Comparing the LMC Complexity of Neural Networks with their Generalization Capability

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Outline

Introduction

Context: The Era of Large Language Models

- **Transformers (2017)**:
  - Introduced by Vaswani et al. [12].
  - Enabled massive parallelization, sparking a "gold rush" in ML.
- **Rapid Adoption**:
  - GPT-3.5 (ChatGPT) became the fastest-growing consumer app in history (2022) [11].
  - Triggered massive investment from Tech Giants (Google, Microsoft, Meta).

The Scaling Paradigm

- **Scaling Laws by Kaplan et al., 2020** [7]:
  - Performance depends strongly on scale:
    - N: Number of Parameters.
    - D: Dataset Size.
    - C: Amount of Compute.
  - Performance depends weakly on shape (depth vs width).
- **Power Laws**:
  - $L(N) \approx (N_c/N)^{\alpha}$
  - **Implication**: Exponential increase in resources is required for constant linear gains in performance.

Problem Statement

- **Diminishing Returns**:
  - Recent models show marginal gains despite massive cost increases.
  - "Data Wall": Running out of high-quality internet data.
- **The Challenge**:
  - Relying solely on scaling (N, D, C) is becoming unsustainable.
  - Need for alternative approaches to improve efficiency.

Motivation & Proposed Solution

- **Two Approaches**:
  1. **Brute Force**: Continue scaling (Current Industry Standard).
  2. **Understanding**: Analyze the learning process to engineer better architectures.
- **Our Focus**:
  - Investigate **LMC Statistical Complexity** [8].
  - A metric combining **Disequilibrium** (Order) and **Entropy** (Randomness).
  - Hypothesis: It might help creating a better model by relating generalization performance and its distribution.

Thesis and Objectives

Work Thesis

"There exists a relationship between model complexity and its generalization capability." (Murta Junior, 2025)

Main Objective:

- Validate the existence of a meaningful relationship between neural network weight complexity and generalization performance.

Secondary Objectives:

- Explore the influence of **Parameter Count**.
- Analyze the impact of **Weight Types** (Bias, Norm, Embedding).
- Determine the effect of **Filtering** outliers.

Methodology

Experimental Setup

- **Hardware Constraints**:
  - **RAM**: 512GB DDR4 (Critical for loading large models).
  - **GPU**: NVIDIA Quadro P5000 (16GB).
  - **CPU**: 2x Intel Xeon Gold 6130 (64 threads).
- **Software Stack**:
  - Python 3.12, PyTorch 2.8, Transformers 4.56.
  - Models loaded in **Main Memory (CPU)** cast to `float32`.

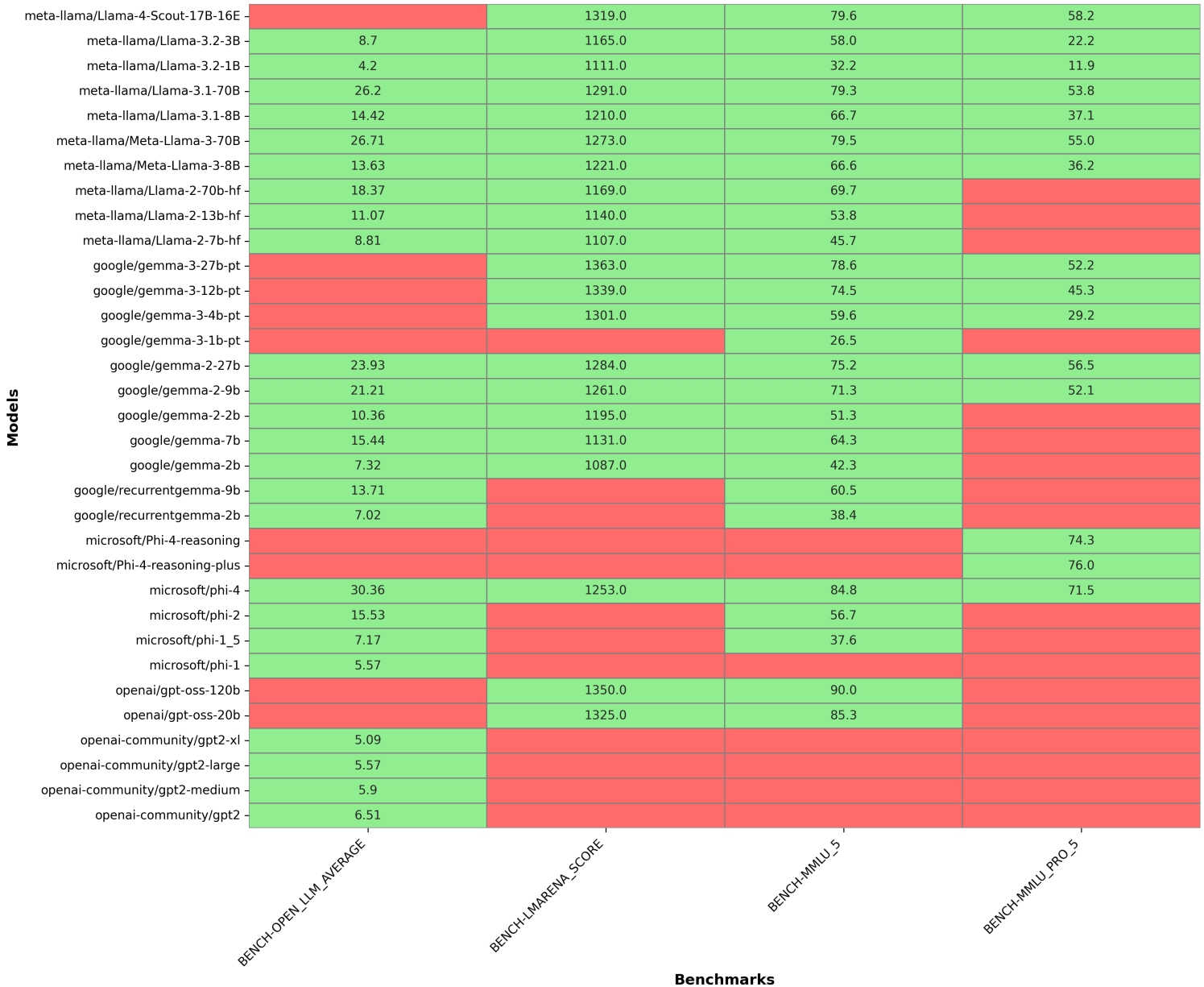
Model Selection Strategy

- **Source**: Hugging Face (Open Weights) [14, 2].
- **Criteria**:
  - Must be available on Hugging Face (official company account).
  - Transformer-based language model.
  - Open weights (including gated access).
  - Text-only (no multimodal inputs).
  - Base model (no fine-tunes).
  - Parameter count < 150 Billion (Hardware limit).
  - Supported by `AutoModel` utility.
  - Has benchmark results available.
- **Selected Models (35 Total)**:
  - **Meta**: Llama 2, 3, 3.1, 3.2, 4 (Scout).
  - **Google**: Gemma 1, 2, 3, RecurrentGemma.
  - **Microsoft**: Phi-1, 1.5, 2, 4 (Mini/Reasoning).
  - **OpenAI**: GPT-2 (Small to XL), GPT-OSS (120B, 20B).

Generalization Capability: Benchmarks

- **Why Benchmarks?**:
  - Proxies for Test Loss (Performance) [10].
  - Training from scratch/Test loss unavailable for all models.
- **Selection Criteria**:
  - **Relevance**: Widely recognized (e.g., MMLU).
  - **Generality**: Covers range of tasks.
  - **Availability**: Results publicly available.
- **Selected Benchmarks**:
  - **MMLU**: 57 tasks, STEM/Humanities. Standard for LLMs [6].
  - **MMLU-Pro**: Enhanced MMLU, harder reasoning [13].
  - **OpenLLM**: Aggregated score of multiple datasets [9].
  - **LMArena**: Crowdsourced Elo ratings based on human preference [1].

Benchmark Availability



LMC Statistical Complexity

Definition

$$C_{LMC} = H \times D$$

- **Disequilibrium (D)**:
  - Measures distance from uniform distribution ("Order").
  - $D = \sum_{i=1}^{n} (p_i - \frac{1}{n})^2$
- **Shannon Entropy (H)**:
  - Measures uncertainty or randomness.
  - $H = -K \sum_{i=1}^{n} p_i \log p_i$

LMC Statistical Complexity Extraction

1. **Weight Extraction**:
   - Flatten tensors from `named_parameters()`.
   - Categorize: Bias, Norm, Embedding, Other.
   - Tested combinations: Power set of categories (15 combinations).
2. **Filtering**:
   - Remove outliers.
   - Range: $\mu \pm \sigma_{\text{filter}} \cdot \sigma$.
   - Tested $\sigma_{\text{filter}} \in \{0.125, \ldots, 20, 40(\text{unfiltered})\}$.
3. **Discretization (Histogram)**:
   - **Freedman-Diaconis Rule** [4]: $h = \frac{2 \times IQR}{N^{1/3}}$.
   - Adapts to distribution spread and sample size (N).
4. **Calculate LMC**:
   - Compute $C_{LMC} = H \times D$ using the histogram probabilities.

Analysis Dimensions: Dataset

- **Dataset Construction**:
  - **Models**: 35 Selected Models.
  - **Weight Combinations**: 15 (Power set of Bias, Norm, Embedding, Other).
  - **Filtering Settings**: 11 (σ_{filter} values).
  - **Total Data Points**: $35 \times 15 \times 11 \approx 5775$.
- **Tuple Structure**:
  - (Model, Params, Weight-Type, Filter, Complexity, Bins, Benchmarks).

Analysis Dimensions: Statistical Tools

- **Correlation Analysis**:
  - **Pearson Correlation (r)**: Measure linear relationship.
  - **T-tests**: Determine statistical significance ($p < 0.05$).
- **Regression Analysis**:
  - **Linear Regression**: $y = ax + b$.
  - **Free Regression**: Curve fitting (Linear, Quadratic, Exponential, Logarithmic, Power).
  - R^2 **Score**: Measure goodness of fit.

