Learning What Matters: Scalable Data Mixing for LLMs

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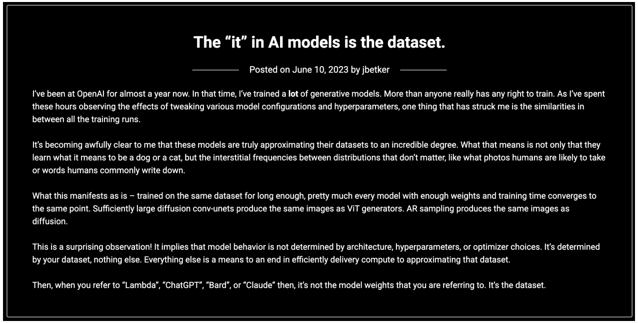
Outline

- What is data mixing?
- Taxonomy
- DoReMi, DoGE, RegMix methods
- The Chameleon framework
- Empirical analysis
- Conclusion

Motivation: Data as a resource

The world's most valuable resource is no longer oil, but data

The data economy demands a new approach to antitrust rules



The "it" in AI models is the dataset.

Posted on June 10, 2023 by jbetker

I've been at OpenAI for almost a year now. In that time, I've trained a **lot** of generative models. More than anyone really has any right to train. As I've spent these hours observing the effects of tweaking various model configurations and hyperparameters, one thing that has struck me is the similarities in between all the training runs.

It's becoming awfully clear to me that these models are truly approximating their datasets to an incredible degree. What that means is not only that they learn what it means to be a dog or a cat, but the interstitial frequencies between distributions that don't matter, like what photos humans are likely to take or words humans commonly write down.

What this manifests as is – trained on the same dataset for long enough, pretty much every model with enough weights and training time converges to the same point. Sufficiently large diffusion conv-unets produce the same images as ViT generators. AR sampling produces the same images as diffusion.

This is a surprising observation! It implies that model behavior is not determined by architecture, hyperparameters, or optimizer choices. It's determined by your dataset, nothing else. Everything else is a means to an end in efficiently delivery compute to approximating that dataset.

Then, when you refer to "Lambda", "ChatGPT", "Bard", or "Claude" then, it's not the model weights that you are referring to. It's the dataset.

Figure: (Left) Economist 2017 article on the importance of data. (Right) The relative importance of data within the model.

- Architectures determine
  - inference resources
  - inference capabilities
- Algorithms determine
  - training resources
  - generalization
- Data determines
  - generalization
  - training resources

Data processing pipeline for LLM pretraining

∘ Modern LLMs (e.g., ChatGPT, Gemini, Claude, DeepSeek,...) employ the following general data pipeline:

1. Data cleaning
   - Deduplication
   - Privacy and copyright
   - Quality filtering
   - Data age
2. Data selection
   - Data masking
   - Document packing
   - Data ordering
   - Synthetic data
3. Data mixing
   - Find optimal domain mixtures
   - Target evaluations
   - Online mixing approaches
   - Offline mixing approaches

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Motivating example: Data mixing in practice

- Large-scale pretraining datasets contain many domains (e.g., Wikipedia, Books, etc.) [11, 26].

Data Source	Train Tokens	Validation Tokens	Train (% of Total)
CommonCrawl	200.82B	214.72M	66.99
C4	44.98B	48.06M	15.00
GitHub	13.51B	14.42M	4.51
Books	13.49B	14.39M	4.50
Wikipedia	13.50B	14.41M	4.50
ArXiv	7.49B	8.01M	2.50
StackExchange	5.99B	6.41M	2.00
Total	299.78B	320.42M	100.00

Table: SlimPajama dataset [26].

- Denote k domains for pretraining as $D^{\text{train}} = \{D_1, D_2, \ldots, D_k\}$.
- The sampling distribution is $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_k) \in \triangle^k$, the probability simplex over k domains.
- *How to set $\boldsymbol{\alpha}$ to improve downstream performance?*

What does data mixture optimize?

- Training a language model involves different loss objectives at different stages.

Example (Examples of relevant losses)

- $\mathcal{L}_{\text{train}}$: *Next-token prediction loss* on mixed data sources (e.g., CommonCrawl, Wikipedia).
  - $\mathcal{L}_{\mathrm{train}} = \sum_{i=1}^{k} \alpha_i f(\mathbf{x}; D_i)$ is the weighted cross-entropy loss over the training domains.
- $\mathcal{L}_{\text{val}}$: *Validation perplexity* on held-out set.
  - $\mathcal{L}_{\mathrm{val}} = \sum_{i=1}^{k} f(\mathbf{x}; D_i^{\text{val}})$ is the validation loss on the training domains.
- $\mathcal{L}_{\text{task}}$: *Downstream loss*, e.g., performance on reasoning benchmarks like ARC or LogiQA.
  - $\mathcal{L}_{\mathrm{task}} = f(\mathbf{x}; D^{\text{target}})$ is the loss on a set of interest.

- These losses guide us in choosing data mixture weights $\boldsymbol{\alpha}$.

Data mixing question

How should we sample data from diverse domains to minimize losses that matter?

Illustrative example: A toy data mixture problem

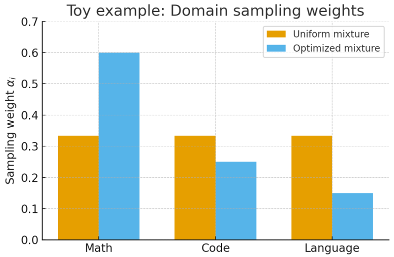
- Suppose we train an LLM on:
  - D_1: Math domain (e.g., problems and proofs)
  - D_2: Code domain (e.g., Python, C++)
  - D_3: Natural language (e.g., Wikipedia, Books)

- We want to optimize model performance on a downstream reasoning benchmark (e.g., LogiQA or ARC).

Question: What is the optimal sampling distribution $(\alpha_1, \alpha_2, \alpha_3)$?

- Uniform might underrepresent math.
- Manual heuristics might overfit and do not scale.

We need a principled optimization method!



Data mixing optimization

∘ Objective: Find optimal data composition over k sources minimizing loss of interest.

