

# 000 001 002 003 004 005 006 007 008 009 010 011 012 BREAKING THE CORRELATION PLATEAU: ON THE OP- TIMIZATION AND CAPACITY LIMITS OF ATTENTION- BASED REGRESSORS

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## ABSTRACT

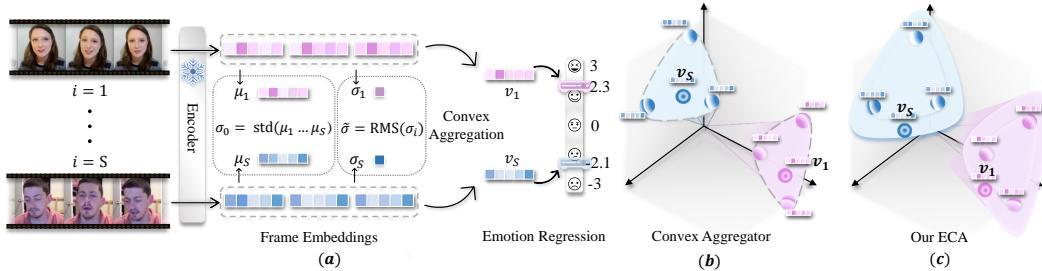
Attention-based regression models are often trained by jointly optimizing Mean Squared Error (MSE) loss and Pearson correlation coefficient (PCC) loss, emphasizing the magnitude of errors and the order or shape of targets, respectively. A common but poorly understood phenomenon during training is the *PCC plateau*: PCC stops improving early in training, even as MSE continues to decrease. We provide the first rigorous theoretical analysis of this behavior, revealing fundamental limitations in both optimization dynamics and model capacity. First, in regard to the flattened PCC curve, we uncover a critical conflict where lowering MSE (magnitude matching) can *paradoxically* suppress the PCC gradient (shape matching). This issue is exacerbated by the softmax attention mechanism, particularly when the data to be aggregated is highly homogeneous. Second, we identify a limitation in the model capacity: we derived a PCC improvement limit for *any* convex aggregator (including the softmax attention), showing that the convex hull of the inputs strictly bounds the achievable PCC gain. We demonstrate that data homogeneity intensifies both limitations. Motivated by these insights, we propose the Extrapolative Correlation Attention (ECA), which incorporates novel, theoretically-motivated mechanisms to improve the PCC optimization and extrapolate beyond the convex hull. Across diverse benchmarks, including challenging homogeneous data setting, ECA consistently breaks the PCC plateau, achieving significant improvements in correlation without compromising MSE performance.

## 1 INTRODUCTION

The attention mechanism is a powerful tool for regression tasks where each input sample comprises multiple elements, such as tokens or image patches, and the elements' embeddings are aggregated using attention mechanism to predict a continuous target (Lee et al., 2019; Martins et al., 2020; Born & Manica, 2023). This paradigm is widely used in areas like digital pathology, time-series prediction and emotional analysis (Jiang et al., 2023; Ni et al., 2023; Zhang et al., 2023). For example, in video-based sentiment analysis, the attention mechanism is used to aggregate frame embeddings within a video clip to predict emotion variables, such as sentiment intensity, arousal, and valence (Truong & Lauw, 2019; Xie et al., 2024).

Two characteristics are common in such applications. First, the in-sample data frequently exhibits **higher homogeneity** than cross-sample data. For example, in pathology images, nearby regions tend to share more similar tissue or cell types than distant regions. Likewise, in video-based sentiment analysis, frames from the same clip are more similar than frames from different clips. Second, the regression performance is not simply evaluated by **magnitude** (e.g., Mean Squared Error (MSE)) but also by **shape**—the relative ordering of predictions, measured by the Pearson Correlation Coefficient (PCC). In many settings, capturing the correct correlations matters more than predicting the exact values (Pandit & Schuller, 2019). For instance, in spatial transcriptomics, capturing the relative trend of gene expression (e.g., co-expression) is more informative than predicting exact magnitudes (Xiao et al., 2024). To emphasize shape while retaining magnitude performance, models are commonly trained with a joint loss function, such as  $\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{MSE}} + \lambda_{\text{PCC}}(1 - \rho)$  where  $\rho$  is the PCC and  $\lambda_{\text{PCC}}$  is a hyperparameter weight (Liu et al., 2022; Zhang et al., 2023; Zhu et al., 2025).

Figure 1: (a) Illustration of a video-based sentiment analysis example. A sample is considered homogeneous when its within-sample dispersion  $\tilde{\sigma}$  is below  $\sigma_0$ . (b) A convex attention yields an aggregated embedding inside the convex hull of the sample’s embeddings. (C) Our ECA extrapolates beyond the hull to amplify within-sample contrasts.



However, such joint training strategy applied to attention-based regression model frequently exhibits a puzzling *PCC plateau*, even with large PCC weight  $\lambda_{\text{PCC}}$ . As shown in Figure 2, the PCC curve's slope flattens early in training, failing to improve further even while the MSE continues to decrease. This empirical phenomenon is particularly severe with high in-sample homogeneity data. The underlying mechanisms driving this plateau remain unclear and it raises a critical question: why does the regression model fail to optimize the correlation effectively?

In this work, we provide the first theoretical investigation into this question, analyzing the limitations of standard attention from two distinct perspectives: **optimization dynamics** and **model capacity**.

**Limitation 1: Conflict in Optimization Dynamics.** Our analysis reveals a direct relation between the decrease of MSE and the flattening of the PCC curve in the attention-based regression model. Using a decomposition of MSE (Proposition 2.1), we show the following. Although training continues to reduce MSE by matching the predictions' mean and standard deviation, the gradient of the correlation term is paradoxically attenuated, flattening the PCC curve. This effect is amplified by *in-sample homogeneity*: when embeddings within a sample are similar, the within-sample dispersion term in the PCC gradient shrinks and further suppresses the magnitude of the gradient.

**Limitation 2: Model Capacity of Convex Aggregation.** Notice that softmax attention is a convex combination of element embeddings; we compare convex attention aggregation to mean-pooling aggregation and derive an upper bound on the achievable PCC gain (Theorem 2.2) depending on the radius of convex hull formed by the in-sample embeddings. Greater in-sample homogeneity will shrink the convex hull and tightens this bound, yielding a fundamental capacity limit for PCC gain.

**Extrapolative Correlation Attention.** Motivated by these theoretical insights, we propose Extrapolative Correlation Attention (ECA), a novel framework designed to overcome these limitations. To mitigate the optimization conflict in Limitation 1, ECA introduces a Dispersion-Normalized PCC loss to counteracts the attenuation effect, restoring the magnitude of correlation gradient. We also employ Dispersion-Aware Temperature Softmax to prevent the gradient collapse and near-uniform attention distribution under in-sample homogeneity. To address Limitation 2, ECA introduces Scaled Residual Aggregation, which allows the model to extrapolate beyond the convex hull, mitigating the PCC gain limitation induced by convex aggregation mechanism.

**Contributions.** We theoretically investigate the PCC plateau when training attention-based regression model with a joint MSE+PCC loss. We identify two limitations in optimization dynamics and in model capacity.

- **Optimization Dynamics.** We identify a conflict in optimization dynamics: as MSE optimization increases  $\sigma_{\hat{y}}$  to match  $\sigma_y$ , the magnitude of the PCC loss gradient scales with  $1/\sigma_{\hat{y}}$  leading to a flattened PCC curve during training. In addition, We show that within-sample

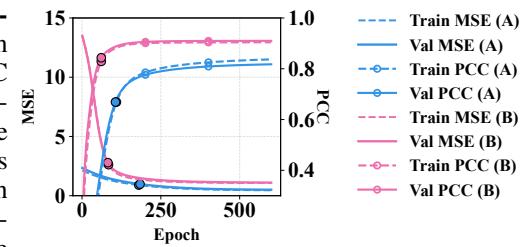


Figure 2: PCC plateau example: PCC flattens at early epoch while MSE continues to decrease. The plateau becomes more noticeable as within-sample homogeneity increases, specifically, dataset A is more homogeneous than B.

108 homogeneity further shrinks the PCC gradient through the Jacobian of softmax attention.  
 109 Both parts contribute to the PCC plateau phenomenon.

110 • **Model Capacity.** We prove that for any convex aggregator (e.g., softmax attention), the  
 111 achievable PCC improvement over mean-pooling can be bounded by the within-sample  
 112 data homogeneity.

113 To address these limitations, we introduce ECA, a novel attention-based regression framework with  
 114 three components:

115 • Motivated by the optimization limitation, we re-scale the PCC objective to counteract the  
 116  $1/\sigma_{\hat{y}}$  factor, restoring correlation gradients magnitude while minimizing MSE.  
 117 • Motivated by the convex aggregator limitation, we incorporate a Scaled Residual Aggregation  
 118 that enables controlled extrapolation beyond the convex hull.  
 119 • To handle within-sample homogeneity, we propose a Dispersion-Aware Temperature Soft-  
 120 max to prevent attention collapse and amplify the informative contrasts within homoge-  
 121 neous samples.

122 Across diverse regression benchmarks, ECA consistently overcomes the PCC plateau and achieves  
 123 higher correlation gains while maintaining competitive MSE. Ablation studies confirm the contribu-  
 124 tion of each component.

## 125 2 THEORETICAL ANALYSIS OF CORRELATION LEARNING IN 126 ATTENTION-BASED AGGREGATION

127 We theoretically analyze why the PCC plateau occurs when training attention-based regression with  
 128 a joint MSE+PCC loss. First, we relate MSE and PCC through a decomposition that motivates joint  
 129 training. Then we prove that softmax attention, as a convex aggregator, limits both the optimization  
 130 dynamics and the model’s expressive capacity. These limits hinder correlation learning and explain  
 131 the observed PCC plateau.

### 132 2.1 PROBLEM SETUP

133 **Data Notation.** We consider a regression dataset with a batch of  $S$  samples  $(x_s, y_s)$ . Each sample  
 134  $x_s$  is a set of  $n_s$  element with embeddings  $\mathbf{h}_s = \{\mathbf{h}_{si}\}_{i=1}^{n_s}$ , where  $\mathbf{h}_{si} \in \mathbb{R}^d$ . Let  $y_s, \hat{y}_s \in \mathbb{R}$  be the  
 135 ground-truth target and model prediction for  $s$ th sample. The batch-level empirical means are  $\mu_y, \mu_{\hat{y}}$   
 136 and standard deviations are  $\sigma_y, \sigma_{\hat{y}}$ . Define centered targets and predictions as  $a_s := y_s - \mu_y$  and  
 $b_s := \hat{y}_s - \mu_{\hat{y}}$ .

137 **Attention-based Aggregation.** The attention-based model processes each input sample to produce  
 138 a scalar prediction. An attention scoring function  $f_{\text{attn}}(\cdot)$  (e.g., KQV dot-product similarity or gating  
 139 mechanism) scores each embedding in  $\mathbf{h}_s$  and produces attention logits  $\mathbf{z}_s = f_{\text{attn}}(\{\mathbf{h}_{si}\}_{i=1}^{n_s}) \in$   
 140  $\mathbb{R}^{n_s}$  with entries  $z_{si} = [\mathbf{z}_s]_i \in \mathbb{R}$ . Softmax converts these logits to positive attention weights  
 141  $\boldsymbol{\alpha}_s = \text{Softmax}(\mathbf{z}_s)$  on the probability simplex with entries  $\alpha_{si} = [\boldsymbol{\alpha}_s]_i \in \mathbb{R}$  and  $\sum_{i=1}^{n_s} \alpha_{si} = 1$ .  
 142 The sample-level embedding is the convex combination  $\mathbf{v}_s = \sum_{i=1}^{n_s} \alpha_{si} \mathbf{h}_{si} \in \mathbb{R}^d$ . Finally, a linear  
 143 regression head with weights  $\mathbf{w} \in \mathbb{R}^d$  and bias  $c \in \mathbb{R}$  produces the scalar prediction:  $\hat{y}_s = \mathbf{w}^\top \mathbf{v}_s + c$ .  
 144 Note that this formulation is backbone-agnostic:  $\{\mathbf{h}_{si}\}$  represents the features at the final layer of  
 145 any deep architecture (e.g., a multi-layer Transformer). Since these models typically derive the  
 146 final prediction with a convex attention pooling (e.g., [CLS] token aggregation) followed by a linear  
 147 projection, our analysis of the attention-based aggregation and its interaction with joint MSE and  
 148 PCC optimization applies regardless of the depth or complexity of the preceding backbone. We  
 149 provide a detailed discussion on the applicability to deep architectures in Appendix E.

150 **Learning Objective.** We measure Pearson correlation between targets and predictions over the  
 151 batch by  $\rho := \frac{\text{Cov}(\mathbf{y}, \hat{\mathbf{y}})}{\sigma_y \sigma_{\hat{y}}}$ . To optimize both magnitude and correlation of the prediction, we use the  
 152 popular joint loss  $\mathcal{L}_{\text{total}} := \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) + \lambda_{\text{PCC}}(1 - \rho)$  where  $\lambda_{\text{PCC}} \geq 0$  balances the two terms.

153 **Homogeneity Measures.** For each sample, let the in-sample mean be  $\boldsymbol{\mu}_s = \frac{1}{n_s} \sum_{j=1}^{n_s} \mathbf{h}_{sj}$ . We  
 154 quantify within-sample homogeneity by (i) the in-sample dispersion  $\sigma_s = \sqrt{\frac{1}{n_s} \sum_{j=1}^{n_s} \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|_2^2}$ ,

162 and (ii) the convex-hull radius  $R_s := \max_i \|\mathbf{h}_{si} - \boldsymbol{\mu}_s\|_2$ . These quantities are related by inequality  
 163  $\sigma_s \leq R_s \leq \sqrt{n_s} \sigma_s$  with proof in Lemma D.3. Cross-sample homogeneity is summarized by the  
 164 root-mean-square (RMS) values  $\tilde{\sigma} := (\frac{1}{S} \sum_{s=1}^S \sigma_s^2)^{1/2}$  and  $\tilde{R} := (\frac{1}{S} \sum_{s=1}^S R_s^2)^{1/2}$ .  
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## 166 2.2 PRELIMINARIES: THE INTERPLAY BETWEEN MSE AND PCC

167 **Proposition 2.1** (MSE Mean–std–correlation Decomposition). *The MSE between  $y$  and  $\hat{y}$  can be  
 168 decomposed as:*

$$171 \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) = \underbrace{(\mu_{\hat{\mathbf{y}}} - \mu_{\mathbf{y}})^2}_{\text{mean matching}} + \underbrace{(\sigma_{\hat{\mathbf{y}}} - \sigma_{\mathbf{y}})^2}_{\text{std matching}} + \underbrace{2 \sigma_{\mathbf{y}} \sigma_{\hat{\mathbf{y}}} (1 - \rho)}_{\text{weighted correlation}}. \quad (1)$$

174 **Lemma 2.1** (Scaling-invariance of PCC). *Let  $m \geq 0$  and  $n \in \mathbb{R}$ .  $\text{PCC}(y, m\hat{y} + n) = \text{PCC}(y, \hat{y})$ .*

175 We defer the proof for Proposition 2.1 and Lemma 2.1 to Appendix A.

176 **Remark 2.1.** *Proposition 2.1 and lemma 2.1 are model-independent and hold for any regressor.*

177 **Remark 2.2** (The PCC Plateau). *By Proposition 2.1, minimizing MSE jointly targets (i) mean matching,  
 178 (ii) standard deviation matching, and (iii) weighted correlation. Because MSE is sensitive to  
 179 affine transformations while PCC is invariant (Lemma 2.1), optimization can reduce MSE by mainly  
 180 adjusting mean and scale, with little improvement on correlation. This explains why MSE may keep  
 181 decreasing while PCC plateaus, and motivates adding the explicit correlation term  $\lambda_{\text{PCC}}(1 - \rho)$  to  
 182 the objective.*

183 The discussion above provides intuitions for the PCC plateau phenomenon. We further empirically validate this phenomenon on 8 UCI regression datasets using multi-layer Transformers (Appendix F). Figure 7 shows a consistent pattern across all tasks: PCC curve flattens before MSE convergence. This consistent pattern confirms that “PCC plateau” is a general correlation learning failure mode under attention-based joint optimization setting. We now provide a formal analysis by characterizing the PCC gradient in attention-based regression models.

## 191 2.3 OPTIMIZATION DYNAMICS: THE CORRELATION GRADIENT BOTTLENECK

192 We study how the gradients propagate through the attention aggregator when optimizing the joint  
 193 loss  $\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{MSE}} + \lambda_{\text{PCC}}(1 - \rho)$ . We derive the gradients of both MSE and PCC with respect to  
 194 the attention logits  $z_{si}$  to understand the optimization dynamics.

