Domain-Aware Scaling Laws Uncover Data Synergy

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Abstract

Machine learning progress is often attributed to scaling model size and dataset volume, yet the composition of data can be just as consequential. Empirical findings repeatedly show that combining datasets from different domains yields non-trivial interactions: adding code improves mathematical reasoning, while certain mixtures introduce interference that suppresses performance. We refer to these effects collectively as data *synergy*—interaction effects whereby the joint contribution of multiple domains exceeds (positive synergy) or falls short of (interference) the sum of their isolated contributions. In this work, we formalize and quantify dataset interactions in large language models. Leveraging observational variation across open-weight LLMs with diverse pretraining mixtures, we estimate both direct domain-to-benchmark synergy (how one domain contributes to performance on another) and pretraining data synergy (capabilities that require co-occurrence of multiple domains). Our framework improves the fit over domain-agnostic scaling laws, recovers stable synergy patterns such as math–code complementarity, and provides interpretable maps of cross-domain transfer.

1 Introduction

Recent improvements in Large Language Models (LLMs) are strongly shaped by their pretraining data [15, 25], yet most formulations abstract away composition and interactions, reducing data into an undifferentiated token count [13, 9]. Practitioners frequently observe that adding data from one domain improves performance on seemingly unrelated tasks–for example, code data enhancing mathematical reasoning [18, 1], while other combinations lead to interference and degraded performance [34, 16]. We refer to these cross-domain interactions as **data synergy**. Such findings suggest that tokens are not interchangeable: what matters is not only how much data we train on, but also *what kinds of data are combined*.

There is growing evidence that interactions matter. Prior works find that continued pretraining on code improves reasoning-heavy benchmarks [32]; and targeted ablations reveal both positive transfer and occasional negative transfer across conceptually related sources [31, 34, 8]. These observations are not isolated anecdotes but point to regularities in how domain composition shapes learned representations; regularities that merit explicit modeling.

Most existing approaches overlook this dimension, and instead treat pretraining corpora as homogeneous. Classical scaling laws, for instance, relate loss to parameter count and total data but are domain-agnostic, since they assume all tokens contribute equally [13, 9]. and mixture-optimization methods often search over weights while implicitly assuming independent returns [30]. What is missing is an explicit, identifiably interaction-aware formulation: a way to separate the aggregate benefit of more data from domain-specific deviations, and to quantify when two domains together yield more (or less) than the sum of their parts.

In this paper, we present a framework for quantifying and modeling data synergy in LLMs. Rather than treating data as homogeneous, we exploit natural variation across open-weight models trained on di-

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Preprint.

verse data mixtures. Our approach formalizes two complementary notions: (i) **Domain→benchmark synergy**, measuring how pre-training data from one domain affects the performance on another, and (ii) **Pretraining data synergy**, capturing domain-domain interaction effects that depend on co-occurrence of multiple domains in the training data. Our estimation procedure jointly fits these effects across many (model, benchmark) observations, provides sparse, interpretable maps of cross-domain interactions that generalize beyond observed mixtures.

Our contributions are as follows:

- We provide an operational definition of dataset synergy that links empirical observations to formal modeling.
- We introduce domain-aware estimators that improve predictive model performance over standard scaling laws by incorporating synergy terms.
- We recover stable, interpretable synergy patterns, such as the recurring complementarity between code and math, that provide actionable insights for data curation and acquisition.

2 Domain and Synergy-Aware Scaling Laws

2.1 Problem Setup

Let $M_1, \ldots, M_m$ denote a set of language models (e.g., open-weight LLMs on Huggingface), and let $D_1, \ldots, D_n$ be evaluation domains. For every model-domain pair we observe the loss value $L = \big[l_{i,j}\big] \in \mathbb{R}^{m \times n}$. Alongside L we collect model-level covariates: parameter count N_i, total pretraining tokens d_i, and composition (mixture shares) of the pretraining data $u_{i,k} \in [0,1]$, the fraction of tokens from training domain D_k that model M_i is pretrained on. Our goal is to quantify *cross-domain data synergy*: how training on pretraining domain(s) affects loss on a benchmark, after accounting for model scale and total tokens.