Results

Data Extraction Statistics

- **Scale**:
  - Total Parameters Processed: **652.8 Billion**.
  - Compute Time: **228 hours** ($\approx$ 9.5 days).
- **Dataset**:
  - Expected: 5775 data points.
  - Actual: **5511 data points**.
  - **Exclusions**: Models exceeding 1 billion bins (unfiltered) or containing NaN/Infinite values (numerical errors).

Filter Dimension: Histogram Bins (Average)

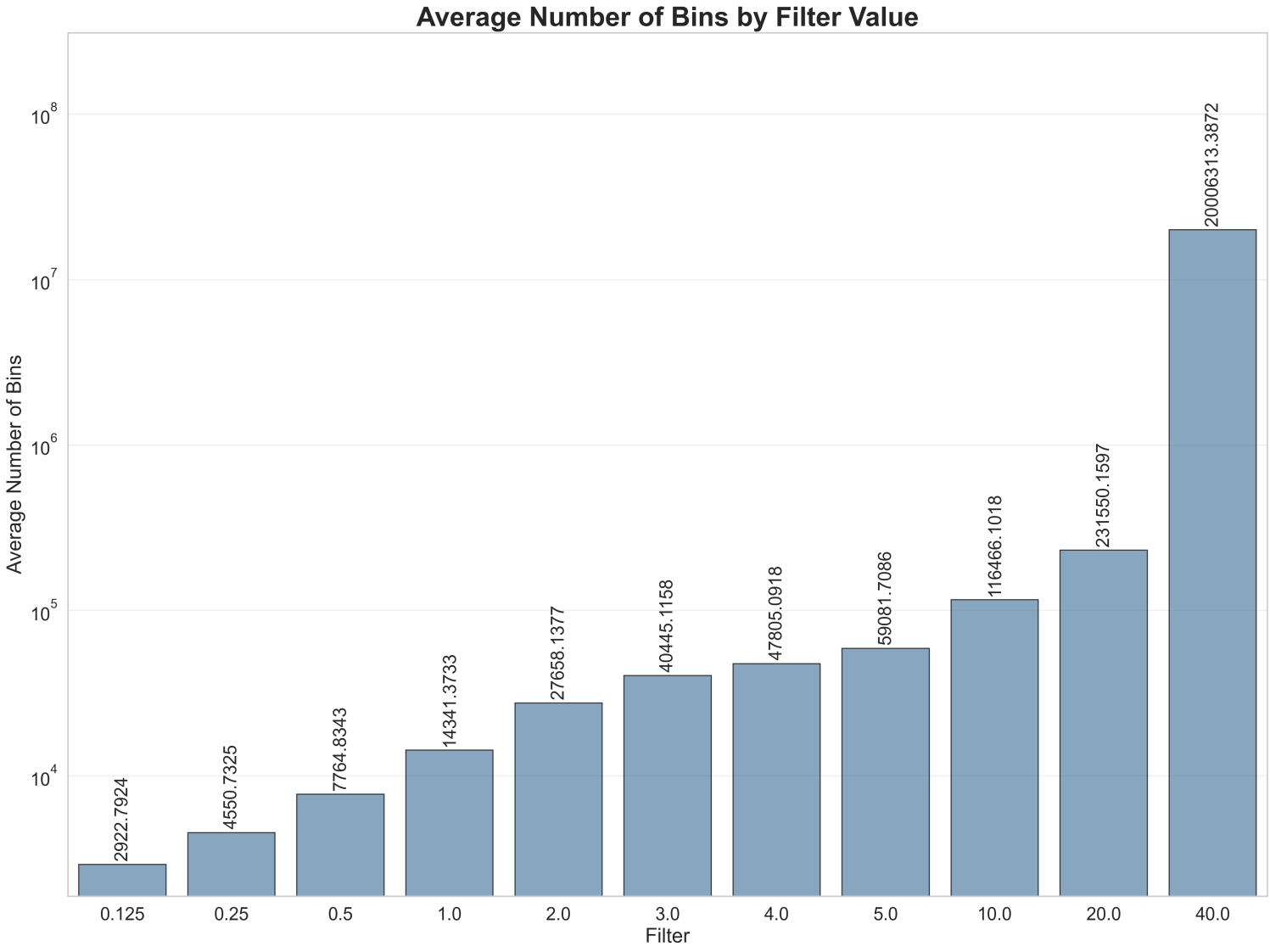


Figure: Average number of histogram bins per filtering setting.

Filter Dimension: Histogram Bins (Maximum)

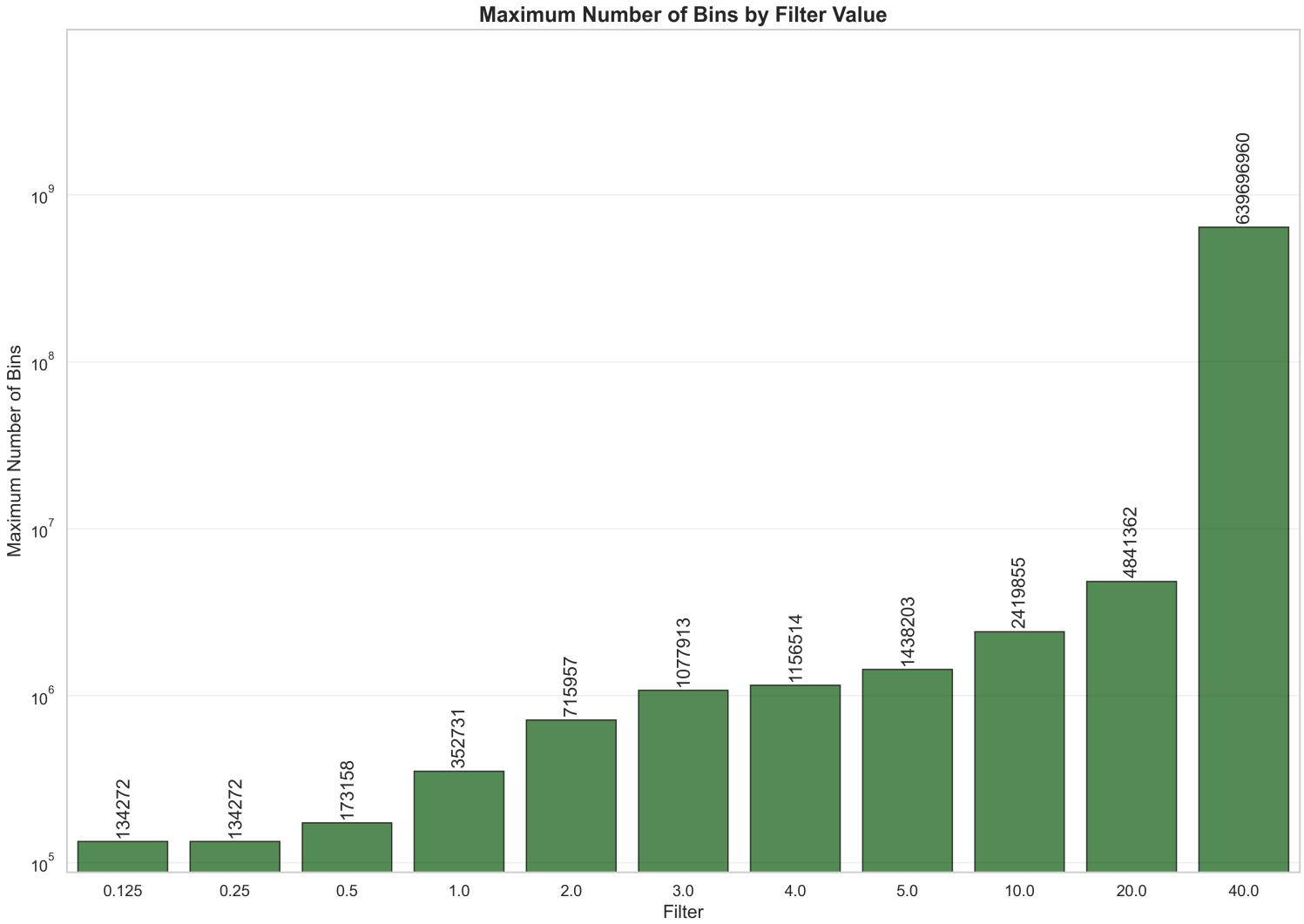


Figure: Maximum number of histogram bins per filtering setting.