Data mixing

The data mixing problem can be written as a bilevel optimization [9]:

$$\min_{\boldsymbol{\alpha} \in \Delta^k} \mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha})) \quad \text{subject to} \quad \mathbf{x}^\star \in \arg\min_{\mathbf{x}} \mathcal{L}_{\text{train}}(\mathbf{x}; \boldsymbol{\alpha}), \tag{1}$$

where $\mathcal{L}_{\text{train}}$ is the next token prediction loss and $\mathcal{L}_{\text{target}}$ is the target loss of interest ($\mathcal{L}_{\text{val}}$ or $\mathcal{L}_{\text{task}}$).

Question

Note that $\mathbf{x}^\star(\boldsymbol{\alpha})$ is the model trained on the dataset re-weighted by $\boldsymbol{\alpha}$. How can we solve this bilevel problem?

Bilevel optimization

◦ We first recall the general bilevel problem:

Bilevel optimization problem [34]

The canonical form of bilevel optimization is given by:

$$\min_{\mathbf{x}_1 \in \mathcal{X}_1} \; f_1(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1)) \quad \text{s.t.} \quad \mathbf{x}_2^*(\mathbf{x}_1) \in \arg\min_{\mathbf{x}_2 \in \mathcal{X}_2} f_2(\mathbf{x}_1, \mathbf{x}_2), \tag{2}$$

where f_1, f_2 are smooth functions.

- $\mathbf{x}_1$ is the outer variable with outer objective f_1.
- $\mathbf{x}_2$ is the inner variable with inner objective f_2.

Example (Data mixing)

The above template captures data mixing with:

- Inner objective: $f_2(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{L}_{\text{train}}(\mathbf{x}; \boldsymbol{\alpha})$.
- Outer objective: $f_1(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1)) = \mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha}))$.

Remarks:

◦ Optimization of f_2 (model training) wrt $\mathbf{x}_2$ depends on $\mathbf{x}_1$ (data mixing).

◦ Hence, (2) is intrinsically hard to solve.

The implicit function approach

◦ Consider the following simplifications:

$$\min_{\mathbf{x}_1 \in \mathcal{X}_1} h(\mathbf{x}_1) \iff \min_{\mathbf{x}_1 \in \mathcal{X}_1} h(\mathbf{x}_1) := f_1(\mathbf{x}_1, \mathbf{x}_2^\star(\mathbf{x}_1)) \quad \text{s.t. } \mathbf{x}_2^\star(\mathbf{x}_1) = \arg\min_{\mathbf{x}_2 \in \mathbb{R}^{p_2}} f_2(\mathbf{x}_1, \mathbf{x}_2),$$

with $f_2(\mathbf{x}_1, \mathbf{x}_2)$ strongly convex in $\mathbf{x}_2$ and unconstrained.

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with $f_2(\mathbf{x}_1, \mathbf{x}_2)$ strongly convex in $\mathbf{x}_2$ and unconstrained.

∘ Let's calculate the gradient for $h(\mathbf{x}_1)$:

$$\nabla h(\mathbf{x}_1) = \nabla_{\mathbf{x}_1} f_1(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1)) + \left(\frac{d\mathbf{x}_2^*}{d\mathbf{x}_1}\right)^\top \nabla_{\mathbf{x}_2} f_1(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1)).$$

Implicit function theorem gives:

$$\frac{d\mathbf{x}_2^*}{d\mathbf{x}_1} = -\left(\nabla^2_{\mathbf{x}_2\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1))\right)^{-1} \nabla^2_{\mathbf{x}_1\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2^*(\mathbf{x}_1)).$$

We obtain:

$$\nabla h(\mathbf{x}_1) = \nabla_{\mathbf{x}_1} f_1(\mathbf{x}_1, \mathbf{x}_2^*) - \nabla^2_{\mathbf{x}_1\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2^*)\left(\nabla^2_{\mathbf{x}_2\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2^*)\right)^{-1} \nabla_{\mathbf{x}_2} f_1(\mathbf{x}_1, \mathbf{x}_2^*).$$

The hyper-gradient

- The gradient requires $\mathbf{x}_2^\star(\mathbf{x}_1)$, i.e., the lower-level problem solved to global min $\Rightarrow$ not possible in most cases.
- We assume access to a surrogate for the unknown original gradient of f_1 at any $\mathbf{x}_1$.

The hyper-gradient

Consider the stationary conditions of the bilevel problem as finding $(\mathbf{x}_1^\star, \mathbf{x}_2^\star)$ such that

$$\bar{\nabla} f_1(\mathbf{x}_1, \mathbf{x}_2) = 0, \qquad \nabla_{\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2) = 0,$$

where the gradient approximation of f_1 is defined as

$$\bar{\nabla} f_1(\mathbf{x}_1, \mathbf{x}_2) = \nabla_{\mathbf{x}_1} f_1(\mathbf{x}_1, \mathbf{x}_2) - \nabla^2_{\mathbf{x}_1\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2)\left[\nabla^2_{\mathbf{x}_2\mathbf{x}_2} f_2(\mathbf{x}_1, \mathbf{x}_2)\right]^{-1} \nabla_{\mathbf{x}_2} f_1(\mathbf{x}_1, \mathbf{x}_2).$$

We call $\bar{\nabla} f_1(\mathbf{x}_1, \mathbf{x}_2)$ the *hyper-gradient*.

The bilevel approximation method

Algorithm 1: The bilevel approximation method

```
Input: $\mathbf{x}_1^{(0)} \in \mathbb{R}^{p1}$, $\mathbf{x}_2^{(0)} \in \mathbb{R}^{p2}$, step sizes $\{a^{(m)}\}, \{b^{(t)}\}$, inner iterations $\{t^{(m)}\}$
for $m = 0, 1, 2, \ldots$ do
    // Inner loop: approximate $\mathbf{x}_2^\star(\mathbf{x}_1^{(m)})$
    for $t = 0, 1, \ldots, t^{(m)} - 1$ do
        $\mathbf{x}_2^{(t+1)} = \mathbf{x}_2^{(t)} - b^{(t)} \nabla_{\mathbf{x}_2} f_2(\mathbf{x}_1^{(m)}, \mathbf{x}_2^{(t)})$
    $\bar{\mathbf{x}}_2^{(m)} = \mathbf{x}_2^{(t^{(m)})}$
    // Outer update using approximate hypergradient
    $\mathbf{x}_1^{(m+1)} = \arg\min_{\mathbf{u} \in \mathcal{X}_1} \left\{ \langle \bar{\nabla} f_1(\mathbf{x}_1^{(m)}, \bar{\mathbf{x}}_2^{(m)}), \mathbf{u} \rangle + \frac{1}{2a^{(m)}} \|\mathbf{u} - \mathbf{x}_1^{(m)}\|^2 \right\}$
Output: $\mathbf{x}_1^{(m+1)}$
```

Remarks:

- [12] derives the convergence rate $f_1(\mathbf{x}_1^{(T)}, \mathbf{x}_2^*(\mathbf{x}_1^{(T)})) - f_1(\mathbf{x}_1^*, \mathbf{x}_2^*(\mathbf{x}_1^*)) = \mathcal{O}(1/T)$.
- More advanced algorithms have been developed [34, 3, 18, 23].
- **Key challenge**: Computing second-order derivatives and Hessian inverse is challenging in LLMs.