2.2 Domain-agnostic scaling law

We begin with a domain-agnostic baseline that explains loss variation using only model size N in terms of number of parameters, and total pretraining tokens D. This serves as the baseline model against which composition- and synergy-aware refinements will be evaluated. Following Chinchilla scaling laws [9], we have the parametric form $L(N, D) = L_\infty + AN^{-\alpha} + BD^{-\beta}$, where L_∞ is the irreducible loss, A, B are scale coefficients for parameter and data terms, and α, β are the parameter and data scaling exponent. In practice we fit this baseline *per benchmark*, and allow these parameters to vary across evaluation domains, after mapping heterogeneous metrics to a common monotone-transformed pseudo-loss. Let $s = \log N$ and $d = \log D$, and for benchmark j define $e_j = \log L_{\infty,j}$, $a_j = \log A_j$, and $b_j = \log B_j$. Writing the parametric form in log-parameters gives the numerically-stable log-sum-exp (LSE) form:

$$\log L_j(s, d) = \mathrm{LSE}\big(e_j,\ a_j - \alpha_j s,\ b_j - \beta_j d\big), \tag{1}$$

where $\mathrm{LSE}(x_1, x_2, x_3) = \log\big(e^{x_1} + e^{x_2} + e^{x_3}\big)$. Equation (1) is our *domain-agnostic* baseline: the expected log-loss depends only on total parameters and total tokens. In the next subsections we enrich the *data* term $b - \beta \log D$ to account for training mixture composition and to estimate cross-domain synergy, while keeping the same overall form of the scaling law recoverable.

2.3 First-order Domain-Benchmark Synergy

We now modify the data term so that *different training domains can reduce loss at different rates* on each benchmark. Recall that $u_{i,k} \in [0,1]$ is the fraction of tokens from training domain D_k that model M_i is pretrained on. It is easy to show that $\log d_i = \sum_k u_{i,k} \log(u_{i,k} d_i) + H(u_i)$, where $H(u_i) = -\sum_k u_{i,k} \log u_{i,k}$. To allow domain–specific data scaling exponent on benchmark j, $\beta_j + \gamma_{j,k}$ (faster if $\gamma_{j,k} > 0$, slower if $\gamma_{j,k} < 0$).

We introduce domain–specific data scaling exponent parameters $\{\gamma_{i,j}\}$, which modify the per-task data scaling exponents additively: $\beta_j + \gamma_{j,k}$. A positive $\gamma_{j,k}$ indicates that data from domain k yields greater-than-expected scaling – i.e, a synergistic effect with benchmark j. Conversely, a negative $\gamma_{j,k}$ implies diminishing returns, where data from domain k contributes less effectively than expected (interference). Substituting the $\log d_i$ decomposition equation into the third argument of the LSE in (1) and introducing these modifiers gives

$$\mathbb{E}[\, l_{i,j}\,] = \mathrm{LSE}\Big(e_j, a_j - \alpha_j s_i, b_j - \big[\beta_j \mathbf{1} + \gamma_{j,\cdot}\big]^\top z_i - \beta_j H(u_i)\Big), \tag{2}$$

with $z_{i,k} = u_{i,k} \log(u_{i,k} d_i)$ and synergy coefficients $\gamma_{j,k} \in \mathbb{R}$.