195 **Lemma 2.2** (Softmax Aggregator Jacobian). *The derivative of the aggregated embedding  $\mathbf{v}_s$  with  
 196 respect to a pre-softmax logit  $z_{si}$  is  $\partial \mathbf{v}_s / \partial z_{si} = \alpha_{si}(\mathbf{h}_{si} - \mathbf{v}_s)$  and consequently,  $\partial \hat{y}_s / \partial z_{si} =$   
 197  $\alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s)$ .*

198 **Theorem 2.1** (Gradient of PCC w.r.t. Attention Logits). *The derivative of Pearson correlation  $\rho$   
 199 with respect to a pre-softmax logit  $z_{si}$  is*

$$200 \frac{\partial \rho}{\partial z_{si}} = \frac{1}{S \sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (2)$$

201 To understand the interplay during joint optimization, we also examine the gradient of the MSE loss.

202 **Lemma 2.3** (Gradient of MSE w.r.t. Attention Logits). *The derivative of MSE with respect to a  
 203 pre-softmax logit  $z_{si}$  is*

$$204 \frac{\partial \mathcal{L}_{\text{MSE}}}{\partial z_{si}} = \frac{2}{S} (\hat{y}_s - y_s) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (3)$$

205 **Gradient Decomposition and the Optimization Conflict.** Comparing the PCC gradient (Equation  
 206 (2)) and the MSE gradient (Equation (3)), we observe they share the same *local* structure factor  
 207  $L_{si} := \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s)$ , which governs attention adjustment within sample  $s$ . The difference lies  
 208 entirely in the *global* scaling factors which depend on overall batch statistics:

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$$\frac{\partial \mathcal{L}_{\text{MSE}}}{\partial z_{si}} = \frac{1}{S} g_s^{\text{MSE}} L_{si}, \quad \text{where } g_s^{\text{MSE}} := 2(\hat{y}_s - y_s), \quad (4)$$

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$$\frac{\partial \rho}{\partial z_{si}} = \frac{1}{S} g_s^{\text{PCC}} L_{si}, \quad \text{where } g_s^{\text{PCC}} := \frac{1}{\sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right). \quad (5)$$

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The relative impact of MSE versus PCC optimization is determined by the ratio of these global factors. We analyze this ratio using their Root Mean Square (RMS) values across the batch.

**Corollary 2.1** (PCC/MSE Gradient Ratio Decay). *Assuming  $\rho \in [0, 1]$ , the RMS ratio of the global scaling factors across the batch is bounded by:*

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Corollary 2.1 identifies a gradient bottleneck where the PCC signal attenuates relative to MSE at a rate of  $\mathcal{O}(1/\sigma_{\hat{y}}^{3/2})$ . This bound is empirically validated in Figure 3 on synthetic dataset , illustrating how magnitude matching dominates the optimization dynamics. We further analyze the magnitude of the PCC gradient alone, which reveals dependence on in-sample homogeneity.

**Corollary 2.2** (PCC Gradient Magnitude Bound). *The magnitude of the PCC gradient in Theorem 2.1 can be bounded by*

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Detailed derivations for Lemma 2.2, Theorem 2.1 are provided in Appendix B.1. Proofs for Lemma 2.3, Corollary 2.1, and Corollary 2.2 are provided in Appendix C.

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**Remark 2.3** (The Two Bottlenecks of Softmax Attention for Correlation). *The gradient analysis reveals two key bottlenecks in optimization dynamics that drive PCC plateaus:*

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**1. Dominance of the MSE Gradient.** Corollary 2.1 reveals a critical conflict in the joint optimization: the ratio of the PCC gradient magnitude relative to the MSE gradient magnitude decays rapidly at a rate of  $\mathcal{O}(1/\sigma_{\hat{y}}^{3/2})$ . Training with the joint loss minimizes the MSE std-matching term in Equation (1), which drives  $\sigma_{\hat{y}}$  toward the target standard deviation  $\sigma_y$ . As  $\sigma_{\hat{y}}$  typically increases during early training (see Figure 4), the relative contribution of the PCC gradient diminishes significantly. Consequently, the optimization becomes dominated by the MSE objective (magnitude matching), effectively downplaying PCC optimization (shape matching) and causing the plateau, even when the PCC loss weight  $\lambda_{\text{PCC}}$  is large. This motivates optimization strategies that counteract this rapid attenuation.

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**2. Dependence on Within-sample Homogeneity.** The gradient bound in Corollary 2.2 is proportional to the in-sample dispersion  $\sigma_s$ . When a sample’s elements are homogeneous,  $\sigma_s$  is small and the PCC gradient magnitude reduces, effectively hindering improvements to PCC via attention adjustment. Furthermore, since attention scoring functions are generally continuous, homogeneous inputs lead to low-variance logits  $z_{si}$ . Under fixed-temperature softmax, this results in near-uniform weights  $\alpha_{si} \approx 1/n_s$ , suppressing per-sample selectivity. These effects motivate mechanisms that adapt attention sensitivity to the in-sample dispersion.

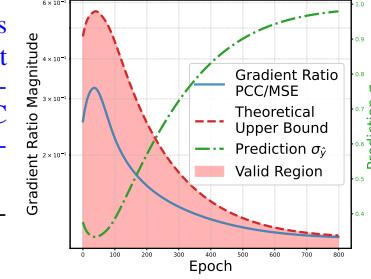


Figure 3: Validation of gradient ratio (PCC/MSE) decay. The RMS ratio of PCC vs. MSE gradients (blue) is strictly constrained by the theoretical upper bound (red). The increase in prediction dispersion  $\sigma_{\hat{y}}$  (green) during training drives the attenuation of the PCC gradient signal relative to the MSE gradient.

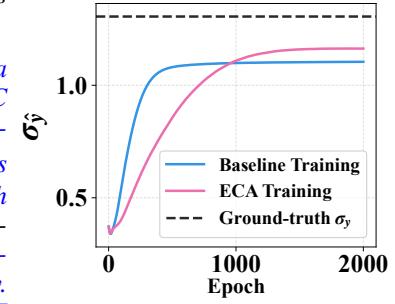


Figure 4: The standard deviation of predictions  $\sigma_{\hat{y}}$  increases during training to match the standard deviation of labels  $\sigma_y$  under MSE loss.

270 2.4 MODEL CAPACITY: THE PCC CEILING OF CONVEX AGGREGATION  
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272 Beyond optimization dynamics, we study the limits of the aggregator’s expressivity. Softmax attention  
273 performs convex combinations, restricting aggregated embedding  $\mathbf{v}_s$  to the convex hull of the  
274 in-sample embeddings  $\{\mathbf{h}_{si}\}$ . We study how much PCC improvement can be achieved by any convex  
275 aggregator over mean-pooling and show a capacity limit governed by in-sample homogeneity.

276 **Prediction Decompositon.** We decompose the sample embedding  $\mathbf{v}_s$  relative to the mean-pooling  
277 embedding  $\boldsymbol{\mu}_s$ . The prediction can be decomposed as:  $\hat{y}_s = \underbrace{(\mathbf{w}^\top \boldsymbol{\mu}_s + c)}_{\bar{y}_s} + \underbrace{\mathbf{w}^\top (\mathbf{v}_s - \boldsymbol{\mu}_s)}_{\Delta \hat{y}_s}$ , where  
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279  $\bar{y}_s$  is the prediction using mean-pooling aggregation, and  $\Delta \hat{y}_s$  is the attention-induced perturbation.

280 **Theorem 2.2** (PCC Gain Bound for Convex Attention). *Let  $\sigma_0 := \text{std}_s(\bar{y}_s)$  be the standard de-  
281 viation of the mean-pooling predictions; define baseline  $\rho_0 := \text{PCC}(\mathbf{y}, \bar{\mathbf{y}})$  and  $\rho$  is the PCC after  
282 applying any convex attention mechanism. Provided  $\|\mathbf{w}\|_2 > 0$  and  $\tilde{R} < \sigma_0/\|\mathbf{w}\|_2$ ,*

$$285 \quad |\rho - \rho_0| \leq \frac{2\tilde{R}}{\sigma_0/\|\mathbf{w}\|_2 - \tilde{R}}. \quad (8)$$

287 Detailed proof is provided in Appendix D.

288 **Remark 2.4.** *Theorem 2.2 shows that the PCC improvement bound of any convex attention de-  
289 pends only on the ratio between convex hull radius  $\tilde{R}$  (reflecting in-sample homogeneity) and the  
290 normalized standard deviation of mean-pooling baseline ( $\sigma_0/\|\mathbf{w}\|_2$ ). The bound is scale-invariant  
291 and independent of the regression head magnitude since  $\sigma_0/\|\mathbf{w}\|_2 = \text{std}_s(\mathbf{w}^\top \boldsymbol{\mu}_s)/\|\mathbf{w}\|_2 =$   
292  $\text{std}_s((\mathbf{w}^\top/\|\mathbf{w}\|_2)\boldsymbol{\mu}_s)$ . When in-sample homogeneity is high ( $\tilde{R}$  is small), no convex attention can  
293 substantially increase correlation. The limitation arises because  $\mathbf{v}_s$  is confined to the convex hull; a  
294 small hull restricts the magnitude of adjustments to the aggregated embedding, thereby limiting the  
295 potential PCC improvement and motivating mechanisms that can extrapolate beyond it.*

297 2.5 SUMMARY OF THEORETICAL INSIGHTS  
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299 Our analysis reveals that the difficulty of optimizing PCC using softmax attention stems from two  
300 aspects: optimization dynamics and model capacity. Remark 2.3 highlights the vanishing PCC gra-  
301 dients due to cross-sample dispersion attenuation  $1/\sigma_{\hat{y}}$  and weak in-sample dispersion. Remark 2.4  
302 further shows that any convex aggregator is restricted to the convex hull, which limits the possible  
303 PCC gain by ratio  $\tilde{R}/(\sigma_0/\|\mathbf{w}\|_2)$ . Together, these effects explain the plateau and motivate a novel  
304 attention mechanism proposed in the next section that addresses the identified bottlenecks accord-  
305 ingly.

306 3 EXTRAPOLATIVE CORRELATION ATTENTION (ECA)  
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309 Our analysis has identified fundamental limitations in softmax attention for optimizing joint  
310 MSE+PCC objective. To address these issues, we propose Extrapolative Correlation Attention  
311 (ECA), a novel drop-in attention module for regression that enhances both optimization and ex-  
312 pressivity. ECA incorporates three components: (i) Scaled Residual Aggregation to break the  
313 convex hull constraint; (ii) Dispersion-Aware Temperature Softmax, to avoid gradient collapse; and (iii)  
314 Dispersion-Normalized PCC Loss, which compensates the  $1/\sigma_{\hat{y}}$  attenuation in correlation gradients.

315 3.1 BREAKING THE CONVEX HULL WITH SCALED RESIDUAL AGGREGATION (SRA)  
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317 Theorem 2.2 shows that any convex attention mechanism is capacity-limited in correlation improve-  
318 ment because the aggregated embedding  $\mathbf{v}_s$  lies inside the convex hull of the in-sample embeddings  
319  $\{\mathbf{h}_{si}\}$ . This PCC gain bound is especially tighter when in-sample dispersion is low. To relax this  
320 limit, we introduce Scaled Residual Aggregation (SRA): instead of a strict convex aggregation, the  
321 model extrapolates along the residual  $(\mathbf{h}_{si} - \boldsymbol{\mu}_s)$ , allowing  $\mathbf{v}_s$  to move beyond the convex hull.

323 Given the mean embedding  $\boldsymbol{\mu}_s = 1/n_s \sum_i \mathbf{h}_{si}$ , we define the residual  $\Delta \mathbf{v}_s$  as the attention-  
324 weighted deviation from the mean:  $\Delta \mathbf{v}_s := \sum_i \alpha_{si}(\mathbf{h}_{si} - \boldsymbol{\mu}_s)$ . SRA scales this residual by a

324 learnable factor  $\gamma_s \geq 1$ :  
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$$\mathbf{v}_s^{\text{ECA}} = \boldsymbol{\mu}_s + \gamma_s \cdot \Delta \mathbf{v}_s = \boldsymbol{\mu}_s + \gamma_s \sum_i \alpha_{si} (\mathbf{h}_{si} - \boldsymbol{\mu}_s). \quad (9)$$

328 We parameterize  $\gamma_s$  using a small, sample-specific MLP conditioned on the mean embedding  $\boldsymbol{\mu}_s$   
 329 and use a shifted Softplus activation to ensure  $\gamma_s \geq 1$ , that is  $\gamma_s = 1 + \text{Softplus}(\text{MLP}_{\theta_\gamma}(\boldsymbol{\mu}_s))$ .  
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331 The factor  $\gamma_s$  allows the model to amplify weak in-sample contrasts. When  $\gamma_s = 1$ , SRA reduces  
 332 to standard convex attention aggregation. For  $\gamma_s > 1$ , the model extrapolates beyond the convex  
 333 hull, and more importantly, it breaks the convexity constraint. In standard attention, the deviation  
 334  $\|\Delta \mathbf{v}_s\|$  is bounded by the radius of the convex hull  $R_s$ . SRA expands the reachable space by increasing  
 335 the effective radius and fundamentally bypasses the capacity limit derived for convex aggregators  
 336 in Theorem 2.2. In practice we optionally clip  $\gamma_s$  at a maximum (e.g.,  $\gamma_{\max} = 2$ ) or add a regularizer  
 337  $\mathcal{L}_\gamma = \frac{\lambda_\gamma}{S} \sum_s (\gamma_s - 1)^2$  to discourage excessive scaling.  
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### 339 3.2 DISPERSION-AWARE TEMPERATURE SOFTMAX (DATS)

340 While SRA enables extrapolation beyond the convex hull, the model still needs a informative direc-  
 341 tion to extrapolate. In homogeneous samples, standard softmax produces flat attention  $\alpha_{si} \approx 1/n_s$   
 342 (Remark 2.3), which pulls the aggregated embedding toward  $\boldsymbol{\mu}_s$  and makes the residual in Equa-  
 343 tion (9) small ( $\Delta \mathbf{v}_s \approx 0$ ). With small residual, SRA provides little benefit. To address this, we  
 344 introduce Dispersion-Aware Temperature Softmax (DATS), which adapts the attention temperature  
 345 to the in-sample dispersion, sharpening attention when homogeneity is high:  
 346

347 We modify the softmax attention for Equation (9) with a sample-specific temperature  $\tau_s$  reflecting  
 348 within-sample dispersion:  
 349

$$\alpha_{si} = \text{softmax}\left(\frac{z_{si}}{\tau_s}\right), \quad \tau_s = T_{\min} + \beta \sqrt{\frac{1}{n_s} \sum_{1 \leq i \leq n_s} \|\mathbf{h}_{si} - \boldsymbol{\mu}_s\|^2}. \quad (10)$$

351 Here  $T_{\min} > 0$  lower-bounds the temperature for stability, and  $\beta \geq 0$  is a hyperparameter that  
 352 controls sensitivity. When embeddings within a sample are homogeneous,  $\tau_s$  has lower value so  
 353 small differences between logits  $z_{si}$  become sharper after attention, yielding a meaningful deviation  
 354  $\Delta \mathbf{v}_s$  that SRA can effectively amplify.  
 355

### 356 3.3 STABILIZING OPTIMIZATION: DISPERSION-NORMALIZED PCC LOSS (DNPL)

358 Theorem 2.1 shows that the correlation gradient is attenuated by  $1/\sigma_{\hat{y}}$ . As MSE optimization im-  
 359 proves standard deviation matching,  $\sigma_{\hat{y}}$  increases, which shrinks the PCC gradient and contributes  
 360 to a PCC plateau. We counteract this attenuation effect with a Dispersion-Normalized PCC Loss  
 361 (DNPL), which rescales the PCC term by the current prediction standard deviation while blocking  
 362 its gradient:  
 363

$$\tilde{\mathcal{L}}_{\text{PCC}} = \text{StopGrad}(\sigma_{\hat{y}}) \cdot (1 - \rho). \quad (11)$$

364 The StopGrad( $\cdot$ ) operation ensures we only adjust the gradient magnitude to counteract the attenu-  
 365 ation, while leaving the learning objective's stationary points unchanged.  
 366

### 367 3.4 OVERALL OBJECTIVE

369 The complete ECA framework, including SRA and DATS, is fully differentiable and can be trained  
 370 end-to-end. The overall learning objective combines the primary regression loss (MSE), the normal-  
 371 ized PCC loss (DNPL), and the extrapolation regularizer:  
 372

$$\mathcal{L}_{\text{Total}} = \mathcal{L}_{\text{MSE}} + \lambda_{\text{PCC}} \cdot \tilde{\mathcal{L}}_{\text{PCC}} + \mathcal{L}_\gamma. \quad (12)$$

## 374 4 RELATED WORKS

375 **Correlation Learning and Optimization.** Correlation is a core metric in biological and medical  
 376 areas (Langfelder & Horvath, 2008; Lawrence & Lin, 1989). In these domains, PCC is a standard  
 377

378 criterion for evaluating regression performance (Kudrat et al., 2025; Long et al., 2023). Because  
 379 PCC is differentiable, it is often optimized directly as a loss in regression pipelines (Kudrat et al.,  
 380 2025; Avants et al., 2008). From a multi-task perspective, many works combine PCC with MSE to  
 381 balance the prediction magnitude and shape (Yang et al., 2023; Liu et al., 2022; Balakrishnan et al.,  
 382 2019). However, the interaction dynamics between MSE and PCC under joint optimization remain  
 383 underexplored, motivating our analysis of gradient coupling and the observed PCC plateau.

384 **Softmax Attention Aggregation.** Softmax attention is a cornerstone component in the backbones of  
 385 many representative regression models (Zhou et al., 2021; Gorishniy et al., 2021; Kim et al., 2019).  
 386 Despite its empirical success, recent theory has revealed expressivity limits of softmax mappings  
 387 in related contexts (Yang et al., 2017; Kanai et al., 2018; Bhojanapalli et al., 2020). However, to  
 388 our knowledge, no prior work analyzes the model capacity of softmax attention in terms of upper  
 389 bounds on achievable PCC improvements, especially with high in-sample homogeneity data.