Data mixing with direct modelling

- Find a mixing function V mapping domain weights to target loss:

$$\boldsymbol{\alpha}^\star = \arg\min_{\boldsymbol{\alpha}} \mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha})) \approx V(\boldsymbol{\alpha})$$

- Goal: estimate the mixing function V.
  1. Sample mixing weights $\boldsymbol{\alpha}_j$, $j = 1, \ldots, n$, where n is the sampling budget
  2. Train n models with each $\boldsymbol{\alpha}_j$ and evaluate their validation loss $\mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha}_j))$
  3. Fit $V(\boldsymbol{\alpha})$ on $\{(\boldsymbol{\alpha}_j, \mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha}_j)))\}_{j=1}^n$ (e.g., linear regression)

- **Problem**: retraining costs at large model and data scales can be expensive.

Proxy-based algorithms

- Key idea: train smaller proxy models to approximate target performance.
- Fit a mixing function V through the proxy models.
- Train large model with $\alpha^\star$ optimized on proxies.

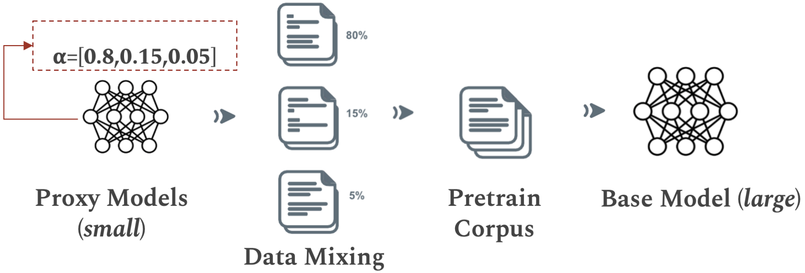


Figure: Proxy-based algorithms' pipeline [9].

What is data mixture *transfer*?

◦ Goal: use mixture $\boldsymbol{\alpha}$ found at a small proxy scale to train a larger model.

Setup

Let s denote the model scale and $\boldsymbol{\alpha} \in \Delta^k$ a domain mixture.

$$\mathbf{x}^\star(\boldsymbol{\alpha}; s) \in \arg\min_{\mathbf{x}} \mathcal{L}_{\text{train}}(\mathbf{x}; \boldsymbol{\alpha}, s), \quad V_s(\boldsymbol{\alpha}) := \mathcal{L}_{\text{target}}\Big(\mathbf{x}^\star(\boldsymbol{\alpha}; s)\Big), \quad \boldsymbol{\alpha}^\star(s) \in \arg\min_{\boldsymbol{\alpha}\in\Delta^k} V_s(\boldsymbol{\alpha}).$$

We ask: how does $\boldsymbol{\alpha}^\star(s)$ change with s?

Two notions of transfer

Strong transfer: $\boldsymbol{\alpha}^\star(s_{\text{small}}) \in \arg\min_{\boldsymbol{\alpha}} V_{s_{\text{large}}}(\boldsymbol{\alpha})$

Effective transfer: $V_{s_{\text{large}}}\Big(\boldsymbol{\alpha}^\star(s_{\text{small}})\Big) \le \min_{\boldsymbol{\alpha}} V_{s_{\text{large}}}(\boldsymbol{\alpha}) + \varepsilon,$ for a small tolerance $\varepsilon > 0$.

Remarks:

◦ In general, $\boldsymbol{\alpha}^\star(s_1) \neq \boldsymbol{\alpha}^\star(s_2)$: capacity, optimization dynamics, and implicit bias vary with s.

◦ Strong transfer is generically *not* expected; in practice, we aim for *effective* transfer.

Optimal weights are scale-dependent...

- Some works [30, 9, 29] empirically show $\alpha^\star$ across model scales.
- Domain weights could change at various scales of proxy model (flatter is more stable).

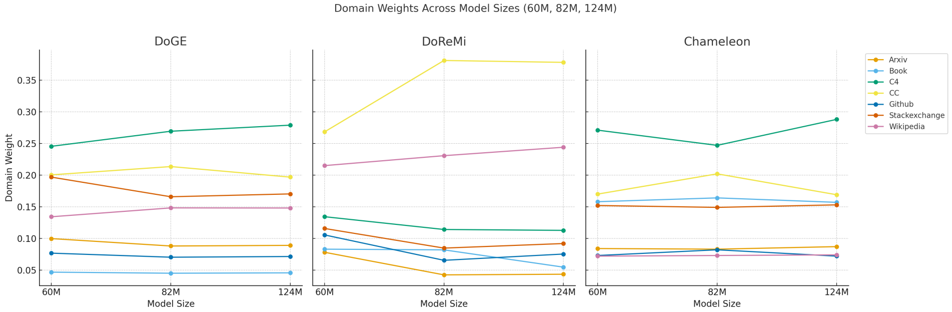
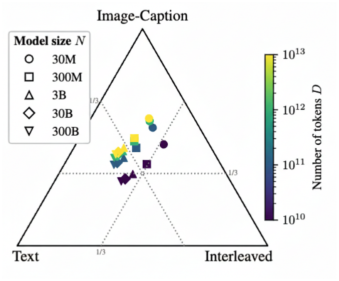


Figure: Optimal domain weights at three proxy model scales for multiple proxy-based methods.

... but effective data mixtures transfer in practice

◦ Can small models reliably select data mixtures for larger models?