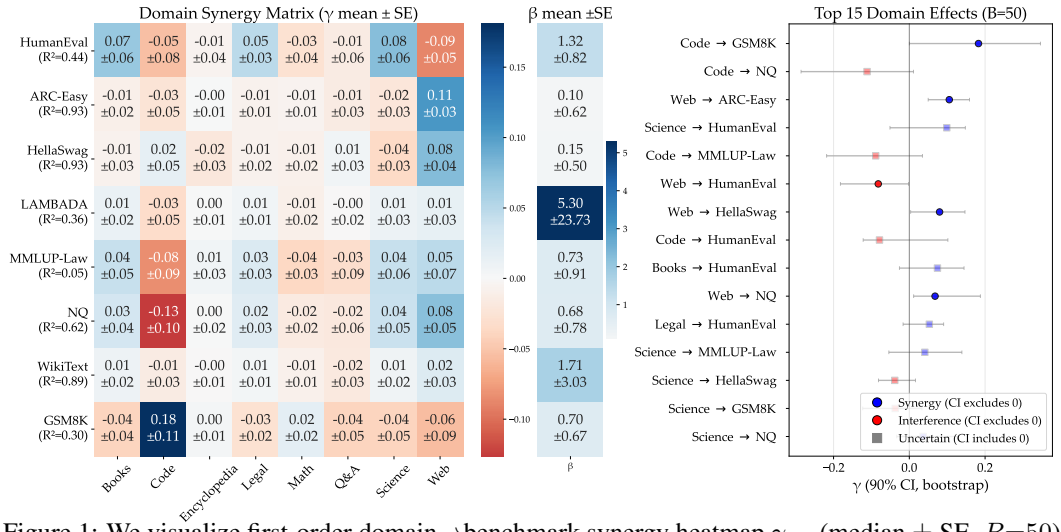

Figure 1: We visualize first-order domain→benchmark synergy heatmap $\gamma_{j,k}$ (median $\pm$ SE, B=50) between pretraining domains (columns) and benchmarks (rows), and right panel shows β_j with 90% CIs. A few synergies (e.g., code → `GSM8K`) are reliably positive, while most synergies are small or uncertain.

2.4 Second-order Pretraining Data Synergy

We hypothesize that certain training domains interact synergistically and intrinsically, such that their joint presence yields learning benefits irrespective of the specific downstream benchmark. These synergies reflect fundamental complementarities between domains, though their effect size is still mediated by the benchmark-specific data scaling coefficient. The gain from such co-occurrence is bottlenecked by the scarcer source and can be understood as producing "additional bonus tokens" only when both domains are present. To capture this, we model synergy with a pairwise term that vanishes if either domain is absent and scales with the smaller per-domain log-token budget.

Let $u_{i,k} \in [0,1]$ be pretraining domain mixture weights and d_i the total token count and define

$$z_{i,k} = u_{i,k}\log(u_{i,k}d_i), \qquad \bar{z}_{i,k} = \log\big(1{+}u_{i,k}d_i\big), \qquad \mathrm{softmin}_\tau(a,b) := -\tau\log\big(e^{-a/\tau}{+}e^{-b/\tau}\big).$$

Start from the first–order data term split into baseline and per–domain parts, $-\beta_j\sum_k z_{i,k} - \sum_k \gamma_{j,k}\, z_{i,k} - \beta_j H(u_i)$, and augment only the base effect with a co-occurrence correction

$$-\beta_j \sum_k \Big[z_{i,k} + \sum_{k'\neq k} \gamma_{j,k}\sigma_{kk'}\ \mathrm{softmin}_\tau\big(\bar{z}_{i,k}, \bar{z}_{i,k'}\big)\Big] - \sum_k \gamma_{j,k} z_{i,k} - \beta_j H(u_i),$$

that is with a cross-domain synergy correction modulated by domain-benchmark synergy strength. Using $\bar{z}$ (nonnegative and $=0$ when $u_{i,k}=0$) ensures the interaction truly vanishes if either domain is absent and preserves the desired $O(\log d_i)$ scaling. We then scale the last term by β_j to ensure that it moves at the same rate as the baseline. Symmetrizing (using $\sigma_{kk'} = \sigma_{k'k}$), gives,

$$\Phi_{i,j} = b_j - \big[\beta_j \mathbf{1}_K + \gamma_{j,\cdot}\big]^\top z_i - \beta_j\, H(u_i) - \beta_j \sum_{k<k'} (\gamma_{j,k} + \gamma_{j,k'})\,\sigma_{kk'}\ \mathrm{softmin}_\tau\big(\bar{z}_{i,k}, \bar{z}_{i,k'}\big) \quad (3)$$

where $\Sigma = [\sigma_{kk'}]$ is symmetric with $\sigma_{kk}=0$. The complete log-space law has the form $\log L_{i,j} = \mathrm{LSE}\big(e_j,\ a_j - \alpha_j s_i,\ \Phi_{i,j}\big)$. In Appendix B.2, we interpret the new data term as "effective" number of pretraining data.

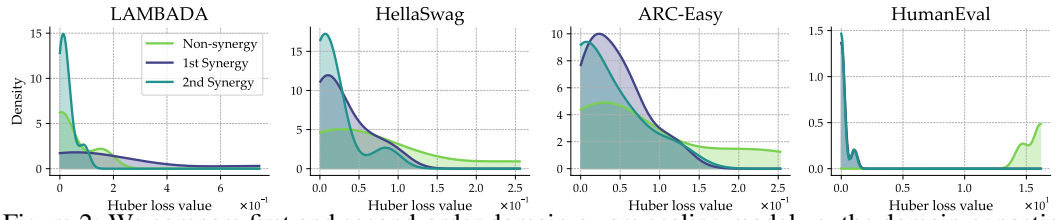

Figure 2: We compare first and second-order domain-aware scaling model vs. the domain-agnostic one (Chinchilla) on a number of benchmarks. The synergy-aware estimators achieves lower test loss on held-out models in these benchmarks.

