)); and (iii) information availability (full dataset vs. data dictionary summarising variable names and types). Each specification suggested by the LLMs is implemented, estimated, and evaluated based on goodnessof-fit metrics, behavioural plausibility, and model complexity. Our findings reveal that proprietary LLMs can generate valid and behaviourally sound utility specifications, particularly when guided by structured prompts (CoT). Open-weight models such as Llama and Gemma struggled to produce meaningful specifications. Claude 4 Sonnet consistently produced the best-fitting and most complex models, while GPT models suggested models with robust and stable modelling outcomes (LL and AIC values). Notably, some LLMs performed better when provided with just data dictionary, suggesting that limiting raw data access may enhance internal reasoning capabilities. Among all LLMs, GPT o3 was uniquely capable of correctly estimating its own specifications by executing self-generated code. Overall, the results demonstrate both the promise and current limitations of LLMs as assistive agents in discrete choice modelling, not only for model specification but also for supporting modelling decision and estimation, and provide practical guidance for integrating these tools into choice modellers' workflows.

Keywords: Large Language Models, Discrete Choice Models, Utility Specification

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1 Introduction

Discrete choice models (DCMs), are widely used across numerous fields for understanding and analysing individual choice behaviour (Hess & Daly, 2024; Mariel et al., 2021; Liebe et al., 2023; Buckell et al., 2022). Modellers use these structures to mathematically represent decision-makers' observed choices, estimate parameters that capture their current preferences, and apply the models to forecast demand in future scenarios.

The process of conducting a choice modelling study involves numerous modeller decisions, drawing on behavioural theories, data constraints, and researcher assumptions (cf. Nova et al., 2024; Van Cranenburgh et al., 2022). Modellers need to make a decision on model family (e.g. random utility vs preference accumulation) and then choose a specific structure within that model family (e.g. multinomial vs nested logit) (Hess et al., 2018). They have to construct functional forms that map observed data, typically including alternative-specific attributes (e.g., travel time, travel cost), individual-specific socioeconomic and contextual variables (e.g., gender, age, income, region, weather), and alternative availabilities, into a formal definition of a value function such as utility, which includes decisions on linearity vs non-linearity, as well as interactions. Modellers often propose a candidate specification, estimate its parameters, examine both goodness-of-fit statistics and theoretical plausibility, and then refine the specification, balancing parsimony, model fit, and behavioural assumptions. Even with a small set of variables, the space of possible specifications grows combinatorially, and despite decades of modelling advancements, specifying Discrete Choice Models remains a time-intensive and expertisedriven task, requiring careful consideration of behavioural theory, statistical diagnostics, and domain knowledge.

Against this backdrop, the present paper explores whether the exponential growth in the development and application of Large Language Models (LLMs) across a wide range of tasks provides a novel opportunity in choice modelling. LLMs have proven themselves as powerful tools for queries that require understanding, generating, and reasoning technical text (Qu et al., 2025). Moreover, recent work has demonstrated that LLMs achieve high performance on a range of tasks. For instance, GPT-4 reaches near-human accuracy on complex reasoning benchmarks and solves most grade-school math problems (Wei et al., 2022), while Claude 3 Opus and DeepSeek-V3 similarly excel on mathematical and coding problems (Anthropic, 2025a; Liu, Feng, Xue, et al., 2024). Although LLMs can parse academic literature, generate code, and even run them based on user prompts across diverse fields (Brown et al., 2020; Mialon et al., 2023; L. Wang et al., 2024), their actual potential to provide assistance in the choice model specification process has not been explored.

This paper evaluates how current LLMs can assist in the specification of and, where technically feasible, the estimation of Discrete Choice Models. Our aim is twofold. First, we seek to understand how modellers should interact with LLMs to obtain useful and behaviourally plausible specifications. Second, we evaluate which LLMs currently perform best in this context. To this end, we design a set of experiments that vary by prompt type (i.e. the instruction given to the LLM), information provided to the LLM (full data vs. data dictionary only), and modelling task (specification vs. estimation). These variations allow us to identify interaction patterns that influence the quality and plausibility

of model specifications. Moreover, by varying the modelling task, we not only evaluate LLMs as assistive agents for specification, but also provide insights into their ability to conduct end-to-end econometric modelling, including the execution of self-generated code for estimation. We then apply this framework to thirteen versions of six prominent LLM families, including OpenAI's GPT variants, Anthropic's Claude series, DeepSeek Chat, Google's Gemini and Gemma, and Meta's Llama series. All LLM-generated specifications are then assessed based on behavioural plausibility (e.g., sign of parameters), goodness-of-fit measures, and overall specification quality, as well as their robustness across experiment configurations (i.e., whether the same LLM consistently generate good specifications) and convergence reliability (i.e., whether generated specifications converge when implemented and reported estimates can be reproduced). By bridging the fields of Discrete Choice Modelling and AI, this study provides, to our knowledge, a first study that investigates the potential benefits of LLMs in behavioural econometric model development. The results not only offer practical insights for researchers seeking to augment their workflows with LLMs but also raise broader questions about the evolving boundary between human expertise and machine intelligence in scientific modeling. Of course, the development of LLMs continues apace, and the models applied in this paper are only current at the time of writing this paper—the broader points remain valid going forward.

The remainder of this paper is organized as follows. Section 2 reviews relevant literature at the intersection of DCMs and LLMs. Section 3 describes the research methodology and presents the different LLMs, prompts, and dataset used in this study. Section 4 reports and analyses the results across all experimental configurations. Finally, Section 5 concludes with a discussion of key findings, limitations, and directions for future research.

2 Literature

Model specification is the main phase of the choice modelling process, characterised by a semi-structured, iterative, demanding workflow that is often time consuming. Rooted in behavioural theories and guided by the modeller's knowledge and prior assumptions, this task involves making decisions on model structure and specification of the value functions (e.g., utility functions) (Van Cranenburgh et al., 2022; Nova et al., 2025). Modelling decisions include choices on the model family and error structure, which attributes to include, how to specify their functional form (e.g., linear, transformed, or interacted either among themselves or with covariates), and how to account for heterogeneity. Even with a modest number of variables, the space of possible model specification expands combinatorially (Rodrigues et al., 2024). In this section, we look at existing work on assisted model specification before turning our attention to LLMs.

2.1 Exisiting work on assisted specification process

To support or automate the model-building phase, recent research has explored a range of approaches, from combinatorial optimisation techniques to machine learning. Initially, researchers used static metaheuristics, such as Simulated Annealing, Bayesian variable selection, neighbourhood search, and bi-level optimisation, to explore the model space iteratively, often incorporating constraints to enhance behavioural plausibility and model fit (Páez & Boisjoly, 2022; Rodrigues et al., 2020; Ortelli et al., 2021; Beeramoole et al., 2023). More recently, grammar-based approaches have emerged, with Grammatical

Evolution used either independently (Haj-Yahia et al., 2024) or in bi-level frameworks to improve predictive consistency (Ghorbani et al., 2025). Lastly, machine learning methods have also been used towards automating this process. For instance, Mesbah & Rafeei (2025) used SHapley Additive exPlanations (SHAP) to inform the construction of behaviourally sound utility functions. Building on these trends, Nova et al. (2025) proposed a reinforcement learning framework that formulates model specification as an adaptative learning process rather than a static one. In their approach, a Deep Q-Network agent learns to propose model candidates through sequential interaction, guided by a reward function that encodes behavioural expectations and modelling outcomes.

2.2 Large Language Models

Large Language Models are generative artificial intelligence models designed to process, understand, and generate human-like text (Naveed et al., 2023). Initially, LLMs were pre-trained on large corpora of text (and more recently, code) to learn representation of lexical elements, syntactic structures, and world knowledge through self-supervised objectives, i.e., mostly predicting the next token in a sequence of source of information Chang et al. (2024). The achievement that enables these capabilities is the Transformer architecture, which replaces convolution or recurrent operation with multi-head self-attention, allowing models to capture long-range dependencies within millions of tokens in a context window (Vaswani et al., 2017).

Early approaches to text representation relied on high-dimensional co-occurrence matrices that produced sparse word embeddings (Turney & Pantel, 2010). Neural language models advanced this by learning dense, low-dimensional embeddings jointly with predictive tasks, improving generalisation and efficiency (Bengio et al., 2003; Collobert & Weston, 2008). Word2Vec and GloVe further improved these representations by capturing semantic patterns through local context and global co-occurrence, respectively (Mikolov et al., 2013; Pennington et al., 2014). However, these static embeddings could not adapt to different contexts or capture long-range dependencies (Chiu et al., 2016). Recurrent Neural Networks allowed to capture sequential dependencies using evolving hidden states (Hochreiter & Schmidhuber, 1997; Chung et al., 2014), yet still struggled with long-sequence memory issues (Bahdanau et al., 2014). Finally, the Transformer architecture enabled parallel processing and high-volume scalability (Vaswani et al., 2017). This paved the ground for pioneer models that demonstrated few-shot generalisation through autoregressive training on large-scale corpora (Devlin et al., 2019; Radford et al., 2019; Brown et al., 2020).