- Similar trend to average bins

Filter Dimension: Histogram Bins Regression

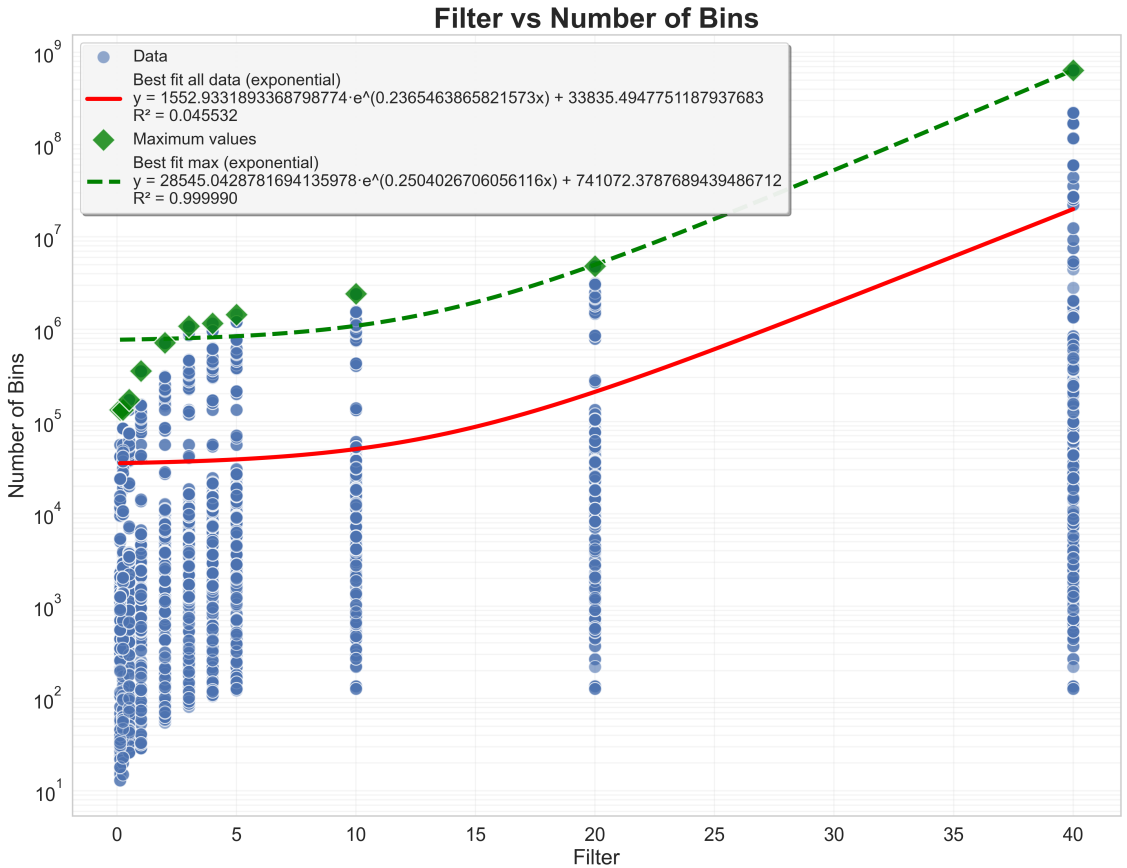


Figure: Regression of histogram bins per filtering setting.

- Maximum bins follow strict exponential trend ($R^2 = 0.999$).
- Average bins show higher variability ($R^2 = 0.045$).

Filter Dimension: Complexity (Average)

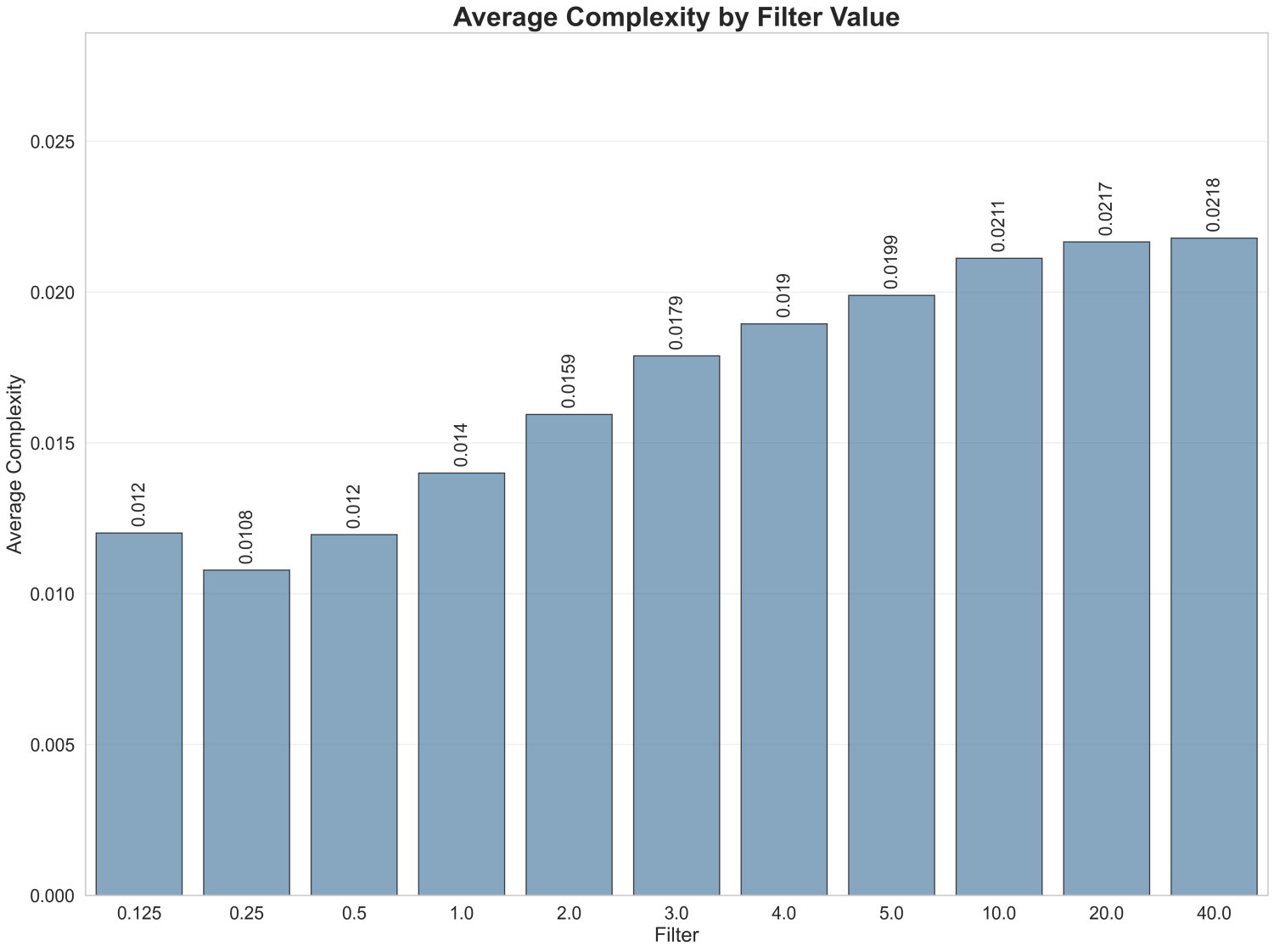


Figure: Average complexity per filtering setting.

Filter Dimension: Complexity (Maximum)

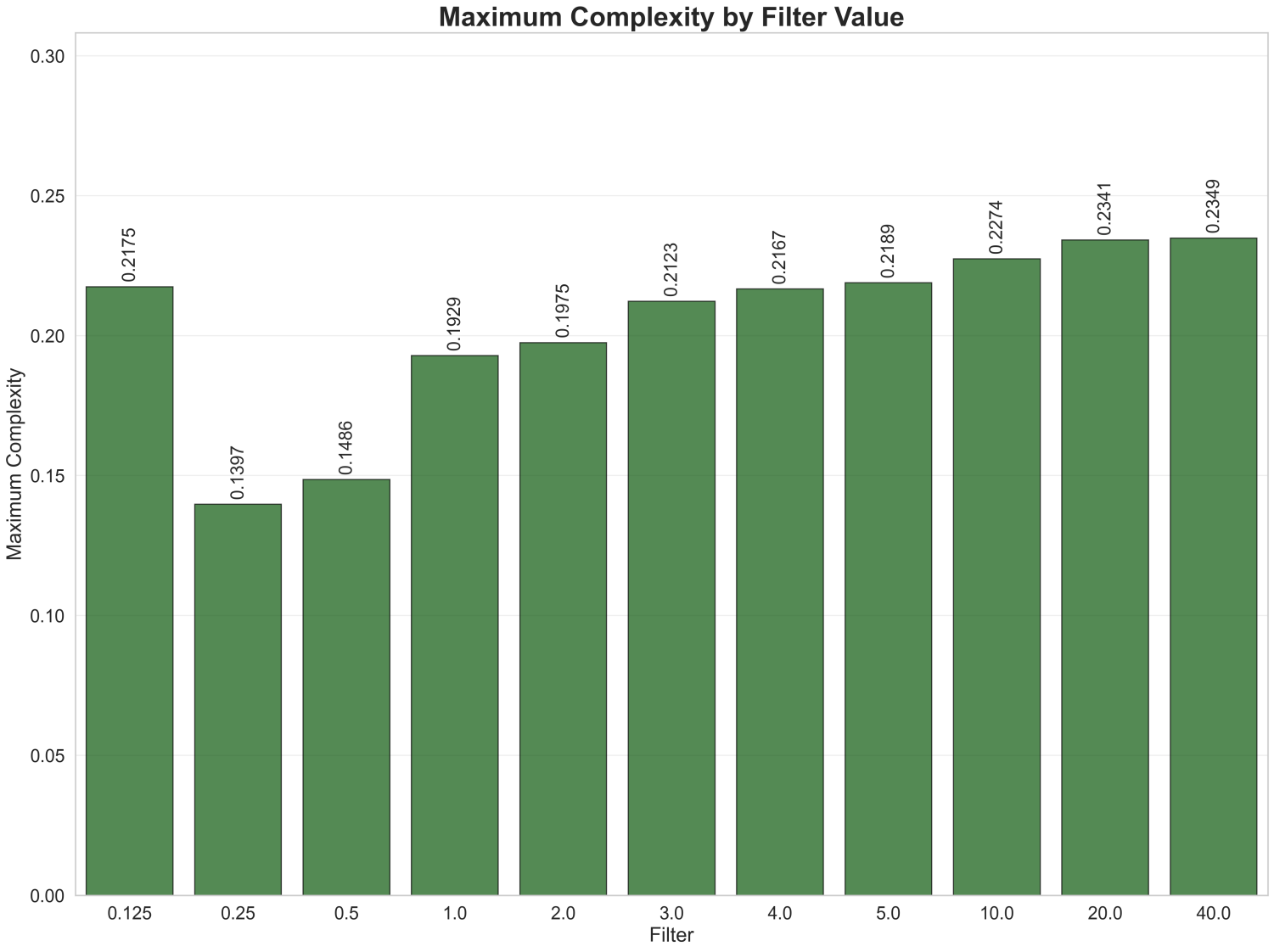


Figure: Maximum complexity per filtering setting.

