CO_2 classification analysis for AI models

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***Abstract*—**

***Index Terms*—Cluster analysis, K-means, Classification models,**

I. Introduction

II. Methodology

Classification methods are applied to the selected dataset. A workflow comprising six procedures is followed: **univariate analysis**, **cluster analysis**, **k-means clustering**, **linear classification**, and **nonlinear classification**. Upon completion of these steps, the results are compared and the best-performing model is identified.

A. Univariate Analysis

In this stage, the dataset **HFCO2.csv**—originating from a CO_2-emissions report on the Hugging Face platform—is profiled to characterize marginal distributions, identify outliers, and screen variables for subsequent modeling. The variables under study are enumerated below. Variables such as `modelId`, `datasets`, `co2_reported`, `createdat`, and `libraryname` are excluded due to limited analytical relevance; `database_efficiency` is removed because it is functionally dependent on `co2_eq_emissions` and `size`. Because no native target is present, classification labels are defined to enable supervised evaluation. First, `model_type` is created to align the `performance_score` with the appropriate metric family (e.g., accuracy, F1, Rouge); rows lacking performance metrics are discarded. Univariate summaries and frequency counts are then computed for qualitative variables (e.g., `model_type`) and proportions are reported for `domain`; variables exhibiting near-constant distributions (e.g., `library_name` = `pytorch`), or extreme sparsity (`geographical_location`, `environment`) are removed. Finally, a fairness-oriented label is introduced to relate predictive performance to environmental impact, yielding four categories—*Fair and Efficient*, *Powerful but Expensive*, *Green but Weak*, and *Inefficient*—and a derived Boolean variable `is_fair`. The resulting curated dataset and label structure provide the basis for the next methodological step, cluster analysis.

B. Cluster analysis

A hierarchical clustering analysis was applied to segment AI models using numeric performance-and-cost variables. Records with N/A/∞ were removed and features were were standardized to z-scores, to mitigate dominance of high skewed counts in features like `downloads` and `likes`, simple transformation (log/winsorzing) were considered. Two distances were evaluated: Euclidean and Mahalanobis, the latter computed with a Ledoit-Wold covariance estimator. Four linkage rules (Ward, average, complete and single) were compared. The dendogram was cut either at a target k (k $\in \{3, 4\}$) to improve size balance or at the k that maximized the average silhouette; the equivalent distance threshold reproducing that partition was also recorded. Internal quality was assessed with the silhouette score, while cophenetic correlation was used descriptively to gauge dendogram fidelity. As external validation, labels (`is_fair`, `fairness_class`, `model_type`) were not used for training and were cotrasted post-hoc via contingency tables, χ^2/Crammer's V, and adjusted Rand index. Cluster interpretation relied on profiles in original units and on z-centroids; a |z| ranking highlighted the most discriminative variables. A comparative summary across configurations (metrics, thresholds, balance) and visualizations (dedongrams with horizontal cut, stacked proportions and heatmaps) were produced for review.Final selection prioritized overall separability and operational usefulness, balancing silhouette with stability, cluster-size balance and consistency with external labels.

K-means analysis: K-means was applied to the same numeric variables used in the hierarchical analysis (*performance_score*, *co2_eq_emissions*, *likes*, *downloads*, *size*). Rows with non-numeric/inf values were removed and features were standardized to z-scores (`StandardScaler`). We explored $k \in \{2, \ldots, 10\}$ with `k-means++` initialization (n_init = 50, `max_iter`=500, `random_state`=42).

For each k we reported: Silhouette (higher is better), Calinski–Harabasz (CH; higher is better), Davies–Bouldin (DBI; lower is better), and the inertia (*elbow* curve). The primary selector was the maximum Silhouette; CH/DBI and the elbow were used as secondary evidence.

For the selected k we exported cluster sizes, original-unit profiles (count/mean/median), z-centroids, and a variable ranking using $\max |z|$ (to highlight the most discriminative features). External labels (*is_fair*, *clasification_fairness*, *model_type*) were held out from training and only used for validation via contingency tables, χ^2/Cramér's V, Fisher's exact test when 2×2, and ARI when applicable.