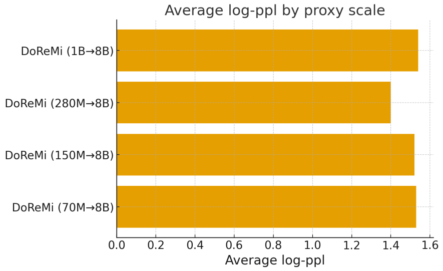


Figure: Figures from [27, 30].

Remarks:

◦ While *optimal* weights change at different scales, the transferred α may still be *effective*.

◦ Optimal α varies with scale, ε-optimal region is broad $\Rightarrow$ proxy mixtures remain effective.

Taxonomy of data mixture methods

Two Main Axes of Classification

- **Temporal Adaptation:** *Offline* (fixed mixture) vs. *Online* (adapt during training).
- **Target Objective:** *General-purpose* (universal generalization $\mathcal{L}_{\text{val}}$) vs. *Task-specific* (downstream target $\mathcal{L}_{\text{task}}$).

Type	General-Purpose	Target Task-Specific
Offline	DoReMi [30] DoGE [9] Data Mixing Laws [33] **Chameleon** [31] ...	RegMix [19] MixMin [28] UtiliMax [14]
Online	ODM [2] ADO [15]	Skill-it! [6] DGA [8]

Proxy-based algorithms: DoReMi [30]

- DoReMi is a three-step algorithm.
  1. Train a small reference model $\mathbf{x}_{\text{ref}}$ with uniform domain weights.
  2. Train proxy model with group distributionally robust optimization to obtain domain weights.
  3. Train large model with new domain weights.

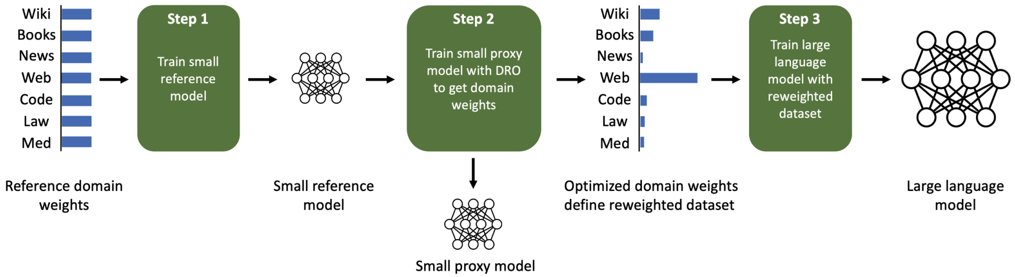

Wiki
Books
News
Web
Code
Law
Med
Reference domain weights
Step 1
Train small reference model
Small reference model
Step 2
Train small proxy model with DRO to get domain weights
Small proxy model
Wiki
Books
News
Web
Code
Law
Med
Optimized domain weights define reweighted dataset
Step 3
Train large language model with reweighted dataset
Large language model

Figure: DoReMi's pipeline [30].

Proxy-based algorithms: DoReMi [30]

◦ Optimize the worst-case loss over domains (Group DRO with *excess loss* [25, 22]):

$$\min_{\mathbf{x}} \max_{\boldsymbol{\alpha}\in\triangle^k} \mathcal{L}(\mathbf{x},\boldsymbol{\alpha}) := \sum_{i=1}^{k} \alpha_i \cdot [f_i(\mathbf{x}) - f_i(\mathbf{x}_{\text{ref}})]$$

DoReMi intuition

Down-weight redundant and noisy domains, up-weight learnable ones.

$$\begin{aligned}
&\textbf{Redundant}: && \text{low } f_i(\mathbf{x}),\ \text{low } f_i(\mathbf{x}_{\text{ref}}) && \Rightarrow \text{low excess loss } \big(f_i(\mathbf{x}) - f_i(\mathbf{x}_{\text{ref}})\big) && \Rightarrow \textbf{down-weighted};\\
&\textbf{Noisy}: && \text{high } f_i(\mathbf{x}),\ \text{high } f_i(\mathbf{x}_{\text{ref}}) && \Rightarrow \text{low excess loss } \big(f_i(\mathbf{x}) - f_i(\mathbf{x}_{\text{ref}})\big) && \Rightarrow \textbf{down-weighted};\\
&\textbf{Learnable}: && \text{high } f_i(\mathbf{x}),\ \text{low } f_i(\mathbf{x}_{\text{ref}}) && \Rightarrow \text{high excess loss } \big(f_i(\mathbf{x}) - f_i(\mathbf{x}_{\text{ref}})\big) && \Rightarrow \textbf{up-weighted}.
\end{aligned}$$

Remarks:

◦ $\boldsymbol{\alpha}$ highly depends on the performance of reference model.

◦ DoReMi is not efficient enough since it requires two auxiliary models.

◦ Mathematically, one-hot weights can be optimal $\boldsymbol{\alpha}^\star$!

Proxy-based algorithms: DoReMi [30]

∘ DoReMi's core problem corresponds to an inner maximization over domain weights, which is *linear* in α:

$$\max_{\boldsymbol{\alpha}\in\triangle^k} \sum_{i\in[k]} \alpha_i\, g_i^{(t)}, \quad \text{where } g_i^{(t)} = f_i(\mathbf{x}^{(t)}) - f_i(\mathbf{x}_{\text{ref}}).$$

Lemma (Optimality of one-hot weights)

The weights placing all mass on the domain(s) with the largest excess loss solve DoReMi's inner maximization.

∘ No exploration! Idea: treat the maximizer as an online learner updating a distribution $\boldsymbol{\alpha}^{(t)}$ over actions.

Hedge [10] update for DoReMi

For each domain $i \in \{1, \dots, k\}$:

$$\boldsymbol{\alpha}_i' \propto \boldsymbol{\alpha}_i^{(t)} \exp\left(\eta\, g_i^{(t)}\right).$$

Remarks:

∘ Implements entropic regularization to the inner maximization [5, 21].

∘ This prevents collapse to a one-hot solution.

∘ Optimistic update can be applied for further smoothing of the domain weights [7, 16].

Proxy-based algorithms: DoReMi [30]

- In the multiplicative-weights regime, probabilities can collapse: $\boldsymbol{\alpha}_i^{(t)} \to 0$.
- DoReMi enforces stability using uniform smoothing via EXP3 [4].