Filter Dimension: Complexity Regression

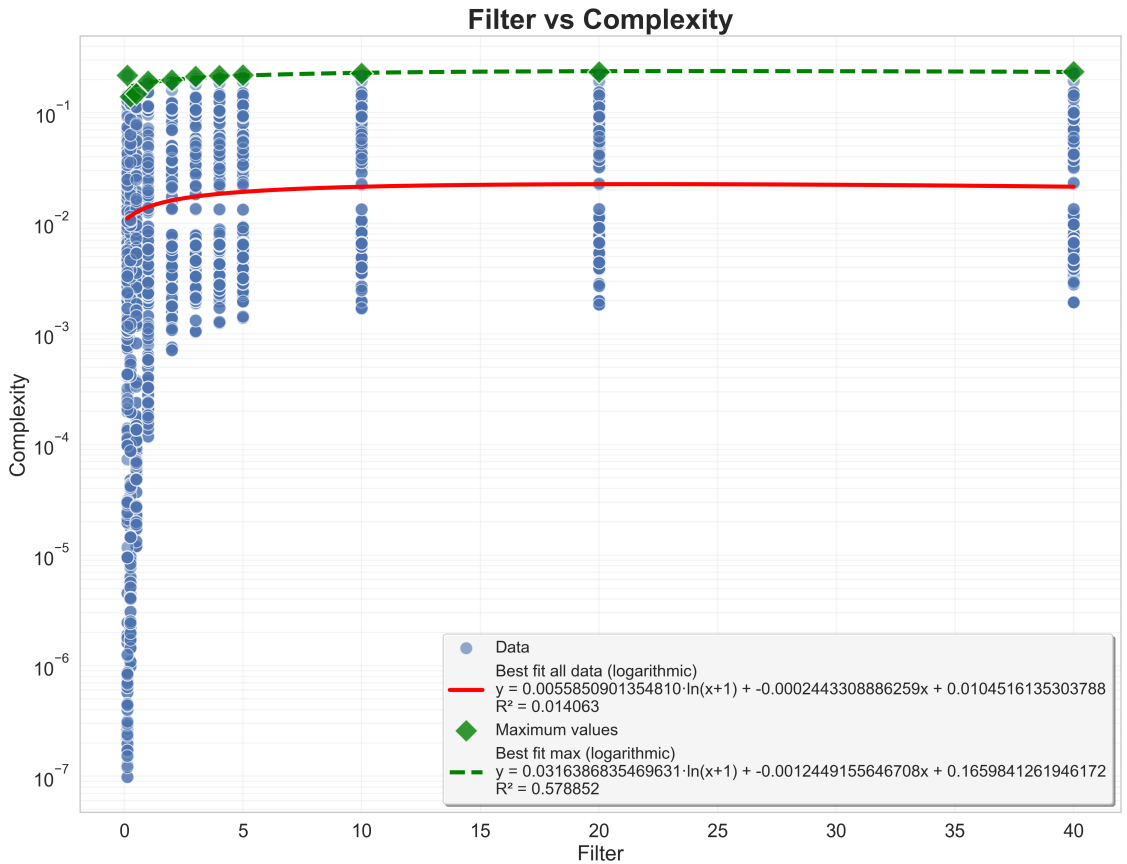


Figure: Regression of complexity per filtering setting.

- Both follow logarithmic trend.
- Maximum fit ($R^2 = 0.578$) is better than average fit ($R^2 = 0.014$).

Filter Selection

Decision: **20** σ chosen.

- Significant bin reduction.
- Complexity values almost identical to unfiltered data.

Weight-Type Dimension: Average Complexity

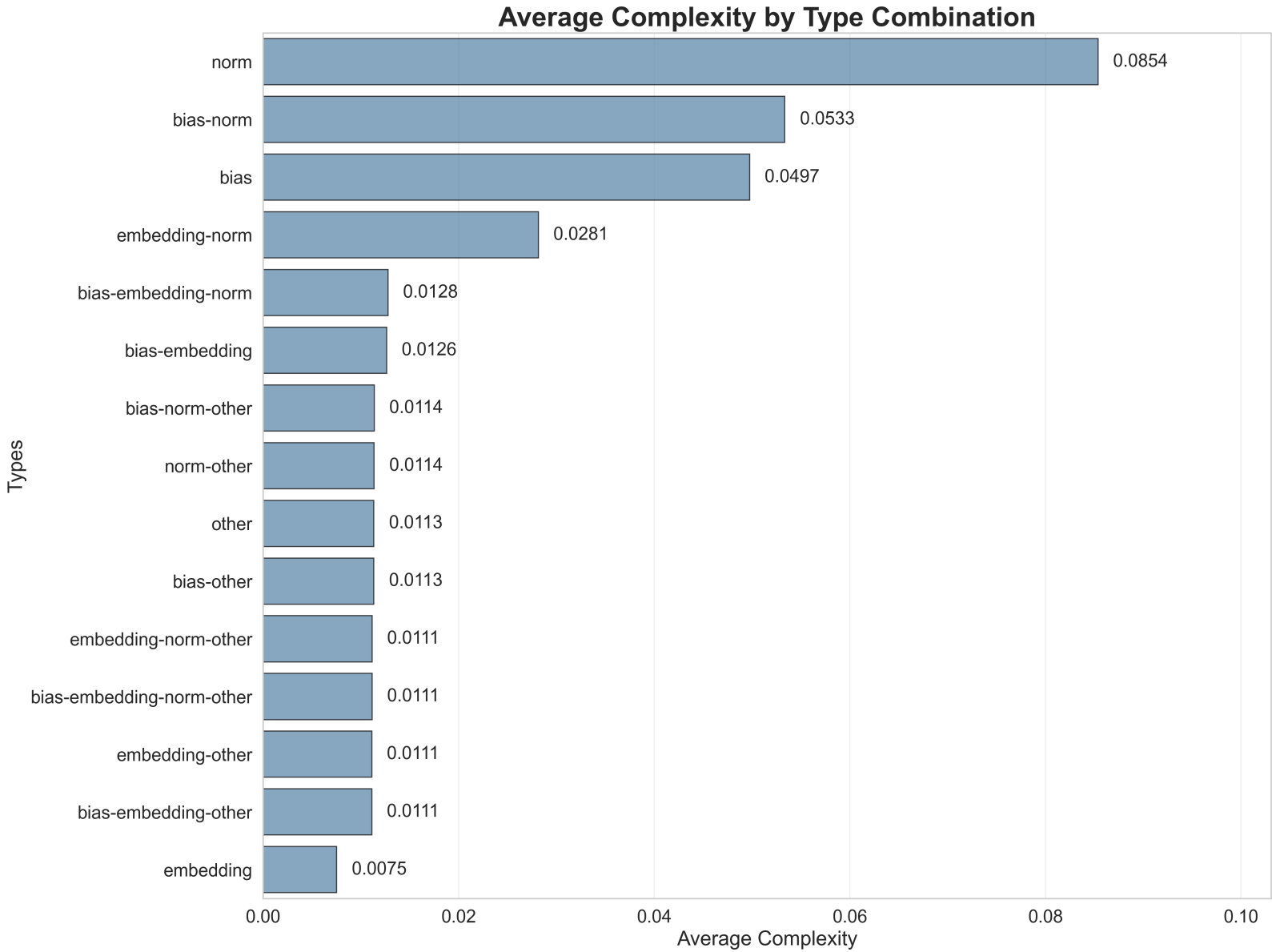


Figure: Average complexity per weight-type combination.

Weight-Type Dimension: Maximum Complexity

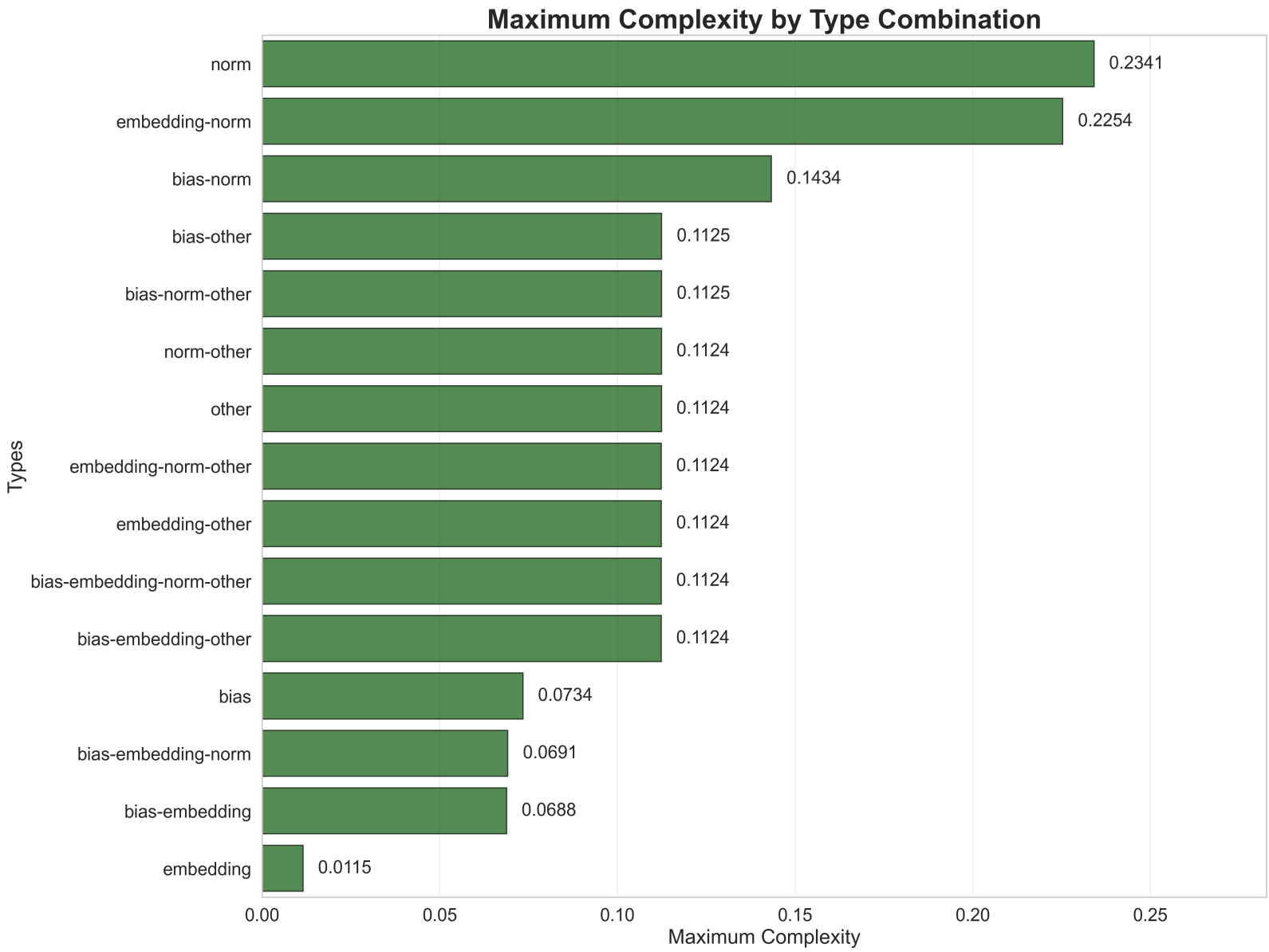


Figure: Maximum complexity per weight-type combination.