3 Results

We estimate composition effects from *observational variation* across open-weight models and their publicly documented pre-training mixtures, rather than training models. Details on models and data are included in Appendix D.

3.1 First-order Domain→Benchmark Synergy

We estimate the first-order synergy of each pre-training domain on each benchmark, as explained in Appendix C. Figure 1 visualizes the estimated matrix $\Gamma = \{\gamma_{j,k}\}$ with the benchmark-specific data exponent β_j. To quantify uncertainty, we report standard errors from B=50 bootstrap resamples (80% subsampling) and show 90% confidence intervals for β_j. The resulting map is sparse and interpretable: a few domain→benchmark synergies are reliably positive, while most γ values are small or statistically indistinguishable from zero synergy. Notably, code pretraining exhibits positive first-order synergy to math reasoning benchmark `GSM8K`, which is consistent with findings of prior work [1, 18].

3.2 Second-order Pre-training Data Synergy

Beyond first-order effects, we estimate *pairwise* data synergy between pre-training domains to capture gains that materialize only when two domains co-occur, across all benchmarks. We fit the symmetric synergy matrix $\Sigma = \{\sigma_{k,k'}\}$ along with other parameters as in Equation 3 evaluate uncertainty via $B = 50$ bootstrap resamples (80% subsampling). Figure 3 summarizes the results the shared pairwise synergy across domains, along with the confidence intervals. Positive entries indicate domain-domain synergy (e.g. the expected *Code*×*Math* synergy), while negative entries show interference. We also observe negative synergy between *Code*×*Encyclopedia*/*Q&A*, which reflects that having both domains present in the pre-training dataset, may hurt average performance on selected domains.

We also assess how predictive the model is on held-out samples. Figure 2 compares our domain-aware estimator with a domain-agnostic ($\gamma_{i,j} = 0$) baseline. Across a number of benchmarks, the synergy-aware models show better loss on residuals of held-out examples, on these datasets. A comparison of all fits is shown in Figure 4 Appendix E.1. These gains show that modeling composition, via a small number of non-zero $\gamma_{j,k}$ (and universal $\sigma_{k,k'}$) adds explanatory power beyond total token count, which is especially effective for benchmarks that are different in distribution from typical pre-training datasets, such as in `HumanEval`, a coding benchmark.

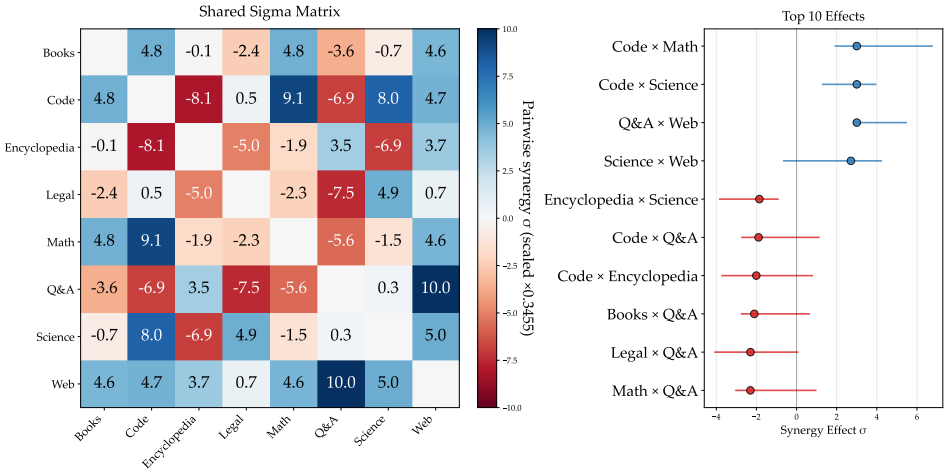

Figure 3: Second-order pretraining domain×domain synergy matrix $\Sigma = \{\sigma_{i,j}\}$ shows positive synergy between domains such as *Code*×*Math*, *Q&A*×*Web*/*Science*.

4 Conclusion

We formalize and quantify data synergy in LLM pretraining, and show that explicitly modeling domain-benchmark and pretraining data interactions can lead to interpretable estimates of data synergy, and improve predictive fit across multiple benchmarks. Our approach is limited by its observational design and future work will validate these measured synergies by training on domains we find to be synergistic. Beyond methodology, our estimates support practical applications in data curation, mixing, and acquisition, and performing synergy-aware mixture optimization to target specific capabilities.