390

## 391 5 EXPERIMENTS

392

393 We evaluate our ECA on four settings, including the challenging high in-sample homogeneity tasks.  
 394 The evaluations consist of: (i) a synthetic regression dataset with controllable in-sample homogene-  
 395 ity; (ii) three representative tabular regression benchmarks from the UCI ML Repository (Asuncion  
 396 et al., 2007); (iii) a clinical pathology dataset for spatial transcriptomic prediction, where nearby  
 397 regions exhibit *high homogeneity*; and (iv) a multimodal sentiment analysis (MSA) dataset, where  
 398 consecutive video frames are *highly homogeneous*.

399

400 As ECA is a drop-in replacement for softmax attention, we integrate it into existing attention-based  
 401 regression models for each benchmark to measure the performance improvement. More details are  
 402 provided in Appendix G.

403

### 404 5.1 EXPERIMENTAL SETUP

405

406 **Synthetic Dataset.** We construct a synthetic dataset to validate our theory and proposed ECA  
 407 method. We synthetic  $N$  samples, each with  $K$  element embeddings in  $D$  dimensions as input  
 408 samples. In each sample, one key element carries signal along a fixed unit direction  $\mathbf{w}^*$ , while the  
 409 remaining  $K-1$  background elements cluster around a shared sample mean. The label  $\mathbf{y}$  is the pro-  
 410 jection of the sample mean onto  $\mathbf{w}^*$  with a term proportional to the key strength and small additive  
 411 noise. We control within-sample homogeneity via  $\eta$  (larger  $\eta$  means the key deviates further from  
 412 the mean), yielding four homogeneity levels  $\tilde{\sigma} \in \{0.10, 0.24, 0.42, 0.73\}$  where lower  $\tilde{\sigma}$  indicates  
 413 higher homogeneity. We compare regression model with one layer of ECA to one layer of standard  
 414 softmax attention and report MSE and PCC.

415

416 **UCI ML Repository Datasets.** We evaluate on three representative tabular regression benchmarks:  
 417 Appliance Energy Prediction (28 features, 1 target) (Candanedo, 2017), Online News Popularity  
 418 (58 features, 1 target) (Fernandes & Sernadela, 2015), and Superconductivity (81 features, 1 target)  
 419 (Hamidieh, 2018). We integrate ECA into the attention layer of the FT-Transformer (Gorishniy  
 420 et al., 2021) and report mean absolute error (MAE), MSE, and PCC.

421

422 **Spatial Transcriptomic Dataset.** We test spatial transcriptomics prediction from pathology images  
 423 on the 10xProteomic dataset (10x Genomics, 2025; Yang et al., 2023), which contains 32,032 slide-  
 424 image patches paired with gene-expression measurements of breast-cancer slides. We follow the  
 425 data processing and experimental settings of the EGN baseline (Yang et al., 2023), which jointly  
 426 optimize MSE+PCC loss. We adopt ECA methods onto the EGN baseline and report MSE, PCC@F,  
 427 PCC@S, and PCC@M as evaluation metrics. The training set exhibits high in-sample embedding  
 428 homogeneity with  $\tilde{\sigma} = 0.068$  versus cross-sample  $\sigma_0 = 0.164$ .

429

430 **Multimodal Sentiment Analysis (MSA) Dataset.** We use MOSI (Zadeh et al., 2016), a standard  
 431 MSA benchmark consists of 2,199 monologue video clips with audio and visual inputs. As il-  
 432 lustrated in Figure 1, consecutive frames within a clip are more similar than frames across clips.  
 433 Quantitatively, the video frames shows strong within-sample homogeneity with  $\tilde{\sigma} = 0.098$  versus  
 434 cross-sample  $\sigma_0 = 0.170$ . We follow the commonly used MOSI processing protocol from THUIAR  
 435 releases (Yu et al., 2020; 2021). Video frame embeddings are extracted with OpenFace (Amos et al.,  
 436 2016). Consistent with prior work, we report F1, PCC, and MAE as evaluation metrics. We include

10 representative baselines. ALMT (Zhang et al., 2023), the leading baseline optimizing with MSE loss, is selected to incorporate the ECA method.

Table 1: Results on three UCI tabular regression tasks. “+ECA” denotes adding ECA onto the FT-Transformer baseline. Rows marked “w/o SRA/DATS/DNPL” are ablation studies that remove the corresponding ECA components. “w/o” = “without” and **bold** indicating best result.

Method	Appliance			Online News			Superconductivity		
	MAE ↓	MSE $\times 10^3$ ↓	PCC ↑	MAE ↓	MSE $\times 10^0$ ↓	PCC ↑	MAE ↓	MSE $\times 10^2$ ↓	PCC ↑
FT-Transformer	39.333	6.108	0.556	0.641	0.724	0.408	8.793	1.772	0.920
+ ECA (full)	<b>38.665</b>	<b>5.790</b>	<b>0.598</b>	<b>0.631</b>	<b>0.712</b>	<b>0.420</b>	<b>7.976</b>	<b>1.582</b>	<b>0.930</b>
+ ECA (w/o SRA)	39.208	5.994	0.575	0.637	0.725	0.410	8.377	1.695	0.920
+ ECA (w/o DATS)	38.906	6.037	0.561	0.645	0.740	0.418	8.630	1.709	0.927
+ ECA (w/o DNPL)	39.742	5.910	0.583	0.640	0.719	0.418	8.466	1.671	0.922

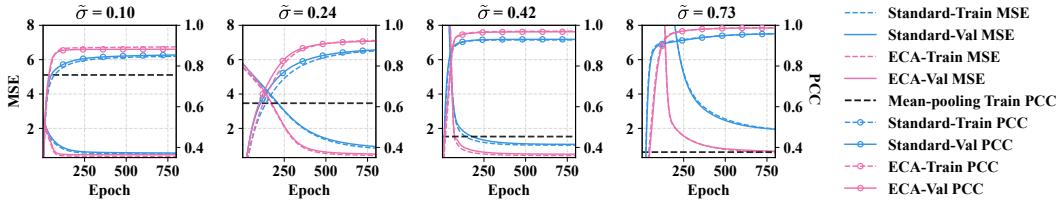


Figure 5: PCC and MSE curves on synthetic datasets with in-sample homogeneity  $\tilde{\sigma} \in [0.10, 0.24, 0.42, 0.73]$ .

## 5.2 RESULTS AND ANALYSIS

**Synthetic Dataset.** Figure 5 shows case studies on the training and validation curves under different in-sample dispersion (with  $\tilde{\sigma} = 0.10, 0.24, 0.42$ , and  $0.73$ ). The horizontal line indicates the PCC achieved by mean-pooling over input embeddings. This result confirms our theoretical study in three ways: 1) as the homogeneity intensifies, both the PCC of our ECA and baseline model decrease and the MSE get higher (task harder), and the achievable PCC improvement of convex (e.g., softmax) attention over mean-pooling decreases (Theorem 2.2). 2) ECA consistently outperforms standard attention in both PCC and MSE across all four  $\tilde{\sigma}$ s, achieving PCC gains of 4.80%, 5.76%, 4.68%, 3.05% and MSE reductions of 20.3%, 40.8%, 54.0%, 66.7% (in order of increasing  $\tilde{\sigma}$ ), showing its ability to explore beyond the convex hull and improving the PCC without compromising the MSE. 3) The PCC curve of ECA keeps improving and converges later and at a higher value than the standard attention baseline, indicating the effectiveness of our proposed DNPL in mitigating the PCC attenuation effect identified in Remark 2.3.

Table 2: Results on MOSI. <sup>†</sup> from THUIAR’s GitHub (Yu et al., 2020; 2021); <sup>\*</sup> from (Hazarika et al., 2020); <sup>\*\*</sup> reproduced from public code with provided hyper-parameters.

Method	F1 ↑	MAE ↓	PCC ↑
TFN <sup>†</sup> (Zadeh et al., 2017)	0.791	0.947	0.673
LMF <sup>*</sup> (Liu et al., 2018)	0.824	0.917	0.695
EF-LSTM <sup>†</sup> (Williams et al., 2018b)	0.785	0.949	0.669
LF-DNN <sup>†</sup> (Williams et al., 2018a)	0.786	0.955	0.658
Graph-MFN <sup>†</sup> (Zadeh et al., 2018)	0.784	0.956	0.649
Mult <sup>*</sup> (Tsai et al., 2019)	0.828	0.871	0.698
MISA <sup>†</sup> (Hazarika et al., 2020)	0.836	0.777	0.778
ICCN <sup>*</sup> (Sun et al., 2020)	0.830	0.860	0.710
DLF <sup>**</sup> (Wang et al., 2025)	0.850	0.731	0.781
ALMT <sup>**</sup> (Zhang et al., 2023)	<u>0.851</u>	<u>0.721</u>	0.783
ALMT+ $\mathcal{L}_{PCC}$	0.834	0.731	<u>0.791</u>
ALMT+ $\tilde{\mathcal{L}}_{PCC}$ + ECA	<b>0.859</b>	<b>0.695</b>	<b>0.806</b>

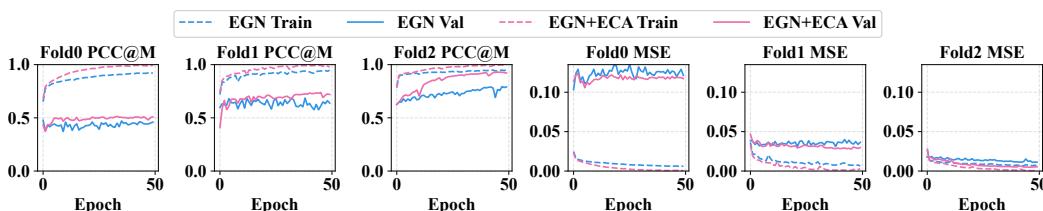
addressing our identified PCC gradient limitation and the convex attention capacity limit substantially

## UCI ML Repository Datasets.

Across three UCI tabular regression tasks, adapting our ECA module into the FT-Transformer yields consistent improvements in both magnitude (MSE and MAE) and shape (PCC) metrics. On Appliance, PCC increases by 0.042 and MSE decreases by  $0.318 \times 10^3$ ; on Online News, PCC increases 0.012 from 0.408 while MSE decreases 0.012 from 0.724; on Superconductivity, PCC 0.920 → 0.930 and MSE  $1.772 \times 10^2 \rightarrow 1.582 \times 10^2$ . MAE also decreases across all datasets. These improvements provide strong evidence that ad-

486 Table 3: Three-fold regression PCC and MSE on 10xProteomic dataset.  
487

488 Method	489 PCC@F $\uparrow$	490 PCC@S $\uparrow$	491 PCC@M $\uparrow$	492 MSE $\downarrow$
493 EGN	494 $0.602 \pm 0.160$	495 $0.647 \pm 0.164$	496 $0.629 \pm 0.135$	497 $0.056 \pm 0.047$
498 EGN+ECA	499 $0.690 \pm 0.202$	500 $0.724 \pm 0.191$	501 $0.716 \pm 0.168$	502 $0.051 \pm 0.048$

500 Figure 6: PCC@M and MSE curves for EGN baseline and EGN+ECA on 10xProteomic dataset  
501 under each fold. Curves for PCC@S and PCC@F please refer to Figure 8 and Figure 9.

502  
503 mitigates the PCC plateau without compromising MSE. The ablations further support the contribu-  
504 tion of each components: removing DATS lowers Appliance PCC to 0.561, while removing SRA  
505 reduces Online News PCC to 0.418 and removing DNPL decreases Superconductivity PCC to 0.922.

506  
507 **Spatial Transcriptomic Dataset.** We follow the EGN (Yang et al., 2023) setting and report three-  
508 fold results. Figure 6 plots PCC and MSE curves for training and validation. Across all folds,  
509 integrating ECA consistently improves both metrics. In fold 2, the EGN baseline’s PCC flattens  
510 near epoch 4, but the MSE keeps decreasing, indicating a clear PCC plateau. In contrast, PCC of  
511 EGN+ECA continues to increase, effectively breaking the PCC plateau and improving final valida-  
512 tion PCC by  $\sim 16.51\%$ . The same pattern holds in folds 0 and 1. Throughout training, EGN+ECA  
513 also achieves comparable or lower MSE than EGN alone, indicating that ECA successfully preserves  
514 magnitude information while achieving better PCC. Table 3 summarizes the overall performance,  
515 where EGN+ECA achieves +14.64% for PCC@F, +11.89% for PCC@S, +13.81% for PCC@M,  
516 and a 9.83% reduction in MSE, showing that ECA effectively and robustly alleviates the PCC plateau  
517 without compromising the MSE.

518 **Multimodal Sentiment Analysis (MSA) Dataset.** Since ALMT optimizes MSE loss only, we test  
519 two settings: (i) ALMT with an additional PCC loss; and (ii) ALMT with ECA adapted into the  
520 video attention encoder and trained with the dispersion-normalized PCC loss. Table 2 reports results  
521 of 10 baselines. Adding a PCC term yields a small PCC gain but degrades F1 and MAE, reflecting  
522 the MSE-PCC conflict under strong in-sample homogeneity. In contrast, adding ECA improves all  
523 metrics, achieving a +2.3% PCC increase without sacrificing F1 or MAE.

## 524 6 CONCLUSION

525 This work presents the first theoretical investigation into the PCC plateau phenomenon observed  
526 when training attention-based regression models with a joint MSE+PCC loss, particularly under  
527 high data homogeneity. Our analysis identified two fundamental limitations in standard softmax at-  
528 tention: conflict in optimization dynamics that attenuate the correlation gradient, and an achievable  
529 PCC bound imposed by convex aggregation. To address these bottlenecks, we introduced ECA, a  
530 novel plug-in framework incorporating mechanisms to stabilize optimization, adapt to homoge-  
531 neity, and extrapolate beyond the convex hull. Comprehensive experiments validate our theoretical  
532 insights and demonstrate that ECA successfully breaks the PCC plateau, achieving significant cor-  
533 relation gains while maintaining competitive magnitude performance.

540 7 REPRODUCIBILITY STATEMENT  
541542 We support reproducibility as follows.  
543544 **Theoretical Study** The appendix has complete proofs for all theorems, lemmas, and corollaries in  
545 the paper. See Appendix A for results from Section 2.2, Appendix B for Section 2.3, and Appendix D  
546 for Section 3.  
547548 **Dataset Processing** Processing details for all datasets (synthetic and real-world) are listed in Ap-  
549 pendix G.  
550551 **Code Reproducibility** We include an anonymous zip file with implementations for the synthetic  
552 and spatial transcriptomics datasets along with the hyperparameters we use for review. For the spa-  
553 tial transcriptomic dataset, we follow the EGN baseline preprocessing protocol. Due to the limited  
554 space, we did not include the dataset. The README.md explains how to get the data and run the  
555 code. We will release the full code publicly upon acceptance.  
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## 756 757 758 759     Appendix

### 760     A PRELIMINARIES

#### 761     A.1 PROOF FOR PROPOSITION 2.1

763 **Proposition A.1** (MSE Mean–std–correlation Decomposition). *Let  $y, \hat{y} \in \mathbb{R}$  be the ground truth  
764 and predictions across  $S$  samples. Let  $\mu_y, \mu_{\hat{y}}$  be the empirical means, and  $\sigma_y, \sigma_{\hat{y}}$  be the empirical  
765 standard deviations. The Mean Squared Error can be decomposed as:*

$$766 \quad \text{MSE}(y, \hat{y}) = (\mu_{\hat{y}} - \mu_y)^2 + (\sigma_{\hat{y}} - \sigma_y)^2 + 2 \sigma_y \sigma_{\hat{y}} (1 - \rho). \quad (13)$$

769 *Proof.* Write the error for sample  $i$  as

$$771 \quad y_i - \hat{y}_i = [(y_i - \mu_y) - (\hat{y}_i - \mu_{\hat{y}})] + (\mu_y - \mu_{\hat{y}}). \quad (14)$$

773 Squaring and averaging over  $i = 1, \dots, S$  give us

$$775 \quad \text{MSE}(y, \hat{y}) = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (15)$$

$$778 \quad = \frac{1}{N} \sum_{i=1}^N \left( (y_i - \mu_y) - (\hat{y}_i - \mu_{\hat{y}}) \right)^2 + (\mu_y - \mu_{\hat{y}})^2 \quad (16)$$

$$781 \quad + \frac{2(\mu_y - \mu_{\hat{y}})}{N} \sum_{i=1}^N \left( (y_i - \mu_y) - (\hat{y}_i - \mu_{\hat{y}}) \right). \quad (17)$$

784 The last sum vanishes since  $\sum_i (y_i - \mu_y) = \sum_i (\hat{y}_i - \mu_{\hat{y}}) = 0$ . Expanding the remaining square  
785 and using the definitions of variances,  $\text{Cov}(y, \hat{y}) = \sigma_y \sigma_{\hat{y}} \rho$ , we obtain

$$787 \quad \text{MSE}(y, \hat{y}) = (\mu_{\hat{y}} - \mu_y)^2 + \sigma_y^2 + \sigma_{\hat{y}}^2 - \frac{2}{N} \sum_{i=1}^N (y_i - \mu_y)(\hat{y}_i - \mu_{\hat{y}}) \quad (18)$$

$$790 \quad = (\mu_{\hat{y}} - \mu_y)^2 + \sigma_y^2 + \sigma_{\hat{y}}^2 - 2\sigma_y \sigma_{\hat{y}} \rho. \quad (19)$$

792 Finally, rearranging  $\sigma_y^2 + \sigma_{\hat{y}}^2 - 2\sigma_y \sigma_{\hat{y}} \rho = (\sigma_{\hat{y}} - \sigma_y)^2 + 2\sigma_y \sigma_{\hat{y}} (1 - \rho)$  yields the claimed decom-  
793 position.  $\square$

#### 795     A.2 PROOF FOR LEMMA 2.1

797 **Lemma A.1** (Scaling Invariance of PCC). *Let  $m \in \mathbb{R} \setminus \{0\}$  and  $n \in \mathbb{R}$ . For any sample  
798  $\{(y_i, \hat{y}_i)\}_{i=1}^S$ ,*

$$800 \quad \text{PCC}(y, m\hat{y} + n) = \text{sign}(m) \text{PCC}(y, \hat{y}). \quad (20)$$

802 *Proof.* Using  $\rho(u, v) = \frac{\text{Cov}(u, v)}{\sigma_u \sigma_v}$  and  $\sigma_{m\hat{y}+n} = |m| \sigma_{\hat{y}}$ ,

$$805 \quad \text{PCC}(y, m\hat{y} + n) = \frac{\text{Cov}(y, m\hat{y} + n)}{\sigma_y \sigma_{m\hat{y}+n}} = \frac{m \text{Cov}(y, \hat{y})}{\sigma_y |m| \sigma_{\hat{y}}} \quad (21)$$

$$807 \quad = \frac{m}{|m|} \text{PCC}(y, \hat{y}) = \text{sign}(m) \text{PCC}(y, \hat{y}) \quad (22)$$

809  $\square$

## 810 B GRADIENT ANALYSIS OF CORRELATION

### 812 B.1 GRADIENT OF PEARSON CORRELATION W.R.T. ATTENTION LOGITS

814 **Lemma B.1** (Softmax Aggregator Jacobian). *The derivative of the aggregated embedding  $\mathbf{v}_s$  with*  
 815 *respect to a pre-softmax logit  $z_{si}$  is  $\partial \mathbf{v}_s / \partial z_{si} = \alpha_{si}(\mathbf{h}_{si} - \mathbf{v}_s)$  and consequently,  $\partial \hat{y}_s / \partial z_{si} =$*   
 816  *$\alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s)$ .*

818 *Proof.* Within a fixed sample  $s$ , the aggregated embedding is  $\mathbf{v}_s = \sum_{j=1}^{n_s} \alpha_{sj} \mathbf{h}_{sj}$ . We first recall  
 819 the derivative of the softmax function. The partial derivative of the  $j$ -th attention weight  $\alpha_{sj}$  with  
 820 respect to the  $i$ -th input logit  $z_{si}$  is given by:

$$821 \quad \frac{\partial \alpha_{sj}}{\partial z_{si}} = \alpha_{sj}(\delta_{ij} - \alpha_{si}), \quad (23)$$

823 where  $\delta_{ij}$  is the Kronecker delta ( $\delta_{ij} = 1$  if  $i = j$ , and 0 otherwise).