This rapid progress has resulted in several families of closed-weight¹ models with different architectures, scales, intended uses, and multimodal capabilities. These models are typically accessed through proprietary user interfaces, allowing non-technical users to interact with them directly. For instance, at the time of writing, OpenAI's GPT models includes the reasoning-optimized GPT-o3 (OpenAI, 2025b) and its cost-efficient variant GPT-o4-mini (OpenAI, 2024b), the general-purpose chat model GPT-4.5 (OpenAI, 2025a), and the multimodal flagship GPT-40 (OpenAI, 2024a), which accepts text, vision, and audio

^{1.} Closed-weight models are LLMs whose internal parameters (weights) are not publicly released. They are typically only accessible via proprietary APIs or interfaces, preventing users from fine-tuning or deploying the model on their own hardware.

inputs. Anthropic's Claude series includes Claude 4 Opus (Anthropic, 2025b), known for achieving high scores on cognitive benchmarks, along with Claude 4 Sonnet (Anthropic, 2025c), a faster, cost-optimized variant, and Claude 3.7 Sonnet, recognised for its reliable language understanding and inference speed (Anthropic, 2025a). Google has also introduced the Gemini models, which are described as a family of highly capable multimodal models. Gemini 1.5 flash was introduced to work and reason using information from over 10 million tokens of context, which overcame existing models like Claude 3.0 (200k) and GPT-4 Turbo (128k) (Gemini et al., 2024). Then, Google introduced a cost-optimized version namely Gemini 2.5 Flash that delivers rapid inference with robust reasoning performance (Google, 2025).

In contrast, leading teams have released open-weight² models that provide full access to model parameters, allow architectural replication, and support fine-tuning on local infrastructure. Meta's LLaMA series is one of the most widely adopted in this category, with LLaMA 2 (Touvron et al., 2023), LLaMA 3 (Grattafiori et al., 2024), and LLaMA 4 (Meta, 2025) offering competitive performance under permissive licences suitable for academic and limited commercial use. Google has similarly released the Gemma family of lightweight, open-weight models (Gemma (Team, Mesnard, et al., 2024), Gemma 2 (Team, Riviere, et al., 2024) and Gemma 3 (Team et al., 2025)), designed to support local workflows and fine-tune on local machines. Similarly, DeepSeek Chat is recognized for its efficient multilingual reasoning and code-generation capabilities. This model is part of an incipient, yet growing family that has introduced models such as DeepSeek-V2 (Liu, Feng, Wang, et al., 2024), a Mixture-of-Experts (MoE) language model that uses a novel innovative Multi-head Latent Attention architecture. Building upon this, DeepSeek-V3 (Liu, Feng, Xue, et al., 2024) is presented as a large MoE model, aiming for performance comparable to leading closed models like GPT-40 and Claude-3.5-Sonnet. This family also has introduced a reasoning model, namely DeepSeek-R1 (Guo et al., 2025). Together, these models exemplify the state of the art in reasoning power, modality support, inference efficiency, and context-length scalability.

2.3 Prompting strategies

A prompt is a structured instruction or query provided to a LLM to guide the form, content, or behaviour of its response. In general, a prompt consists of textual input, contextual information, system role (e.g., defining the model as a helpful assistant, a tutor, etc.), or examples that define the task the model is expected to perform and/or specify the format the response should follow. Some LLMs are capable of handling multimodal inputs, such as images, audio, files, or even code.

To be able to interpret prompts, LLMs decompose them into discrete units known as tokens, which are the basic units for computation. These tokens are mapped into high-dimensional latent spaces and passed through multiple layers of transformer-based neural architectures that predict the next most likely tokens in the output sequence. Consequently, the quality and structure of the input prompt highly influence the relevance, coherence, and robustness of the model's output (Jin et al., 2020; Minaee et al.,

^{2.} Open-weight models are LLMs for which the trained model weights are publicly released. This allows users to run, fine-tune, or integrate the models into their own systems, although the original training data and/or training code are not always disclosed.

2021). Moreover, without adequate context, these LLMs can also manifest undesirable behaviours (Bommasani et al., 2021), biased responses (Gehman et al., 2020), provide false or incorrect information, or even generate hallucinatory content (Welleck et al., 2019).

The quality, relevance, and factual consistency of model responses can be significantly impacted by structure, content, and context of prompts. For example, Kojima et al. (2022) show that models benefit from prompts that contains chain of thought instructions, enabling them to outperform the same prompt-task. Similarly, Min et al. (2022) provide evidence that prompt context—including examples, step-by-step reasoning patterns, or structural templates—plays a more critical role than the prompt length or wording alone. This process, referred to as prompt engineering nowadays, is the practice of designing input prompts that effectively obtain accurate and context-aware responses from generative AI systems Reynolds & McDonell (2021); Brown et al. (2020).

Prompt engineering can therefore take many forms depending on the degree of structure, domain knowledge, and contextual information integrated into the input. The two most extensively used prompting paradigms are Zero-Shot Prompting (ZSP) and Chain-of-Thought (CoT) prompting. ZSP relies solely on the model's pre-trained knowledge and requires no additional context, examples, or step-by-step instructions (Brown et al., 2020). Although ZSP is versatile and straightforward to use, it often generates generic responses that lack detailed thoughts, especially in tasks that require specific domain knowledge. In contrast, CoT prompting guides the model through intermediate reasoning steps, encouraging more structured and coherent outputs (Wei et al., 2022). It has been shown to significantly improve performance on tasks involving logical inference, arithmetic, and structured decision-making (Zhou et al., 2022). A key contribution of the present paper is to investigate the importance of the type of prompt used when deploying LLMs for choice modelling.

3 Research methodology and empirical setup

This section outlines the experimental framework used to evaluate the ability of LLMs to specify and, where technically feasible, estimate MNL models. This latter point relates to gaining insight into whether LLMs can conduct the entire process, i.e. including estimation, rather than just providing suggestions for how to analyse the data. In the present work, we limit our focus to MNL models only as the work serves as a proof of concept. Extensions to more complex specifications remains an avenue for future work. We start by looking at the overall methodological framework before looking at the specific context of our application.

3.1 General framework

Our framework evaluates the performance of LLMs using two prompting strategies, Zero-Shot Prompt (ZSP) and Chain-of-Thoughts (CoT). In our context, the ZSP template asked the LLM to suggest and estimate (where feasible) model specifications without detailed contextual guidance. In contrast, the CoT template instructs the LLM to (i) perform a descriptive analysis of the dataset, (ii) apply behavioural constraints commonly used in discrete choice modelling (e.g., negative cost sensitivity), and (iii) generate

a structured utility specification using a predefined code syntax (e.g., consistent with Apollo or Biogeme). This strategy simulates common choice modelling workflows (Nova et al., 2024).

We use two information settings illustrated in Figures 1 and 2. In the Full Information setting (Figure 1), the LLM is provided with a structured input consisting of (i) choice dataset in CSV format, (ii) a structured markdown data description explaining the dataset and its variables, and (iii) a textual prompt (either ZSP or CoT). The LLM is instructed through the provided prompt to either suggest and estimate MNL models to indentify the best-fitting MNL specification or to suggest plausible specifications based on the provided data. In the Limited Information setting (Figure 2), the LLM is provided only with (i) the data description and (ii) a ZSP prompt strategy. In this setting, the LLM is asked to suggest MNL specifications that are both theoretically sound and expected to perform well empirically, despite not having access to the raw data. Thus, these experiments vary along three dimensions — information setting, prompting strategy, and modelling goal — resulting in a total of five experimental configurations, as summarized in Table (1).

Table 1: Experiment Setup Overview

Experiment	Information Setting	Prompting Strategy	Modelling Goal
1	Full	ZSP	Suggest & Estimate
2	Full	CoT	Suggest & Estimate
3	Full	ZSP	Suggest
4	Full	CoT	Suggest
5	Limited	ZSP	Suggest

All MNL specifications generated by the LLMs, whether they are estimated by the LLMs or not, are then implemented and estimated also outside the LLMs. This serves two purposes. First, to verify in the case of "Suggest & Estimate" scenarios that the LLM is estimating the generated specifications correctly and not hallucinating or fabricating the log-likelihood values, as well as the parameter estimates and their significance. Second, for the "Suggest" scenarios, all generated specifications are implemented and estimated to assess their empirical performance. Across both goals, all resulting models are evaluated based on goodness-of-fit measures (e.g., log-likelihood, AIC), behavioural plausibility, (e.g., sign and significance of relevant parameters) and expert judgment concerning the overall quality and interpretability of the specifications.

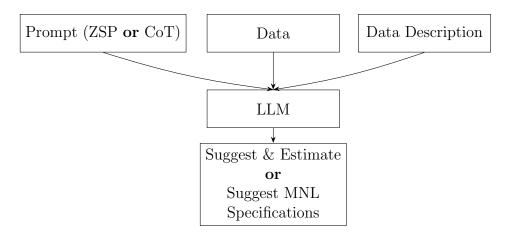


Figure 1: Full Information Setting

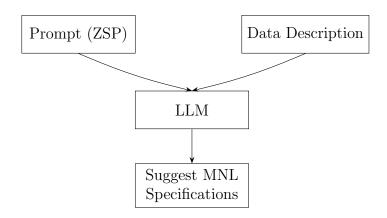


Figure 2: Limited Information Setting

3.2 Case study setup

This section presents the different LLMs evaluated, the dataset used, and the prompts we implemented.