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A Related Work

Scaling laws. A line of work shows that LLM loss follows smooth power laws as model capacity and data grow. Early results characterize scaling trends across parameters, data, and compute [13], while subsequent analyses refine the compute–data trade-off and argue that many models were under-trained for their size and recommend that token counts scale roughly with parameters to remain compute-optimal [9]. We treat these as the domain-agnostic baseline and study differences induced by heterogeneous data mixtures.

Domain-aware scaling and mixture optimization. Beyond total token count, several works show that *which* tokens matter. Data pruning and curation can "beat" naive power-law scaling by shifting the effective constants and exponents in favorable ways [26]. Mixture-optimization approaches explicitly treat domain composition as a control variable: AutoScale automates scaling-law fitting and uses the fitted laws to recommend data-mixture and broader training-design choices with minimal additional training [12]. RegMix frames mixture selection as a regression problem with regularization to stabilize estimates under limited supervision [17]. More recently, "data mixing laws" relate performance to mixture weights and document nonlinear returns, including phase-transition-like effects as specific domains are increased [31]. Our formulation contributes to this line by modeling domain effects via the empirical domain frequencies $u_{i,k}$ (fraction of tokens from domain k in the dataset used for model i), which allows the data term's exponent to vary for different domains and compositions, rather than only with D.

Observational inference of skills and benchmark structure. Orthogonal to controlled pretraining, a complementary literature uses observational variation across many (model, task) points to infer latent capability structure and transfer patterns. Perplexity-correlation methods identify promising upstream corpora for a target benchmark using only readily available statistics, providing a zero-shot signal for mixture selection [28]. Hierarchical latent-variable models on leaderboard matrices recover shared factors that explain co-movement of benchmark scores across models, offering a data-driven map of "skills" without interventional training runs [11]. Our estimator follows this observational spirit but focuses on predicting performance under counterfactual mixtures by leveraging the fraction of tokens in pre-training data from a specific domain.

Evidence for data synergy. Multiple empirical studies report positive transfer between code and mathematical reasoning. Continued pretraining on math+code corpora improves math benchmarks beyond either domain alone [1, 18]. Controlled ablations further indicate that injecting code during pretraining (rather than only SFT) yields broader reasoning gains with minimal negative transfer [19]. These findings motivate sparse, domain-specific parameters that can capture synergy between conceptually related domains.

B Additional Details

B.1 First-order Domain→ Benchmark Synergy

De-confounding global and domain effects. To decouple the aggregate data-scaling coefficient β_j from domain synergies $\gamma_{j,\cdot}$, we impose the mean-zero (orthogonality) constraint $\mathbf{1}^\top \gamma_{j,\cdot} = 0$. Let $P_\perp := I - \frac{1}{K}\mathbf{1}\mathbf{1}^\top$ be the projector onto the subspace orthogonal to $\mathbf{1}$. We enforce this either by *reparameterization* $\gamma_{j,\cdot} = P_\perp \eta_{j,\cdot}$ with free $\eta_{j,\cdot}$. Using $z_{i,k} = u_{i,k}\log(u_{i,k}d_i)$ and $H(u_i) = -\sum_k u_{i,k}\log u_{i,k}$, recall $\mathbf{1}^\top z_i = \log d_i - H(u_i)$. Without the constraint, the data term

$$(\beta_j \mathbf{1} + \gamma_{j,\cdot})^\top z_i + \beta_j H(u_i)$$

lets the mean of $\gamma_{j,\cdot}$ shift the effective coefficient on $\log d_i$ and spuriously couple to $H(u_i)$. Enforcing $\mathbf{1}^\top \gamma_{j,\cdot} = 0$ removes this confounding and reduces the data term to

$$D_{i,j} = \beta_j \log d_i + \gamma_{j,\cdot}^\top z_i,$$

so β_j is identifiable as the aggregate token-scaling coefficient while $\gamma_{j,\cdot}$ captures only domain-specific deviations. We apply sparsity and shrinkage penalties to the projected coefficients $P_\perp \gamma_{j,\cdot}$.