EXP3 [4] update for DoReMi

DoReMi adds uniform smoothing for each domain $i \in \{1, \ldots, k\}$:

$$\boldsymbol{\alpha}_i^{(t+1)} = (1-\gamma)\frac{\boldsymbol{\alpha}_i'}{\sum_{j=1}^{k} \boldsymbol{\alpha}_j'} + \gamma u_i, \qquad \boldsymbol{u} = \frac{1}{k}\mathbf{1}.$$

Remarks:
- DoReMi formulates domain reweighting as an adversarial online learning problem.
- Uniform exploration prior prevents any domain weight from vanishing.

Proxy-based algorithms: DoGE [9]

- DoGE gets rid of training the reference model.
- DoGE is a two-step algorithm.

1. Train a small-scale proxy model to find optimal domain weights.
   - Formulate domain reweighting as the bilevel problem:

$$\min_{\boldsymbol{\alpha} \in \triangle^k} \sum_{i \in [k]} f_i(\mathbf{x}^\star(\boldsymbol{\alpha})) \quad \text{s.t.} \quad \mathbf{x}^\star(\boldsymbol{\alpha}) \in \arg\min_{\mathbf{x}} \sum_{i \in [k]} \alpha_i f_i(\mathbf{x}). \tag{3}$$

2. Train large-scale base LLM with resampled pretrain corpus according to the finalized domain weights.

Proxy-based algorithms: DoGE [9]

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  2. Train large-scale base LLM with resampled pretrain corpus according to the finalized domain weights.

Lemma (Optimality of uniform weights)

The uniform domain weight vector $\boldsymbol{\alpha} = \left(\frac{1}{k}, \dots, \frac{1}{k}\right)$ *is a global minimizer of* (3).

Proxy-based algorithms: DoGE [9]

- ◦ DoGE gets rid of training the reference model.
- ◦ DoGE is a two-step algorithm.

1. Train a small-scale proxy model to find optimal domain weights.
   - ▶ Formulate domain reweighting as the bilevel problem:

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Lemma (Optimality of uniform weights)

The uniform domain weight vector $\boldsymbol{\alpha} = \left(\frac{1}{k}, \ldots, \frac{1}{k}\right)$ is a global minimizer of (3).

Remarks:
- ◦ Uniform weights can be optimal, although we aim to improve over uniform...
- ◦ Alternatively, one can choose outer loss ≠ inner loss, e.g., $\mathcal{L}_{\text{val}}$ or $\mathcal{L}_{\text{task}}$ [8].

Proxy-based algorithms: DoGE [9]

◦ Inner-loop: model update at step t:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta \sum_{i \in [k]} \alpha_i^{(t)} \nabla f_i(\mathbf{x}^{(t)}), \qquad \boldsymbol{\alpha}^{(t)} \in \Delta^k. \tag{1}$$

◦ Outer-loop: one-step greedy expansion. Minimize the average loss across domains at the next step $(t+1)$:

$$\begin{aligned} \boldsymbol{\alpha}^{(t)\star} &= \arg \min_{\boldsymbol{\alpha} \in \Delta^k} \sum_{i \in [k]} \left[f_i(\mathbf{x}^{(t+1)}) - f_i(\mathbf{x}^{(t)}) \right] \\ &= \arg \min_{\boldsymbol{\alpha} \in \Delta^k} \sum_{i \in [k]} \left\langle \nabla f_i(\mathbf{x}^{(t)}), \mathbf{x}^{(t+1)} - \mathbf{x}^{(t)} \right\rangle + \epsilon^{(t)} \\ &= \arg \min_{\boldsymbol{\alpha} \in \Delta^k} \sum_{i \in [k]} \left\langle \nabla f_i(\mathbf{x}^{(t)}), -\eta \sum_{j \in [k]} \alpha_j \nabla f_j(\mathbf{x}^{(t)}) \right\rangle + \epsilon^{(t)}. \end{aligned}$$

Remark: ◦ The domain weight update uses approximations based on "influence functions" [13, 17].

Proxy-based algorithms: DoGE [9]

◦ Define the generalization estimation function of domain j as the *gradient alignment*:

$$W_j^{(t)} \triangleq \left\langle \nabla f_j(\mathbf{x}^{(t)}), \sum_{i\in[k]} \nabla f_i(\mathbf{x}^{(t)}) \right\rangle.$$

◦ The outer problem becomes:

$$\boldsymbol{\alpha}^{(t)} = \arg\min_{\boldsymbol{\alpha}\in\Delta^k} -\eta^{(t)}\boldsymbol{\alpha}^\top \boldsymbol{\mathcal{W}}^{(t)} + \mu\, D_\Psi(\boldsymbol{\alpha}\|\boldsymbol{\alpha}^{(t-1)}), \qquad \boldsymbol{\mathcal{W}}^{(t)} = [W_1^{(t)}, \ldots, W_k^{(t)}] \in \mathbb{R}^k,$$

where the Bregman divergence $D_\Psi(\boldsymbol{\alpha}\|\boldsymbol{\alpha}^{(t-1)})$ with $\Psi(\boldsymbol{\alpha}) = \sum_i \alpha_i \log(\alpha_i)$ is used to remain on the simplex.

◦ DoGE's domain weights update rule:

$$\boldsymbol{\alpha}^{(t)} \propto \boldsymbol{\alpha}^{(t-1)} \odot \exp\left(\frac{\eta}{\mu} \boldsymbol{\mathcal{W}}^{(t)}\right).$$

Remark: ◦ The proxy model requires k gradient computations per update, slowing training.

◦ DoGE is sensitive to the choice of μ [31].

Proxy-based algorithms: RegMix [19]

- RegMix grid searches domain proportions and predicts optimal weights via regression.
- RegMix follows four steps.

1. Train a large number of small proxy models.
   - Generate n random mixtures $\boldsymbol{\alpha}_j$.
   - For each $\boldsymbol{\alpha}_j$, train proxy $\mathbf{x}^\star(\boldsymbol{\alpha}_j)$ and compute target metric $y_j = \mathcal{L}_{\text{target}}(\mathbf{x}^\star(\boldsymbol{\alpha}_j))$.
   - Example settings: $n = 512$ of scale $1M$.
2. Fit regression model.
   - Fit a regression model $V(\boldsymbol{\alpha}) : \Delta^k \to \mathbb{R}$ on $\{(\boldsymbol{\alpha}_j, y_j)\}_{j=1}^n$ (e.g., linear regression or tree model).
3. Simulate and predict.
   - Find $\boldsymbol{\alpha}^\star = \arg\min_{\boldsymbol{\alpha}} V(\boldsymbol{\alpha})$.
   - Solved by random search over $1,000,000$ candidates.
4. Train large-scale model.