3.2.1 Large Language Models

We evaluate a diverse set of Large Language Models to investigate how differences in architecture, training scale, openness, and provider influence their ability to support discrete choice model specification. Our selection balances coverage across major proprietary providers (OpenAI, Anthropic, Google, DeepSeek) and includes open-source models (Meta and Google) to ensure transparency and replicability. Moreover, models were chosen based on their performance, accessibility via browser-based user interfaces or API, and relevance to real-world application scenarios in research and practice. These include GPT-o3 (OpenAI, 2025b), GPT-o4-mini-high (OpenAI, 2025b), GPT-4.5 (OpenAI, 2025a), and GPT-4o (OpenAI, 2025a), Claude 4 Opus (Anthropic, 2025b), Claude 4 Sonnet (Anthropic, 2025c), Claude 3.7 Sonnet (Anthropic, 2025a), DeepSeek Chat (Liu, Feng, Xue, et al., 2024), Gemini 2.5 Flash (Google, 2025), Gemma 3 (Team et al., 2025), Llama 3 (Grattafiori et al., 2024), Llama 4 Maverick, and Llama 4 Scout (Meta, 2025).

Table 2 summarises the capabilities of LLMs evaluated in this study, based on metrics reported by the LLM Leaderboard (Tamales, 2024). This comparison provides context on each model's general reasoning ability (e.g., MMLU-Pro, GPQA), coding proficiency (e.g., LiveCodeBench, HumanEval), and performance on human judgement tasks (e.g., HLE) (Y. Wang et al., 2024; Rein et al., 2024; Phan et al., 2025; Tian et al., 2024; Liang et al., 2022)³.

Table 2: Evaluation metrics for selected LLMs

Model	Creator	Release	License	Context	MMLU	MMLU-Pro	GPQA	HumanEval	LIVECODEBENCH	SCICODE	HLE
GPT 4o	OpenAI	06/08/24	Proprietary	128k	86%	75%	46%	87%	63.5%	25%	84%
GPT o4-mini	OpenAI	16/04/25	Proprietary	200k	82%	65%	40%	_	52.7%	-	71%
GPT o3	OpenAI	16/04/25	Proprietary	200k	_	_	83%	_	57.1%	33%	-
GPT 4.5	OpenAI	27/02/25	Proprietary	128k	91%	_	70%	88%	-	23%	83%
Claude 4 Opus	Anthropic	22/05/25	Proprietary	200k	-	_	83%	_	24.1%	-	81%
Claude 4 Sonnet	Anthropic	22/05/25	Proprietary	200k	_	_	84%	_	26.6%	-	77%
Claude 3.7 Sonnet	Anthropic	24/02/25	Proprietary	200k	-	80%	85%	_	-	26%	75%
DeepSeek R1	Deepseek	28/05/25	Open	131k	_	85%	81%	_	50.7%	28.5%	76%
Gemini 2.5 Flash	Google	20/05/25	Proprietary	$1 \mathrm{m}$	_	80%	83%	_	50.2%%	36%	80%
Llama 3	Meta	06/12/24	Open	128k	86%	69%	51%	88%	52.2%	19.8%	74%
Llama 4 Maverick	Meta	05/04/25	Open	$1 \mathrm{m}$	86%	81%	70%	_	-	-	79%
Llama 4 Scout	Meta	05/04/25	Open	$10 \mathrm{m}$	80%	74.3%	57%	_	-	-	76%
Gemma 3 27B	Google	12/03/25	Open	131k	_	68%	42%	88%	-	-	73%

Interaction with these LLM models was performed mostly via their official browser-based user interfaces, where available (e.g., ChatGPT, Claude, DeepSeek, Gemini). To minimise potential contamination from prior user interactions and ensure greater reproducibility, we took precautions for each LLM. For ChatGPT variants, we disabled memory settings and avoided assigning persistent roles or naming the conversation, ensuring that the model could not accumulate session-specific knowledge. For Claude, Gemini, and DeepSeek, we created new accounts with no prior chat or profile history. These steps were taken to reduce any influence of user-specific context on model outputs. For open-weight models such as Gemma and Llama, interaction was conducted via API calls within local environments to ensure consistency across runs. Moreover, we control by their temperature and probability for suggesting the tokens (see appendix 5).

Given the inherently probabilistic nature of LLMs, it cannot be guaranteed that repeated queries will produce identical results. However, to improve replicability, each query was executed exactly once per model and per experiment, without regeneration or manual sampling. In addition, we controlled key generation parameters, such as temperature and token probability, when possible (see Appendix 5). Our approach prioritises comparability between models under consistent conditions, while recognising that minor variability in results is an expected feature of LLM behaviour.

3.2.2 Dataset

We evaluate the LLMs using a subset of the inter-city mode choice dataset distributed with the Apollo software (Hess & Palma, 2019). The dataset contains synthetic revealed preference (RP) data from 500 individuals, each reporting two inter-city trip observations, which yield a total of 1,000 choice responses. The choice set consists of four transport alternatives labelled as car, bus, air, and rail, with at least two of them available per

 $^{3. \ \} The \ leaderboard \ compiles \ and \ standardizes \ results \ from \ a \ wide \ range \ of \ benchmark \ papers, \ including: arXiv:2501.12948, \ 2405.04434, \ 2412.19437, \ 2412.10302, \ 2312.11805, \ 2403.05530, \ 2303.08774, \ 2408.12570, \ 2501.12599, \ 2410.01257, \ 2502.00203, \ 2404.14219, \ 2412.08905, \ 2503.01743, \ 2504.21233, \ 2504.21318, \ 2407.10671, \ 2409.12186, \ 2309.00071, \ 2409.12191, \ 2503.20215, \ 2502.13923, \ and \ 2412.15115.$

choice situation. Each alternative is characterised by in-vehicle travel time (in minutes), travel cost (in pounds), and access-time (in minutes), the latter only for non-car modes. In addition, the dataset includes information on each individual's gender, income, and whether the journey was a business trip or not.

3.2.3 Prompts design

Prompt design is a critical part of the methodology, as it defines how tasks are framed and used by the LLMs to guide their outputs (White et al., 2023). In this study, prompts were developed through iterative trial-and-error by the authors, drawing on both domain expertise in discrete choice modelling and prior experience interacting with LLMs. While no formal optimisation was conducted, prompts were refined to ensure clarity, internal consistency, and alignment with common modelling workflows (Nova et al., 2024; Van Cranenburgh et al., 2022). Once established, the final prompt templates were kept fixed across experiments and LLMs to ensure comparability. We acknowledge the growing body of literature on prompt engineering, and agree that systematic prompt development is an important direction for future research (Schulhoff et al., 2024). However, this lies beyond the scope of the present study, which focuses on evaluating the modelling capabilities of LLMs under clearly defined and consistently applied prompting strategies. The full prompt texts used for the five different experiment (Table 1) are presented below.

Experiment 1

- Information Setting: Data & Data Description
- Prompting Strategy: Zero-Shot
- Modelling Goal: Suggest & Estimate

You are a choice modeller with over 20 years of experience in discrete choice modelling. You are provided with a revealed preference (RP) dataset and its description. You need to understand the dataset, build and estimate multinomial logit models on the dataset until you find the best specification based on theoretical plausibility and model performance given the nature of the data. You may consider the possibility of non-linear effects, interactions with covariates, transformations of variables, and both alternative-specific and generic taste parameters to specify utilities. Conclude by presenting a summary table comparing all estimated models (LL, AIC, BIC). Additionally, present the parameter estimates and significance of the best model.

Experiment 2

- Information Setting: Data & Data Description
- Prompting Strategy: Chain-of-Thoughts
- Modelling Goal: Suggest & Estimate

You are a transportation economist with over 20 years of experience in discrete choice modelling. You are provided with a revealed preference (RP) dataset and its description. Your target is to find the best Multinomial Logit (MNL) model specification by relying on this workflow:

- 1. Understand the structure of the dataset and its variables.
- 2. Propose, justify, and estimate several utility specifications for a Multinomial

Logit (MNL) model until you find the best specification based on theoretical plausibility and model performance in terms of log-likelihood. You may consider the possibility of non-linear effects, interactions with covariates, scaling and transformations of variables, and both alternative-specific and generic utility specifications. Do not split the data into train and test sets.

- 3. Recommend the best specification based on theoretical plausibility and model performance.
- 4. Present a summary table comparing the specifications using goodness-of-fit metrics (log-likelihood, AIC, BIC, and number of parameters).
- 5. Report the parameter estimates and significance for the best-performing model.

Experiment 3

• Information Setting: Data & Data Description

• Prompting Strategy: Zero-Shot

• Modelling Goal: Suggest

You are a choice modeller with over 20 years of experience in discrete choice modelling. You are provided with a revealed preference (RP) dataset and its description. You need to understand the dataset and propose Multinomial Logit (MNL) model specifications that are both theoretically sound and likely to perform well empirically. The goal is to suggest the best MNL specification based on theoretical plausibility and potential model performance given the nature of the data. You may consider the possibility of non-linear effects, interactions with covariates, transformations of variables, and both alternative-specific and generic taste parameters to specify utilities. Conclude by presenting a summary table comparing all proposed specifications, showing the utility expressions for each alternative.

Experiment 4

- Information Setting: Data & Data Description
- Prompting Strategy: Chain-of-Thoughts
- Modelling Goal: Suggest

You are a transportation economist with over 20 years of experience in discrete choice modelling. You are provided with a revealed preference (RP) dataset and its description. Your target is to find the best Multinomial Logit (MNL) model specification by relying on this workflow:

- 1. Understand the structure of the dataset and its variables.
- 2. Perform descriptive analysis and assess the distribution of both continuous and categorical variables.
- 3. Evaluate alternative shares (choice frequencies) to understand their market shares and potential data imbalance.
- 4. Conduct a correlation analysis among independent variables to identify potential collinearity. Discuss how collinearity issues, if identified, should be managed.

