Squeezing Your Fine-Tuning Data to the Last Drop

From Selection to Rebalancing

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About Me

- Final-year Ph.D. candidate at Monash University
- Research focus: Large Language Models, Multilinguality, Machine Translation
- 20+ papers in top-tier venues (ICML, ACL, EMNLP, COLING, TACL, etc.)
- Outstanding Paper Award at ACL 2025
- Visit/Intern experience: Huawei, Tencent, Alibaba, MBZUAI
- `https://minghao-wu.github.io/`

Overview

1. Introduction
2. GraphFilter: Static Data Selection
3. Mixture-of-Skills: Dynamic Data Rebalancing
4. Conclusion

The Data Challenge in LLM Fine-Tuning

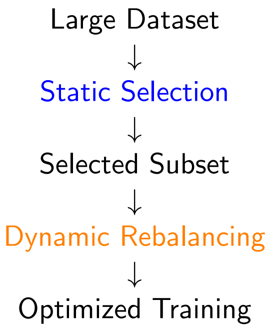
Why does data matter in LLM fine-tuning?

- Training data directly shapes model capabilities
- Quality determines how well the model learns
- Diversity ensures comprehensive skill coverage
- Scale vs. efficiency trade-offs

Key Challenges:

- Selection: What data to train on?
- Composition: How to mix datasets?
- Optimization: When to use what data?

The Pipeline



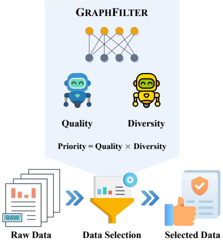
Large Dataset
↓
Static Selection
↓
Selected Subset
↓
Dynamic Rebalancing
↓
Optimized Training

Two complementary approaches

Two Complementary Approaches

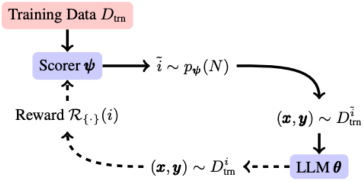
Study 1: GraphFilter

- Static Data Selection
- Bipartite graph representation
- Set cover optimization
- Quality × Diversity priority



Study 2: Mixture-of-Skills

- Dynamic Rebalancing
- Reinforcement learning framework
- Adaptive data rebalancing
- Skill-aware training


Training Data D_{trn}
Scorer $\boldsymbol{\psi}$
$\tilde{i} \sim p_{\boldsymbol{\psi}}(N)$
$(\boldsymbol{x}, \boldsymbol{y}) \sim D_{\text{trn}}^{\tilde{i}}$
LLM $\boldsymbol{\theta}$
$(\boldsymbol{x}, \boldsymbol{y}) \sim D_{\text{trn}}^{i}$
Reward $\mathcal{R}_{\{\cdot\}}(i)$

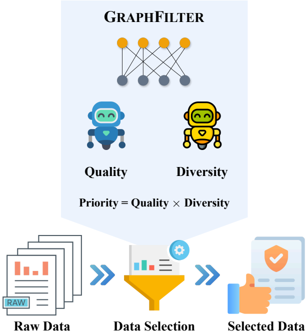
The Best of Both Worlds: Bridging Quality and Diversity in Data Selection with Bipartite Graph

Minghao Wu, Thuy-Trang Vu, Lizhen Qu, Gholamreza Haffari

2025 Forty-Second International Conference on Machine Learning

Key Contributions:

- Novel formulation as set cover problem
- Bipartite graph representation
- Multiplicative priority function
- Outperforms 9 baselines on 6 benchmarks



The Quality-Diversity Dilemma

Existing Methods Fall Short:

- Quality-focused: Select high-scoring examples
- Diversity-focused: Maximize coverage
- Problem: One aspect sacrificed for the other

Real-world Analogy:

- Curating a library collection
- Want both high-quality books *and* diverse topics
- Balance is key for comprehensive learning

The Challenge

Quality ↑

↓

Diversity ↓

GraphFilter: Best of Both Worlds

What is the Set Cover Problem?