B.2 Second-order Pre-Training Data Synergy

Scaling–law interpretation (effective tokens). Define the benchmark-specific *effective tokens*

$$\log D_{i,j}^{\text{eff}} := \log d_i \; + \; \sum_{k<k'} (\gamma_{j,k} + \gamma_{j,k'})\, \sigma_{kk'}\, s_{i,kk'}, \quad D_{i,j}^{\text{eff}} = d_i \exp\Big(\sum_{k<k'} (\gamma_{j,k} + \gamma_{j,k'})\, \sigma_{kk'}\, s_{i,kk'} \Big),$$

so that

$$\exp(\Phi_{i,j}) = \exp\big(b_j - \gamma_{j,\cdot}^{\top} z_i\big) \, \big(D_{i,j}^{\text{eff}}\big)^{-\beta_j}.$$

In a Chinchilla-style view,

$$L_{i,j}(N_i, d_i) \;\approx\; L_{\infty,j} + A_j N_i^{-\alpha_j} + \underbrace{\widetilde{B}_{i,j}}_{=\exp(b_j - \gamma_{j,\cdot}^{\top} z_i)} \big(D_{i,j}^{\text{eff}}\big)^{-\beta_j},$$

and for small interactions, $\big(D_{i,j}^{\text{eff}}\big)^{-\beta_j} \approx d_i^{-\beta_j} \left[1 - \beta_j \sum_{k<k'} (\gamma_{j,k} + \gamma_{j,k'})\, \sigma_{kk'} \; \text{softmin}_{\tau}(\bar{z}_{i,k}, \bar{z}_{i,k'})\right]$, which makes explicit the benchmark-gated "bonus tokens" contributed by co-occurence through the universal Σ.

C Training and Uncertainty

Loss and optimizer. We fit all parameters by minimizing a single Huber$_\delta$ risk [10] over the LSE scaffold (Section 2):

$$\min_{\Theta} \sum_{j=1}^{n} \sum_{i=1}^{m} \text{Huber}_\delta\Big(\text{LSE}\big(e_j,\; a_j - \alpha_j s_i,\; \Phi_{i,j}\big) - l_{i,j}\Big) \;+\; \lambda_1 \sum_j \|\gamma_{j,\cdot}\|_1 \;+\; \lambda_2 \sum_j \|\gamma_{j,\cdot}\|_2^2,$$

where $s_i = \log N_i$ and $\Phi_{i,j}$ is either from the *domain-benchmark* data term (i.e., $\Sigma = 0$) or the *pretraining data synergy* term in Eq. (3). We optimize with full-batch L-BFGS [22] The pretraining domain synergy matrix Σ is parameterized on the upper triangle only ($\sigma_{kk'} = \sigma_{k'k}$, $\sigma_{kk} = 0$). In all reported runs we use $\delta = 0.5$, $\tau = 0.1$, $\lambda_1 = 0.01$, and $\lambda_2 = 10^{-5}$. For the synergy model we first optimize $(e_j, a_j, b_j, \alpha_j, \beta_j, \gamma_{j,\cdot})$ with Σ fixed to 0 and then continuing optimizing all parameters (including Σ) jointly.

Uncertainty via bootstrap. *first-order fits.* We estimate variability by resampling 80% of models (without replacement) $B = 50$ times and refitting; we report percentile intervals for $(e_j, a_j, b_j, \alpha_j, \beta_j, \gamma_{j,\cdot})$.

second-order fits. We warm-start with training on all models, and then we cluster bootstrap over model families: each replicate resamples families with replacement, retains all domains per sampled model, and refits the full objective from the warm start. With $B = 50$ replicates we report 90% percentile intervals for (α_j, β_j), the per-domain effects $\gamma_{j,k}$, and the shared pairwise coefficients $\sigma_{kk'}$.

D Observational Data: Models and Data

We estimate composition effects from *observational variation* across open-weight models and their publicly documented pre-training mixtures, rather than training models. This provides variation in both scale and composition, and enables identifying of domain-specific returns using our framework. Throughout we denote by $u_{i,k}$ the fraction of tokens from training domain k in the dataset used for model i.

Model families Our panel spans six open-weight families with heterogeneous scales and training mixtures: `GPT-Neo/J/NeoX` [24] (125M–20B; 5 checkpoints), `Pythia` [2] (70M–12B; 8 checkpoints), `DataDecide` [20] (150M–1B; 30 checkpoints across Dolma variants with systematic ablations: *no-code*, *no-flan*, *no-math-code*, *no-reddit*), `OLMo` [7] (1B–13B; 5 checkpoints), `OpenLLaMA` [6] (3B–13B; 5 checkpoints), and `RedPajama-INCITE` [29] (3B–7B; 2 checkpoints). The DataDecide ablations provide controlled composition shifts that are especially informative for informing counterfactual domain effects. We map each subset in each model's pretraining data to one of the following domains: books, code, encyclopedia, legal, math, Q&A, Science, and Web.