- 5. Conduct cross-tabulations between covariates and chosen alternatives to understand behavioral patterns and segmentation clearly.
- 6. Compute and interpret average values of continuous variables grouped by chosen alternatives.
- 7. Based on your descriptive analysis and understanding of the data, propose and justify several utility specifications for a Multinomial Logit (MNL) model that would fit the data best based on theoretical plausibility and potential model performance. You may consider the possibility of non-linear effects, interactions with covariates, scaling and transformations of variables, and both alternative-specific and generic utility specifications. Do not split the data into train and test sets.
- 8. Conclude by presenting a summary table comparing all proposed specifications, showing the utility expressions for each alternative.

Experiment 5

• Information Setting: Data Description

• Prompting Strategy: Zero-Shot

• Modelling Goal: Suggest

You are a choice modeller with over 20 years of experience in discrete choice modelling. You are provided a description of a dataset that contains revealed preference (RP) observations. You need to understand the dataset and propose Multinomial Logit (MNL) model specifications that are both theoretically sound and likely to perform well empirically. The goal is to suggest the best MNL specification based on theoretical plausibility and potential model performance given the nature of the data. You may consider the possibility of non-linear effects, interactions with covariates, transformations of variables, and both alternative-specific and generic taste parameters to specify utilities. Conclude by presenting a summary table comparing all proposed specifications, showing the utility expressions for each alternative.

4 Results

This section presents the empirical results. Section 4.1 provides a detailed evaluation of the performance of the different LLMs in each experimental configuration, with particular attention to how prompting strategies and information availability influence the quality of suggested model specifications. Section 4.2 offers an overall evaluation of the utility specifications generated by each LLM, independent of experimental setting.

4.1 Evaluation by Experiment

4.1.1 Goal: Suggest & Estimate

We start by presenting the outcomes of the two "Suggest & Estimate" experiments, which differ in their prompting strategies. The first experiment is executed with a Zero-Shot prompt while the second experiment applies a Chain-of-Thoughts prompt (Table 1).

Among all the LLMs, only **ChatGPT o3** successfully suggested valid MNL specifications and accurately estimated their parameters by executing self-generated Python code, that generated the same results as our own estimations⁴. In contrast, every other LLM either mis-estimated specifications it suggested or hallucinated the results by returning Log-Likelihood values, parameter estimates and standard deviations that we could not reproduce in our independent re-estimations. This finding highlights the current limitations of most LLMs in performing faithful end-to-end model estimation, particularly in tasks that require domain-specific knowledge and executed outputs. It also puts a responsibility on the modeller to verify the results reported by LLMs.

Tables 3 and 4 summarise the results of the specifications suggested and estimated by ChatGPT o3 across the first and second experiments. The Zero-Shot prompt generated and estimated three specifications, while the Chain-of-Thoughts prompt produced five. Despite the difference in prompt, both experiments converged to the same best-performing specification in terms of Log-Likelihood (LL), Akaike Information Criterion (AIC), and Bayesian Information Criterion (BIC) (S2 in Table 3 and S4 in Table 4). The utility functions of the best-performing model follows a linear-in-parameter specification. They include generic taste parameters for travel time, travel cost, and access time (the latter for all modes except car), as well as a generic interaction coefficient between travel time and a business trip variable. The specification also incorporates alternative-specific constants, with the constant for the car alternative normalised to zero for identification.

Table 3: Experiment 1 (Full Information, ZSP, Suggest & Estimate)

Specification (ChatGPT o3)	LL	AIC	BIC	VOT
S1	-1,031.82	2,073.63	2,098.17	0.197
S2	-981.80	1,977.61	2,011.96	0.198
S3	-1,083.68	$2,\!177.36$	2,201.90	0.262

Table 4: Experiment 2 (Full Information, CoT, Suggest & Estimate)

Specification (ChatGPT o3)	LL	AIC	BIC	VOT
S1	-1,031.82	2,073.63	2,098.17	0.197
S2	-1,030.97	2,073.93	$2,\!103.38$	0.198
S3	-1,026.81	2,065.62	2,095.06	0.262
S4	-981.80	1,977.61	$2,\!011.96$	0.198
S5	-993.30	2,000.59	$2,\!034.95$	0.364

4.1.2 Goal: Suggest

Next, we discuss the results of the "Suggest" experiments, which explore how different prompting strategies and information availability influence the quality of model specifications generated by LLMs. Experiments 3 and 4 are both under the same full information

 $^{4. \} See\ ChatGPT\ o3\ transcript\ of\ Experiment\ 1:\ https://chatgpt.com/share/6887d3a6-815c-8009-9b40-78be528ef4f7abberged.$

setup (providing the model with both the raw dataset and a structured data description) but differ in prompting strategies (ZSP for Experiment 3 and CoT for Experiment 4). In contrast, Experiment 5 is conducted with limited information, providing only the data description, and a ZSP (Table 1). Note that the Llama models (Llama 3, Llama 4 Maverick, and Llama 4 Scout) were not included in Experiments 3 and 4, as their API interface did not support loading raw data files at the time of evaluation. As a result, these models were only evaluated under the limited-information setting in Experiment 5.

The results from Experiment 3 demonstrate that LLMs, when prompted under a ZSP strategy and provided with full information, are capable of generating plausible and wellperforming model specifications; though not without limitations. Tables 5 and 6 present the LL and AIC values, respectively, for all specifications generated by ten LLM variants in Experiment 3. Notably, the Claude family (Claude 4 Opus, 4 Sonnet, and 3.7 Sonnet) and DeepSeek produced a greater number of specifications than any ChatGPT or Gemini variant, which reflects a relative higher capacity for exploring the modelling space. However, all specifications suggested by DeepSeek and ChatGPT 40 systematically omitted alternative-specific constants, which are important in the case of labelled alternatives. As a result, these specifications obtained far inferior fit and were excluded from further comparison. In addition, some specifications generated by Claude 4 Opus, Claude 4 Sonnet, and DeepSeek failed to converge during estimation and were likewise disregarded. Moreover, two specifications — specifically S6 from Claude 3.7 Sonnet and S4 from Gemini 2.5 Flash — yielded at least one positive coefficient for travel time and/or travel cost, which violates economic behaviour expectations. These were also excluded. All excluded specifications are shown in gray font within the tables for transparency. In contrast, all specifications generated by ChatGPT o4-mini-high, ChatGPT o3, ChatGPT 4.5, Claude 4 Sonnet, and Gemma 3 passed both convergence and behavioural plausibility checks. Among the valid specifications, specification 3 (S3) from ChatGPT 4.5 has the best LL (LL = -974.95), while specification 4 (S4) and specification 5 (S5) from Claude 4 Sonnet have the lowest AIC (AIC = 1.976.75), demonstrating a more favourable balance between model complexity and fit.

Overall, the valid specifications generated in the "Suggest" experiment exhibit slightly improved goodness-of-fit relative to those identified in the "Suggest & Estimate" configurations. This suggests that, when LLMs are tasked solely with proposing specifications, without the additional workload involved in estimating them, they may provide models with marginal better goodness-of-fit metrics. One possible explanation is that separating specification task from estimation enables the LLMs to fully allocate their computational resources and internal reasoning capabilities to generating behaviourally plausible and empirically well-performing model specifications. In contrast, executing the estimation process introduces substantial computation demands, including data handling, code generation, syntax validation, and numerical optimisation, all of which may detract from the LLM's ability to focus on the specification task itself.

Table 5: Experiment 3 (Full Information, ZSP, Suggest) - LL

							•	- /		
Spec.	ChatGPT 40	ChatGPT o4-mini-high	ChatGPT o3	ChatGPT 4.5	Claude 4 Opus	Claude 4 Sonnet	Claude 3.7 Sonnet	DeepSeek R1	Gemini 2.5 Flash	Gemma 3
S1	-1,106.23*	-1,031.82	-1,031.00	-1,030.97	-1,030.97	-1,031.00	-1,030.98	-1,089.94*	-1,031.82	-1,030.97
S2	-1,027.57*	-1,030.97	-1,030.97	-1,024.48	$-1,048.30^{\dagger}$	-1,025.91	-1,025.00	-1,025.82*	-1,030.97	-999.70
S3	-1,022.32*	-1,025.00	-1,036.49	-974.95	-1,026.10	-1,017.58	-978.15	-1,080.08*	-983.45	-1,000.05
S4	-1,023.33*	-999.72	-1,011.22	-1,024.18	-982.15	-978.37	-1,025.36	$-68,386.87^{\dagger}$	$-1,028.78^{\ddagger}$	-998.60
S5	-1,123.26*	-1,036.38	-977.37	_	$-1,033.34^{\dagger}$	-978.37	$-4,991.18^{\dagger}$	-1,026.19*	_	_
S6	_	_	_	_	-1,027.99	-1,030.78	-967.80^{\ddagger}	−963.94 *	_	_

^{*}No ASCs included. †Model did not converge. ‡Positive Beta Cost and/or Beta Time.