Weight-Type Selection

Decision: Use **Bias + Norm + Other** (No Embeddings).

- Embeddings have very low complexity (near zero).

Complexity vs. Number of Parameters

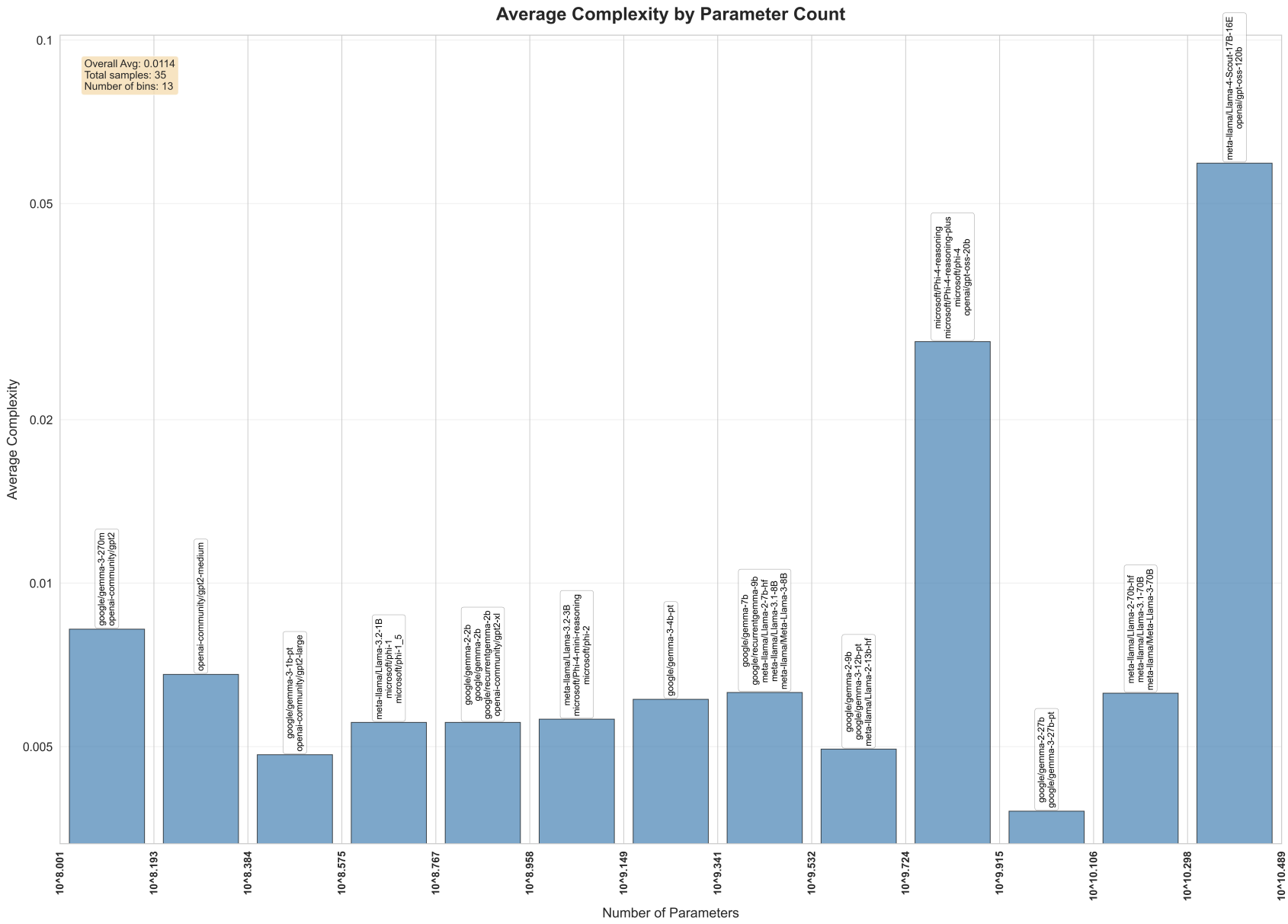


Figure: Average complexity vs number of parameters

Complexity vs. Number of Bins

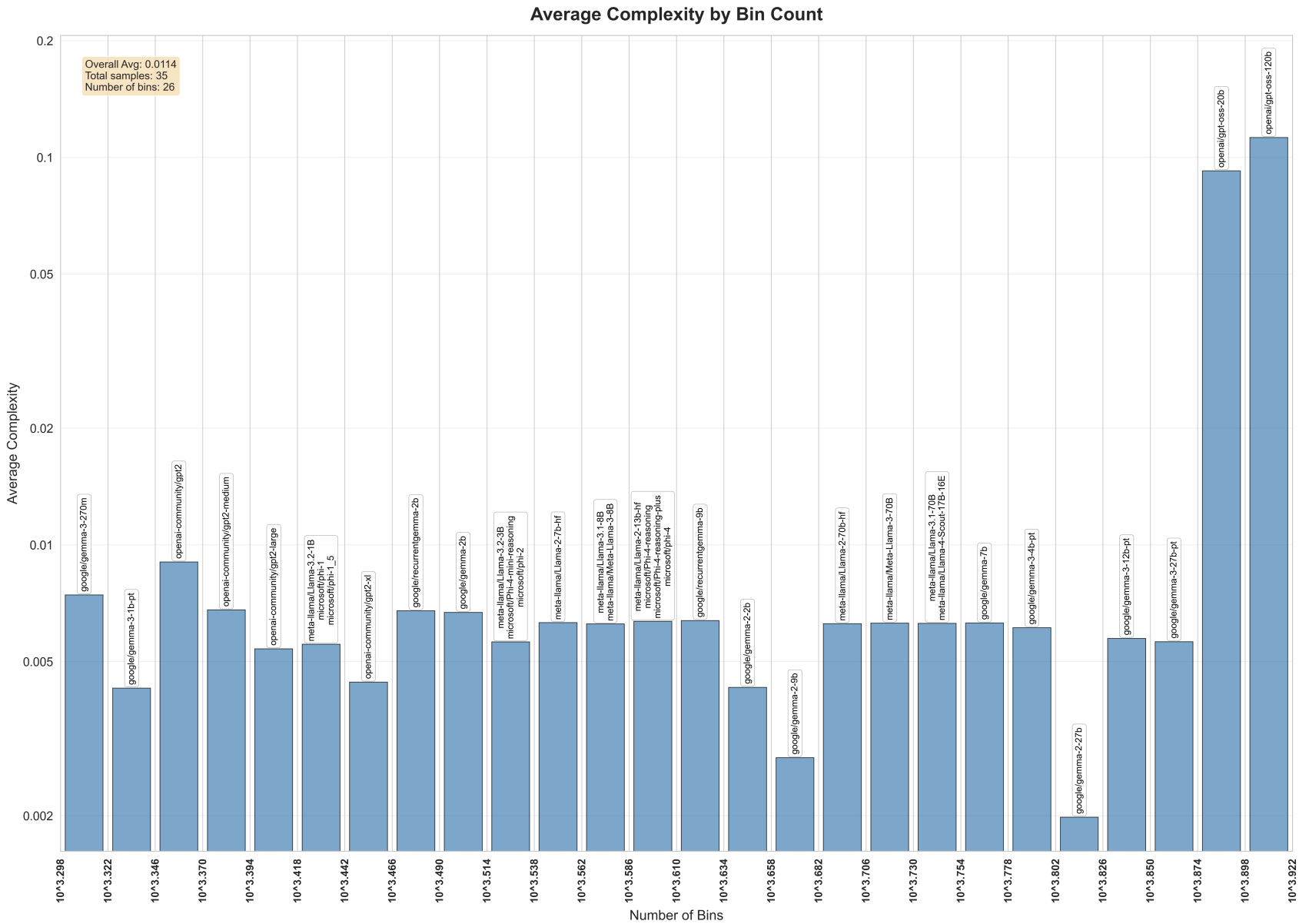


Figure: Average complexity vs number of histogram bins

Control: Parameters vs. Benchmarks (Correlation)