825 We can now compute the derivative of  $\mathbf{v}_s$  with respect to  $z_{si}$  using the chain rule:

$$827 \quad \frac{\partial \mathbf{v}_s}{\partial z_{si}} = \sum_{j=1}^{n_s} \frac{\partial \alpha_{sj}}{\partial z_{si}} \mathbf{h}_{sj} \quad (24)$$

$$830 \quad = \sum_{j=1}^{n_s} \alpha_{sj}(\delta_{ij} - \alpha_{si}) \mathbf{h}_{sj} \quad (25)$$

$$832 \quad = \sum_{j=1}^{n_s} \alpha_{sj} \delta_{ij} \mathbf{h}_{sj} - \sum_{j=1}^{n_s} \alpha_{sj} \alpha_{si} \mathbf{h}_{sj}. \quad (26)$$

835 The first term simplifies because  $\delta_{ij}$  is non-zero only when  $j = i$ :

$$837 \quad \sum_{j=1}^{n_s} \alpha_{sj} \delta_{ij} \mathbf{h}_{sj} = \alpha_{si} \mathbf{h}_{si}. \quad (27)$$

840 In the second term,  $\alpha_{si}$  is independent of the summation index  $j$  and can be factored out:

$$842 \quad \sum_{j=1}^{n_s} \alpha_{sj} \alpha_{si} \mathbf{h}_{sj} = \alpha_{si} \sum_{j=1}^{n_s} \alpha_{sj} \mathbf{h}_{sj} = \alpha_{si} \mathbf{v}_s. \quad (28)$$

844 Combining these results, we obtain:

$$846 \quad \frac{\partial \mathbf{v}_s}{\partial z_{si}} = \alpha_{si} \mathbf{h}_{si} - \alpha_{si} \mathbf{v}_s = \alpha_{si}(\mathbf{h}_{si} - \mathbf{v}_s). \quad (29)$$

848 Consequently, since the prediction is  $\hat{y}_s = \mathbf{w}^\top \mathbf{v}_s + c$ , its derivative is:

$$850 \quad \frac{\partial \hat{y}_s}{\partial z_{si}} = \mathbf{w}^\top \frac{\partial \mathbf{v}_s}{\partial z_{si}} = \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (30)$$

852  $\square$

853 **Theorem B.1** (Gradient of PCC w.r.t. Attention Logits). *For any  $s$ , the derivative of Pearson cor-*  
 854 *relation  $\rho$  with respect to a pre-softmax logit  $z_{si}$  is*

$$856 \quad \frac{\partial \rho}{\partial z_{si}} = \frac{1}{S \sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (31)$$

859 *Proof.* We express the Pearson correlation  $\rho$  as the ratio  $\rho = N/D$ , where  $N$  is the covariance and  
 860  $D$  is the product of standard deviations.

$$862 \quad N := \text{Cov}(y, \hat{y}) = \frac{1}{S} \sum_{t=1}^S a_t b_t, \quad D := \sigma_y \sigma_{\hat{y}}. \quad (32)$$

864 Recall that  $a_t := y_t - \mu_y$  and  $b_t := \hat{y}_t - \mu_{\hat{y}}$  are the centered targets and predictions, respectively,  
 865 satisfying  $\sum_t a_t = 0$  and  $\sum_t b_t = 0$ .  
 866

867 By the quotient rule, the derivative of  $\rho$  is:

$$868 \quad \frac{\partial \rho}{\partial z_{si}} = \frac{1}{D} \frac{\partial N}{\partial z_{si}} - \frac{N}{D^2} \frac{\partial D}{\partial z_{si}} = \frac{1}{D} \left( \frac{\partial N}{\partial z_{si}} - \rho \frac{\partial D}{\partial z_{si}} \right). \quad (33)$$

871 We compute the derivatives of  $N$  and  $D$  separately. Note that the logit  $z_{si}$  only directly affects the  
 872 prediction of sample  $s$ , i.e.,  $\partial \hat{y}_t / \partial z_{si} = 0$  if  $t \neq s$ .  
 873

874 **Step 1: Derivative of the Covariance ( $N$ ).**  
 875

$$876 \quad \frac{\partial N}{\partial z_{si}} = \frac{1}{S} \sum_{t=1}^S a_t \frac{\partial b_t}{\partial z_{si}}. \quad (34)$$

879 We expand the derivative of the centered prediction  $b_t = \hat{y}_t - \mu_{\hat{y}}$ :  
 880

$$881 \quad \frac{\partial b_t}{\partial z_{si}} = \frac{\partial \hat{y}_t}{\partial z_{si}} - \frac{\partial \mu_{\hat{y}}}{\partial z_{si}} = \frac{\partial \hat{y}_t}{\partial z_{si}} - \frac{1}{S} \sum_{u=1}^S \frac{\partial \hat{y}_u}{\partial z_{si}}. \quad (35)$$

884 Substituting this back into the expression for  $\partial N / \partial z_{si}$ :

$$886 \quad \frac{\partial N}{\partial z_{si}} = \frac{1}{S} \sum_t a_t \left( \frac{\partial \hat{y}_t}{\partial z_{si}} - \frac{1}{S} \sum_{u=1}^S \frac{\partial \hat{y}_u}{\partial z_{si}} \right) \quad (36)$$

$$889 \quad = \frac{1}{S} \left( \sum_t a_t \frac{\partial \hat{y}_t}{\partial z_{si}} \right) - \frac{1}{S^2} \left( \sum_t a_t \right) \left( \sum_{u=1}^S \frac{\partial \hat{y}_u}{\partial z_{si}} \right). \quad (37)$$

892 Since the targets are centered ( $\sum_t a_t = 0$ ), the second term vanishes:

$$893 \quad \frac{\partial N}{\partial z_{si}} = \frac{1}{S} \sum_t a_t \frac{\partial \hat{y}_t}{\partial z_{si}}. \quad (38)$$

896 Since  $\partial \hat{y}_t / \partial z_{si} = 0$  for  $t \neq s$ , the summation collapses to a single term:  
 897

$$898 \quad \frac{\partial N}{\partial z_{si}} = \frac{1}{S} a_s \frac{\partial \hat{y}_s}{\partial z_{si}}. \quad (39)$$

901 **Step 2: Derivative of the Standard Deviation Product ( $D$ ).** Since  $\sigma_y$  is constant with respect  
 902 to  $z_{si}$ , we have  $\partial D / \partial z_{si} = \sigma_y (\partial \sigma_{\hat{y}} / \partial z_{si})$ . To find the derivative of  $\sigma_{\hat{y}}$ , we first differentiate the  
 903 variance  $\sigma_{\hat{y}}^2 = \frac{1}{S} \sum_t b_t^2$ .

$$905 \quad \frac{\partial \sigma_{\hat{y}}^2}{\partial z_{si}} = \frac{\partial}{\partial z_{si}} \left( \frac{1}{S} \sum_t b_t^2 \right) = \frac{1}{S} \sum_t 2b_t \frac{\partial b_t}{\partial z_{si}}. \quad (40)$$

908 Similar to Step 1, we substitute the expression for  $\partial b_t / \partial z_{si}$  and use the fact that the predictions are  
 909 centered ( $\sum_t b_t = 0$ ):

$$911 \quad \frac{\partial \sigma_{\hat{y}}^2}{\partial z_{si}} = \frac{2}{S} \sum_t b_t \left( \frac{\partial \hat{y}_t}{\partial z_{si}} - \frac{1}{S} \sum_{u=1}^S \frac{\partial \hat{y}_u}{\partial z_{si}} \right) \quad (41)$$

$$914 \quad = \frac{2}{S} \left( \sum_t b_t \frac{\partial \hat{y}_t}{\partial z_{si}} \right) - \frac{2}{S^2} \left( \sum_t b_t \right) \left( \sum_{u=1}^S \frac{\partial \hat{y}_u}{\partial z_{si}} \right) \quad (42)$$

$$916 \quad = \frac{2}{S} \sum_t b_t \frac{\partial \hat{y}_t}{\partial z_{si}}. \quad (43)$$

918 Again, since  $\partial \hat{y}_t / \partial z_{si} = 0$  for  $t \neq s$ :

$$\frac{\partial \sigma_{\hat{y}}^2}{\partial z_{si}} = \frac{2}{S} b_s \frac{\partial \hat{y}_s}{\partial z_{si}}. \quad (44)$$

922 We now use the chain rule:  $\frac{\partial \sigma_{\hat{y}}^2}{\partial z_{si}} = 2\sigma_{\hat{y}} \frac{\partial \sigma_{\hat{y}}}{\partial z_{si}}$ . Equating the two expressions and solving for  $\frac{\partial \sigma_{\hat{y}}}{\partial z_{si}}$  (assuming  $\sigma_{\hat{y}} > 0$ ):

$$925 \quad 2\sigma_{\hat{y}} \frac{\partial \sigma_{\hat{y}}}{\partial z_{si}} = \frac{2}{S} b_s \frac{\partial \hat{y}_s}{\partial z_{si}} \implies \frac{\partial \sigma_{\hat{y}}}{\partial z_{si}} = \frac{b_s}{S\sigma_{\hat{y}}} \frac{\partial \hat{y}_s}{\partial z_{si}}. \quad (45)$$

927 Therefore, the derivative of the denominator  $D$  is:

$$928 \quad \frac{\partial D}{\partial z_{si}} = \sigma_y \frac{\partial \sigma_{\hat{y}}}{\partial z_{si}} = \frac{\sigma_y b_s}{S\sigma_{\hat{y}}} \frac{\partial \hat{y}_s}{\partial z_{si}}. \quad (46)$$

931 **Step 3: Combining the results.** We substitute the derivatives of  $N$  (Equation (39)) and  $D$  (Equation 932 (46)) back into the quotient rule formula (Equation (33)).

$$933 \quad \frac{\partial \rho}{\partial z_{si}} = \frac{1}{D} \left( \frac{\partial N}{\partial z_{si}} - \rho \frac{\partial D}{\partial z_{si}} \right) \quad (47)$$

$$936 \quad = \frac{1}{\sigma_y \sigma_{\hat{y}}} \left( \frac{a_s}{S} \frac{\partial \hat{y}_s}{\partial z_{si}} - \rho \frac{\sigma_y b_s}{S\sigma_{\hat{y}}} \frac{\partial \hat{y}_s}{\partial z_{si}} \right) \quad (48)$$

$$938 \quad = \frac{1}{S\sigma_y \sigma_{\hat{y}}} \left( a_s - \rho \frac{\sigma_y b_s}{\sigma_{\hat{y}}} \right) \frac{\partial \hat{y}_s}{\partial z_{si}} \quad (49)$$

$$940 \quad = \frac{1}{S\sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right) \frac{\partial \hat{y}_s}{\partial z_{si}}. \quad (50)$$

942 Finally, we substitute the expression for  $\partial \hat{y}_s / \partial z_{si}$  derived in Lemma B.1 (Equation (30)):

$$944 \quad \frac{\partial \rho}{\partial z_{si}} = \frac{1}{S\sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (51)$$

946 This concludes the proof.  $\square$

## C PROOFS FOR OPTIMIZATION DYNAMICS ANALYSIS

### C.1 PROOF OF LEMMA 2.3 (GRADIENT OF MSE W.R.T. ATTENTION LOGITS)

952 *Proof.* The Mean Squared Error (MSE) loss is defined as:

$$954 \quad \mathcal{L}_{\text{MSE}} = \frac{1}{S} \sum_{k=1}^S (y_k - \hat{y}_k)^2. \quad (52)$$

956 We compute the derivative with respect to the attention logit  $z_{si}$  using the chain rule:

$$958 \quad \frac{\partial \mathcal{L}_{\text{MSE}}}{\partial z_{si}} = \sum_{k=1}^S \frac{\partial \mathcal{L}_{\text{MSE}}}{\partial \hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_{si}}. \quad (53)$$

961 The derivative of the loss w.r.t. the prediction  $\hat{y}_k$  is:

$$962 \quad \frac{\partial \mathcal{L}_{\text{MSE}}}{\partial \hat{y}_k} = \frac{1}{S} \cdot 2(y_k - \hat{y}_k) \cdot (-1) = \frac{2}{S} (\hat{y}_k - y_k). \quad (54)$$

964 The derivative of the prediction  $\hat{y}_k$  w.r.t. the logit  $z_{si}$  is non-zero only if  $k = s$ . From Lemma 2.2, 965 we have:

$$966 \quad \frac{\partial \hat{y}_s}{\partial z_{si}} = \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (55)$$

968 Combining these results:

$$969 \quad \frac{\partial \mathcal{L}_{\text{MSE}}}{\partial z_{si}} = \frac{2}{S} (\hat{y}_s - y_s) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (56)$$

$\square$

972 C.2 PROOF OF COROLLARY 2.1 (PCC/MSE GRADIENT RATIO DECAY)  
973974 *Proof.* We analyze the ratio of the global scaling factors  $g_s^{\text{MSE}}$  and  $g_s^{\text{PCC}}$  identified in Section 2.3:  
975

976 
$$g_s^{\text{MSE}} = 2(\hat{y}_s - y_s), \quad (57)$$

977 
$$g_s^{\text{PCC}} = \frac{1}{\sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right). \quad (58)$$
  
978

980 We analyze their typical scale across samples using their Root Mean Square (RMS) values. We  
981 denote the empirical average over the batch as  $\mathbb{E}_s[\cdot]$ .  
982983 **Step 1: RMS scale of the PCC global factor.** We define normalized variables  $A_s := a_s/\sigma_y$   
984 and  $B_s := b_s/\sigma_{\hat{y}}$ . By construction,  $A_s$  and  $B_s$  have zero mean and unit variance ( $\text{Var}(A_s) =$   
985  $\text{Var}(B_s) = 1$ ), and their covariance is the PCC ( $\text{Cov}(A_s, B_s) = \rho$ ). The term inside the parenthesis  
986 of  $g_s^{\text{PCC}}$  is  $A_s - \rho B_s$ . Its variance is:  
987

988 
$$\text{Var}(A_s - \rho B_s) = \text{Var}(A_s) + \rho^2 \text{Var}(B_s) - 2\rho \text{Cov}(A_s, B_s) \quad (59)$$

989 
$$= 1 + \rho^2 - 2\rho^2 = 1 - \rho^2. \quad (60)$$

990 Since the mean of  $A_s - \rho B_s$  is zero, the RMS magnitude of  $g_s^{\text{PCC}}$  across samples is:  
991

992 
$$\text{RMS}_s(g_s^{\text{PCC}}) = \sqrt{\mathbb{E}_s[(g_s^{\text{PCC}})^2]} = \frac{1}{\sigma_{\hat{y}}} \sqrt{\text{Var}(A_s - \rho B_s)} = \frac{\sqrt{1 - \rho^2}}{\sigma_{\hat{y}}}. \quad (61)$$
  
993

995 **Step 2: RMS scale of the MSE global factor.** For the MSE global factor, we have:  
996