Benchmarks and normalization. We evaluate on eight benchmarks chosen to roughly cover our domains: mathematical reasoning (`GSM8K` [5]), code generation (`HumanEval` [3]), science/general-knowledge MC (`ARC-Easy`[4]), commonsense inference (`HellaSwag` [33]), broad-context cloze (`LAMBADA` [23]), professional legal knowledge (`MMLU-Pro-Plus, Law` [27]), open-domain QA (`Natural Questions` [14]), and encyclopedia (`WikiText` [21]). To compare different evaluation metrics, we convert accuracy-/pass@1-type scores to error (1−success), and apply a per-task rank transform to obtain the pseudo-loss used for fitting.

Evaluation. In most benchmarks we do not directly observe direct loss $l_{i,j}$ but a task metric $m_{i,j}$ (accuracy, pass@1, etc.). We map metrics to a *pseudo log-loss* via a domain-specific monotone transform g_j (e.g., rank–Gaussian (inverse normal) transform $g_j(m) = \Phi^{-1}\big(\hat{F}_j(m)\big)$, where $\hat{F}_j$ is the empirical CDF of metric values on D_j and Φ^{-1} is the standard normal quantile function):

$l_{i,j} = g_j(m_{i,j}) \;\propto\; \log L_{i,j}$, so different metrics lie on a common (log-loss) scale.

E Additional Results

E.1 Comparison Results

We also assess how predictive the model is on held-out samples. Figure 2 compares our domain-aware estimator with a domain-agnostic ($\gamma_{i,j} = 0$) baseline. Across a number of benchmarks, the synergy-aware models show better loss on residuals of held-out examples, on these datasets.

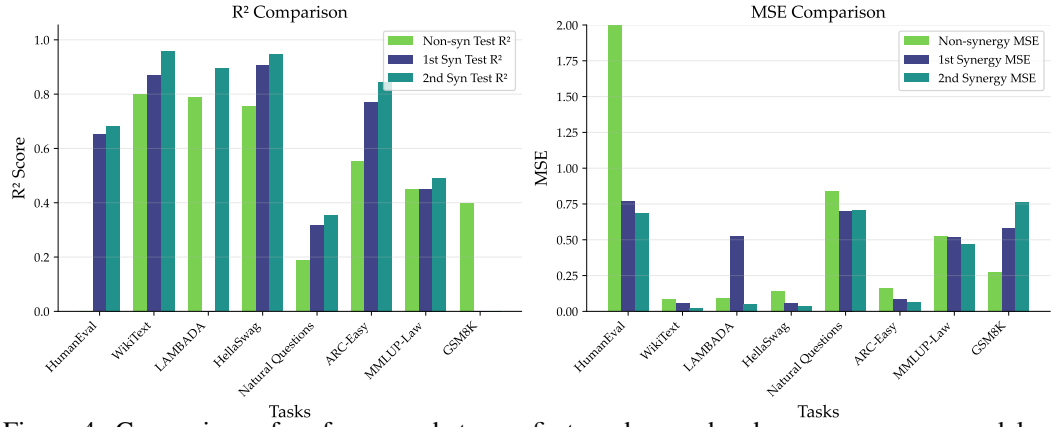


Figure 4: Comparison of performance between first- and second-order synergy-aware model vs. non-synergy-aware model