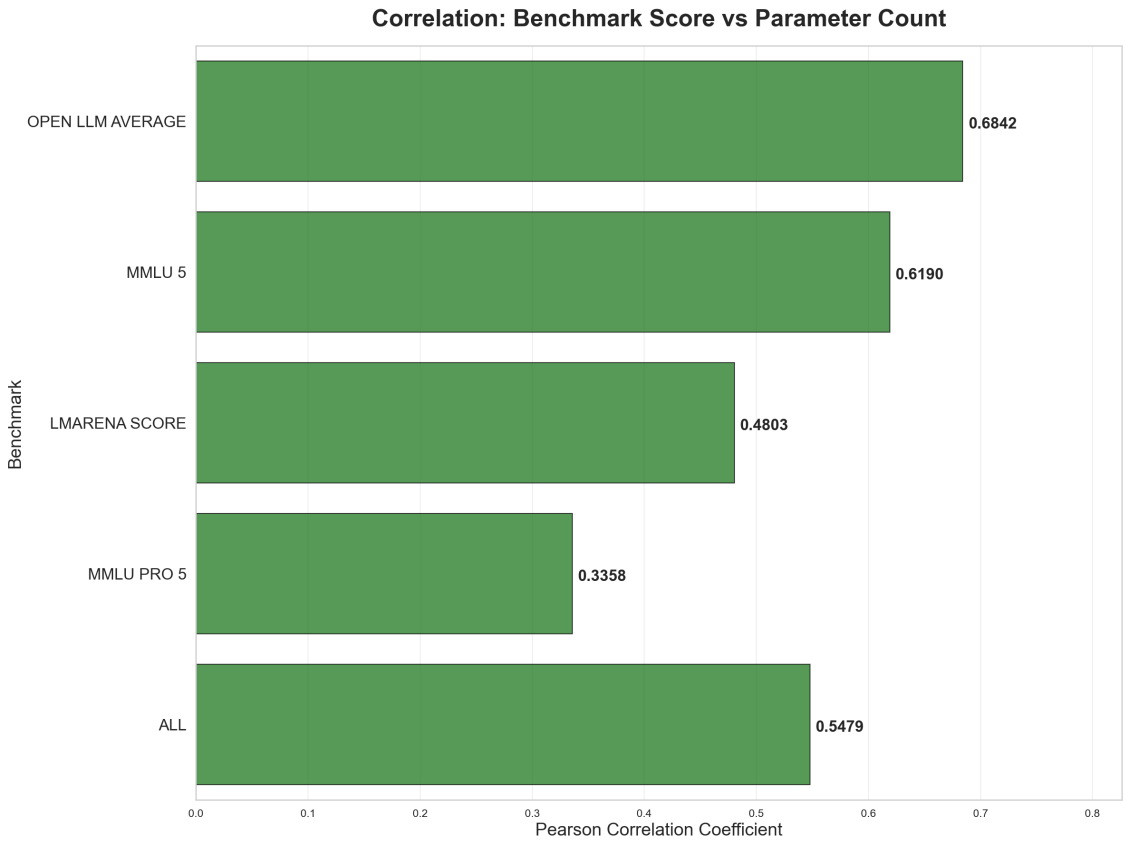


Figure: Pearson correlation for parameter count vs benchmark performance [3].

- All benchmarks show **positive correlation**.
- Validates methodology and scaling laws.

Control: Parameters vs. Benchmarks (R^2)

Figure: R^2 values for parameter count vs benchmark performance.

- Low R^2 values indicate non-linear relationship.
- Consistent with Power Laws.

Complexity vs. Benchmarks: Correlation

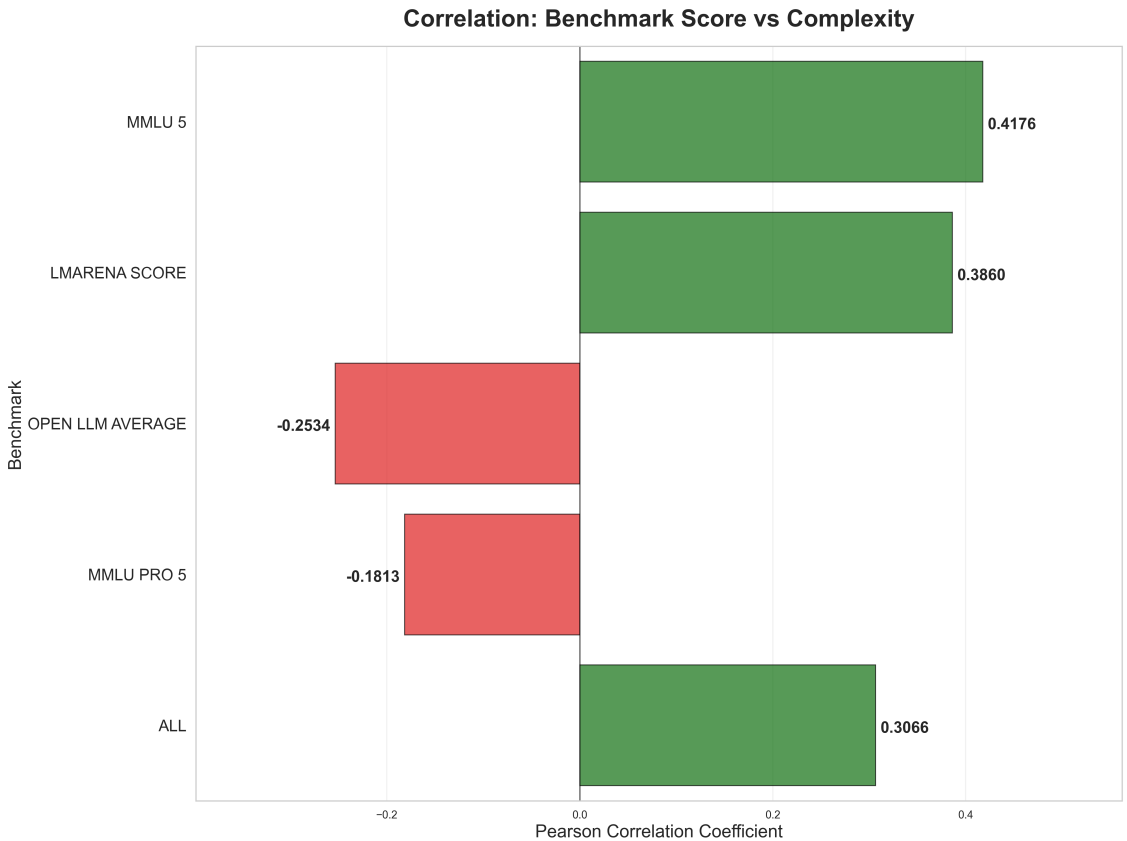


Figure: Pearson correlation for Complexity vs benchmark performance.

- **Inconsistent**: Positive (MMLU, LMArena) vs Negative (MMLU-Pro, OpenLLM).
- Lower correlations than Control.

Complexity vs. Benchmarks: R^2

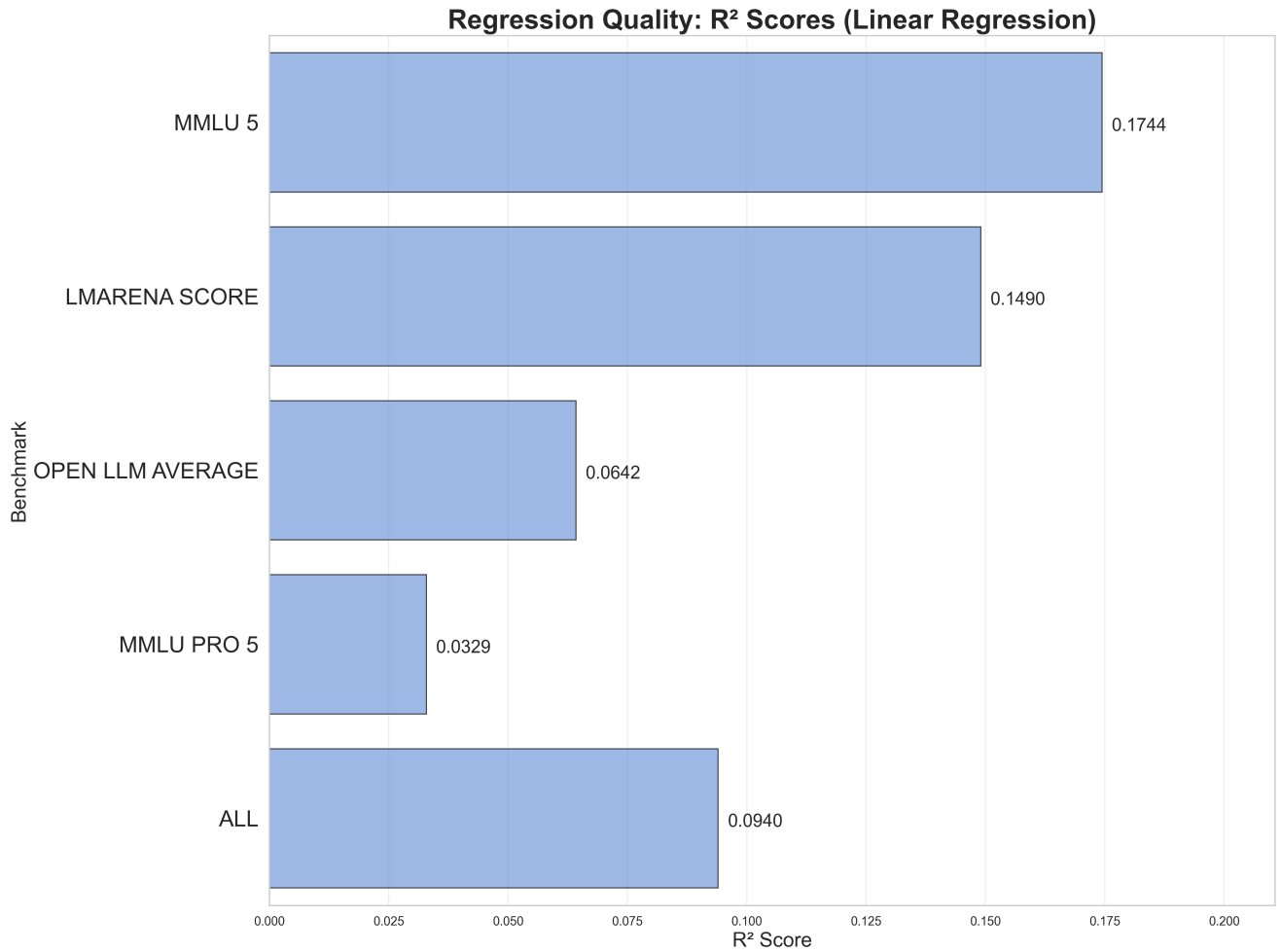


Figure: R^2 values for complexity vs benchmark performance.

- Very low R^2 values.
- Indicates weak predictive power.