Proxy-based algorithms: RegMix [19]

- Perplexity average may not directly relate to downstream tasks' performance.
  - RegMix finds that Common Crawl (CC) is highly relevant to downstream tasks' performance.
  - It uses the validation loss of Pile-CC [11] as $\mathcal{L}_{\text{target}}$ objective.

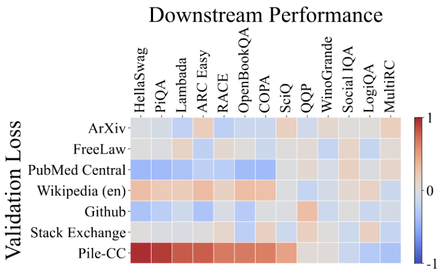


Figure: Correlation between validation loss by domains of the Pile and downstream performance.

From proxy-based methods to a data-centric view

So far: DoReMi, DoGE, RegMix

- All critically rely on proxy training runs and challenging bilevel-style optimization.
- Domain weights are tightly coupled to the training dynamics.
- Any change in domains $\Rightarrow$ retrain proxy models.

Our goal with Chameleon:

- Domain weights from a **single, well-understood least-squares problem**...

A least-squares view of domain importance

We equip each domain with a vector embedding $\boldsymbol{v}_i \in \mathbb{R}^p$. Let $\mathbf{V} = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k]^\top \in \mathbb{R}^{k \times p}$.

Min-norm reconstruction problem

For each domain i, consider:

$$S_i = \min_{\mathbf{y} \in \mathbb{R}^k} \left\{ \| \mathbf{y} \|_2^2 + \frac{1}{\lambda} \| \mathbf{V}^\top \mathbf{y} - \boldsymbol{v}_i \|_2^2 \right\}.$$

The S_i is called the *ridge leverage score* of row $\boldsymbol{v}_i$ in matrix $\mathbf{V}$ [20].

Remarks:

- If $\boldsymbol{v}_i$ is a simple linear combination of other rows of $\mathbf{V}$, a small-norm $\mathbf{y}$ can exist $\Rightarrow S_i$ is **small**.
- If $\boldsymbol{v}_i$ is hard to reconstruct from other domains, then $\mathbf{y}$ must have larger norm $\Rightarrow S_i$ is **large**.
- Interpretation: S_i measures how *unique* domain i is in the geometry of the embedded dataset.

Illustrative examples of leverage scores

Example (2D example)

Let $\boldsymbol{v}_1 = (1, 0),\ \boldsymbol{v}_2 = (1, 0.1),\ \boldsymbol{v}_3 = (0, 1)$ be three domain embeddings.

- $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are nearly collinear, $\boldsymbol{v}_3$ is orthogonal to $\boldsymbol{v}_1$ and nearly orthogonal to $\boldsymbol{v}_2$.
- To reconstruct $\boldsymbol{v}_1$: a balanced mix of $\boldsymbol{v}_1$ and $\boldsymbol{v}_2 \Rightarrow$ as $\lambda \to 0$, $\| \mathbf{y}^\star \|_2^2 \approx 0.5$ (low leverage).
- Same for $\boldsymbol{v}_2$.
- To reconstruct $\boldsymbol{v}_3$: one must put almost all weight to itself $\Rightarrow \| \mathbf{y}^\star \|_2^2 \approx 1$ (high leverage).

Example (NLP example)

Consider three domains: D_1 (Common Crawl), D_2 (C4), and D_3 (Arxiv). We expect embeddings $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ to be highly similar, while $\boldsymbol{v}_3$ is relatively orthogonal.

$$\boldsymbol{v}_1 \approx \boldsymbol{v}_2, \quad \boldsymbol{v}_3^\top \boldsymbol{v}_1 \approx 0, \quad \boldsymbol{v}_3^\top \boldsymbol{v}_2 \approx 0$$

Consequently, we anticipate: S_1, S_2 are low and S_3 is high.

Computing domain affinity

∘ We construct the kernel matrix of domain embeddings as $\mathbf{\Omega} = [\kappa(\boldsymbol{v}_i, \boldsymbol{v}_j)]_{i,j=1}^{k} \in \mathbb{R}^{k \times k}$.

Definition: Kernel Ridge Leverage Scores (KRLS)

The KRLS [1] of domain D_i is the i-th diagonal element of the kernel *hat matrix* with regularization $\lambda > 0$:

$$S_i = \left[\mathbf{\Omega}(\mathbf{\Omega} + \lambda \boldsymbol{I})^{-1}\right]_{ii}. \tag{4}$$

∘ Eigendecomposition perspective. Let $\mathbf{\Omega} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^\top$ with $\mathbf{\Sigma} = \operatorname{diag}(\sigma_1, \ldots, \sigma_k)$ be the reduced SVD, then

$$S_i = \sum_{j=1}^{k} \frac{\sigma_j}{\sigma_j + \lambda} U_{ij}^2.$$

Remark: ∘ For $\lambda > 0$, the contribution of directions with small eigenvalues is damped.

Least-squares view of KRLS

◦ Primal problem of KRLS of domain i:

$$\boxed{\text{P}} \quad \min_{\boldsymbol{w},\boldsymbol{e}} \frac{1}{2}\sum_{j=1}^{k} e_j^2 + \frac{\lambda}{2}\|\boldsymbol{w}\|^2 \quad \text{s.t. } e_j = \delta_j - \boldsymbol{w}^\top \boldsymbol{v}_j \ \ \forall j, \tag{5}$$

where

$$\delta_j = \begin{cases} 1 & \text{if } j = i, \\ 0 & \text{otherwise.} \end{cases}$$

◦ Lagrangian:

$$\mathcal{L}(\boldsymbol{w}, \boldsymbol{e}; \boldsymbol{\alpha}) = \frac{1}{2}\sum_{j=1}^{k} e_j^2 + \frac{\lambda}{2}\|\boldsymbol{w}\|^2 - \sum_{j=1}^{k} \alpha_j (e_j - \delta_j + \boldsymbol{w}^\top \boldsymbol{v}_j). \tag{6}$$

◦ Elimination of $\boldsymbol{w}, \boldsymbol{e}$ in the optimality conditions gives:

$$\boxed{\text{D}} \quad (\boldsymbol{\Omega} + \lambda \boldsymbol{I})\boldsymbol{\alpha} = \lambda \boldsymbol{\delta},$$

with linear kernel matrix $\boldsymbol{\Omega}$.