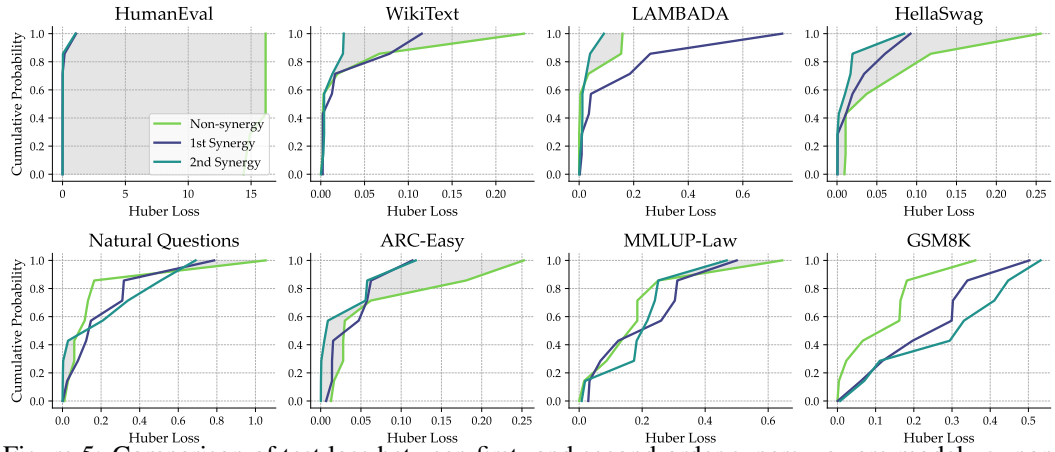


Figure 5: Comparison of test loss between first- and second-order synergy-aware model vs. non-synergy-aware model

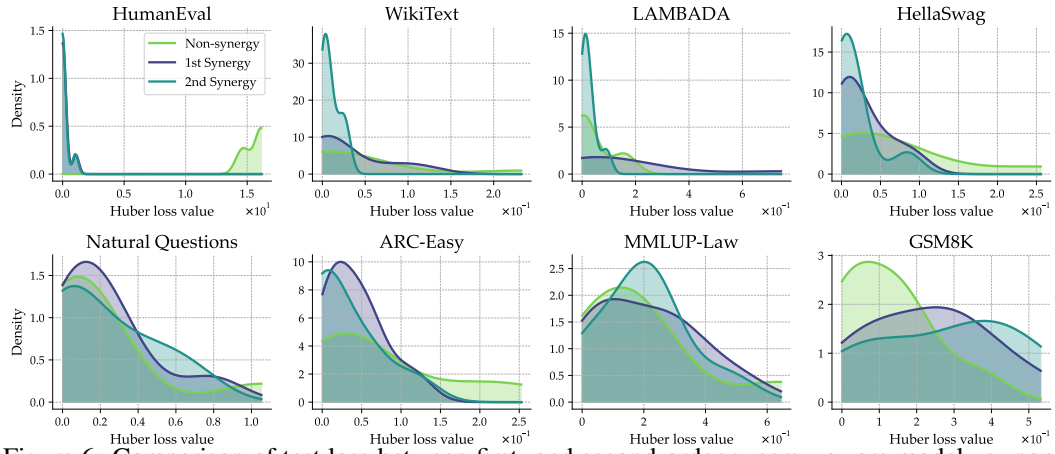
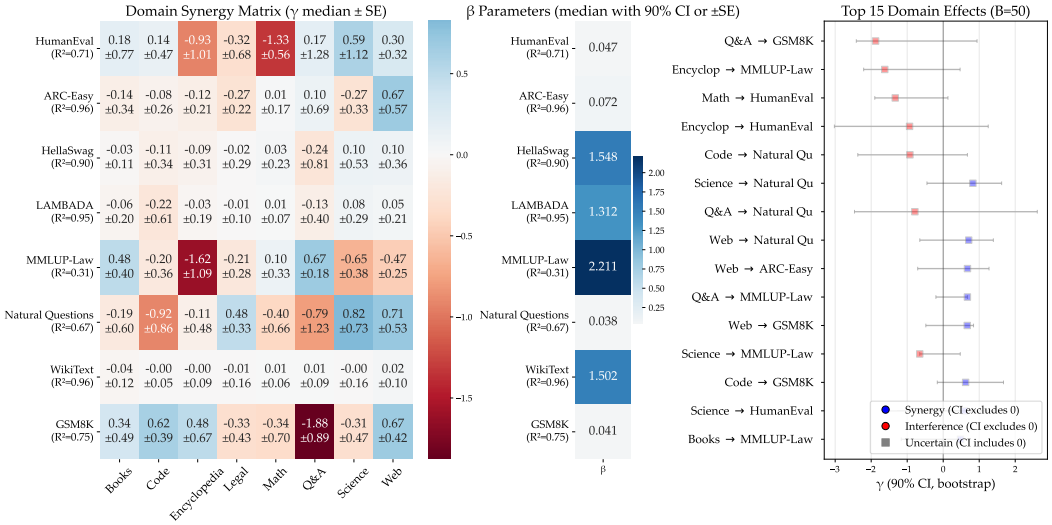


Figure 6: Comparison of test loss between first- and second-order synergy-aware model vs. non-synergy-aware model

E.2 Second-order Pre-training Synergy

We provide γ and β values for the second-order synergy model.