Table 6: Experiment 3 (Full Information, ZSP, Suggest) - AIC

Spec.	ChatGPT 40	ChatGPT o4-mini-high	ChatGPT o3	ChatGPT 4.5	Claude 4 Opus	Claude 4 Sonnet	Claude 3.7 Sonnet	DeepSeek R1	Gemini 2.5 Flash	Gemma 3
S1	2,216.47*	2,073.63	2,071.99	2,073.94	2,073.93	2,071.99	2,073.95	2,185.87*	2,073.63	2,073.93
S2	2,071.14*	2,073.94	2,073.93	2,076.97	$2{,}108.60^{\dagger}$	2,065.82	2,074.01	2,073.65*	2,073.93	2,033.39
S3	2,060.64*	2,074.01	2,084.98	1,987.91	2,070.19	2,053.15	1,978.30	2,166.17*	1,986.90	2,034.10
S4	2,062.67*	2,029.44	2,036.44	2,082.36	1,980.31	1,976.75	2,068.72	$136,783.74^{\dagger}$	2,073.56 [‡]	2,037.19
S5	2,250.53*	2,084.77	1,984.74	_	$2,090.67^{\dagger}$	1,976.75	10,016.36 [†]	2,064.38*	_	_
S6	_	_	_	_	2,067.98	2,073.56	1,963.60 [‡]	1,961.87*	_	_

^{*}No ASCs included. †Model did not converge. ‡Positive Beta Cost and/or Beta Time.

Next, we present the LL and AIC of all specifications generated in Experiment 4 (Tables 7 and 8). Unlike the Zero-Shot prompt in Experiment 3, this experiment employed a structured Chain-of-Thoughts (CoT) prompting strategy, encouraging the LLMs to perform preliminary analyses before suggesting utility specifications. The results of Experiment 4 demonstrate that structured prompting, in the form of Chain-of-Thoughts strategies, can substantially improve the quality of LLM-suggested model specifications. By guiding LLM models through intermediate analysis steps before suggesting model specifications, CoT prompting encourages more behaviourally plausible and complex utility forms.

As shown in Tables 7 and 8, this approach led to consistent improvements across various aspects compared to the ZSP baseline used in Experiment 3. Most notably, the use of CoT resolved a recurring issue from Experiment 3 in which alternative-specific constants were sometimes omitted; now, all generated specifications included them. Furthermore, CoT prompting improved the overall model fit across all LLMs, with the exception of the open-weight Gemma 3 model. Specifically, all closed-weight LLMs achieved better AIC values under CoT prompting (Experiment 4, Table 8) than under the ZSP condition (Experiment 3, Table 6). Moreover, ChatGPT o4-mini-high, Claude 4 Opus and 4 Sonnet, and Gemini 2.5 suggested better specifications in terms of LL values. Despite these gains, certain limitations persisted. One specification from Claude 3.7 Sonnet and two specifications from DeepSeek failed to converge during estimation. In addition, one specification from ChatGPT 40 and two specifications from Gemini 2.5 Flash led to at least one positive coefficient for travel time and/or travel cost, contradicting expected economic behaviour. Surprisingly, all specifications generated by the open-weight Gemma 3 from Google Deepmind failed to converge during estimation. Despite these limitations, the best-performing model overall, Specification 5 from Claude 4 Sonnet, achieved the highest log-likelihood (-967.53) and the lowest AIC (1,963.05) overall, demonstrating the potential of CoT prompts to guide LLMs toward more effective and interpretable model structures.

Table 7: Experiment 4 (Full Information, CoT, Suggest) - LL

Spec.	ChatGPT 40	ChatGPT o4-mini-high	ChatGPT o3	ChatGPT 4.5	Claude 4 Opus	Claude 4 Sonnet	Claude 3.7 Sonnet	DeepSeek R1	Gemini 2.5 Flash	Gemma 3
S1	-1,024.48	-1,030.97	-1,030.97	-1,031.00	-1,024.48	-1,019.18	-1,024.48	-1,030.97	-1,031.42	$-1,030.97^{\dagger}$
S2	-979.47	-1,024.48	-980.62	-978.34	-1,030.97	-1,010.30	-1,030.97	-1,025.76	-1,024.36 [‡]	$-1,030.97^{\dagger}$
S3	-1,024.97	-987.79	-1,026.00	-1,037.28	-973.34	-1,019.76	$-1,030.96^{\dagger}$	$-1,083.58^{\dagger}$	-968.29	$-1,024.84^{\dagger}$
S4	-1,017.16 [‡]	-1,036.49	-1,035.45	-1,030.97	-1,035.14	-1,024.00	-979.02	-993.95^{\dagger}	-1,024.48	$-1,028.78^{\dagger}$
S5	-	-1,014.87	_	-975.11	-1,040.96	-967.53	-1,035.94	-1,499.58	-1,030.97	_
S6	-	-	_	-	-980.82	-1,019.32	-1,021.88	-	-960.07^{\ddagger}	_
S7	-	_	-	-	-	-	-981.80	_	-	_

[†]Model did not converge. [‡]Positive Beta Cost and/or Beta Time.

Table 8: Experiment 4 (Full Information, CoT, Suggest) - AIC

			1	(,	, 0	<i>3</i> /		
Spec.	ChatGPT 40	ChatGPT o4-mini-high	ChatGPT o3	$\begin{array}{c} {\rm ChatGPT} \\ {\rm 4.5} \end{array}$	Claude 4 Opus	Claude 4 Sonnet	Claude 3.7 Sonnet	DeepSeek R1	Gemini 2.5 Flash	Gemma 3
S1	2,076.96	2,073.93	2,073.94	2,071.99	2,076.96	2,056.37	2,076.95	2,073.93	2,074.84	2,079.93
S2	1,992.94	2,076.95	1,979.23	1,970.68	2,073.93	2,038.61	2,073.93	2,069.51	$2,080.72^{\ddagger}$	$2,081.93^{\dagger}$
S3	2,077.94	1,993.59	2,070.01	2,084.57	1,970.69	2,055.52	$2,075.93^{\dagger}$	$2,179.16^{\dagger}$	1,966.59	$2,067.67^{\dagger}$
S4	$2,068.32^{\ddagger}$	2,084.98	2,082.89	2,073.93	2,082.28	2,066.01	1,978.04	2,003.90†	2,076.95	$2,077.56^{\dagger}$
S5	_	2,043.74	_	1,966.22	2,091.92	1,963.05	2,083.87	3,011.16	2,079.93	_
S6	_	_	_	_	1,977.63	2,052.64	2,057.76	_	1,972.14	_
S7	_	_	_	-	_	_	1,977.61	_	-	_

[†]Model did not converge. [‡]Positive Beta Cost and/or Beta Time.

The results of Experiment 5 indicate that LLMs are capable of generating well-performing model specifications even under limited information conditions, where only a dataset description is provided. Despite the absence of raw data, several LLM models produced specifications that equalled or even surpassed those they generated under full information conditions in previous experiments. As shown in Tables 9 and 10, Claude variants and DeepSeek continued to show stronger generative capacity, producing a greater number of specifications than any of the GPT or Gemini models. Although some results were promising, they were excluded due to specification or estimation issues. Specifically, one specification from GPT-o4-mini-high was omitted for lacking ASCs, which led to poor model fit. Five additional specifications, three from Claude 3.7 Sonnet, one from DeepSeek R1, and one from Llama 4 Scout, were excluded due to convergence failures. Moreover, none of the specifications generated by the open-weight Gemma 3 model converged during estimation and were therefore excluded from further analysis. Among the valid results, Specification 2 (S2) from ChatGPT 40 achieved the best log-likelihood (-969.73), while Specification 4 (S4) from Claude 4 Opus delivered the lowest AIC (1,960.80), indicating a favourable trade-off between model fit and parsimony. Notably, ChatGPT 40, 04-mini-high, Claude 4 Opus, and DeepSeek all produced better-fitting specifications in this limited information setting than in their respective full information experiments (Experiments 3 and 4). These findings suggest that, under certain conditions, LLMs may benefit from simplified input structures, enabling them to focus more effectively on the model specification process itself.

Finally, open-weight models (Gemma 3 and Llama variants) showed noticeably weaker performance in Experiment 5. While the limited information setup reduced the task complexity, these models struggled to deliver viable or competing specifications. As previously mentioned, none of the specifications generated by Gemma 3 converged. The

Llama family performed somewhat better, with Llama 4 Scout generating a specification (S5) with a moderately competitive LL (-981.98) and AIC (1,997.96), though still weaker than most specifications generated by closed-weight models. However, the best specifications from the other two Llama versions (3 and 4 Maverick) produced the worst best specifications in terms of LL and AIC compared to all closed-weight models. These findings confirm that current open-weight LLMs, while valuable for transparency and local deployment, are still far from matching the end-to-end reliability and modeling capacity of closed-weight models in discrete choice modeling tasks, even under simplified tasks with limited information conditions.