997 
$$\text{RMS}_s(g_s^{\text{MSE}}) = \sqrt{\mathbb{E}_s[2(\hat{y}_s - y_s)^2]} = 2\sqrt{\mathbb{E}_s[(\hat{y}_s - y_s)^2]} \quad (62)$$

998 
$$= 2\sqrt{\text{MSE}(\mathbf{y}, \hat{\mathbf{y}})}. \quad (63)$$
  
999

1000 **Step 3: Bounding the ratio of RMS global factors.** The ratio  $r_{\text{global}}$  is defined as:  
1001

1002 
$$r_{\text{global}} = \frac{\text{RMS}_s(g_s^{\text{PCC}})}{\text{RMS}_s(g_s^{\text{MSE}})} = \frac{\sqrt{1 - \rho^2}}{2\sigma_{\hat{y}}\sqrt{\text{MSE}}}. \quad (64)$$
  
1003

1004 We use the MSE decomposition (Theorem 2.1):  
1005

1006 
$$\text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) = (\mu_{\hat{\mathbf{y}}} - \mu_{\mathbf{y}})^2 + (\sigma_{\hat{\mathbf{y}}} - \sigma_{\mathbf{y}})^2 + 2\sigma_{\mathbf{y}}\sigma_{\hat{\mathbf{y}}}(1 - \rho). \quad (65)$$
  
1007

1008 Since all terms are non-negative, we obtain a lower bound for MSE:  
1009

1010 
$$\text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) \geq 2\sigma_{\mathbf{y}}\sigma_{\hat{\mathbf{y}}}(1 - \rho). \quad (66)$$
  
1011

1012 We assume  $\rho \in [0, 1]$ , which is typical during training. We use the inequality:  
1013

1014 
$$1 - \rho^2 = (1 - \rho)(1 + \rho) \leq 2(1 - \rho) \implies \sqrt{1 - \rho^2} \leq \sqrt{2}\sqrt{1 - \rho}. \quad (67)$$
  
1015

1016 Plugging the bounds from equation 66 and equation 67 into the ratio definition equation 64:  
1017

1018 
$$r_{\text{global}} \leq \frac{\sqrt{2}\sqrt{1 - \rho}}{2\sigma_{\hat{y}}\sqrt{2\sigma_{\mathbf{y}}\sigma_{\hat{\mathbf{y}}}(1 - \rho)}} \quad (68)$$
  
1019

1020 
$$= \frac{\sqrt{2}\sqrt{1 - \rho}}{2\sigma_{\hat{y}} \cdot \sqrt{2}\sqrt{\sigma_{\mathbf{y}}\sigma_{\hat{\mathbf{y}}}\sqrt{1 - \rho}}} \quad (69)$$
  
1021

1022 
$$= \frac{1}{2\sigma_{\hat{y}}\sqrt{\sigma_{\mathbf{y}}\sigma_{\hat{\mathbf{y}}}}} = \frac{1}{2\sqrt{\sigma_{\mathbf{y}}}} \cdot \frac{1}{\sigma_{\hat{y}}^{3/2}}. \quad (70)$$
  
1023

1024 This completes the proof.  $\square$   
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## C.3 DERIVATION OF THE GRADIENT MAGNITUDE BOUND

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**Lemma C.1** (Within-sample Dispersion Bound). *Recall the definitions  $\boldsymbol{\mu}_s = \frac{1}{n_s} \sum_{j=1}^{n_s} \mathbf{h}_{sj}$  (within-sample mean) and  $\sigma_s^2 = \frac{1}{n_s} \sum_{j=1}^{n_s} \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|^2$  (within-sample variance). Also recall  $\mathbf{v}_s = \sum_{j=1}^{n_s} \alpha_{sj} \mathbf{h}_{sj}$  where  $\alpha_{sj} \geq 0$  and  $\sum_j \alpha_{sj} = 1$ . Then for every  $i \in \{1, \dots, n_s\}$ ,*

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1033

$$\|\mathbf{h}_{si} - \mathbf{v}_s\| \leq 2\sqrt{n_s} \sigma_s.$$

1034  
1035

*Proof.* Fix sample  $s$  and index  $i$ . We use the triangle inequality by inserting the within-sample mean  $\boldsymbol{\mu}_s$ :

1036

$$\|\mathbf{h}_{si} - \mathbf{v}_s\| = \|\mathbf{h}_{si} - \boldsymbol{\mu}_s + \boldsymbol{\mu}_s - \mathbf{v}_s\| \leq \|\mathbf{h}_{si} - \boldsymbol{\mu}_s\| + \|\mathbf{v}_s - \boldsymbol{\mu}_s\|. \quad (71)$$

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1039

We bound each term on the right-hand side separately.

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1041

**Term 1:  $\|\mathbf{h}_{si} - \boldsymbol{\mu}_s\|$ .** We first bound the deviation by the maximum deviation within the sample:

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1043

$$\|\mathbf{h}_{si} - \boldsymbol{\mu}_s\| \leq \max_j \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|. \quad (72)$$

1044  
1045  
1046

The maximum of non-negative numbers is bounded by the square root of the sum of their squares (i.e.,  $x_k^2 \leq \sum_j x_j^2$  implies  $x_k \leq \sqrt{\sum_j x_j^2}$ ):

1047  
1048  
1049  
1050

$$\max_j \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\| \leq \sqrt{\sum_{j=1}^{n_s} \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|^2}. \quad (73)$$

1051

By the definition of  $\sigma_s^2$ , the sum of squares is  $n_s \sigma_s^2$ . Thus,

1052

$$\|\mathbf{h}_{si} - \boldsymbol{\mu}_s\| \leq \sqrt{n_s \sigma_s^2} = \sqrt{n_s} \sigma_s. \quad (74)$$

1054

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**Term 2:  $\|\mathbf{v}_s - \boldsymbol{\mu}_s\|$ .** We express the deviation of the aggregated embedding  $\mathbf{v}_s$  from the mean  $\boldsymbol{\mu}_s$ . Since  $\sum_j \alpha_{sj} = 1$ , we have  $\boldsymbol{\mu}_s = \sum_j \alpha_{sj} \boldsymbol{\mu}_s$ .

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$$\mathbf{v}_s - \boldsymbol{\mu}_s = \sum_{j=1}^{n_s} \alpha_{sj} \mathbf{h}_{sj} - \sum_{j=1}^{n_s} \alpha_{sj} \boldsymbol{\mu}_s = \sum_{j=1}^{n_s} \alpha_{sj} (\mathbf{h}_{sj} - \boldsymbol{\mu}_s). \quad (75)$$

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Using the convexity of the norm (Jensen's inequality):

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1063  
1064

$$\|\mathbf{v}_s - \boldsymbol{\mu}_s\| = \left\| \sum_{j=1}^{n_s} \alpha_{sj} (\mathbf{h}_{sj} - \boldsymbol{\mu}_s) \right\| \leq \sum_{j=1}^{n_s} \alpha_{sj} \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|. \quad (76)$$

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This weighted average is bounded by the maximum element:

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1068  
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$$\sum_{j=1}^{n_s} \alpha_{sj} \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\| \leq \max_j \|\mathbf{h}_{sj} - \boldsymbol{\mu}_s\|. \quad (77)$$

1070  
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As established for Term 1 (Equation (74)), the maximum deviation is bounded by  $\sqrt{n_s} \sigma_s$ . Therefore,

1072  
1073

$$\|\mathbf{v}_s - \boldsymbol{\mu}_s\| \leq \sqrt{n_s} \sigma_s. \quad (78)$$

1074  
1075

**Conclusion.** Substituting the bounds from Equation (74) and Equation (78) into Equation (71):

1076

$$\|\mathbf{h}_{si} - \mathbf{v}_s\| \leq \sqrt{n_s} \sigma_s + \sqrt{n_s} \sigma_s = 2\sqrt{n_s} \sigma_s. \quad \square$$

1077  
1078  
1079

**Lemma C.2** (Magnitude Bound of a Centered, Unit-variance Vector). *Let  $x_1, \dots, x_S \in \mathbb{R}$  satisfy  $\sum_{s=1}^S x_s = 0$  and  $\frac{1}{S} \sum_{s=1}^S x_s^2 = 1$  (equivalently  $\sum_{s=1}^S x_s^2 = S$ ). Then for every  $j \in \{1, \dots, S\}$ , we have  $|x_j| \leq \sqrt{S-1}$ .*

1080 *Proof.* Fix an index  $j$ . Since the vector is centered ( $\sum_{s=1}^S x_s = 0$ ), we can express  $x_j$  in terms of  
 1081 the other elements:  $x_j = -\sum_{s \neq j} x_s$ . We analyze the squared magnitude  $x_j^2$  using the Cauchy-  
 1082 Schwarz inequality and view the summation as a dot product between a vector of ones  $\mathbf{1} \in \mathbb{R}^{S-1}$   
 1083 and the vector  $(x_s)_{s \neq j} \in \mathbb{R}^{S-1}$ .  
 1084

$$1085 \quad x_j^2 = \left( \sum_{s \neq j} 1 \cdot x_s \right)^2 \leq \left( \sum_{s \neq j} 1^2 \right) \left( \sum_{s \neq j} x_s^2 \right) = (S-1) \sum_{s \neq j} x_s^2. \quad (79)$$

1088 We use the unit-variance condition,  $\sum_{s=1}^S x_s^2 = S$ . Therefore,  $\sum_{s \neq j} x_s^2 = S - x_j^2$ . Substituting this  
 1089 into the inequality:  
 1090

$$1091 \quad x_j^2 \leq (S-1)(S - x_j^2) = S(S-1) - (S-1)x_j^2. \quad (80)$$

1092 Rearranging the terms to isolate  $x_j^2$ :  
 1093

$$1094 \quad x_j^2 + (S-1)x_j^2 \leq S(S-1) \quad (81)$$

$$1095 \quad S x_j^2 \leq S(S-1). \quad (82)$$

1097 Dividing by  $S$  (which is positive) gives  $x_j^2 \leq S-1$ . Taking the square root yields the desired bound:  
 1098

$$1099 \quad |x_j| \leq \sqrt{S-1}. \quad \square$$

1101 **Corollary C.1** (Gradient Magnitude Bound). *The magnitude of the PCC gradient in Theorem 2.1  
 1102 can be bounded by*

$$1103 \quad \left| \frac{\partial \rho}{\partial z_{si}} \right| \leq \frac{1}{\sigma_{\hat{y}}} \frac{4\sqrt{n_s(S-1)}}{S} \|\mathbf{w}\| \sigma_s. \quad (83)$$

1106 *Proof.* We start from the expression for the PCC gradient derived in Theorem B.1:

$$1108 \quad \frac{\partial \rho}{\partial z_{si}} = \frac{1}{S\sigma_{\hat{y}}} \left( \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right) \alpha_{si} \mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s). \quad (84)$$

1111 We analyze the magnitude of this expression by applying the triangle inequality and the Cauchy-  
 1112 Schwarz inequality ( $|\mathbf{w}^\top \mathbf{x}| \leq \|\mathbf{w}\| \|\mathbf{x}\|$ ):

$$1113 \quad \left| \frac{\partial \rho}{\partial z_{si}} \right| \leq \frac{|\alpha_{si}|}{S\sigma_{\hat{y}}} \left| \frac{a_s}{\sigma_y} - \rho \frac{b_s}{\sigma_{\hat{y}}} \right| \|\mathbf{w}^\top (\mathbf{h}_{si} - \mathbf{v}_s)\| \quad (85)$$

$$1116 \quad \leq \frac{|\alpha_{si}|}{S\sigma_{\hat{y}}} \left( \left| \frac{a_s}{\sigma_y} \right| + |\rho| \left| \frac{b_s}{\sigma_{\hat{y}}} \right| \right) \|\mathbf{w}\| \|\mathbf{h}_{si} - \mathbf{v}_s\|. \quad (86)$$

1118 We now bound the individual components.

- 1121 1. **Attention weight:** Since  $\alpha_s$  is a probability from Softmax,  $0 \leq \alpha_{si} \leq 1$
- 1122 2. **Correlation coefficient:** By definition,  $-1 \leq \rho \leq 1$ , so  $|\rho| \leq 1$
- 1124 3. **Standardized scores:** The terms  $\frac{a_s}{\sigma_y}$  and  $\frac{b_s}{\sigma_{\hat{y}}}$  are the standardized scores (z-scores) of the  
 1125 target and prediction for sample  $s$ . They form centered, unit-variance vectors across the  $S$   
 1126 samples. By applying Lemma C.2, we have:

$$1128 \quad \left| \frac{a_s}{\sigma_y} \right| \leq \sqrt{S-1} \quad \text{and} \quad \left| \frac{b_s}{\sigma_{\hat{y}}} \right| \leq \sqrt{S-1}.$$

- 1131 4. **Within-sample dispersion:** The term  $\|\mathbf{h}_{si} - \mathbf{v}_s\|$  represents the deviation of the embedding  
 1132  $\mathbf{h}_{si}$  from the aggregated embedding  $\mathbf{v}_s$ . By applying Lemma C.1, we have:

$$1133 \quad \|\mathbf{h}_{si} - \mathbf{v}_s\| \leq 2\sqrt{n_s} \sigma_s.$$

1134 Substituting these bounds into the inequality:  
 1135

$$1136 \quad \left| \frac{\partial \rho}{\partial z_{si}} \right| \leq \frac{1}{S\sigma_{\hat{y}}} \left( \sqrt{S-1} + 1\sqrt{S-1} \right) \|\mathbf{w}\| (2\sqrt{n_s}\sigma_s) \quad (87)$$

$$1138 \quad = \frac{1}{S\sigma_{\hat{y}}} (2\sqrt{S-1}) \|\mathbf{w}\| (2\sqrt{n_s}\sigma_s) \quad (88)$$

$$1140 \quad = \frac{4\sqrt{n_s(S-1)}}{S\sigma_{\hat{y}}} \|\mathbf{w}\| \sigma_s. \quad (89)$$

1143 Rearranging the terms to highlight the key factors identified in the main text:  
 1144

$$1145 \quad \left| \frac{\partial \rho}{\partial z_{si}} \right| \leq \underbrace{\frac{1}{\sigma_{\hat{y}}}}_{\substack{\text{prediction} \\ \text{deviation}}} \cdot \underbrace{\frac{4\sqrt{n_s(S-1)}}{S}}_{\substack{\text{batch scale}}} \cdot \underbrace{\|\mathbf{w}\|}_{\substack{\text{regression} \\ \text{weights}}} \cdot \underbrace{\sigma_s}_{\text{in-sample dispersion}}. \quad (90)$$

1149 This concludes the proof.  $\square$   
 1150

## 1152 D ACHIEVABLE PCC BOUND OF CONVEX ATTENTION MODELS

1154 This section provides the detailed analysis and proof of an intrinsic upper bound on the PCC gain  
 1155 that any convex attention mechanism can achieve compared to a simple mean-pooling baseline. This  
 1156 analysis formalizes the capacity limitation imposed by the convex hull constraint.  
 1157

1158 **Setup and Decomposition.** We consider a dataset of  $S$  samples. For sample  $s$ , we have element  
 1159 embeddings  $\mathbf{h}_s = \{\mathbf{h}_{si}\}_{i=1}^{n_s}$  where  $\mathbf{h}_{si} \in \mathbb{R}^d$ . Let  $\boldsymbol{\mu}_s := \frac{1}{n_s} \sum_{i=1}^{n_s} \mathbf{h}_{si}$  be the mean-pooling embed-  
 1160 ding. A convex attention mechanism computes weights  $\{\alpha_{si}\}_{i=1}^{n_s}$  such that  $\alpha_{si} \geq 0$  and  $\sum_i \alpha_{si} = 1$ .  
 1161 The aggregated embedding is  $\mathbf{v}_s = \sum_i \alpha_{si} \mathbf{h}_{si}$ . The prediction is given by a linear regression head  
 1162 ( $\mathbf{w}, b$ ):  $\hat{y}_s = \mathbf{w}^\top \mathbf{v}_s + c$ .

1163 We decompose the prediction relative to the mean-pooling baseline:  
 1164

$$1165 \quad \hat{y}_s = \underbrace{(\mathbf{w}^\top \boldsymbol{\mu}_s + c)}_{\bar{y}_s} + \underbrace{\mathbf{w}^\top (\mathbf{v}_s - \boldsymbol{\mu}_s)}_{\Delta \hat{y}_s}. \quad (91)$$

1167 Here,  $\bar{y}_s$  is the baseline prediction, and  $\Delta \hat{y}_s$  is the attention-induced perturbation.  
 1168

1169 **Quantifying Dispersion and Variation.** We introduce measures for within-sample dispersion (re-  
 1170 lated to in-sample homogeneity) and across-sample variation. Throughout this section,  $\|\cdot\|_2$  denotes  
 1171 the  $\ell_2$  norm. We assume the empirical definition for standard deviation (normalized by  $1/S$ ).  
 1172

1173 **Definition D.1** (Intrinsic Dispersion and Baseline Variation). *For each sample  $s$ , define the maxi-  
 1174 mum within-sample deviation (the radius of the convex hull centered at the mean):*

$$1175 \quad R_s := \max_{1 \leq i \leq n_s} \|\mathbf{h}_{si} - \boldsymbol{\mu}_s\|_2. \quad (92)$$

1177 Define the intrinsic within-sample dispersion  $\tilde{R}$  as the root mean square (RMS) of these radii across  
 1178 the dataset:  
 1179

$$1180 \quad \tilde{R} := \sqrt{\frac{1}{S} \sum_{s=1}^S R_s^2}. \quad (93)$$

1183 Let  $\sigma_0 := \text{std}_s(\bar{y}_s)$  denote the standard deviation of the baseline predictions across samples.  
 1184

1185 **Remark D.1.**  $\tilde{R}$  measures the intrinsic homogeneity of the embeddings within samples, independent  
 1186 of the regression head  $\mathbf{w}$ .  $\sigma_0$  captures the variation of the mean embeddings projected onto the  
 1187 regression space. By the scaling property of the standard deviation,  $\sigma_0 = \|\mathbf{w}\|_2 \text{std}_s(\hat{\mathbf{w}}^\top \boldsymbol{\mu}_s)$ ,  
 1188 where  $\hat{\mathbf{w}} := \mathbf{w}/\|\mathbf{w}\|_2$ .