Statistical Significance

Benchmark	r	n	**p-value**	**Sig. (< 0.05)**
LMArena	0.3860	21	0.0839	No
MMLU	**0.4176**	**26**	**0.0338**	**Yes**
MMLU-Pro	-0.1813	15	0.5179	No
OpenLLM	-0.2534	24	0.2322	No
All (Aggregated)	**0.3066**	**86**	**0.0041**	**Yes**

- **MMLU** and **Aggregated (All)** are significant (T-test [5]).
- Negative correlations are not significant.

Regression Analysis: LMArena

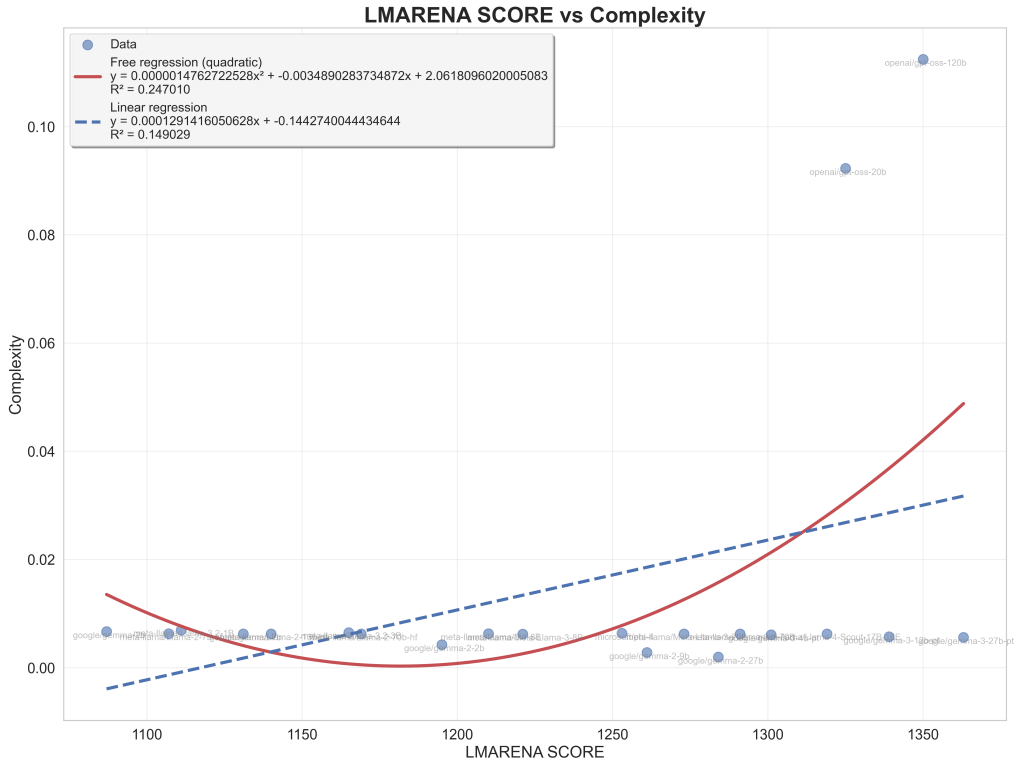


Figure: LMC complexity vs LMArena benchmark.

- Constant trend with outliers.
- Outliers (GPT-OSS) drive positive correlation.

Regression Analysis: MMLU

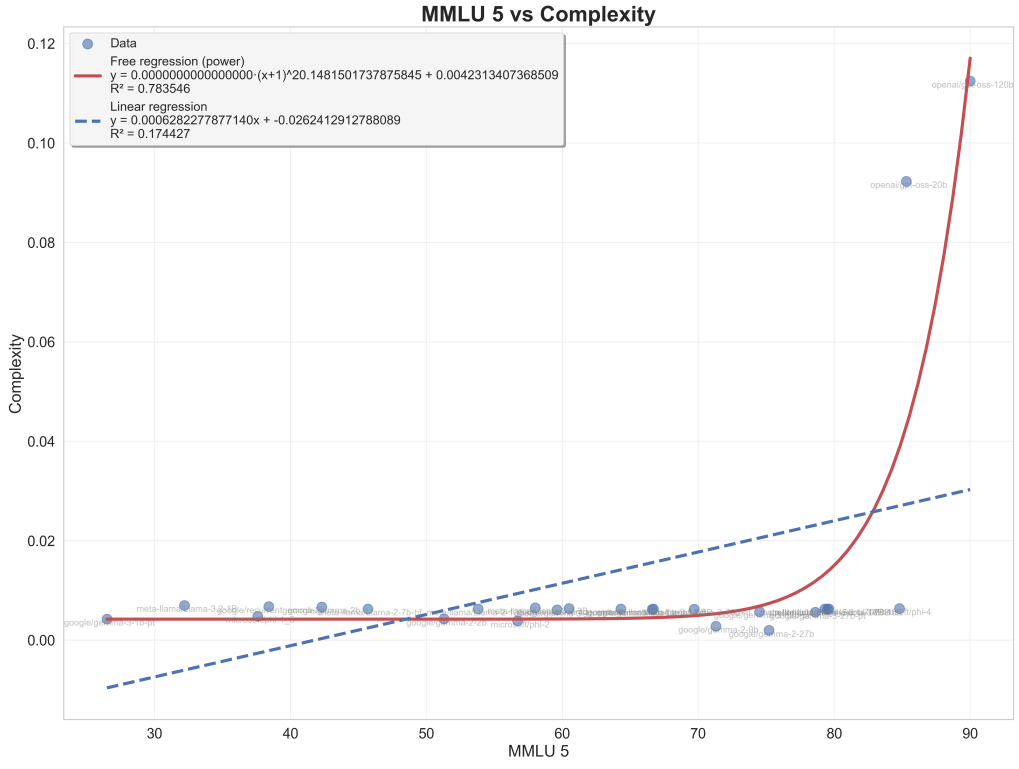


Figure: LMC complexity vs MMLU benchmark.

- Similar to LMArena.
- Exponential fit suggested, but driven by outliers.

Regression Analysis: MMLU-Pro

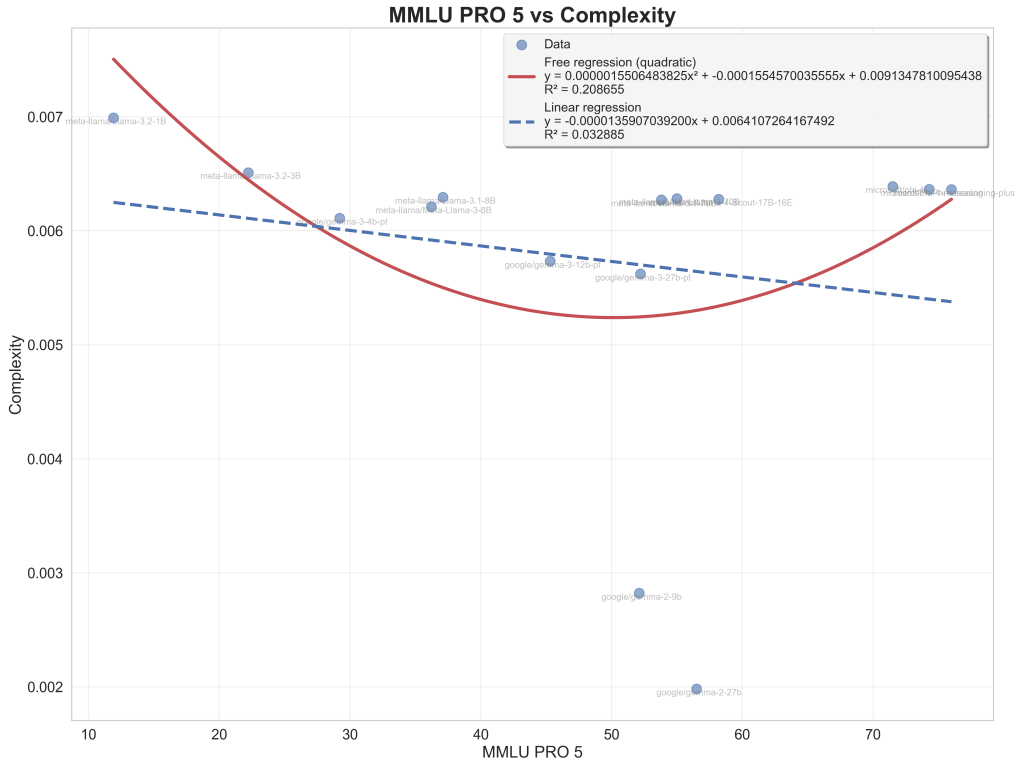


Figure: LMC complexity vs MMLU-Pro benchmark.

- Slight downward trend.
- Outliers (Gemma-2) drive negative correlation.