KRLS: Model representation

◦ Model-based approach of KRLS:

$$\begin{tikzcd} & \boxed{\text{P}}\ S_i = \boldsymbol{w}^\top \boldsymbol{v}_i \\ \text{KRLS of } \boldsymbol{v}_i \arrow[ur] \arrow[dr] & \\ & \boxed{\text{D}}\ S_i = \boldsymbol{\delta}^\top \left[\boldsymbol{\Omega}(\boldsymbol{\Omega} + \lambda \boldsymbol{I})^{-1}\right] \boldsymbol{\delta} \end{tikzcd}$$

Remarks:

◦ The dual $\boxed{\text{D}}$ recovers the standard definition of KRLS in (4).

◦ The primal $\boxed{\text{P}}$ provides the interpretation of KRLS as finding a vector $\boldsymbol{w}$ that "picks out" $\boldsymbol{v}_i$.

◦ Leads to a natural way to extend KRLS to **multiple modalities** (see our recent preprint [32]).

From data domains to geometric embeddings

- How to learn meaningful embeddings of data domains?
- A proxy model $h_{\mathbf{x}_p}$ is first trained with uniform domain weights.

Definition: Domain embedding

The embedding for a domain D_i is defined as the *centroid* of the representations of its constituent data points, extracted from the L-th hidden layer of the proxy model $h_{\mathbf{x}_p}$.

$$\boldsymbol{v}_i = \frac{1}{|D_i|} \sum_{\mathbf{a} \in D_i} h_{\mathbf{x}_p}^{(L)}(\mathbf{a}) \in \mathbb{R}^p.$$

Remarks:

- In practice, this expectation is estimated using a sufficiently large batch $B_i \subseteq D_i$.
- Proximity between vectors $\boldsymbol{v}_i$ and $\boldsymbol{v}_j$ in the embedding space corresponds to a high degree of semantic similarity between domains D_i and D_j.

The Chameleon pipeline

[Xie, Tonin, Cevher; ICML'25]

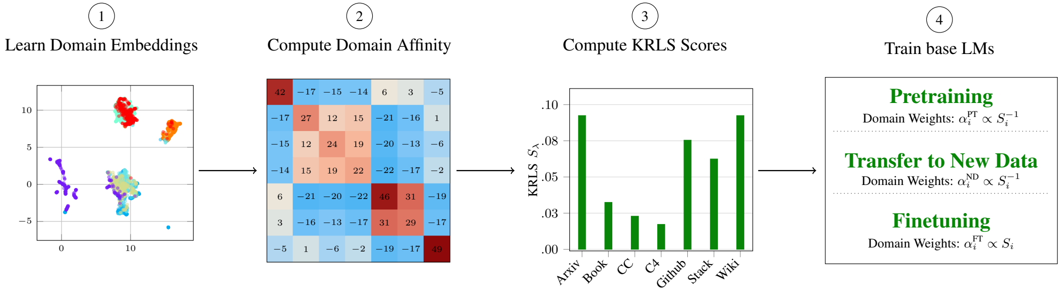


Figure: CHAMELEON's pipeline.

Remarks:

- We use a linear kernel $\kappa(\boldsymbol{v}_i, \boldsymbol{v}_j) = \boldsymbol{v}_i^\top \boldsymbol{v}_j$ as the LLM embeddings are already highly non-linear.
- Chameleon is more stable since domain weights are decoupled from the training process.
- The time for step 1-3 in the above figure is negligible compared to proxy model training.

Using KRLS differently for pretraining vs finetuning

- We propose distinct weighting strategies for pretraining and finetuning.
- One geometric score, two regimes: generalization vs. specialization.

Pretraining: learn broad, shared knowledge.

- Upweight *representative* (low-score) domains.
- Learn general-purpose representations.

$$\alpha_i^{\mathsf{PT}} \propto \frac{1}{S_i}$$

Example

In the SlimPajama dataset, broad domains like 'Common Crawl (CC)' and 'C4' lie in denser regions of the embedding space. Our α^{PT} upweights them.

Finetuning: specialize to a target.

- Upweight *novel* (high-score) domains.
- Focus on features underrepresented in pretraining.

$$\alpha_i^{\mathsf{FT}} \propto S_i$$

Example

When finetuning on the 'Stack' code dataset, the 'Go' domain might be distant from 'Python' or 'Java' Our α^{FT} upweights 'Go' to learn its distinct syntax.

Direct extension to new data

◦ Chameleon allows direct weight computation for new domains.

Out-of-sample extension

1. Given a new set of domains $D' = \{D_1, \ldots, D_{k'}\}$.
2. Generate embeddings for new domains using the *existing* proxy: $\boldsymbol{v}'_j = \mathbb{E}_{\mathbf{a} \in D_j}[h_{\mathbf{x}}(\mathbf{a})]$.
3. Construct the new affinity matrix $\boldsymbol{\Omega}'$.
4. Calculate the new KRLS scores:

$$S'_j = \left[\boldsymbol{\Omega}'(\boldsymbol{\Omega}' + \lambda \boldsymbol{I})^{-1}\right]_{jj} .$$

Remarks: ◦ In existing methods, any change to the dataset D requires costly retraining from scratch.

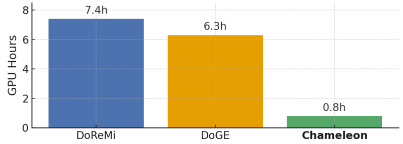
◦ Our method is decoupled from the proxy model's optimization loop.

Experiments: Universal generalization on SlimPajama

Setup: Pretraining a 684M model on SlimPajama (7 domains). Weights derived from an 82M proxy model.

Domain	**Uniform**	DoReMi	DoGE	**Chameleon**	RegMix
Arxiv	8.16	9.16	9.07	8.31	11.35
Book	42.55	46.48	40.30	39.23	41.52
CC	45.26	40.62	38.99	40.11	37.32
C4	49.00	43.92	40.65	42.59	43.85
Github	3.99	4.10	4.09	4.20	4.99
Stackexchange	7.99	8.35	7.39	7.94	10.63
Wikipedia	12.42	10.78	15.74	13.90	20.88
Avg. PPL (↓)	24.20	23.34	22.32	**22.31**	24.36

Perplexity (PPL) results on the SlimPajama dataset. Lower is better.