Classic Computer Science Problem:

- Given a universe of elements U
- Given a collection of sets $\mathcal{S} = \{S_1, S_2, ..., S_m\}$
- Each set $S_i \subseteq U$
- **Goal**: Find minimum number of sets that cover all elements in U

NP-Hard Problem:

- No polynomial-time exact solution
- Greedy approximation works well
- Widely applicable in real-world scenarios

Mathematical Formulation

$$\min \textstyle\sum_{i=1}^{m} x_i$$

subject to:

$$\textstyle\sum_{i:e\in S_i} x_i \geq 1, \forall e \in U$$

$$x_i \in \{0, 1\}$$

where $x_i = 1$ if set S_i is selected

From Set Cover to Data Selection

The Connection:

- Universe U: All possible n-grams
- Sets $\mathcal{S}$: Training sentences
- Coverage: Each sentence covers its n-grams
- Goal: Select sentences that cover diverse n-grams

Why This Makes Sense:

- N-grams represent linguistic patterns
- Diverse n-gram coverage = diverse training data
- Natural formulation for diversity

Data Selection as Set Cover

Sentence 1: "How to cook pasta"

N-grams: {how, to, cook, pasta, how_to, to_cook, ...}

Sentence 2: "How to bake bread"

N-grams: {how, to, bake, bread, how_to, to_bake, ...}

Bipartite Graph Representation

Graph Components:

- Left nodes: Sentences $u_1, u_2, \ldots, u_5$
- Right nodes: N-grams $v_1, v_2, \ldots, v_5$
- Edges: Connect sentences to their n-grams

Selection Process:

- Select sentence with highest priority
- Remove covered n-grams from graph
- Update priorities dynamically
- Repeat until budget exhausted

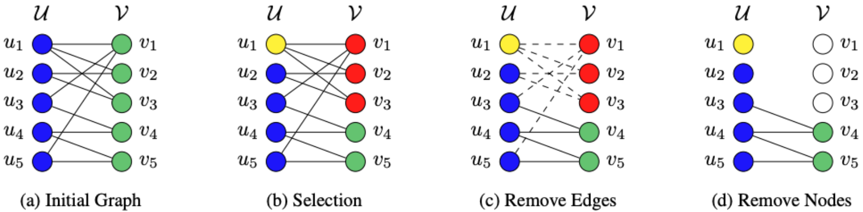


Figure: Example: Selecting u_1 covers n-grams $\{v_1, v_2, v_3\}$, then selecting u_4 covers remaining n-grams

But wait... This only considers diversity, not quality!

Incorporating Quality: The Priority Function

Priority Function Design:

$$\phi(u) = \text{Quality}(u) \times \max(1, \text{Diversity}(u))$$

Quality Metric - IFD Score:

$$\text{Quality}(u) = \text{PPL}(y|x)/\text{PPL}(y)$$

Diversity Metric - TF-IDF:

$$\text{Diversity}(u) = \sum_{v \in \mathcal{V}_u} \text{TF-IDF}(v)$$

Why Multiplicative?

High Quality + Low Diversity
⇒ Low Priority

Low Quality + High Diversity
⇒ Low Priority

High Quality + High Diversity
⇒ **High Priority**

Both aspects must be strong for selection!

GraphFilter Algorithm in Action

Iterative Selection Process:

1. **Initialize**: Empty selection $\mathcal{S} = \emptyset$
2. **Compute**: Priority $\phi(u)$
3. **Select**: u^* with highest priority
4. **Update**: Remove u^* and n-grams
5. **Repeat**: Until budget k is reached

Dynamic Priority Updates:

- Priorities change as n-grams are covered
- Encourages selection of complementary sentences
- Balances quality and remaining diversity

Computational Efficiency

- Max-heap $\mathcal{O}(\log N)$ per iteration
- Localized priority updates
- Scalable to large datasets

N-gram Selection

- Use n-grams up to length 3
- Balances granularity and efficiency
- Captures meaningful linguistic patterns
- Empirically effective

Experimental Setup

Training Dataset:

- **Magpie** dataset (300K instances)
- High-quality instruction-response pairs
- Select 10K subset

Model Backbones:

- Gemma-2-2B
- Mistral-7B-v0.3
- Llama-3-8B

Baseline Methods (9 total):

- **Heuristic**: Random, Longest
- **Quality-based**: PPL, ArmoRM, AlpaGasus, DEITA, IFD
- **Diversity-based**: K-means, InsTag

Evaluation Benchmarks (6 total):