C. Multivariate Normality & LDA Feasibility — Methods

Check whether the feature vector X=`performance_score`, `co2_eq_emissions`, `likes`, `downloads`, `size` is (approximately) multivariate normal—globally and within classes—so that classical LDA is justified.

Preprocessing. Remove rows with NA/inf; standardize all variables to z–scores.

Robust scatter & distances. Fit a shrinkage (Ledoit–Wolf) covariance $\widehat{\Sigma}$ to mitigate outliers. Compute squared Mahalanobis distances $d_i^2 = (x_i - \widehat{\mu})^\top \widehat{\Sigma}^{-1}(x_i - \widehat{\mu})$ (i) globally and (ii) per class.

Normality diagnostic. Under MVN with p variables, $d_i^2 \sim \chi_p^2$. Compare empirical quantiles of $\{d_i^2\}$ against χ_p^2 using QQ–plots: global and class–conditional. Large, systematic upward deviations (heavy tails/mixtures) indicate non–normality.

Optional formal checks. (a) Mardia or Henze–Zirkler tests on z–scores; (b) Box's M (or visual comparison) for equality of class covariances.

Decision rule. nosep,leftmargin=*

1) *Proceed with classical LDA* if QQ–plots track the χ_p^2 line reasonably well (globally *and* by class) and class covariances appear similar.
2) *Prefer robust/regularized LDA or nonparametric classifiers* (e.g., shrinkage LDA, logistic regression, tree–based) if tails inflate, classes differ in scatter, or tests reject MVN/homoscedasticity.

D. LDA

Multivariate normality was examined via Mahalanobis Q–Q diagnostics (globally and by class). Because clear departures from normality were observed, regularized discriminants were preferred. Linear Discriminant Analysis (LDA) with automatic shrinkage (and, for projections, the `eigen` solver) and Quadratic Discriminant Analysis (QDA) with mild regularization were fit on a stratified train/test split. Performance was summarized with confusion matrices, precision/recall/F1, ROC–AUC, and 5–fold stratified cross–validation. Model parameters (priors, class means, coefficients, scalings), LD scores, and plots (ROC, score histograms, dendrograms) were exported to files to enable reporting and reproducibility.

III. Results and discussions

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A. Univariate Analysis

The database **HFCO2.csv** is a product of the CO_2 emissions report generated on the Hugging Face platform. In this case, the analysis is focused on the following variables:

1) `co2_eq_emissions`: the resulting carbon footprint
2) `downloads`: number of model downloads
3) `likes`: number of model likes
4) `performance_metrics`: (accuracy, F1, Rouge-1, Rouge-L)
5) `performance_score`: the harmonic mean of the normalized performance metrics
6) `size`: size of the final trained model in MB

Variables like `modelId`, `datasets`, `co2_reported`, `createdat`, and `libraryname` were removed because of their lack of importance in the analysis. `database_efficiency` was also removed because it is a dependent variable of `co2_eq_emissions` and `size`. The first step was to choose metrics for classification, as the database *per se* does not have a relevant dependent variable to be classified. Therefore, some labels were created with the aim of creating a dependent variable to be predicted by a couple of machine learning models. Accordingly, `model_type` is the label used to determine which metric the model uses for its performance score, because not all models use the same metric for evaluation. After applying this classification, some rows were unusable because hundreds of them do not have performance metrics at all, so they were deleted. After the redundant rows were erased, a count was made on the qualitative variables, as shown in the following table:

TABLE I: model_type counts

model type	count
type1 (accuracy & f1)	773
type2 (rouge)	228
type3 (accuracy)	72
type4 (rouge1)	3
type5 (f1)	2

In an effort to find relationships between model types and the other categories, a summary of the other variables was prepared, focusing on the `domain` variable, which is the model's use case. The following table shows each domain and the associated percentage:

TABLE II: percentage of domains

model type	count
NLP	81,5%
Computer Vision	16,0%
Not specified	2,5%

In conclusion, there are only two major types of domain models. For the purpose of this analysis, this is not an influential variable, so it was removed. Other variables, like `library_name`, revealed that all models use `pytorch` as a library, so this was also removed. The same reasoning applied to `geographical_location`: the analysis revealed that 99% of the models do not specify the training location. Similarly, 99.7% of the models do not report the hardware used in `environment`. After applying analysis upon the mean of performance metrics and CO_2 emissions, the analysis revealed that those models could be labeled again with a more precise metric: *fairness*, defined as a relation between performance score and CO_2 emissions. The following are the labels chosen for the models

1) Fair and Efficient
2) Powerful but Expensive
3) Green but Weak
4) Inefficient

Finally, models were classified by a new boolean variable "is_fair", and those that were previously labeled with respective performance metrics, were evaluated: Results are consigned in the route: `/notebooks/part2/1-univarated-analysis.ipynb` Those classifications are required for the next step in the methodology, Cluster analysis.

TABLE III: Model Classification based on their fairness and performance metrics

Model Type	Classification Fairness	Count
type1 (accuracy & f1)	Fair and Efficient	229
	Powerful but Expensive	214
	Green but Weak	181
	Inefficient	142
	Incomplete data	7
type2 (rouge)	Inefficient	140
	Green but Weak	57
	Powerful but Expensive	18
	Fair and Efficient	9
	Incomplete data	4
type3 (accuracy)	Fair and Efficient	50
	Powerful but Expensive	9
	Green but Weak	7
	Incomplete data	4
	Inefficient	2
type4 (f1)	Incomplete data	2
type5 (rouge1)	Incomplete data	3

B. Cluster Analysis

A grid over *distance* × *linkage* found that the highest internal separation was achieved by **Single–Euclidean** with $k = 3$ (silhouette $\approx$ 0.62, cophenetic $\approx$ 0.71). Close contenders were *Complete–Mahalanobis* ($k = 3$, silhouette ≈ 0.52, cophenetic ≈ 0.71) and *Average–Mahalanobis* ($k = 3$, silhouette $\approx$ 0.43, cophenetic $\approx$ 0.81). Among the "non-single" options, **Average–Euclidean** with $k = 4$ offered a more conservative structure (silhouette $\approx$ 0.34, cophenetic $\approx$ 0.81). *Ward–Euclidean* showed the lowest separation (silhouette ≈ 0.20, cophenetic ≈ 0.44).

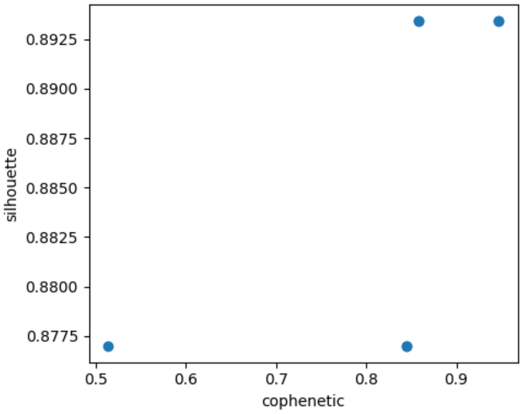

Fig. 1: Cophenetic vs. silhouette for all configurations. Top-right indicates better fidelity and separation.

Because *single* linkage may form chaining clusters, we report two complementary views: (i) the best-silhouette solution (**Single–Euclid,** $k = 3$) and (ii) a robust alternative without single linkage (**Average–Euclid,** $k = 4$). The horizontal cut at the recorded equivalent threshold reproduces the same k in the dendrogram.

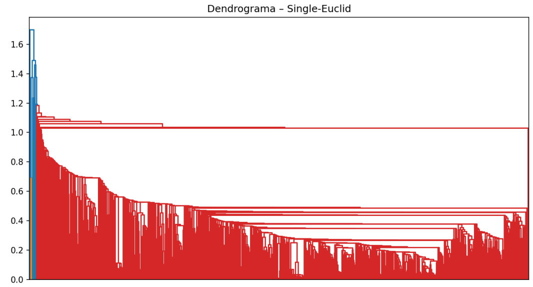

Fig. 2: Dendrogram—Single–Euclidean. The horizontal cut at the equivalent threshold yields $k = 3$.