Regression Analysis: OpenLLM

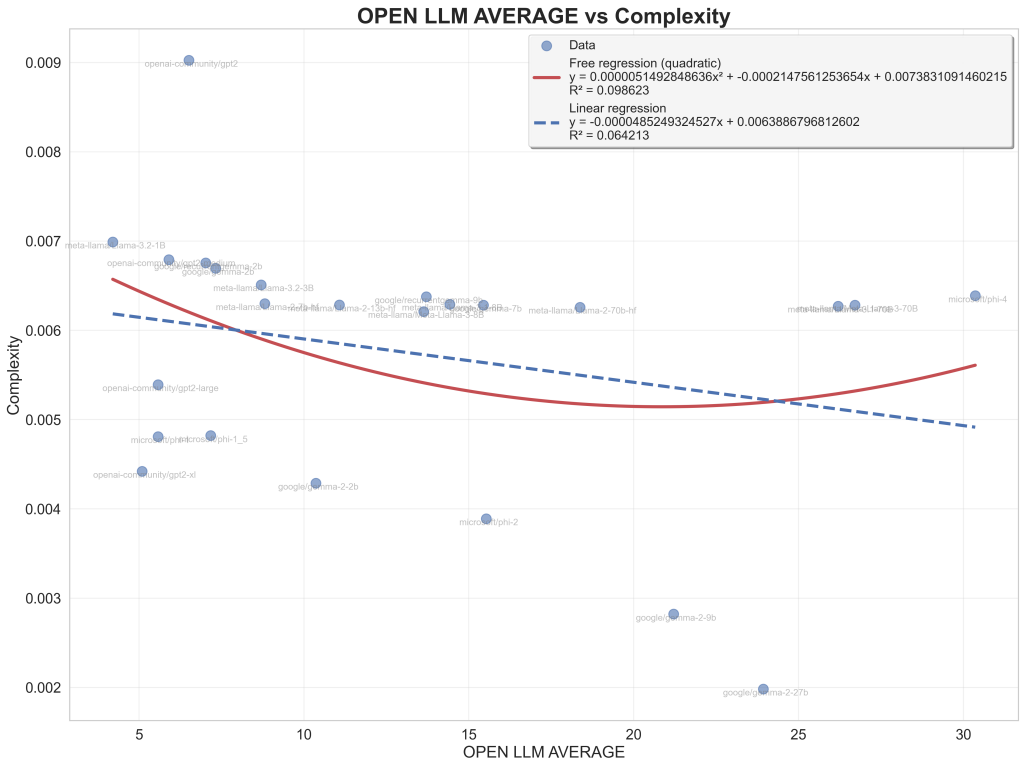


Figure: LMC complexity vs OpenLLM benchmark.

- **Dual Trend**: Upward (LLaMA, Phi-4) vs Downward (Gemma-2, Phi-1.5).

Regression Analysis: All Benchmarks

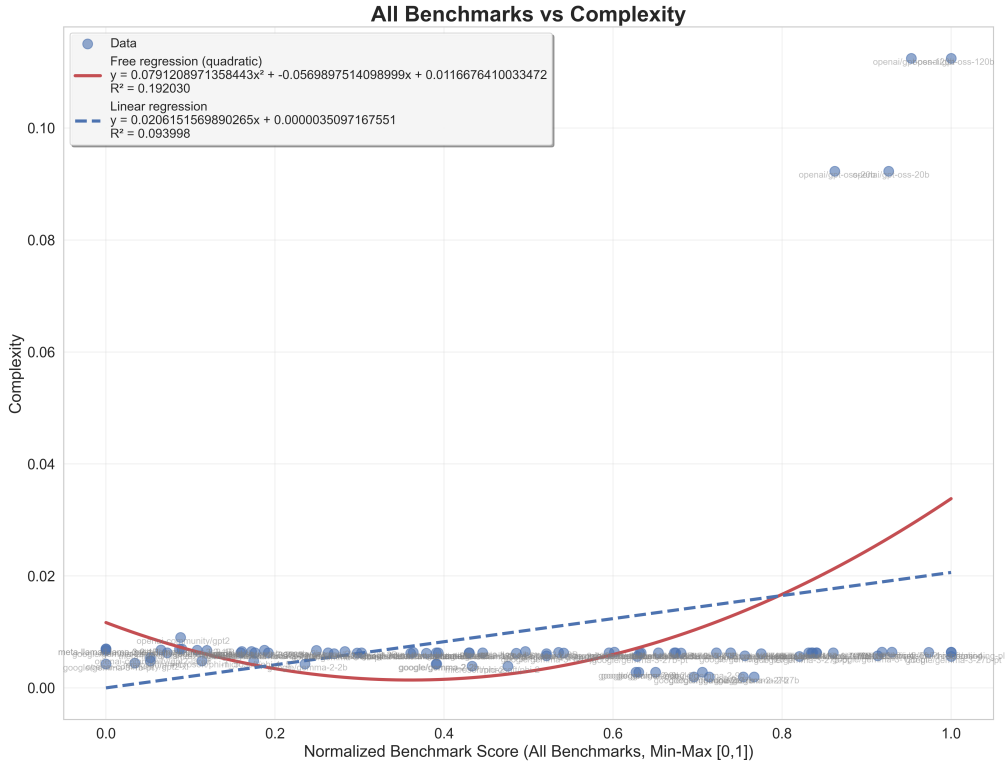


Figure: LMC complexity vs all benchmarks aggregated.

- Follows the "Constant + Outlier" pattern.
- Statistically significant positive correlation.

Top 20 Correlations

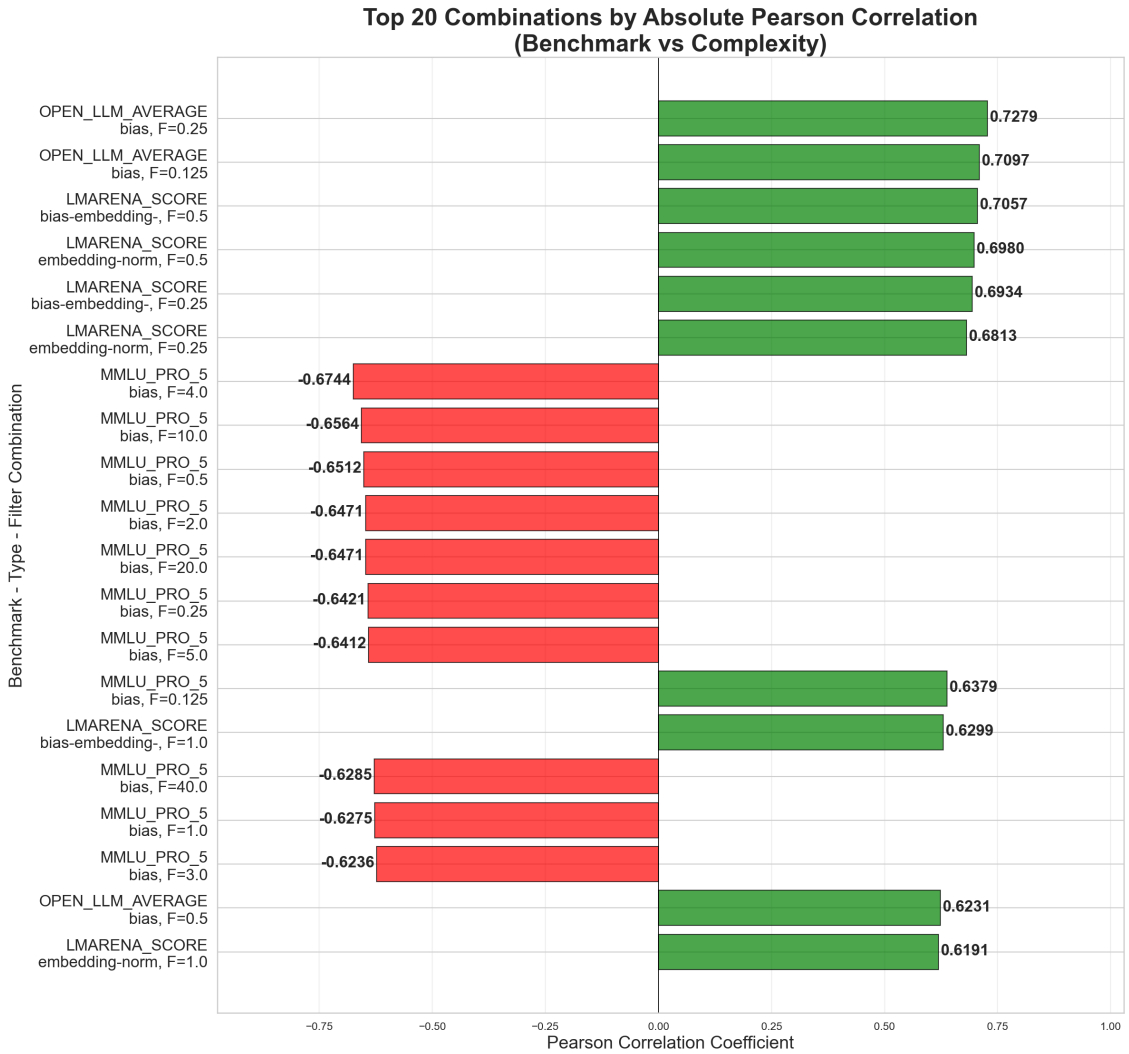


Figure: Top 20 configurations by Pearson correlation.

- Dominated by high filtering (0.25 σ).

Conclusion

Main Conclusion

Finding

A general correlation between LMC Complexity and Generalization Capability cannot be confirmed.

- While statistical significance was found in aggregated data, the relationship is inconsistent across individual benchmarks.
- The results suggest that LMC Complexity, in its current form, is not a reliable universal predictor of model performance.

Evidence Supporting the Hypothesis

- **Aggregated Significance**:
  - The aggregated dataset (**All**) showed a statistically significant positive correlation ($p < 0.05$).
- **Positive Bias**:
  - Positive correlations (e.g., MMLU) were stronger and more significant than negative ones.
- **Parameter Relation**:
  - Complexity tends to increase with parameter count, which is a known predictor of performance.

Evidence Against the Hypothesis

- **Outlier Dependence**:
  - Positive trends were heavily driven by specific outliers (e.g., GPT-OSS family).
  - Removing outliers often reduced correlations to near zero.
- **Inconsistency**:
  - Different benchmarks yielded contradictory results (Positive vs. Negative correlations).
  - Regression shapes varied widely (Constant, Linear, Dual-trend).
- **Predictive Power**:
  - Low R^2 values compared to the control (Parameter Count).

Future Work

1. **Controlled Training & Optimization**:
   - Train models from scratch to compare Test Loss vs. Complexity directly (Intra-Model Analysis).
   - Eliminates the noise and inconsistency of public benchmarks.
   - Investigate if maximizing LMC complexity improves performance.
2. **Filtering Refinement**:
   - Explore less aggressive filtering (e.g., 30 σ) and the complexity spike at 0.125 σ.
3. **Outlier Investigation**:
   - Investigate why the GPT-OSS family is an outlier for LMC complexity.
4. **Alternative Hypothesis**:
   - Complexity might measure "distance to performance ceiling" (Early Stopping Criterion).

Thank You!

Questions?

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