- MMLU, ARC, HellaSwag, GSM8K
- AlpacaEval-2.0, MT-Bench using GPT-4o

Main Results: GraphFilter Outperforms All Baselines

Consistent Improvements Against Random:

- **Gemma-2-2B**: Up to +2.03
- **Mistral-7B**: Up to +2.83
- **Llama-3-8B**: Up to +2.46

Key Findings:

- GraphFilter achieves best/second-best on most benchmarks
- Quality-only methods show benchmark bias (e.g., ArmoRM good on AlpacaEval, poor elsewhere)

	Standard	LLM	ALL
Random	47.75	41.04	45.51
Longest	46.91	39.96	44.59
Perplexity	48.27	40.28	45.61
ArmoRM	48.21	42.66	46.36
AlpaGasus	48.96	41.90	46.60
DEITA	48.78	41.70	46.42
SuperFilter	49.10	41.91	46.70
Kmeans	48.90	41.72	46.51
InsTag	49.93	41.72	47.19
GraphFilter (Ours)	**50.55**	**42.79**	**47.97**

Table: Main results given by Llama-3-8B on the standardized benchmarks and LLM-as-a-Judge benchmarks. The best results are highlighted in **bold**, and the second-best results are highlighted in underline.

Main Results: GraphFilter is Computationally Efficient

Computational Efficiency

- Max-heap $\mathcal{O}(\log N)$ per iteration
- Localized priority updates
- Scalable to large datasets

	Runtime (hrs)
Perplexity	0.92
ArmoRM	5.93
AlpaGasus	32.34
DEITA	22.65
SuperFilter	1.95
Kmeans	2.26
InsTag	25.48
GraphFilter (Ours)	2.48
w/o priority $\phi(u)$	0.53†

Table: Runtime (in hours) for selecting 10K training instances. † indicate the CPU-only method.

Analysis: GraphFilter Balances Quality and Diversity

Visualization Analysis:

- **Lexical Diversity**: Measured by MTLD metric
- **Data Quality**: Assessed by SkyworkRM

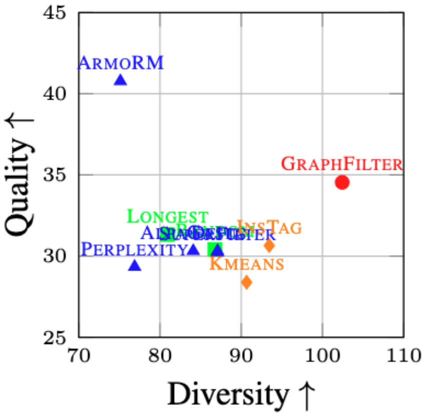
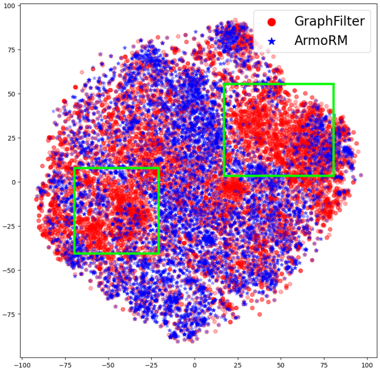


Figure: GraphFilter achieves highest lexical diversity and **second-best data quality** among all methods.

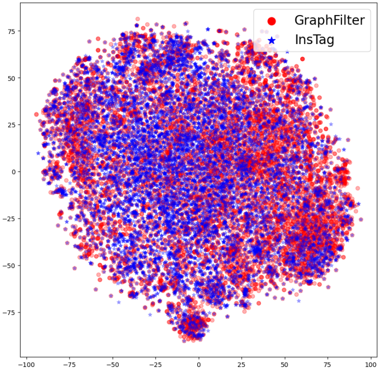
Analysis: GraphFilter Balances Quality and Diversity

Semantic Visualization: t-SNE plots using BGE embeddings

- Selects instructions not chosen by quality-only methods
- Similar semantic diversity to diversity-focused methods



(a) GraphFilter vs. ArmoRM (Quality only)



(b) GraphFilter vs. InsTag (Diversity only)

Analysis: N-gram Combinations Capture Multi-Level Features

Different N-grams Capture Different Patterns:

- **Unigrams (n=1)**: Individual words, basic vocabulary
- **Bigrams (n=2)**: Local word relationships
- **Trigrams (n=3)**: Phrasal patterns, syntax

Key Finding:

- Combining 1-grams + 2-grams + 3-grams significantly outperforms individual n-gram types
- Each level provides complementary information
- Integration consolidates features effectively

Performance by N-gram Type

N-gram	ALL
1-gram only	46.48
2-gram only	46.63
3-gram only	47.15
1+2+3-grams	**47.97**

Multi-level features are essential!