Across configurations, a *dominant* "catalog" cluster concentrates the bulk of models near global means, while 1–3 *small* "elite" clusters group items with markedly higher *downloads/likes/performance* and (on average) lower *size/CO*$_2$. Variable importance from z–centroids is consistent: the most discriminative feature is **downloads** (max $|z| \approx 5.39$), followed by **likes** (≈ 2.03), then *CO*$_2$ and *performance* (moderate), with *size* contributing less (≈ 1.32).

External validation against labels was limited, as expected (labels were not used to train the clustering): ARI vs. `is_fair` stayed near zero across settings; however, cluster–label contingency showed reasonable purities (mean $\sim$ 0.73–0.90 depending on the configuration), with `is_fair=True` enriched in one of the small clusters and scarce in the large catalog group.

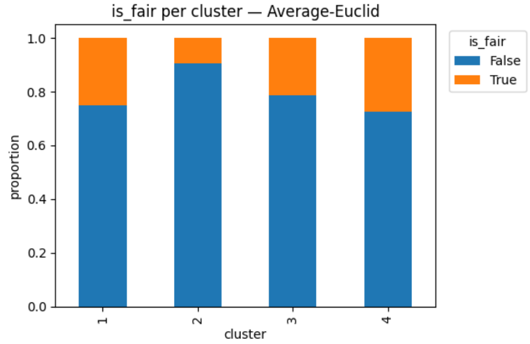

Fig. 3: Stacked proportions of `is_fair` per cluster (Average–Euclid, $k = 4$).

a) Cluster profiles.: Tables IV–VI report *original-unit* profiles (count/mean/median) for *performance_score*, *co2_eq_emissions*, *likes*, *downloads* and *size*. For brevity, we include the robust alternative (*Average–Euclid,* $k = 4$); the z–centroids and the $|z|$ ranking (downloads → likes) appear in the Supplement.

b) Overall quality.: Across linkages and distances, the highest internal separation was obtained by *Single–Euclid* with $k = 3$ (silhouette $\approx$ 0.62, cophenetic $\approx$ 0.71), followed by *Complete–Mahalanobis* (silhouette $\approx$ 0.52). Average-based variants trailed behind (silhouette $\approx$ 0.30–0.44) and *Ward–Euclid* showed the lowest separation (silhouette $\approx$ 0.20).

TABLE IV: Cluster profiles (original units): performance and CO_2

	performance_score			co2_eq_emissions	
cluster	**n**	**mean**	**median**	**mean**	**median**
1	4	0.988	0.991	49.974	3.189
2	1 029	0.727	0.822	71.382	2.749

TABLE V: Cluster profiles (original units): likes and downloads

		likes		downloads	
cluster	**n**	**mean**	**median**	**mean**	**median**
1	4	2.250	0.500	104 439.25	102 572.50
2	1 029	0.181	0.000	65.245	5.00

c) Cluster profiles (what differentiates groups).: Tables IV–V report original-unit profiles for a robust reference solution. Consistent with the winning configuration, a small cluster concentrates very high *downloads*/*likes* (and comparatively lower *size*/CO_2), while a large “catalog” cluster sits near the global mean. In z–space, *downloads* shows the largest between-cluster contrast ($\max|z| \approx 5.39$), followed by *likes* (≈ 2.03); CO_2, performance and size contribute more modestly (≈ 1.3–1.7).

d) External validation (not used for training).: Contingency tables indicate a small–to–moderate association between clusters and external labels. For *Single–Euclid* ($k = 3$), the largest cluster concentrates the majority of *is_fair=False* (share of *True* ≈ 0.27), whereas minor clusters show either higher *True* share or are too small to be conclusive. (mean/weighted), χ^2 with Cramér’s V (≈ 0.03–0.07 across configs), and Fisher’s exact test when applicable, together with ARI vs. *is_fair* (near zero, as expected for weak alignment). Figure 3 visualizes the *is_fair* proportions per cluster.

e) Sensitivity and limitations.: The pattern is robust across $k \in [2, 6]$ and across distance/linkage families that avoid overly compact (*ward*) or overly chained (*single*) artifacts; nonetheless, cluster sizes remain unbalanced and the *single* linkage can induce chaining in dense regions. These caveats do not affect the substantive finding that *downloads* (and, secondarily, *likes*) drive the segmentation.