1188    **Centered Notation.** We define the vectors of predictions across the  $S$  samples:  $\hat{\mathbf{y}}, \bar{\mathbf{y}}, \Delta\hat{\mathbf{y}} \in \mathbb{R}^S$ .  
 1189    From Equation (91), we have  $\hat{\mathbf{y}} = \bar{\mathbf{y}} + \Delta\hat{\mathbf{y}}$ .  
 1190

1191    We denote the centered versions of these vectors (by subtracting their respective means  $\mu_{\hat{\mathbf{y}}}, \mu_{\bar{\mathbf{y}}}, \mu_{\Delta\hat{\mathbf{y}}}$ )  
 1192    as  $\mathbf{b}, \bar{\mathbf{b}}, \Delta\mathbf{b}$ . By linearity, the decomposition holds for centered vectors:  $\mathbf{b} = \bar{\mathbf{b}} + \Delta\mathbf{b}$ . We denote  
 1193    the centered ground-truth targets as  $\mathbf{a}$ , where  $a_s = y_s - \mu_y$ .

1194    The Pearson correlation coefficient (PCC) is the cosine similarity between centered vectors. Let  
 1195     $\rho = \text{PCC}(\mathbf{a}, \mathbf{b})$  and  $\rho_0 = \text{PCC}(\mathbf{a}, \bar{\mathbf{b}})$ .  
 1196

1197    **Bounding the Attention Perturbation.** We first establish bounds on the magnitude of the pertur-  
 1198    bation  $\Delta\hat{\mathbf{y}}$  and its centered counterpart  $\Delta\mathbf{b}$ .  
 1199

1200    **Lemma D.1** (Bound on Prediction Perturbation). *For any convex attention weights  $\{\alpha_{si}\}$ , the per-  
 1200    turbation for sample  $s$  is bounded by:*

$$1201 \quad |\Delta\hat{y}_s| \leq \|\mathbf{w}\|_2 R_s.$$

1202    *Consequently, the L2 norm of the centered perturbation vector is bounded by:*

$$1204 \quad \|\Delta\mathbf{b}\|_2 \leq \sqrt{S} \|\mathbf{w}\|_2 \tilde{R}.$$

1206    *Proof.* We analyze the perturbation term. Since  $\sum_i \alpha_{si} = 1$ , we can write  $\boldsymbol{\mu}_s = \sum_i \alpha_{si} \boldsymbol{\mu}_s$ .  
 1207

$$1208 \quad \Delta\hat{y}_s = \mathbf{w}^\top (\mathbf{v}_s - \boldsymbol{\mu}_s) = \mathbf{w}^\top \left( \sum_{i=1}^{n_s} \alpha_{si} \mathbf{h}_{si} - \sum_{i=1}^{n_s} \alpha_{si} \boldsymbol{\mu}_s \right) = \mathbf{w}^\top \sum_{i=1}^{n_s} \alpha_{si} (\mathbf{h}_{si} - \boldsymbol{\mu}_s).$$

1211    Taking the absolute value:

$$\begin{aligned} 1212 \quad |\Delta\hat{y}_s| &\leq \|\mathbf{w}\|_2 \left\| \sum_i \alpha_{si} (\mathbf{h}_{si} - \boldsymbol{\mu}_s) \right\| \quad (\text{Cauchy-Schwarz}) \\ 1213 \\ 1214 \quad &\leq \|\mathbf{w}\|_2 \sum_i \alpha_{si} \|\mathbf{h}_{si} - \boldsymbol{\mu}_s\| \quad (\text{Convexity of norm / Triangle inequality}) \\ 1215 \\ 1216 \quad &\leq \|\mathbf{w}\|_2 \sum_i \alpha_{si} R_s \quad (\text{Definition of } R_s) \\ 1217 \\ 1218 \quad &= \|\mathbf{w}\|_2 R_s. \\ 1219 \end{aligned}$$

1220    To bound the L2 norm of the uncentered perturbation vector  $\Delta\hat{\mathbf{y}}$ , we sum the squared bounds across  
 1221    samples:

$$1223 \quad \|\Delta\hat{\mathbf{y}}\|_2^2 = \sum_{s=1}^S |\Delta\hat{y}_s|^2 \leq \sum_{s=1}^S (\|\mathbf{w}\|_2 R_s)^2 = \|\mathbf{w}\|_2^2 \sum_{s=1}^S R_s^2.$$

1225    Using the definition of the RMS dispersion  $\tilde{R}^2 = \frac{1}{S} \sum_s R_s^2$ , we get:

$$1227 \quad \|\Delta\hat{\mathbf{y}}\|_2^2 \leq S \|\mathbf{w}\|_2^2 \tilde{R}^2 \implies \|\Delta\hat{\mathbf{y}}\|_2 \leq \sqrt{S} \|\mathbf{w}\|_2 \tilde{R}.$$

1228    Finally,  $\Delta\mathbf{b}$  is the centered vector of  $\Delta\hat{\mathbf{y}}$ . Centering a vector (projecting onto the subspace or-  
 1229    thogonal to the constant vector (Arefidamghani et al., 2022; Wang et al., 2010)) is a non-expansive  
 1230    operation on  $\ell_2$  space, hence  $\|\Delta\mathbf{b}\|_2 \leq \|\Delta\hat{\mathbf{y}}\|_2 \leq \sqrt{S} \|\mathbf{w}\|_2 \tilde{R}$ .  $\square$   
 1231

1232    **General Correlation Perturbation Lemma.** We utilize a general result bounding the change in  
 1233    the cosine similarity when one vector is perturbed.

1234    **Lemma D.2** (Correlation perturbation). *For any  $\mathbf{a}, \mathbf{b}, \delta \in \mathbb{R}^S$  with  $\|\delta\|_2 < \|\mathbf{b}\|_2$ ,*

$$1236 \quad \left| \frac{\mathbf{a} \cdot (\mathbf{b} + \delta)}{\|\mathbf{a}\|_2 \|\mathbf{b} + \delta\|_2} - \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{a}\|_2 \|\mathbf{b}\|_2} \right| \leq \frac{2 \|\delta\|_2}{\|\mathbf{b}\|_2 - \|\delta\|_2}.$$

1239    *Proof.* Let  $\hat{\mathbf{a}} = \mathbf{a}/\|\mathbf{a}\|_2$ . Using triangle inequality, we have:

$$1241 \quad \left| \frac{\hat{\mathbf{a}} \cdot (\mathbf{b} + \delta)}{\|\mathbf{b} + \delta\|_2} - \frac{\hat{\mathbf{a}} \cdot \mathbf{b}}{\|\mathbf{b}\|_2} \right| = \left| \frac{\hat{\mathbf{a}} \cdot \mathbf{b}}{\|\mathbf{b} + \delta\|_2} - \frac{\hat{\mathbf{a}} \cdot \mathbf{b}}{\|\mathbf{b}\|_2} + \frac{\hat{\mathbf{a}} \cdot \delta}{\|\mathbf{b} + \delta\|_2} \right| \quad (94)$$

$$1242 \leq \underbrace{(\hat{\mathbf{a}} \cdot \mathbf{b}) \left( \frac{1}{\|\mathbf{b} + \delta\|_2} - \frac{1}{\|\mathbf{b}\|_2} \right)}_{T_1} + \underbrace{\frac{\hat{\mathbf{a}} \cdot \delta}{\|\mathbf{b} + \delta\|_2}}_{T_2}. \quad (95)$$

1246 We analyze each term. For  $T_2$ , by Cauchy–Schwarz ( $|\hat{\mathbf{a}} \cdot \delta| \leq \|\delta\|_2$ ) and the reverse triangle  
1247 inequality ( $\|\mathbf{b} + \delta\|_2 \geq \|\mathbf{b}\|_2 - \|\delta\|_2$ ), we have  $T_2 \leq \frac{\|\delta\|_2}{\|\mathbf{b}\|_2 - \|\delta\|_2}$ .

1249 For  $T_1$ , we rewrite the expression:  $T_1 = |\hat{\mathbf{a}} \cdot \mathbf{b}| \left| \frac{\|\mathbf{b}\|_2 - \|\mathbf{b} + \delta\|_2}{\|\mathbf{b}\|_2 \|\mathbf{b} + \delta\|_2} \right|$ .

1251 Using Cauchy–Schwarz ( $|\hat{\mathbf{a}} \cdot \mathbf{b}| \leq \|\mathbf{b}\|_2$ ), and the reverse triangle inequality ( $|\|\mathbf{b}\|_2 - \|\mathbf{b} + \delta\|_2| \leq$   
1252  $\|\delta\|_2$ ) again, we get:  $T_1 \leq \|\mathbf{b}\|_2 \frac{\|\delta\|_2}{\|\mathbf{b}\|_2 (\|\mathbf{b}\|_2 - \|\delta\|_2)} = \frac{\|\delta\|_2}{\|\mathbf{b}\|_2 - \|\delta\|_2}$ . Summing  $T_1$  and  $T_2$  completes the  
1254 proof.  $\square$

## 1257 D.1 MAIN RESULT: ACHIEVABLE PCC GAIN

1259 We now combine these lemmas to prove the main theorem regarding the capacity ceiling of convex  
1260 attention.

1261 **Theorem D.1** (Achievable PCC Gain Bound for Convex Attention). *Let  $\rho_0$  be the PCC achieved  
1262 by the mean-pooling baseline  $\bar{\mathbf{y}}$ , and  $\rho$  the PCC achieved by any convex attention mechanism  $\hat{\mathbf{y}}$ .  
1263 Assume  $\|\mathbf{w}\|_2 > 0$ . If the intrinsic dispersion is small relative to the baseline variation such that  
1264  $\tilde{R} < \sigma_0/\|\mathbf{w}\|_2$ , then:*

$$1265 \quad |\rho - \rho_0| \leq \frac{2 \|\mathbf{w}\|_2 \tilde{R}}{\sigma_0 - \|\mathbf{w}\|_2 \tilde{R}} = \frac{2 \tilde{R}}{\sigma_0/\|\mathbf{w}\|_2 - \tilde{R}}.$$

1269 *Proof.* We apply Lemma D.2 using the centered vectors:  $\mathbf{m} = \mathbf{a}$  (centered targets),  $\mathbf{n} = \bar{\mathbf{b}}$  (centered  
1270 baseline predictions), and  $\delta = \Delta \mathbf{b}$  (centered attention perturbation).

1271 First, we relate the L2 norms of the centered vectors to the defined dispersion measures. By the  
1272 definition of the empirical standard deviation  $\sigma_0$ , we have:

$$1274 \quad \|\bar{\mathbf{b}}\|_2 = \sqrt{\sum_s (\bar{y}_s - \mu_{\bar{y}})^2} = \sqrt{S} \sigma_0.$$

1277 By Lemma D.1, the perturbation is bounded by:

$$1278 \quad \|\Delta \mathbf{b}\|_2 \leq \sqrt{S} \|\mathbf{w}\|_2 \tilde{R}.$$

1280 Next, we verify the condition required for Lemma D.2,  $\|\delta\|_2 < \|\mathbf{n}\|_2$ . The assumption  $\tilde{R} <$   
1281  $\sigma_0/\|\mathbf{w}\|_2$  implies  $\|\mathbf{w}\|_2 \tilde{R} < \sigma_0$ . Multiplying by  $\sqrt{S}$ , we get:

$$1283 \quad \sqrt{S} \|\mathbf{w}\|_2 \tilde{R} < \sqrt{S} \sigma_0.$$

1285 Therefore,  $\|\Delta \mathbf{b}\|_2 < \|\bar{\mathbf{b}}\|_2$ , satisfying the prerequisite.

1286 Now, applying Lemma D.2:

$$1287 \quad |\rho - \rho_0| \leq \frac{2 \|\Delta \mathbf{b}\|_2}{\|\bar{\mathbf{b}}\|_2 - \|\Delta \mathbf{b}\|_2}.$$

1289 Since the function  $f(x) = 2x/(C - x)$  is monotonically increasing for  $x < C$  (where  $C = \|\bar{\mathbf{b}}\|_2$ ),  
1290 we substitute the upper bound for  $\|\Delta \mathbf{b}\|_2$ :

$$1292 \quad |\rho - \rho_0| \leq \frac{2 (\sqrt{S} \|\mathbf{w}\|_2 \tilde{R})}{\sqrt{S} \sigma_0 - (\sqrt{S} \|\mathbf{w}\|_2 \tilde{R})} \\ 1293 \quad = \frac{2 \|\mathbf{w}\|_2 \tilde{R}}{\sigma_0 - \|\mathbf{w}\|_2 \tilde{R}}.$$

1296 Dividing the numerator and denominator by  $\|\mathbf{w}\|_2$  (which is positive by assumption) yields the  
 1297 scale-invariant form:

$$1298 \quad 1299 \quad 1300 \quad 1301 \quad 1302 \quad 1303 \quad 1304 \quad 1305 \quad 1306 \quad 1307 \quad 1308 \quad 1309 \quad 1310 \quad 1311 \quad 1312 \quad 1313 \quad 1314 \quad 1315 \quad 1316 \quad 1317 \quad 1318 \quad 1319 \quad 1320 \quad 1321 \quad 1322 \quad 1323 \quad 1324 \quad 1325 \quad 1326 \quad 1327 \quad 1328 \quad 1329 \quad 1330 \quad 1331 \quad 1332 \quad 1333 \quad 1334 \quad 1335 \quad 1336 \quad 1337 \quad 1338 \quad 1339 \quad 1340 \quad 1341 \quad 1342 \quad 1343 \quad 1344 \quad 1345 \quad 1346 \quad 1347 \quad 1348 \quad 1349$$

$$|\rho - \rho_0| \leq \frac{2 \tilde{R}}{\sigma_0 / \|\mathbf{w}\|_2 - \tilde{R}}.$$

□

## D.2 CONNECTION BETWEEN IN-SAMPLE DISPERSION AND RADIUS

**Lemma D.3** (Dispersion–Radius Connection). *For each sample  $s$ ,  $R_s / \sqrt{n_s} \leq \sigma_s \leq R_s$ . Consequently, we denote  $\tilde{\sigma} := \left( \frac{1}{S} \sum_{s=1}^S \sigma_s^2 \right)^{1/2}$  with  $n_{\max} = \max_s n_s$ , we have  $\tilde{R} / \sqrt{n_{\max}} \leq \tilde{\sigma} \leq \tilde{R}$ .*

## E GENERALITY OF THEORETICAL ANALYSIS REGARDING ARCHITECTURE DEPTH

A potential concern regarding our theoretical analysis is whether the findings derived for attention aggregation apply to deep, multi-layer architectures. In this section, we clarify that our analysis focuses on the aggregation mechanism at the readout stage, which dictates the final prediction behavior regardless of the depth of the preceding backbone.

**Backbone-Agnostic Formulation.** Our theoretical model assumes input embeddings  $\mathbf{h}_s = \{\mathbf{h}_{si}\}_{i=1}^{n_s}$ . In the context of deep learning, these are not raw inputs but rather the latent representations produced by a backbone function  $f_\theta(\cdot)$  (comprising multiple Transformer blocks, FFNs, residual connections, and LayerNorms). The final prediction is modeled as  $\hat{y}_s = \mathbf{w}^\top \mathbf{v}_s + c$ , where  $\mathbf{v}_s$  is a convex combination of these final-layer representations. This formulation exactly matches the standard architectural paradigm used in modern Transformers:

- **[CLS] Token Aggregation:** In models like BERT or ViT, the prediction is often derived from a specific [CLS] token. However, in a standard Transformer layer, the output embedding of the [CLS] token is computed via the attention mechanism, which is a convex combination (softmax) of the element embeddings from the previous layer. Thus, the readout remains a convex aggregation of the backbone’s features, subject to the analysis we present.
- **Global Average Pooling:** Many regression heads utilize global average pooling over token embeddings, which is a special case of convex attention where uniform weights are applied ( $\alpha_{si} = 1/n_s$ ).

**The Readout Bottleneck.** Our analysis (Theorem 2.2) establishes that the achievable PCC gain is bounded by the convex hull of the input embeddings. Even with a highly expressive deep backbone  $f_\theta$ , if the final aggregation step is convex, the prediction  $\hat{y}_s$  is geometrically constrained to the interior of the simplex formed by the final-layer features  $\{\mathbf{h}_{si}\}$ . Crucially, deep backbones do not inherently solve the *homogeneity* issue. In fact, models pre-trained with contrastive objectives often produce highly homogeneous embeddings for in-sample elements (semantically similar tokens or patches), which shrinks the convex hull radius  $R_s$  and exacerbates the capacity limitation.

**Empirical Validation on Deep Architectures.** Our experimental evaluation in Section 5.1 and Table 2 utilizes deep, multi-layer architectures, not shallow regressors.