Analysis: Trigrams Provide Optimal Balance

N-gram Size Analysis (n_{max}=1 to 5):

- **Performance**: Peaks at trigrams ($n_{max}=3$)
- **Efficiency**: Decreases with larger n_{max}
- **Diminishing returns**: Beyond $n_{max}=3$

Why Trigrams Work Best:

- Capture meaningful linguistic patterns
- Balance granularity and computational cost
- Avoid over-specification of larger n-grams

N-gram Size Trade-offs

n_{max}	ALL	Time (hrs)
1	46.48	2.12
2	47.31	2.30
3	**47.97**	**2.48**
4	47.43	3.38
5	47.85	4.58

Sweet spot at n=3

# N-grams Nodes:
0.1M (1-gram) → 7.4M (5-gram)

Analysis: Instruction Diversity Matters Most

What to Apply GraphFilter To?

- Each training instance has instruction + response
- Tested three scenarios:
  - Instructions only
  - Responses only
  - Both instructions and responses

Surprising Result:

- **Instructions only performs best**
- Instruction diversity more impactful than response diversity
- Quality remains similar
- Rethinking: Response diversity also matters!

Type	Benchmarks			Lexical Diversity		Quality
	Standard	LLM	ALL	Instruction	Response	
Instruction	**50.55**	**42.79**	**47.97**	**102.43**	71.74	**81.54**
Response	47.16	39.71	44.68	90.22	**73.57**	81.52
Inst. + Resp.	48.03	41.20	45.76	90.13	72.60	81.52

Analysis: Budget Determines Quality vs. Diversity Priority

When to Prioritize What?

- **Small budgets (1K, 5K)**: Quality methods (SuperFilter) excel
- **Large budgets (10K+)**: Diversity methods (InsTag) catch up
- **All budgets**: GraphFilter consistently demonstrates performance gains

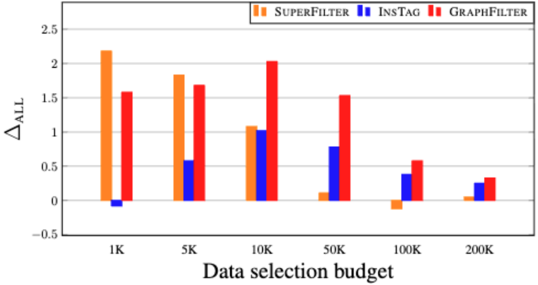


Figure: Relative gains against Random. Budget size affects strategy effectiveness

From Static Selection to Dynamic Optimization

GraphFilter Insights:

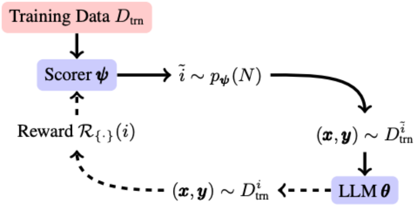
- Quality × Diversity balance is crucial
- Static selection has limitations
- What about during training?

New Challenge:

- Models learn different skills at different rates
- Static data mixing may not be optimal
- Finding the right data mix is expensive

The Next Question

Can we optimize data usage dynamically during fine-tuning?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LLM $\boldsymbol{\theta}$
$(\boldsymbol{x}, \boldsymbol{y}) \sim D_{\text{trn}}^{i}$

Enter: Mixture-of-Skills

Study 2: Mixture-of-Skills

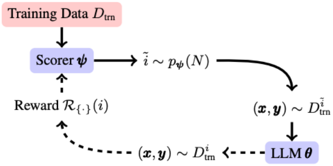
Mixture-of-Skills: Learning to Optimize Data Usage for Fine-Tuning Large Language Models

Minghao Wu, Thuy-Trang Vu, Lizhen Qu, Gholamreza Haffari

2024 Conference on Empirical Methods in Natural Language Processing

Key Contributions:

- Reinforcement learning framework for data rebalancing
- Model-agnostic dynamic optimization
- Adaptive skill development during training
- MoSpec extension for task-specific fine-tuning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LLM $\boldsymbol{\theta}$
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The Data Mixing Challenge

LLMs Need Multiple Skills:

- Writing, coding, mathematics, chatting, etc.
- Each skill requires different training data
- Datasets are heterogeneous and imbalanced

Current Problems:

- **Static mixing**: Ignores learning dynamics
- **Data capping**: Limits large dataset utilization
- **Cost**: Finding optimal ratios is costly

Example Challenge

- Math: 10K samples
- Code: 100K samples
- Chat: 1M samples

Learning Dynamics:

- Some skills learned quickly
- Others need more exposure
- Skills can interfere

Mixture-of-Skills: Bilevel Optimization

The Framework:

- Outer level: Optimize LLM parameters $\boldsymbol{\theta}$
- Inner level: Optimize data sampling via scorer network $\boldsymbol{\psi}$
- **Goal**: Learn optimal data usage automatically

Mathematical Formulation:

$$\boldsymbol{\psi} = \operatorname*{argmin}_{\boldsymbol{\psi}} \mathcal{J}(D_{\mathrm{trn}}; \boldsymbol{\theta}(\boldsymbol{\psi}))$$

$$\boldsymbol{\theta}(\boldsymbol{\psi}) = \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E}_{i \sim p_{\boldsymbol{\psi}}(N)}[\mathcal{L}(D^{i}_{\mathrm{trn}}; \boldsymbol{\theta})]$$

Why RL?

- Bilevel optimization not directly differentiable
- REINFORCE algorithm handles discrete sampling
- Enables dynamic adaptation

MoS Algorithm: Step-by-Step Walkthrough

Algorithm Overview:

1. **Initialize**: Start with uniform sampling ($\tau = \infty$)
2. **Training Loop**: For each step t:
   - Sample dataset $\tilde{i} \sim p_{\boldsymbol{\psi}}(N)$
   - Sample batch from $D^{\tilde{i}}_{\text{trn}}$
   - Update LLM: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{L}$
3. **Scorer Update** (every S steps):
   - Sample batch from each dataset
   - Compute rewards $\mathcal{R}(i)$ for each dataset
   - Update scorer: $\boldsymbol{\psi} \leftarrow \boldsymbol{\psi} + \gamma \sum_i \mathcal{R}(i) \nabla_{\boldsymbol{\psi}} \log p_{\boldsymbol{\psi}}(i)$

Key Components:

- **Scorer Network $\boldsymbol{\psi}$**: Simple 2-layer MLP
- **Update Frequency S**: Computational efficiency
- **Rewards $\mathcal{R}(i)$**: Guide optimization

Dynamic Adaptation:

- Sampling probabilities change over time
- Responds to current model state
- Balances different skills automatically

But how do we design rewards?

Reward Design: Three Perspectives

1. **Transferability ($\mathcal{R}_{\textbf{cosine}}$):**
   - Measure similarity between datasets
   - Use mini-batch embeddings from LLM
   - Higher similarity = better transferability

$$\mathcal{R}_{\text{cosine}}(i) = \frac{1}{N}\sum_{n=1}^{N} \frac{\mathbf{z}^i \cdot \mathbf{z}^n}{\|\mathbf{z}^i\| \cdot \|\mathbf{z}^n\|}$$

2. **Difficulty ($\mathcal{R}_{\textbf{diff}}$):**
   - Relative perplexity decrease after fine-tuning
   - Higher values = more difficult datasets need more attention

$$\mathcal{R}_{\text{diff}}(i) = \frac{1}{L}\sum_{j=1}^{L} \frac{\text{PPL}(\mathbf{y}^i_j; \mathbf{x}^i_j, \boldsymbol{\theta})}{\text{PPL}(\mathbf{y}^i_j; \mathbf{x}^i_j, \boldsymbol{\theta}_0)}$$

3. **Learning Trajectory:**
   - Exponential Moving Average (EMA) for stability
   - Smooths reward signals over time
   - Prevents oscillations

$$\mathcal{R}(i) = \beta\mathcal{R}'(i) + (1-\beta)\mathcal{R}''(i)$$

Design Principles:

- **Transferability**: Knowledge sharing
- **Difficulty**: Learning progress
- **Trajectory**: Stability

Rewards guide the scorer network to make informed sampling decisions

Experimental Setup

Datasets (4 Skills):

- **Mathematics**: MathInstruct (comprehensive collection)
- **Medicine**: MedInstruct (medical instructions)
- **General**: ShareGPT (diverse, high-quality conversations)
- **NLP**: P3 (660 subsets, diverse NLP tasks)

Model Backbones (3 total):

- Qwen1.5-0.5B
- Gemma-2B
- Llama-3-8B

Baselines:

- **Heuristic**: Temperature sampling

$$q_\tau(i) = \frac{q(i)^{1/\tau}}{\sum_{n=1}^{N} q(n)^{1/\tau}}$$

  - Proportional ($\tau = 1$), Temperature ($\tau = 10$), Uniform ($\tau = \infty$)
- **Dynamic**: MultiDDS, MultiUAT

Evaluation:

- **MMLU**: 57 subjects (Math, Medicine, Others)
- **MT-Bench**: 8 skills (Coding, Writing, etc.)

Main Results: MoS Consistently Outperforms Baselines

Consistent Improvements:

- **Qwen1.5-0.5B**: +0.96 improvement
- **Gemma-2B**: +1.15 improvement
- **Llama-3-8B**: +2.45 improvement

Key Findings:

- Larger models benefit more from MoS
- No universally optimal temperature τ
- Different rewards work better for different models
- EMA consistently helps performance

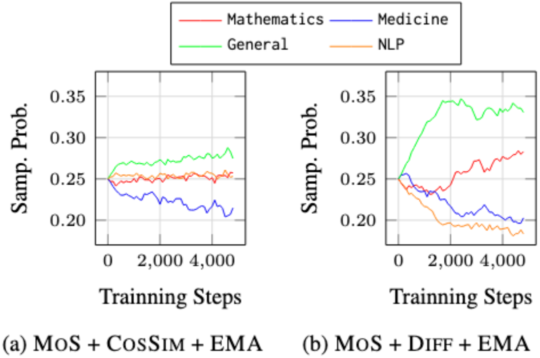
	MMLU	MT	ALL
Prop. ($\tau = 1$)	56.78	6.52	60.97
Temp. ($\tau = 10$)	56.17	6.66	61.40
Uni. ($\tau = \infty$)	55.72	6.63	60.99
MultiDDS	56.65	6.69	61.77
MultiUAT	55.66	6.67	61.18
MoS + cos	56.95	6.80	62.49
MoS + cos + EMA	$\underline{58.08}$	**6.96**	**63.85**
MoS + diff	57.93	6.81	63.00
MoS + diff + EMA	**58.34**	$\underline{6.82}$	$\underline{63.26}$

Table: Results on MMLU and MT-Bench given by Llama-3-8B. Best results in **bold**, second-best $\underline{\text{underlined}}$.

Analysis: MoS Adapts Data Usage Dynamically

Dynamic Sampling Behavior:

- Sampling probabilities evolve over training
- Reflects changing model needs
- Balances skill development



(a) MoS + CosSim + EMA (b) MoS + Diff + EMA

Figure: Sampling probabilities for each dataset over training steps. MoS adjusts focus dynamically.

Analysis: MoS is Robust to Sampling Priors

Initialization Sensitivity:

- MoS starts with uniform sampling ($\tau = \infty$)
- What if we start with different priors?
- **Key Finding**: MoS consistently outperforms best heuristic baseline regardless of initialization

Robustness Analysis:

- All MoS variants beat Temperature ($\tau = 10$) baseline
- Proper prior selection can further enhance performance
- **MoS is robust and effective**

	Prior τ	MMLU	MT	ALL
Heuristic	10	56.17	6.66	61.40
MultiDDS	1	56.65	6.69	61.77
	10	56.88	6.58	61.34
	∞	55.66	6.67	61.18
MoS	1	56.51	6.81	62.29
	10	58.22	**6.91**	**63.66**
	∞	**58.34**	6.82	63.26

Table: MoS performance with different sampling priors using Llama-3-8B. All variants outperform the best heuristic baseline.