C. Univariate Analysis

We ran k-means on the standardized variables (*performance_score*, *co2_eq_emissions*, *likes*, *downloads*, *size*) for $k \in \{2, \dots, 10\}$ with `k-means++`, n_{init}=50, `max_iter`=500. Model selection combined four internal criteria:

- **Silhouette (max is best).** The curve peaked at $\mathbf{k = 2}$ with $\approx \mathbf{0.286}$, and decreased thereafter (Fig. 4).
- **Calinski–Harabasz (max is best).** The maximum occurred at k=3 (≈ 330), with k=2 close behind (≈ 290) (Fig. 4).
- **Davies–Bouldin (min is best).** DBI decreased monotonically with k, reaching ≈ 1.21 at k=10 (Fig. 5).

TABLE VI: Cluster profiles (original units): size ($\times 10^8$)

cluster	n	mean	median
1	4	2.649	2.654
2	1 029	8.953	4.987

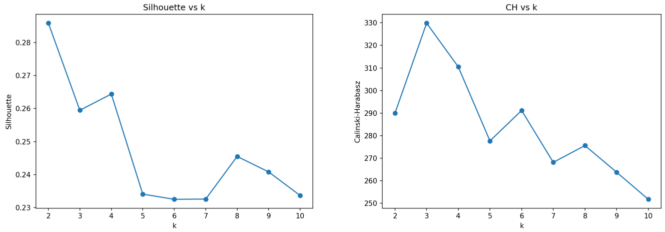

Fig. 4: Silhouette and Calinski–Harabasz across k.

- **Elbow (inertia).** Inertia dropped rapidly up to $k{\sim}6$ and then flattened, with no sharp elbow afterwards (Fig. 5).

Given the primary criterion (silhouette), we selected $\mathbf{k = 2}$. The resulting partition produced **unbalanced cluster sizes** (about $n{\sim}740$ vs. $n{\sim}300$; Fig. 6). Cluster profiles (in original units) and z–centroids were computed; the ranking by $\max|z|$ again highlighted *downloads* as the most discriminative variable, followed by *likes*, with the remaining variables contributing less. Cross-tabs against the external labels (*is_fair*, *clasification_fairness*, *model_type*) were generated for k=2 (see Supplement for the full tables).

The internal criteria point to different trade-offs: silhouette clearly favors k=2, Calinski–Harabasz prefers k=3, and Davies–Bouldin keeps improving as k grows. In this context, we prioritized silhouette because it balances compactness and separation and is less biased by the growth of k than CH/DBI. The *elbow* curve shows diminishing returns beyond $k{\sim}6$, supporting the choice of a small number of groups.

The k=2 solution is *interpretable* and *stable* (across restarts) but *unbalanced*: one major segment (catalog-like) and a smaller, high-intensity segment. The profile tables indicate that the minor cluster concentrates substantially higher *downloads* and *likes* (and slightly higher *performance*), while medians for *size*/CO_2 are not dominant—consistent with the hierarchical analysis. The $\max|z|$ ranking confirms *downloads* (then *likes*) as the strongest separators, which aligns with the business intuition that usage/engagement variables drive the segmentation more than footprint or size.

Regarding *external* labels, the cross-tabs for k=2 show heterogeneous mixes rather than perfectly pure clusters, i.e., they are useful for characterization but should not be read as supervised classes. This is expected because those labels were not used for training. Overall, the k-means segmentation complements the hierarchical results: it recovers the same two-segment story (catalog vs. high-traction niche), is easier to deploy, and preserves the same ordering of discriminative variables. If more granularity is needed, k=3 is a reasonable alternative per CH, though with a slight loss in silhouette and added complexity.