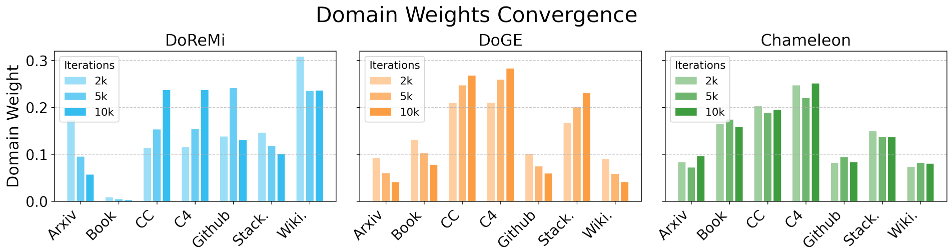


GPU hours for proxy training.

Remarks:
- ○ Chameleon achieves the best perplexity on SlimPajama.
- ○ Chameleon is significantly more efficient, requiring only 1/10th of the FLOPs of DoReMi.

Experiments: Score convergence

- Domain weights across methods during proxy training.



Remarks:

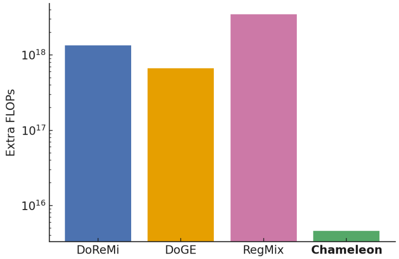
- Chameleon converges quickly.
- DoReMi and DoGE require more iterations to stabilize.
- Chameleon is also robust to training steps, proxy scales, λ, and embedding sample size.

Experiments: Zero-shot transfer to new domains

- The Scalability Test: Can we adapt to a new dataset (The Pile, 17 domains) without retraining?
  - Baselines (DoReMi, DoGE, RegMix) must retrain a proxy from scratch on The Pile.
  - Chameleon simply performs inference using the *same proxy model* trained on SlimPajama.

Benchmark	**Uniform**	DoReMi	DoGE	**Chameleon**	RegMix
ARC-E	37.5	39.3	35.3	39.2	39.5
COPA	56.8	61.5	54.7	60.9	61.2
HellaSwag	26.7	27.3	26.1	27.4	27.3
Lambada	12.5	15.8	9.3	15.9	15.4
LogiQA	22.5	21.2	22.1	23.8	21.9
MultiRC	56.7	56.5	57.2	57.3	56.2
OpenBook	13.3	13.1	13.1	14.2	14.5
PiQA	57.8	59.3	55.9	59.7	60.4
QQP	37.5	36.8	36.8	37.2	37.6
RACE	25.8	27.2	24.9	26.8	27.2
SciQ	64.1	65.7	58.1	66.0	67.1
Social IQA	35.0	36.0	34.2	36.6	36.3
WinoGrande	50.7	51.2	49.8	50.9	49.9
Average (↑)	38.2	39.3	36.7	**39.7**	39.6

Downstream reasoning accuracies. Higher is better (↑).



Extra FLOPs for mixing new domains.

Experiments: Extending data mixing to finetuning

Setup: Finetune a pretrained model on two specialized datasets:

1. Wiki40b: 7 natural languages
2. The Stack: 7 programming languages

Finetuning on Wiki40b

Domain	**Uniform**	**Chameleon**
French	6.86	6.51
German	10.12	8.78
Italian	13.29	12.42
Spanish	8.41	8.04
Portuguese	8.00	7.78
Dutch	13.98	12.30
Polish	5.07	4.21
Average PPL (↓)	9.43	**8.58**
# Domains Over Uniform	-	7/7

Finetuning on The Stack

Domain	**Uniform**	CHAMELEON
Python	19.98	16.53
Java	19.27	15.53
C	28.24	22.58
C++	25.16	21.09
Go	30.25	19.26
Ruby	21.78	17.83
PHP	9.45	7.43
Average PPL (↓)	22.02	**17.18**
# Domains Over Uniform	-	7/7

Remarks:

- ○ Data mixing is effective for finetuning.
- ○ Embeddings can be easily extracted directly from the pretrained model.
- ○ Chameleon demonstrates its flexibility in both pretraining and finetuning phases.

The effect of data mixing on Scion [24]

- Chameleon: optimizes mixtures of pretraining data domains.
- Scion+Chameleon: 40% less steps or 3% better performance on SlimPajama dataset.

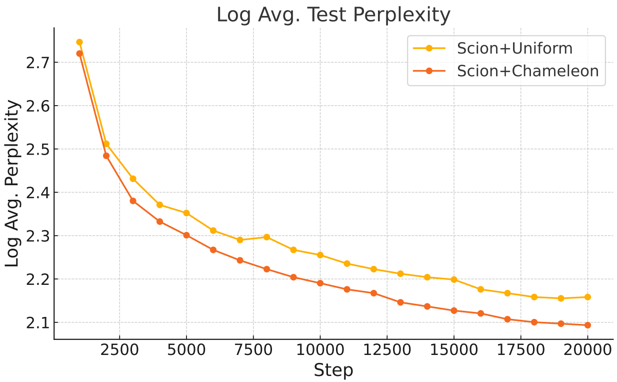


Figure: Significant accelerations in pretraining a 210M LM combining Scion with Chameleon data mixing.

Conclusion

- ◦ Chameleon is a novel, efficient, and flexible data-mixing framework based on Kernel Ridge Leverage Scores.
- ◦ Zero-shot transfer: Adapts to new data domains without costly retraining.
- ◦ Flexibility: Provides a unified, principled approach for both pretraining and finetuning data mixing.

🔔 **NEW** : **Compute grant** – Awarded 50k GPU-hours (NVIDIA GH200) from Swiss AI for:

- ▶ Online adaptation: Extend to online settings where domain weights are adjusted during training.
- ▶ Geometry-aware optimization: Analyze the impact of data mixing on a new class of geometry-aware optimizers — such as Scion and Muon.

Thank you. Questions?

Code: `https://github.com/LIONS-EPFL/Chameleon`

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