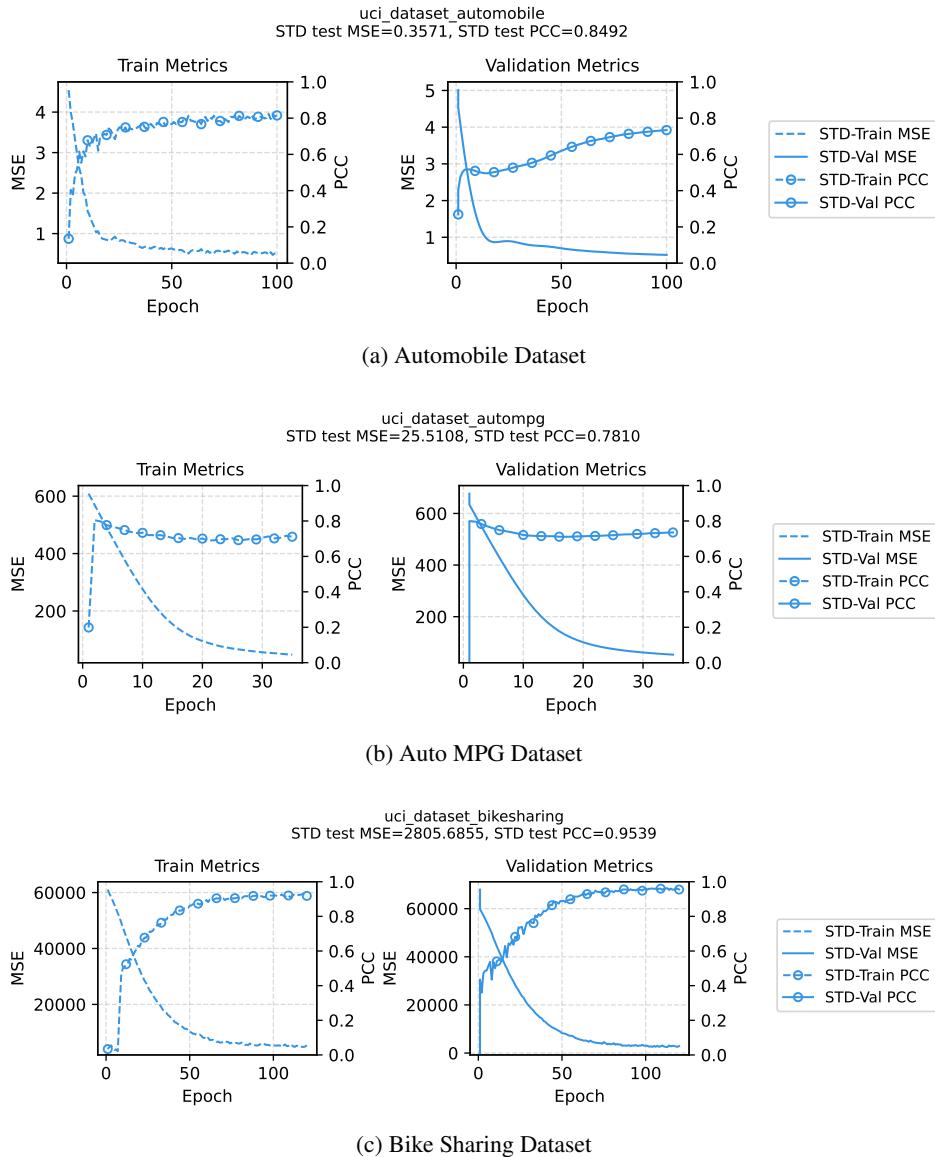
- **FT-Transformer:** A deep tabular Transformer with multiple attention layers.
- **ALMT:** A complex multimodal Transformer for sentiment analysis.
- **EGN:** A multi-layer vision Transformer model for spatial transcriptomics.

In all these deep settings, we observed the PCC plateau phenomenon. The consistent improvement provided by ECA confirms that the convex readout mechanism acts as a bottleneck even in deep models, and that relaxing this constraint via extrapolative mechanisms is necessary for optimal correlation learning.

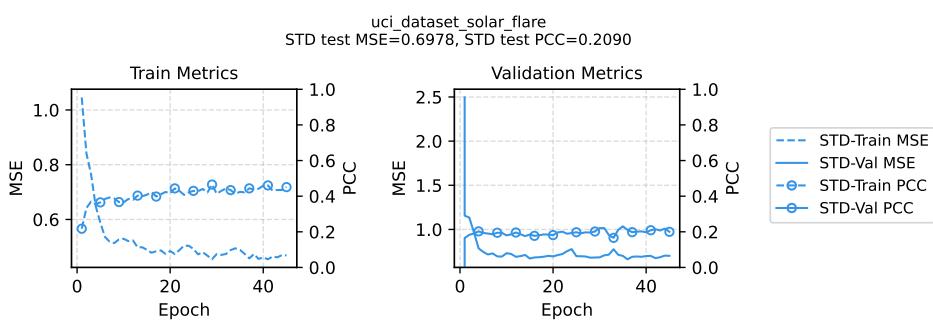
1350 **F EXTENDED EMPIRICAL EVIDENCE OF THE PCC PLATEAU**  
1351  
1352

1353 To rigorously address the universality of the PCC plateau phenomenon and demonstrate that it is not  
1354 an artifact of specific datasets or architectures, we conducted extensive additional experiments on 8  
1355 diverse regression benchmarks from the UCI Machine Learning Repository (Asuncion et al., 2007).  
1356 We utilized a multi-layer FT-Transformer (Gorishniy et al., 2021) as the backbone to represent mod-  
1357 ern, high-capacity attention-based regression models.

1358 Figure 7 illustrates the training (left) and validation (right) trajectories for both MSE and PCC. The  
1359 curves marked with circles represent PCC metric, while the curves without circle represent MSE.  
1360  
1361

1362 Figure 7: Training and validation curves for multi-layer FT-Transformer on 8 UCI regression  
1363 datasets. **Left:** Training set metrics. **Right:** Validation set metrics. The curves with **circles** in-  
1364 dicate PCC (maximizing shape matching), while curves **without circles** indicate MSE (minimizing  
1365 magnitude error). In all instances, PCC hits a ceiling (plateau) significantly earlier than MSE, which  
1366 continues to descend, highlighting the optimization gap.






### (h) Solar Flare Dataset

## Observations and Analysis:

- **Decoupling of MSE and PCC:** Across all 8 datasets, we observe a distinct decoupling of the two metrics. In the early stages of training, both MSE and PCC improve. However, a distinct inflection point: the “PCC Plateau” consistently appears where the correlation gain flattens.
- **Persistent MSE Reduction:** Crucially, after the PCC plateaus, the MSE continues to decrease significantly. This confirms the optimization conflict identified in our theoretical analysis (Remark 2.3): the gradient dynamics of MSE minimization (specifically standard deviation matching) actively suppress the correlation gradient magnitude. The model continues to learn magnitude information (lowering MSE) but loses the ability to optimize the shape/ordering of predictions (PCC).
- **Universality:** Despite varying noise levels and feature dimensions across these diverse real-world datasets, the optimization pattern in correlation learning remains identical. This provides robust empirical evidence that the PCC plateau is a fundamental failure mode in joint MSE-PCC training with attention-based models, which calls for a specific architectural improvement as we proposed in Section 3.

## G DETAILED EXPERIMENTAL SETTINGS

## G.1 SYNTHETIC EXPERIMENT DETAILS

### G.1.1 DETAILED DATA GENERATION PROCESS

We provide a detailed description of the synthetic dataset generation process (DGP). The DGP is parameterized by the embedding dimension  $D$ , the number of elements per sample  $K$ , the signal contrast  $\eta$ , the noise level  $\nu$ , the ground truth extrapolation factor  $\gamma^* \geq 1$ , the cross-sample variation scale  $\sigma_B$ , and a noise floor  $\sigma_{\text{floor}}$ .

**1. Defining Ground Truth Directions.** We first establish the direction of the signal and the direction of the noise.

1. Sample the ground truth regression vector (signal direction)  $\mathbf{w}^* \sim \mathcal{N}(0, \mathbf{I}_D)$ . Normalize  $\|\mathbf{w}^*\|_2 = 1$ .
2. Sample a noise direction vector  $\mathbf{w}^\perp$ . We ensure orthogonality  $(\mathbf{w}^*)^\top \mathbf{w}^\perp = 0$  using the Gram-Schmidt process and normalize  $\|\mathbf{w}^\perp\|_2 = 1$ .

**2. Generating Sample Centers.** For each sample  $s \in \{1, \dots, S\}$ , we sample the sample center (mean embedding) from an isotropic Gaussian distribution, controlling the cross-sample variation:

$$\boldsymbol{\mu}_s \approx \mathcal{N}(\mathbf{0}, \sigma_B^2 \mathbf{I}_D). \quad (96)$$

**3. Generating Elements.** We generate  $K$  elements for each sample  $s$ , distinguishing between  $K - 1$  background samples and one key sample.

1512 **Background Elements** ( $i = 1, \dots, K - 1$ ): These elements are generated by adding small isotropic  
 1513 noise (noise floor) to the sample center:

$$1514 \quad \mathbf{h}_{si} = \boldsymbol{\mu}_s + \boldsymbol{\epsilon}_{si}, \quad \boldsymbol{\epsilon}_{si} \sim \mathcal{N}(0, \sigma_{\text{floor}}^2 \mathbf{I}_D). \quad (97)$$

1516 **Key Element** ( $i = K$ ): The key element is generated by explicitly injecting signal contrast along  
 1517  $\mathbf{w}^*$  and uninformative noise along  $\mathbf{w}^\perp$ :

$$1519 \quad \mathbf{h}_{sK} = \boldsymbol{\mu}_s + \underbrace{\eta \cdot \mathbf{w}^*}_{\text{Signal Contrast}} + \underbrace{\nu \cdot \mathbf{w}^\perp}_{\text{Uninformative Noise}} + \boldsymbol{\epsilon}_{sK}. \quad (98)$$

1522 **4. Defining the Target Variable.** The target variable is defined based on an optimal representation  
 1523  $\mathbf{v}_s^*$  that extrapolates the *signal component* by the factor  $\gamma^*$ :

$$1524 \quad \mathbf{v}_s^* = \boldsymbol{\mu}_s + \gamma^* \cdot (\eta \cdot \mathbf{w}^*). \quad (99)$$

1526 The target label  $y_s$  is generated by applying the ground truth regression vector  $\mathbf{w}^*$  to this optimal  
 1527 representation, with added label noise  $\boldsymbol{\epsilon}'_s \sim \mathcal{N}(0, \sigma_{\text{label}}^2)$ :

$$1528 \quad y_s = (\mathbf{w}^*)^\top \mathbf{v}_s^* + \boldsymbol{\epsilon}'_s. \quad (100)$$

### 1530 G.1.2 EXPERIMENTAL SETUP AND HYPERPARAMETERS

1532 **Model Architecture.** We use a simple gating attention architecture. The element embeddings  
 1533  $\mathbf{h}_{si}$  are generated directly by the DGP (no pre-trained encoder). The attention logits are computed  
 1534 via a linear layer parameterized by  $\mathbf{w}_{\text{attn}} \in \mathbb{R}^{D \times 1}$ :  $z_{si} = \mathbf{h}_{si}^\top \mathbf{w}_{\text{attn}}$ . The aggregated sample-level  
 1535 representation  $\mathbf{v}_s$  is computed using  $\mathbf{v}_s = \sum_{i=1}^{n_s} \text{Softmax}(\{z_{si}\}_{i=1}^{n_s}) \mathbf{h}_{si}$ . The final prediction is  
 1536 computed via a regression head  $\mathbf{W}_{\text{reg}} \in \mathbb{R}^{D \times 1}$  and bias  $b$ :  $\hat{y}_s = \mathbf{v}_s^\top \mathbf{w} + b$ .

1537 **Optimization.** We train the models using the Adam optimizer (Kingma, 2014) with standard pa-  
 1538 rameters ( $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$ ). The objective function is the joint loss  $\mathcal{L}_{\text{total}} =$   
 1539  $\mathcal{L}_{\text{MSE}} + \lambda_{\text{PCC}} \mathcal{L}_{\text{PCC}}$  (or  $\tilde{\mathcal{L}}_{\text{PCC}}$  in Equation (11) for DNPL).

1541 **Hyperparameters.** The default hyperparameters used in the synthetic experiments are summa-  
 1542 rized in Table 4.

1543 Table 4: Hyperparameters for Synthetic Experiments

1545	Parameter	Value
<i>DGP Settings</i>		
1548	$D$ (Embedding dimension)	16
1549	$K$ (Elements per sample)	10
1550	$N_{\text{train}} / N_{\text{val}}$	2000 / 300
1551	$\sigma_B$	1.0
1552	$\sigma_{\text{floor}} / \sigma_{\text{label}}$	0.01 / 0.01
<i>Training Settings</i>		
1553	Optimizer	Adam
1554	Learning Rate	0.001-0.01
1555	Epochs	1000
1556	$\lambda_{\text{PCC}}$ (PCC loss weight)	0.3-0.8
<i>ECA Settings</i>		
1558	DATS $T_{\min} / \beta$	0-0.8 / 0.5-3
1559	SRA $\lambda_\gamma / \gamma_{\max}$	0.001 / 2

### 1561 G.2 UCI ML REPOSITORY DATASETS

1563 For each dataset, We report PCC, MSE and MAE between predictions  $\hat{y}_i$  and ground-truth targets  
 1564  $y_i$  over all samples in test set is

$$1565 \quad \text{PCC}(\hat{y}, y) = \frac{\text{cov}(\hat{y}, y)}{\sigma(\hat{y}) \sigma(y)}.$$

1566 Mean squared error (MSE) and mean absolute error (MAE) are computed sample-wise and averaged  
 1567 over all gene–window pairs:

$$1569 \text{MSE}(\hat{y}, y) = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2, \quad \text{MAE}(\hat{y}, y) = \frac{1}{N} \sum_{i=1}^N |\hat{y}_i - y_i|.$$

1571 **1. Appliance Dataset** The Appliances Energy Prediction dataset from the UCI Machine Learning  
 1572 Repository contains experimental data collected over 4.5 months in a low-energy building. It  
 1573 includes 19,735 instances with 28 real-valued features, including indoor temperature, humidity, and  
 1574 weather conditions. These attributes are recorded at 10-minute intervals. The goal is to predict  
 1575 appliance energy usage as an integer value in watt-hours (Wh).

1577 We replace the attention layer in the FT-Transformer (Gorishniy et al., 2021) with our ECA module  
 1578 and keep the remaining components unchanged. We use the following hyperparameters during training:  
 1579 “batch\_size=128”, “dropout\_rate=0.1”, “embedding\_dim=256” and “num\_heads=8” for both the  
 1580 FT-Transformer baseline and the FT-Transformer+ECA model. We use MSE and MAE to evaluate  
 1581 magnitude matching and PCC to evaluate correlation matching.

1582 **2. Online News Dataset** The Online News Popularity dataset contains 39,797 news articles from  
 1583 Mashable, each described by 58 numeric features (with the URL and timedelta features excluded).  
 1584 Its target is the article’s number of social-media shares (popularity) and we applied the log transfor-  
 1585 mation on the target to reduce the large range of data.

1586 We replace the attention layer in the FT-Transformer (Gorishniy et al., 2021) with our ECA module  
 1587 and keep the remaining components unchanged. We use the following hyperparameters during training:  
 1588 “batch\_size=128”, “dropout\_rate=0.1”, “embedding\_dim=256” and “num\_heads=8” for both the  
 1589 FT-Transformer baseline and the FT-Transformer+ECA model. We use MSE and MAE to evaluate  
 1590 magnitude matching and PCC to evaluate correlation matching.

1592 **3. Superconductivity Dataset** The UCI Superconductivity dataset contains 21,263 superconduc-  
 1593 tors with 81 real-valued features, where the target is the critical temperature.

1595 We replace the attention layer in the FT-Transformer (Gorishniy et al., 2021) with our ECA module  
 1596 and keep the remaining components unchanged. We use the following hyperparameters during training:  
 1597 “batch\_size=128”, “dropout\_rate=0.1”, “embedding\_dim=256” and “num\_heads=8” for both the  
 1598 FT-Transformer baseline and the FT-Transformer+ECA model. We use MSE and MAE to evaluate  
 1599 magnitude matching and PCC to evaluate correlation matching.

### 1600 G.3 SPATIAL TRANSCRIPTOMIC DATASET

1602 **Data Processing.** We follow the data processing as the EGN baseline (Yang et al., 2023). The  
 1603 10xProteomic dataset contains  $\sim 32,032$  image–patch/expression pairs curated from 5 whole-slide  
 1604 images (10x Genomics, 2025; Yang et al., 2023). Prediction targets are restricted to the 250 genes  
 1605 with the largest mean expression across the dataset (computed over all patches). For each target gene,  
 1606 we apply a log transform to expression values and then perform per-gene min–max normalization  
 1607 to map values into  $[0, 1]$ . We use the dataset-provided image patches without modifying tiling or  
 1608 slide-level grouping.

1609 **Evaluation Metric.** We report PCC aggregated across genes and sample-wise error metrics. For  
 1610 each gene  $g$ , PCC between predictions  $\hat{y}_g$  and ground truths  $y_g$  over all evaluation windows is

$$1612 \text{PCC}(g) = \frac{\text{cov}(\hat{y}_g, y_g)}{\sigma(\hat{y}_g) \sigma(y_g)}.$$

1614 We summarize  $\{\text{PCC}(g)\}$  across all target genes using: PCC@F (25th percentile), PCC@S (me-  
 1615 dian), and PCC@M (mean). Higher is better.