Table 9: Experiment 5 (Limited Information, ZSP, Suggest) - LL

	Table 9. Experiment 9 (Elimited Information, 201, 5488600) EE									
C	ChatGPT	ChatGPT	ChatGPT	ChatGPT	Claude	Claude	Claude	DeepSeek	Gemini	Gemma
Spec.	40	o4-mini-high	03	4.5	4 Opus	4 Sonnet	3.7 Sonnet	R1	2.5 Flash	3
S1	-1,031.00	-1,121.16*	-1,031.00	-1,031.00	-1,031.82	-1,030.97	-1,030.97	-1,047.71	-1,031.82	$-1,024.48^{\dagger}$
S2	-969.73	-1,030.97	-1,030.97	-1,030.97	-1,030.97	-1,026.81	-1,024.48	-1,036.03	-1,030.97	$-1,022.34^{\dagger}$
S3	-976.60	-1,036.47	-1,020.74	-1,035.77	-1,022.61	-1,023.22	$-1,038.05^{\dagger}$	-982.10	-981.57	-960.90^{\dagger}
S4	_	-981.12	-982.49	-991.62	-972.40	-971.33	-990.18	$-1,071.10^{\dagger}$	-1,024.48	-955.06^{\dagger}
S5	_	-1,018.80	-1,020.41	-994.39	-1,035.14	-978.89	$-1,013.76^{\dagger}$	-1,025.00	_	-955.18^{\ddagger}
S6	_	_	_	_	-1,030.26	-972.07	-1,030.29	-1,046.18	_	-
S7	_	_	_	_	-1,006.36	_	-1,027.52	_	_	-
S8	-	_	_	-	-	_	-976.31^{\dagger}	_	-	
C	Llama	Llama	Llama							
Spec.	3	4 Maverick	4 Scout							
S1	-1,024.48	-1,030.97	-1,031.82							_
S2	-991.85	-1,024.48	-1,012.41							
S3	-1,024.44	-1,021.96	-1,012.41							
S4	-1,000.18	_	$-1,010.09^{\dagger}$							
S5	_	_	-981.98							

^{*}No ASCs included. †Model did not converge. ‡Positive Beta Cost and/or Beta Time.

Table 10: Experiment 5 (Limited Information, ZSP, Suggest) - AIC

		310 10: E 11	P	me o (Emmeed información, Est, suggest)						
Spec.	ChatGPT	ChatGPT	ChatGPT	ChatGPT	Claude	Claude	Claude	DeepSeek	Gemini	Gemma
	40	o4-mini-high	03	4.5	4 Opus	4 Sonnet	3.7 Sonnet	R1	2.5 Flash	3
S1	2,071.99	2,246.32*	2,071.99	2,071.99	2,073.64	2,073.94	2,073.94	2,107.42	2,073.64	2,078.95
S2	1,973.46	2,073.94	2,073.93	2,073.93	2,073.94	2,065.62	2,076.96	2,084.06	2,073.94	$2,090.68^{\dagger}$
S3	1,987.19	2,084.93	2,057.48	2,081.54	2,059.22	2,064.44	$2,092.10^{\dagger}$	1,978.20	1,983.14	$1,969.80^{\dagger}$
S4	_	1,980.24	1,990.98	2,005.25	1,960.80	1,972.66	2,000.36	$2,154.20^{\dagger}$	2,076.96	$1,974.12^{\dagger}$
S5	_	2,053.61	2,058.82	2,012.78	2,082.28	1,987.78	$2,047.52^{\dagger}$	2,074.00	-	1,986.36 [‡]
S6	-	_	_	-	2,078.52	1,972.14	2,078.58	2,106.36	_	_
S7	_	_	_	_	2,028.72	_	2,067.04	_	_	_
S8	-	_	_	-	-	_	$1,986.62^{\dagger}$	-	_	_
Cnas	Llama	Llama	Llama							
Spec.	3	4 Maverick	4 Scout							
S1	2,076.95	2,073.97	2,073.63							
S2	2,021.70	2,076.95	2,058.82							
S3	2,076.88	2,057.92	2,058.82							
S4	2,036.36	_	$2,070.18^{\dagger}$							
S5	_	_	1,997.96							

^{*}No ASCs included. † Model did not converge. ‡ Positive Beta Cost and/or Beta Time.

4.1.3 Best Specifications by Experiment and/or LLM

To evaluate the capabilities of each Large Language Model across experimental conditions, we analyse the best-performing model specifications in terms of Log-Likelihood (LL), Akaike Information Criterion (AIC), and Bayesian Information Criterion (BIC).

This analysis offers an overview of how LLMs perform when tasked with either suggesting or estimating MNL models under varying information and prompt settings. Tables 11, 12, and 13 summarise the best specifications by experiment and by LLM.

In the "Suggest & Estimate" experiments (Exp. 1 and 2), only GPT-o3 successfully specified theoretically sound specifications and estimated them correctly through self-generated Python code, regardless of the prompting strategy. All other LLMs either mis-estimated their own specifications or returned fabricated estimation outputs. In contrast, when LLMs were tasked solely with specification (Exp. 3 to 5), the competitive performance among LLMs improved in terms of LL, AIC, and BIC. Under the full information and ZSP condition (Exp. 3), GPT 4.5 generated the specification with the best log-likelihood (LL = -974.95). With a structured CoT prompt in Experiment 4, Claude 4 Sonnet produced not only the best model of that experiment but the best specification across all experiments, achieving a log-likelihood of -967.53. Lastly, in the limited information setting (Exp. 5), GPT 40 generated the specification with the best model performance (LL = -969.73). Surprisingly, four LLMs (GPT 40, GPT o4-mini-high, Claude 4 Opus, and DeepSeek) achieved their best performance under this limited-input configuration, suggesting that withholding full data access may, in some cases, prompt stronger theoretical reasoning.

In terms of AIC (Table 12), Claude variants provided the best AIC values in all "Suggest" experiments (Exp. 3 to 5), which suggest a balance between model fit and parsimony. Moreover, Claude 4 Opus, with limited information (Exp. 5), generated the specification with the overall lowest AIC (1,960.80). Similarly to the LL results, the same four LLMs (GPT 40, GPT o4-mini-high, Claude 4 Opus, and DeepSeek) achieved their respective best performances in the limited information experiment.

Table 11: Experiments Results - LL

	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 5	Best Exp. Per LLM	Best LL Per LLM
GPT 40	_	_	_	-979.47	-969.73	Exp. 5	-969.73
GPT o4minihigh	_	_	-999.72	-987.79	-981.12	Exp. 5	-981.12
GPT o3	-981.80	-981.80	-977.37	-980.62	-982.49	Exp. 3	-977.37
GPT 4.5	_	_	-974.95	-975.11	-991.62	Exp. 3	-974.95
Claude 4 Opus	_	_	-982.15	-973.34	-972.40	Exp. 5	-972.40
Claude 4 Sonnet	_	_	-978.37	-967.53	-971.33	Exp. 4	-967.53
Claude 3.7 Sonnet	_	_	-978.15	-979.02	-990.18	Exp. 3	-978.15
DeepSeek	_	_	_	-1,025.76	-982.10	Exp. 5	-982.10
Gemini 2.5 Flash	_	_	-983.45	-968.29	-981.57	Exp. 4	-968.29
Gemma 3	_	_	-998.60	_	_	Exp. 3	-998.60
Llama 3	_	_	_	_	-991.85	Exp. 5	-991.85
Llama 4 Maverick	_	_	_	_	-1,021.96	Exp. 5	-1,021.96
Llama 4 Scout	_	_	_	_	-981.98	Exp. 5	-981.98
Best LLM Per Exp.	GPT o3	GPT o3	GPT 4.5	Claude 4 S.	GPT 4o	_	_
Best LL Per Exp.	-981.80	-981.80	-974.95	-967.53	-969.73	_	_

Exp. 1: Full/ZS/Estimate, Exp. 2: Full/CoT/Estimate, Exp. 3: Full/ZS/Suggest, Exp. 4: Full/CoT/Suggest, Exp. 5: Limited/ZS/Suggest.

Table 12: Experiments Summary - AIC

	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 5	Best Exp. Per LLM	Best AIC Per LLM
ChatGPT 4o	_	_	_	1,992.94	1,973.46	Exp. 5	1,973.46
ChatGPT o4minihigh	_	_	2,029.44	1,993.59	1,980.24	Exp. 5	1,980.24
ChatGPT o3	1,977.61	1,977.61	1,984.74	1,979.23	1,990.98	Exp. 1	1,977.61
ChatGPT 4.5	_	_	1,987.91	1,966.22	2,005.25	Exp. 4	1,966.22
Claude 4 Opus	_	-	1,980.31	1,970.69	1,960.80	Exp. 5	1,960.80
Claude 4 Sonnet	_	_	1,976.75	1,963.05	1,972.14	Exp. 4	1,963.05
Claude 3.7 Sonnet	_	-	1,978.30	1,977.61	2,000.36	Exp. 4	1,977.61
DeepSeek	_	_	_	2,069.51	1,978.20	Exp. 5	1,978.20
Gemini 2.5 Flash	_	_	1,986.90	1,966.59	1,983.14	Exp. 4	1,966.59
Gemma 3	_	_	2,033.39	_	_	Exp. 3	2,033.39
Llama 3	_	_	_	_	2,021.70	Exp. 5	2,021.70
Llama 4 Maverick	_	-	_	_	2,057.92	Exp. 5	2,057.92
Llama 4 Scout	_	_	_	_	1,997.96	Exp. 5	1,997.96
Best LLM Per Exp.	GPT o3	GPT o3	Claude 4 S.	Claude 4 S.	Claude 4 O.	_	_
Best AIC Per Exp.	1,977.61	1,977.61	1,976.75	1,963.05	1,960.80	_	

Exp. 1: Full/ZS/Estimate, Exp. 2: Full/CoT/Estimate, Exp. 3: Full/ZS/Suggest, Exp. 4: Full/CoT/Suggest, Exp. 5: Limited/ZS/Suggest.