Takeaway: MoS learns to adapt regardless of how you start!

Analysis: MoS is Compatible with Data Selection Methods

Combining MoS with Instance Selection:

- Use Instruction-Following Difficulty (IFD) to select top 10% instances
- Apply MoS dynamic rebalancing on selected data
- **Best of both worlds**: Quality selection + dynamic optimization

Complementary Effects:

- Static selection improves data quality
- MoS optimizes usage of selected data
- **Complementary approaches** enhance final performance

	MMLU	MT	ALL
Random			
Temp. ($\tau = 10$)	54.89	6.63	60.62
MoS	55.21	6.72	61.15
IFD Selection			
Temp. ($\tau = 10$)	55.13	6.69	61.02
MoS	**56.43**	**6.77**	**62.05**

Table: Combining MoS with instance selection (IFD) further improves performance using Llama-3-8B.

Key Insight: Static selection and dynamic rebalancing address different aspects of data optimization!

MoSpec: Fine-tuning from Generalist to Specialist

The Specialization Challenge:

- Large general-purpose models are costly to deploy
- Many applications need only narrow functionalities
- Smaller specialized models often outperform larger generalist ones

MoSpec Approach:

- Harnesses diverse datasets to enhance target task performance
- Assigns higher rewards to target domain (e.g., mathematics)
- Learns optimal dataset distribution for specific capabilities

Example: Math Specialization

- Target: Mathematics dataset
- Supporting: General, Medicine, NLP datasets
- **MoSpec + cosine**: Compute similarity between Math and other datasets
- **MoSpec + diff**: Double reward for Math dataset

Key Insight: *SFT datasets from other domains are beneficial for the target task, especially when target dataset is incomplete*

MoSpec Results: Math Specialization Performance

Experimental Setup:

- **Target**: Math specialization
- **Baselines**:
  - Temp. ($\tau = 10$)
  - MathLlama (trained only on Math)
- **Evaluation**: GSM8K, MATH, MMLU-math (M-math) benchmarks

Key Findings:

- **MathLlama performs worst**
- **Other datasets are beneficial**
- **MoSpec learns optimal mixing** for specialization

	GSM8K	MATH	M-math	ALL
Generalist				
Temp. ($\tau = 10$)	49.62	9.54	28.36	29.17
MoS + cos + EMA	50.40	9.78	27.60	29.26
MoS + diff + EMA	49.58	10.26	**32.81**	30.88
Math Specialist				
MathLlama	41.02	9.76	30.34	27.04
MoSpec + cos + EMA	51.10	10.64	30.16	30.63
MoSpec + diff + EMA	**52.10**	**11.40**	32.24	**31.91**

Table: Math specialization results. MoSpec outperforms both generalist models and math-only training.

+4.87 improvement over math-only training!

MoSpec Results: Sampling Behavior Analysis

Dynamic Data Usage:

- MoSpec adjusts dataset sampling over training
- Increases focus on target domain (Math)
- Leverages supporting datasets effectively

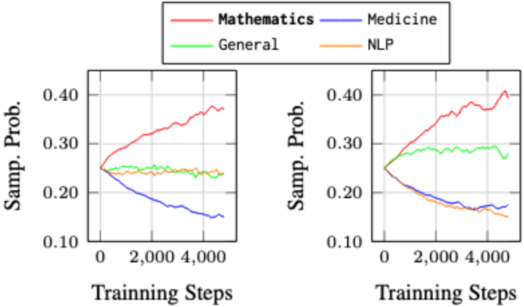


Figure: Sampling probabilities during Math specialization. **Left**: MoSpec + cos + EMA; **Right**: MoSpec + diff + EMA. Both increase focus on Math over time.

Summary of Contributions

GraphFilter: Principled Static Selection

- Novel set cover formulation for data selection
- Bipartite graph representation balancing quality × diversity
- Consistent improvements across models and benchmarks
- Computationally efficient and scalable

MoS: Intelligent Dynamic Optimization

- Model-agnostic RL framework for data rebalancing
- Adaptive skill development during fine-tuning
- Substantial performance improvements
- MoSpec extension for task specialization

Comprehensive solution covering the entire data optimization pipeline

Thank You

Questions & Discussion

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