1616 Mean squared error (MSE) and mean absolute error (MAE) are computed sample-wise and averaged  
 1617 over all gene–window pairs:

$$1619 \text{MSE} = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2, \quad \text{MAE} = \frac{1}{N} \sum_{i=1}^N |\hat{y}_i - y_i|.$$

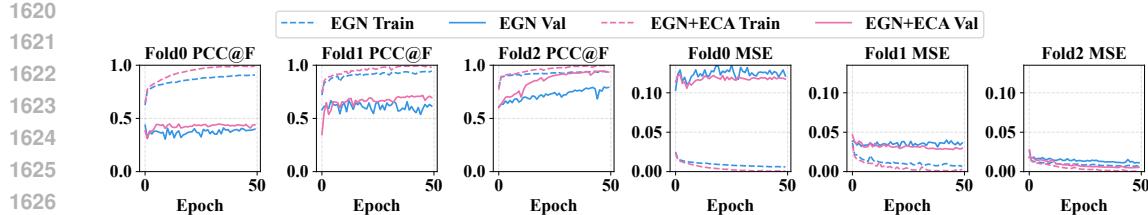


Figure 8: Per-fold PCC@F comparison of EGN and EGN+ECA on 10xProteomic dataset.

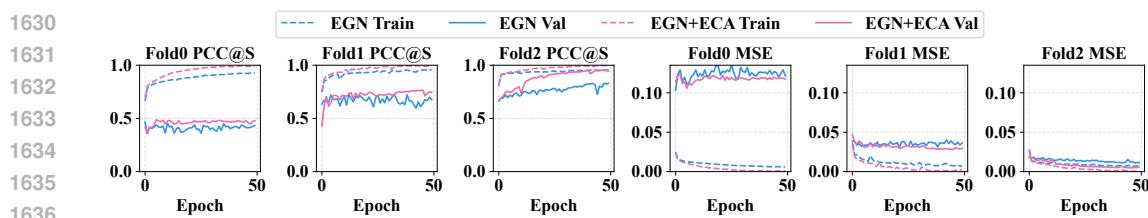


Figure 9: Per-fold PCC@S comparison of EGN and EGN+ECA on 10xProteomic dataset.

**Implementation.** The EGN and ECA improved version are implemented in PyTorch. The visual backbone is a ViT with patch size 32, embedding dimension 1024, MLP dimension 4096, 16 attention heads, and depth 8. We interleave the proposed Exemplar Block (EB) every two ViT blocks. Each EB uses 16 heads with head dimension 64, retrieving the  $k=9$  nearest exemplars. Results are reported on a three-fold cross-validation with the same experimental setting in EGN. We train for 50 epochs with a batch size of 32. Experiments run on  $2 \times$  A6000 GPUs. We apply the same pre-processing and gene-selection protocol throughout and keep dataset-provided tiles and slide/patient groupings intact for fair comparison.

**Extra Results.** Figure 8 and Figure 9 provide extra visualization results on PCC@S and PCC@F metrics for each fold.

#### G.4 MULTIMODAL SENTIMENT ANALYSIS (MSA) DATASET

**Data Processing** We conduct multimodal sentiment analysis (MSA) experiments on the CMU-MOSI dataset (Zadeh et al., 2016), a standard benchmark comprising 2,199 opinion-centric video segments. Each segment pairs a short monologue clip with synchronized *language*, *acoustic*, and *visual* modalities and is annotated with a continuous sentiment intensity score on a seven-point scale from  $-3$  (strongly negative) to  $+3$  (strongly positive). Following the widely adopted split, the data are partitioned into 1,284 / 229 / 686 segments for train/validation/test. In line with community practice and THUIAR’s public releases (Yu et al., 2020; 2021), we use pre-extracted, unaligned features where acoustic streams are sampled at 12.5 Hz and visual streams at 15 Hz; text features are aligned to the same timeline.

**Task formulation and metrics.** We evaluate models in the regression setting (predicting the continuous sentiment score) while also reporting the standard classification metric used in prior MSA work. Concretely, we report: (i) MAE: mean absolute error between predicted and ground-truth sentiment; (ii) PCC: Pearson’s correlation coefficient between predictions and ground truth, measuring rank/linear consistency; and (iii) F1: the binary F1 score computed under the standard MOSI protocol from prior work and THUIAR’s toolkit (Yu et al., 2020; 2021). This suite jointly captures absolute deviation (MAE), correlation structure (PCC), and discrete decision quality (F1) and is consistent with the prevailing MOSI evaluation practice.

**Baselines.** To situate our method among representative approaches, we compare against widely cited MSA baselines that span tensor fusion, low-rank factorization, recurrent and deep feed-forward fusion, graph-based memory models, and cross-modal transformers. Below we list each baseline with its canonical citation (the superscripts indicate the source of numbers when we report them in

1674 tables: <sup>†</sup> from THUIAR’s GitHub/toolkit, <sup>\*</sup> from the original paper, and <sup>\*\*</sup> reproduced by us with  
 1675 released code/hyperparameters):  
 1676

- 1677 • **TFN**<sup>†</sup> (Zadeh et al., 2017): Tensor Fusion Network introducing explicit multimodal tensor  
 1678 interactions.
- 1679 • **LMF**<sup>\*</sup> (Liu et al., 2018): Low-Rank Multimodal Fusion reducing TFN’s cubic complexity  
 1680 via factorization.
- 1681 • **EF-LSTM**<sup>†</sup> (Williams et al., 2018b): Early-fusion recurrent model that concatenates  
 1682 modalities prior to sequence modeling.
- 1683 • **LF-DNN**<sup>†</sup> (Williams et al., 2018a): Late-fusion deep network combining modality-specific  
 1684 predictors at the decision level.
- 1685 • **Graph-MFN**<sup>†</sup> (Zadeh et al., 2018): Graph-structured Memory Fusion Network for cross-  
 1686 view temporal reasoning.
- 1687 • **MuLT**<sup>\*</sup> (Tsai et al., 2019): Cross-modal Transformer that performs directional attention  
 1688 across modalities.
- 1689 • **MISA**<sup>†</sup> (Hazarika et al., 2020): Modality-Invariant/Specific representations with con-  
 1690 trastive objectives to disentangle factors.
- 1691 • **ICCN**<sup>\*</sup> (Sun et al., 2020): Cross-modal correlation networks leveraging canonical corre-  
 1692 lation constraints.
- 1693 • **DLF**<sup>\*\*</sup> (Wang et al., 2025): A recent strong multimodal baseline emphasizing deep latent  
 1694 fusion.
- 1695 • **ALMT**<sup>\*\*</sup> (Zhang et al., 2023): Attention-based latent model trained with MSE; we use  
 1696 ALMT as the host architecture for our ECA augmentation.

1700 **Implementation.** Unless otherwise noted, we follow the standard MOSI preprocessing and the  
 1701 train/validation/test partition described above. For baselines, we adhere to the configuration choices  
 1702 recommended by the original authors or by THUIAR’s toolkit (Yu et al., 2020; 2021). Our primary  
 1703 report includes F1, PCC, and MAE on the held-out test set, with validation used solely for early  
 1704 stopping and hyperparameter selection. The model training is with 2 A6000 GPUs.

1705 We adopt ALMT as the base architecture and keep the optimizer and data pipeline fixed across all  
 1706 runs to ensure a clean ablation. We train for 100 epochs with a batch size of 64, using AdamW with  
 1707 lr=1e-4 and batching and loading use num\_workers=8. Other hyperparameters are shown in Table 5.

1709 ALMT, in its original form, is trained with MSE loss only. To probe correlation-aware training and  
 1710 our correlation-aware aggregation, we evaluate two controlled settings (all other hyperparameters  
 1711 are held constant):

1712 1. **ALMT + PCC loss (no architectural change).** We augment the training objective with a  
 1713 differentiable PCC term, yielding a weighted sum

$$1715 \mathcal{L} = \lambda_{\text{MSE}} \cdot \text{MSE} + \lambda_{\text{PCC}} \cdot \mathcal{L}_{\text{PCC}},$$

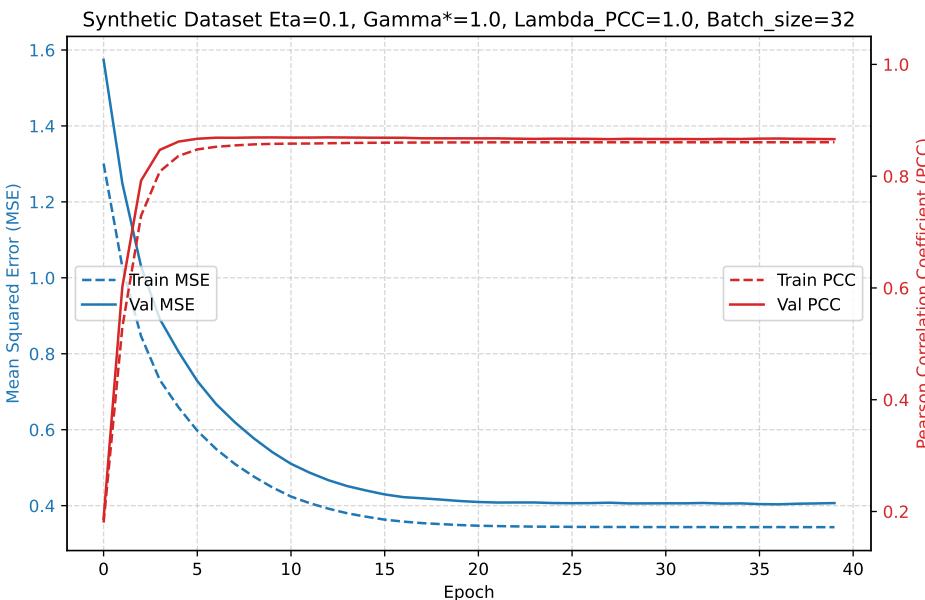
1716 where  $\lambda_{\text{MSE}}=1.0$  and  $\lambda_{\text{PCC}}=1.0$ . This setting isolates the effect of explicitly encouraging  
 1717 high Pearson correlation during training while leaving the model architecture unchanged.

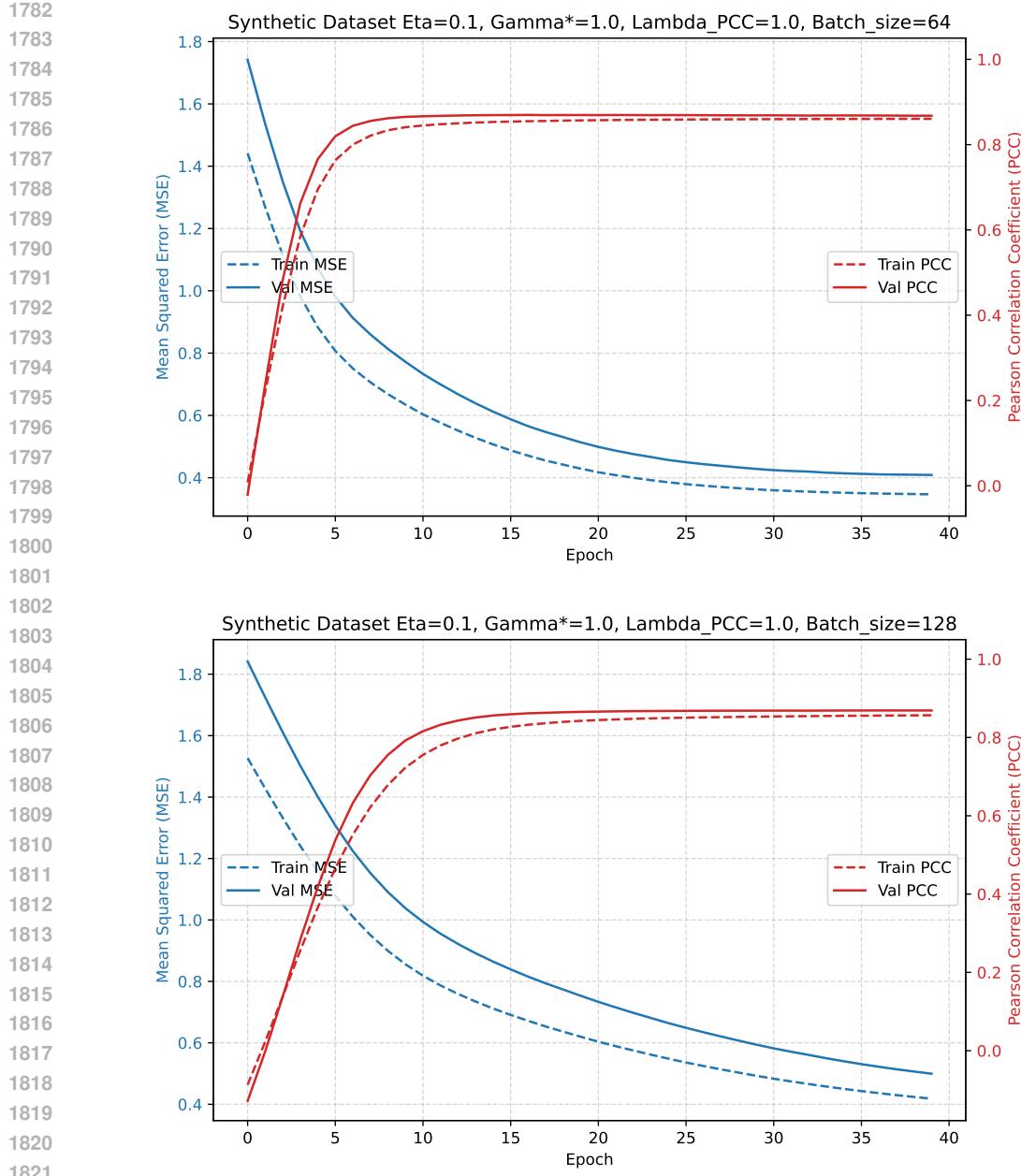
1719 2. **ALMT + PCC loss + ECA (ours).** In addition to the above loss, we adopt our proposed  
 1720 ECA method in the vision stream by modifying the ViT-style token aggregation step.

1722 **Extra Results Analysis.** By comparing Setting 1 to the MSE-only ALMT, we measure the gain  
 1723 from correlation-aware training alone. Comparing Setting 2 to Setting 1 isolates the benefit of  
 1724 ECA’s vision-token aggregation. As summarized in Table 2, adding PCC improves correlation-  
 1725 oriented metrics without harming classification quality, and coupling PCC with our ECA aggregation  
 1726 *further* improves all three metrics (F1, PCC, MAE). These results indicate that ECA enhances the  
 1727 multimodal pipeline beyond loss-level changes, demonstrating tangible benefits for *multimodality*  
 1728 on MOSI.

1728  
1729  
1730 Table 5: Configuration for MOSI experiments (ALMT backbone).

1730 <b>Param</b>	1730 <b>Value</b>
1731 Optimizer / weight decay / lr	1731 AdamW / $1 \times 10^{-4}$ / $1 \times 10^{-4}$
1732 Batch size / epochs	1732 64 / 100
1733 Text / audio / vision dims	1733 768 / 5 / 20
1734 Projection dim (all modalities)	1734 128
1735 Token count / token dim	1735 8 / 128
1736 Seq. lengths (l/a/v)	1736 50 / 375 / 500
1737 Projection transformer (depth/heads/MLP)	1737 1 / 8 / 128
1738 Text encoder (heads/MLP)	1738 8 / 128
1739 Hyper-layer (depth/heads/head-dim/dropout)	1739 3 / 8 / 16 / 0
1740 Loss weights (MSE / PCC)	1740 1.0 / 1.0
1741 ECA module	1741 ✓ in Setting 2

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1744 H BATCH SIZE EFFECT ON PCC PLATEAU  
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17471748  
1749 A potential concern regarding the joint optimization of MSE and PCC is whether the batch size  $S$   
1750 influences the optimization dynamics, specifically the onset of the PCC plateau. Theoretically, as  
1751 discussed in Section 2.3 and the Equation (6), both the MSE and PCC gradient magnitudes scale  
1752 proportionally with  $1/S$ . Consequently, the ratio between the two gradients that determines the  
1753 effective optimization direction is invariant to the batch size. This suggests that the conflict causing  
1754 the plateau is fundamental to the gradient properties (specifically the  $1/\sigma_{\hat{y}}$  attenuation) and the  
1755 homogeneous PCC bound, rather than batch statistics.1756 To empirically validate this independence, we conducted an ablation study using the synthetic  
1757 dataset described in Section 5.1, training the standard attention regression model with varying batch  
1758 sizes  $S \in \{32, 64, 128\}$ .  
1759  
17601761 Figure 10: MSE and PCC curve under various batch size settings.  
1762



Appendix H presents the learning curves for these settings. The results align with our theoretical analysis:

- **Consistent Plateau Behavior:** Across all batch sizes, we observe the characteristic decoupling of the metrics. The PCC curves (red) flatten and plateau significantly earlier than the MSE curves (blue), which continue to decrease steadily throughout training.
- **Generalization Gap:** Both training (dashed) and validation (solid) curves exhibit similar trends, indicating that this phenomenon is an optimization issue rather than a generalization issue.

These results confirm that increasing or decreasing the batch size does not resolve the PCC plateau, further validating the necessity of the architectural interventions proposed in our ECA to explicitly counteract gradient attenuation.

1836 **I DISCLOSURE OF LLM USAGE**  
18371838 A large language model (LLM) was used only for language refinement (grammar, phrasing, and  
1839 clarity) in the main paper and the appendix. The LLM did not contribute to the research ideas,  
1840 mathematical derivations, theorems, proofs, or experimental design. All technical content was inde-  
1841 pendently produced and reviewed by the authors.  
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