Table 13: Experiments Summary - BIC

	ICIC	ло 10. да	apermients	DIC			
	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 5	Best Exp. Per LLM	Best BIC Per LLM
ChatGPT 4o	_	_	2,099.91	2,076.37	2,056.89	Exp. 5	2,056.89
ChatGPT o4minihigh	_	-	2,098.17	2,037.76	2,024.41	Exp. 5	2,024.41
ChatGPT o3	2,011.96	2,011.96	2,058.36	2,023.40	2,054.78	Exp. 1	2,011.96
ChatGPT 4.5	_	_	2,081.16	2,005.03	2,059.23	Exp. 4	2,005.03
Claude 4 Opus	_	_	2,019.57	2,016.90	2,000.06	Exp. 5	2,000.06
Claude 4 Sonnet	_	_	2,025.82	2,031.76	2,040.85	Exp. 3	2,025.82
Claude 3.7 Sonnet	_	_	2,032.28	2,011.96	2,049.44	Exp. 4	2,011.96
DeepSeek	_	_	2,045.30	$2,\!103.38$	2,012.55	Exp. 5	2,012.55
Gemini 2.5 Flash	_	_	2,035.97	2,040.21	2,032.22	Exp. 5	2,032.22
Gemma 3	_	_	2,103.38	_	_	Exp. 3	2,103.38
Llama 3	_	_	_	_	2,114.94	Exp. 5	2,114.94
Llama 4 Maverick	_	_	_	_	2,092.28	Exp. 5	2,092.28
Llama 4 Scout	_	_	_	_	2,081.39	Exp. 5	2,081.39
Best LLM Per Exp.	GPT o3	GPT o4	Claude 4 O.	GPT 4.5	Claude 4 O.	_	_
Best BIC Per Exp.	2,011.97	2,011.96	2,019.57	2,005.03	2,000.06	_	_

Exp. 1: Full/ZS/Estimate, Exp. 2: Full/CoT/Estimate, Exp. 3: Full/ZS/Suggest, Exp. 4: Full/CoT/Suggest, Exp. 5: Limited/ZS/Suggest.

Finally, analysing the best-performing specifications in terms of BIC, which imposes a stronger penalty on model complexity than AIC, we observe consistent patterns with some notable shifts (Table 13). Claude 4 Opus again generated the specification with the lowest BIC value (2,000.06) in Experiment 5 (limited information). This reinforces previous findings from the AIC analysis, highlighting Claude's ability in generating high-quality specifications under limited information conditions. GPT variants also performed well in terms of BIC. In addition to Experiments 1 and 2 where GPT-o3 was the only LLM to successfully estimate its own specification, GPT 4.5 achieved the lowest BIC in Experiment 4 (2,005.03), further confirming that structured prompts (CoT) can guide

LLMs towards statistically efficient specifications. Once again, the same four LLMs (GPT 40, GPT o4-mini-high, Claude 4 Opus, and DeepSeek), as well as Gemini 2.5 Flash, achieved their best BIC performance in Experiment 5. These results further support the emerging pattern that simplified/limited inputs may encourage LLMs to focus more on utility structure and behavioural reasoning rather than being distracted by complex data analysis.

4.2 Overall Evaluation of LLM Performance

To complement the experiment-level analysis, this subsection provides a broader evaluation of each LLM's overall performance across all configurations. Table 14 summarizes the performance and characteristics of the utility specifications generated by each LLM across all experiments, offering a broader view of their modelling capabilities. Note that open-weight models (Gemma 3 and Llama variants) are excluded from this overall evaluation as they produced few valid specifications across expriments (Gemma 3 only in Exp. 3 and Llama variants only in Exp. 5), which renders average-based comparisons unreliable.

Table 14: Overall Evaluation of Generated Specifications by LLM

LLM	Av. Nb of Spec.	Models Converged	Av. Nb of Vars	Av. Nb of Params	Generic Params	Alt-Spec. Params	ASC Included	Av. Nb of Socioeconomics	Av. Nb of Transformations	Av. Nb of Interactions
ChatGPT 4o	2.58	100%	4.00	10.75	23%	77%	58%	0.50	0.50	0.42
ChatGPT o4-mini-high	3.00	100%	3.53	7.80	47%	53%	93%	0.33	0.73	0.40
ChatGPT o3	2.77	100%	3.68	7.18	47%	53%	100%	0.27	0.59	0.59
ChatGPT 4.5	2.86	100%	3.93	9.00	35%	65%	100%	0.64	0.50	0.29
Claude 4 Opus	3.68	89%	3.68	7.74	43%	57%	100%	0.37	0.26	0.53
Claude 4 Sonnet	3.50	100%	4.67	9.33	36%	64%	100%	1.22	0.33	0.72
Claude 3.7 Sonnet	4.05	76%	3.90	9.81	33%	67%	100%	0.57	0.33	0.67
DeepSeek R1	3.35	76%	3.53	7.29	50%	50%	65%	0.18	0.29	0.47
Gemini 2.5 Flash	2.93	100%	3.50	10.71	32%	68%	100%	0.36	0.43	0.43

Across all experiments, Claude variants generated on average more specifications compared to GPT, DeepSeek, and Gemini variants, as we already discussed. Specifically, Claude 3.7 Sonnet generated on average the highest number of specifications (4.05), though only 76% of these converged during estimation. Other models, such as Claude 4 Opus and DeepSeek also had convergence issues, with rates of 89% and 79%, respectively. In contrast, all GPT variants and Gemini 2.5 Flash achieved a perfect 100% convergence rate, demonstrating greater robustness in suggesting estimable specifications.

With respect to model complexity, Claude 4 Sonnet stands out as the LLM model that generated, on average, the most complex specifications. This included the highest number of variables (4.67), a relatively high number of parameters (9.33), the highest number of socioeconomic variables (1.22), and the highest number of interactions between socioeconomic variables and attributes (0.72). Conversely, GPT-o3, despite being OpenAI's most advanced reasoning model, proposed relatively simpler specifications, with the lowest average number of parameters (7.18) and few socioeconomic variables (0.27). This outcomes is likely influenced by the fact that GPT-o3 had to allocate its reasoning capabilities both to suggesting specifications and estimating them in Experiments 1 and 2, rather than allocating all its resources to generating more complex specifications.

While GPT 40 and Gemini 2.5 suggest specifications with the highest number of parameters (10.75 and 10.71, respectively), GPT 40 struggled with including alternative-specific

constants, with only 58% of its specifications incorporating them. DeepSeek encountered a similar issue, with ASCs included in just 68% of its specifications. However, GPT 40 had a strong inclination towards modelling behavioural heterogeneity across alternatives, with 77% of its parameters specified in alternative-specific form. GPTs, Claudes, and Gemini showed a moderate preference for alternative-specific parameters (ranging between 53 and 68%), while DeepSeek showed an equal distribution (50% generic and 50% alternative-specific taste parameters).

In terms of representing systematic observed heterogeneity, Claude 4 Sonnet again led with the highest average use of socioeconomic variables (1.22 per specification), whereas Deepseek incorporated these variables far less frequently (0.18 on average). This shows differences across LLM families in their capability for capturing behavioural heterogeneity across different population segments. The use of functional transformations, such as logarithmic, Box-Cox, and piece-wise forms, was generally limited across all LLMs. However, GPT-o4-mini-high (0.73) and GPT-o3 (0.59) applied them slightly more often, suggesting a better tendency toward including non-linear relationships in their utility functions.

While the summary of utility specifications for each LLM provides a static overview of model complexity and specification trends, the distribution of modelling outcomes also provides a better understanding of the LLMs' overall performance. Figures 3, 4, and 5 display the full distributions of LL, AIC, and BIC values of all specifications that did converge by each LLM. These plots enable comparison not only in terms of central tendency, but also in the consistency and reliability of each LLM's specification quality.

Two main insights emerge from these visualisations. First, the vertical position of each distribution and its corresponding median confirm the earlier numerical findings. Claude 4 Sonnet has, by a slight margin, the uppermost position in the LL plot and the lowest position in the AIC and BIC plots, indicating that it generates, on average, the best-fitting and most efficient specifications. The distributions of the other Claudes, all GPTs, and Gemini 2.5 Flash and their corresponding medians cluster just below Claude 4 Sonnet, indicating a good and comparable empirical fit. By contrast, the DeepSeek distributions occupy the lower end of the LL scale and the upper end of the AIC and BIC scales, signalling systematically poorer fit. Second, the shapes of the violins highlight differences in consistency. All Claudes, Gemini, GPT o3, and GTP 4.5 exhibit relatively large widths around their medians and short tails, suggesting that they regularly reach good solutions with little variability. By contrast, GPT 40, GPT o4-mini-high, and DeepSeek show narrower widths around their medians and longer tails, implying a greater proportion of weaker specifications in terms of LL, AIC, and BIC.

Finally, Figure 6 presents the distribution of the mean Value of Time (VoT) estimates derived from all valid specifications generated by each LLM. For each specification, the VoT is calculated as the ratio of the travel-time coefficient to the cost coefficient, averaged across all alternatives. The blue dashed line indicates the true mean VoT from the synthetic dataset. Most LLMs yielded VoT estimates closely centred around the true value with narrow distributions, indicating that the generated specifications were effective at accurately capturing the trade-off between time and cost in individuals' decision-making. However, Claude 4 Opus and Claude 4 Sonnet show greater variability, with some

specifications yielding high values (e.g., ¿2.0). However, in some of these specifications, cost coefficients were statistically insignificant, resulting in unreliable VoT estimates.

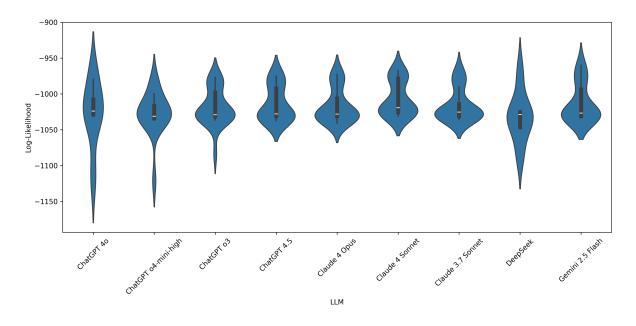


Figure 3: Log-Likelihood Distributions of Generated Specifications across LLMs

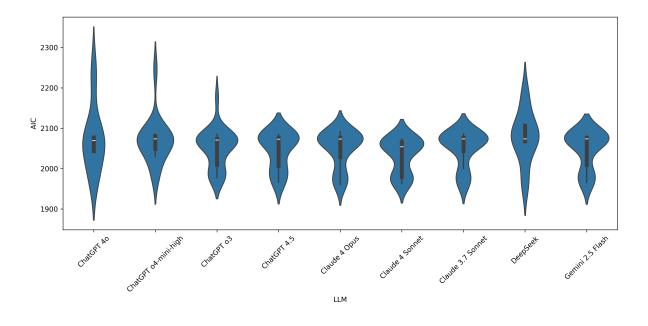


Figure 4: AIC Distributions of Generated Specifications across LLMs

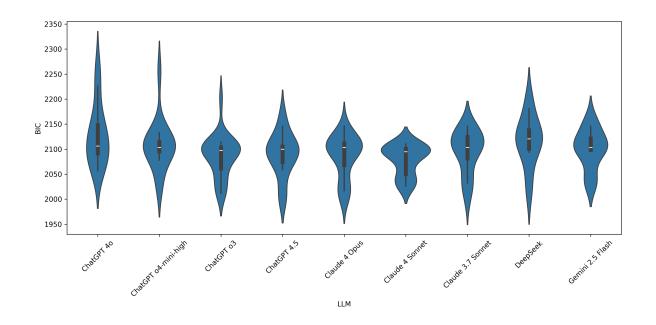


Figure 5: BIC Distributions of Generated Specifications across LLMs

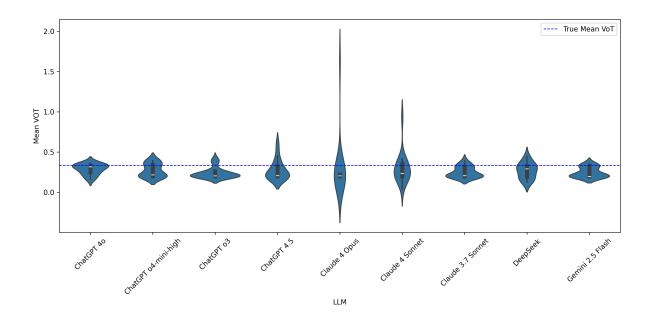


Figure 6: VOT Distributions of Generated Specifications across LLMs

5 Conclusion

This study provides a systematic evaluation of how current Large Language Models (LLMs) can assist in the specification and, where technically feasible, the estimation of Multinomial Logit (MNL) models. Our aim was twofold: to understand how modelling goals, prompting strategies, and information conditions affect model quality, and to assess which LLMs currently perform best in discrete choice modelling tasks. To do so, we designed five experimental configurations that vary along three key dimensions — prompting strategy (Zero-Shot vs. Chain-of-Thoughts), information availability (full data vs. data dictionary), and modelling task (suggestion vs. estimation). Moreover, we benchmarked thirteen versions of six leading LLM families: ChatGPT, Claude, DeepSeek, Gemini, Gemma, and Llama. Across all configurations, we assessed the empirical performance, behavioural plausibility, and complexity of each utility specification generated.

Our findings offer three main insights. First, prompt structure plays a critical role in shaping specification quality. Structured Chain-of-Thought (CoT) prompts led, on average, to higher-quality and better-performing specifications than unstructured Zero-Shot prompts. Second, limited access to raw data did not reduce—and in some cases improved—LLM performance. This suggests that constraining input complexity may allow LLMs to allocate more of their reasoning and computational resources toward behavioural and theoretical reasoning rather than parsing data structure. Third, model capabilities vary significantly across LLM families. Claude 4 Sonnet generated the best-fitting and most complex specifications overall, while GPT o3 was uniquely capable of estimating its own models through executable, verifiable code—demonstrating the potential for partial automation of the entire modelling pipeline. Moreover, Claude variants consistently excelled in terms of AIC, while GPT variants performed better in terms of LL under both full and limited information conditions.

These findings demonstrate the potential of incorporating LLMs into choice modelling workflows. However, several limitations remain. Most LLMs struggled with estimation tasks, either hallucinating results or producing non-reproducible outputs. Additionally, some specifications omitted alternative-specific constants, failed to converge, or produced counter-intuitive parameter signs. These limitations underscore the continued necessity of expert oversight in model development, interpretation, and validation.

In particular, open-weight models such as LLaMA and Gemma revealed significant limitations in supporting end-to-end choice modelling workflows. Unlike proprietary (closed-weight) models, these models lack user-friendly interfaces and must be run locally, which adds a layer of technical complexity. In practice, both models frequently failed to produce plausible utility specifications or convergent results. Gemma only produced usable outputs in one experimental configuration (Experiment 3), and only after unbehavioural specifications were manually filtered out. LLaMA succeeded in generating estimable specifications only in Experiment 5, where only prompt and data dictionary were used as inputs. These models tended to return very few specifications due to limited output length and often lacked access to or understanding of database structure (choice modelling context). Overall, open-weight LLMs, in their current form, remain inadequate for end-to-end assistance in discrete choice modelling. Nonetheless, these models may still

play a useful role within hybrid workflows that leverage their strengths—such as language understanding, reasoning, domain knowledge, and prompt-based guidance—without relying on them for full automation (see (Cao et al., 2024) for a detailed taxonomy of LLM-enhanced reinforcement learning framework, which could be extended to discrete choice modelling (Nova et al., 2025)).

In summary, our findings offer several practical insights for how to best use LLMs in specifying and estimating MNL models:

- **Prompt structure matters:** Structured prompting (Chain-of-Thoughts) significantly enhances specification quality compared to unstructured (Zero-Shot) prompts.
- Less can be more: Limiting LLM access to raw detailed data access can sometimes lead to stronger theoretical reasoning by LLMs, enhancing their performance in generating better utility specifications.
- End-to-end automation remains rare: Only GPT-o3 was capable of both proposing theoretically sound MNL specifications and correctly estimating them, by generating valid Python code, executing it, and returning verifiable log-likelihood values and parameter estimates. This demonstrates a unique strength in supporting both specification and estimation tasks end-to-end.

Regarding model-specific performance, our findings suggest the following:

- Claude models, especially Claude 4 Sonnet, consistently generated more complex, interaction-rich specifications, though some of its variants encountered convergence issues.
- **GPT variants** showed robustness in convergence and consistency in generating reliable specifications, although GPT 40 omitted ASCs from a larger share of its specifications.
- Gemini 2.5 Flash also showed robustness in convergence and consistency in generating reliable specifications, albeit generally less complex than Claude's.
- **DeepSeek** balanced its generated specifications but suffered from convergence issues and omitting ASCs.
- Open-weight models (Llama and Gemma) underperformed overall. They produced very few valid specifications, and even those were rarely competitive with the outputs of closed-weight models in terms of LL, AIC, and BIC.

Finally, this work illustrates both the potential and the current boundaries of LLMs in discrete choice modelling. While these models can assist in utility specification, they should be viewed as support tools rather than autonomous agents. Future research should explore how to refine prompt engineering to improve specifications quality and build hybrid workflows that effectively combine human expertise with LLM-driven support.

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Appendix

Algorithm 1 GROQ API Completion Flow

```
# Initialize Groq client with API key
from groq import Groq
import os
# Get a key at www.groq.com
key = user_key # copy from groq
# Select prompt
prompt = prompt_zero_shot_suggest # or prompt_CoT_suggest
client = Groq(api_key=os.environ.get("GROQ_API_KEY", key),)
# Configure output location
output_dir = "llama_4_scout_17b" # Options:
# output_dir = "llama_4_maverick_17b"
# output_dir = "llama_3_70b_8192"
file_name = "Z_suggest.txt" # or CoT_suggest.txt
full_path = os.path.join(output_dir, file_name)
# Generate completion
llama_output = ""
completion = client.chat.completions.create(
    model="meta-llama/llama-4-scout-17b-16e-instruct",
    # You may find other models such as:
    # model="meta-llama/llama-4-maverick-17b-128e-instruct",
    # model="llama3-70b-8192",
    messages=[{"content": prompt}],
    temperature=1.2, # Control creativity
    top_p=0.95,
                            # Control diversity
    max_completion_tokens=8192, # Max response length
stop=None, # No early stopping )
# Process and save output
for chunk in completion:
    content = chunk.choices[0].delta.content or ""
llama_output += content
with open(full_path, "w", encoding="utf-8") as f:
    f.write(llama_output)
```

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