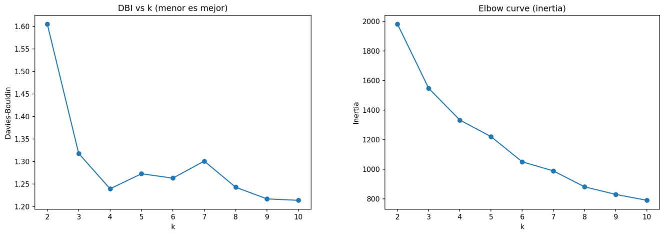

Fig. 5: Davies–Bouldin (lower is better) and inertia (elbow) across k.

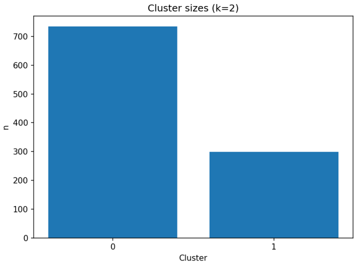

Fig. 6: Cluster sizes for the selected solution (k=2).

D. Multivariate Normality & LDA Feasibility

Visual diagnostics. Mahalanobis QQ–plots (global and by class) depart markedly from the χ^2_p reference line in the upper tail. The global plot shows a pronounced upward bend, indicating heavy–tailed behavior and/or mixture structure. Class–conditional plots (for `is_fair=False/True`) display the same pattern rather than aligning with the diagonal, so non–normality is not restricted to a single group.

Likely drivers. The heaviest deviations coincide with variables that are naturally skewed and highly dispersed in this domain (e.g., `downloads`, `likes`, and `size`). Even after z–scoring, extreme observations inflate the robust Mahalanobis distances, consistent with long right tails.

Implications for LDA. Classical LDA assumes (i) multivariate normality within each class and (ii) equal covariance matrices across classes. The QQ–plots provide clear evidence against (i), and the differing tail behavior between classes suggests that (ii) may also be questionable. Consequently, a standard LDA fit would risk biased boundaries and over–optimistic error estimates.

Recommended course. If a linear boundary is desired, prefer *regularized/shrinkage LDA* (e.g., Ledoit–Wolf within–class covariance) and consider mild preprocessing (log or $\log(1+x)$ transforms for strictly positive features; winsorization of top quantiles). As a distribution–free baseline, *penalized logistic regression* provides a linear separator without normality assumptions. If class scatters differ substantially, *QDA with regularization* or tree–based methods are more appropriate.

Summary. The MVN assumption is *not* supported for these features (globally nor within classes). Standard LDA is therefore not recommended without transformations and regularization; robust or nonparametric alternatives are better aligned with the observed data structure.

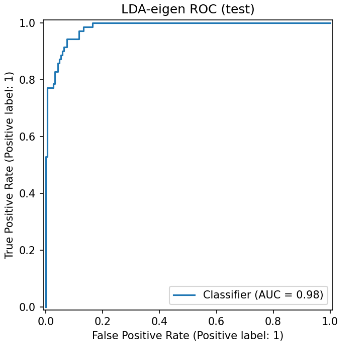

Fig. 7: ROC curve on the test set (AUC ≈ 0.98).

a) Results and discussion (LDA).: An LDA classifier was trained on a stratified train/test split using a `log1p`–standardization preprocessing pipeline and the `eigen` solver with automatic shrinkage. Class priors reflected moderate imbalance (False: 72.9%, True: 27.1%) and were preserved during training. On the held-out test set ($n = 259$), the model reached an overall accuracy of **0.919**; the ROC curve achieved an **AUC of 0.983** (Fig. 7), indicating excellent ranking performance across thresholds. Five-fold stratified cross-validation over the full dataset yielded a mean accuracy of **0.925** (± 0.021), supporting stability under resampling.

Inspection of the linear discriminants $\delta_k(x) = x^\top A_k + b_k$ showed the largest absolute coefficients in A_k for *performance_score*, *co2_eq_emissions*, and *size*, in that order, which identifies these variables as the principal drivers of separation once features are transformed. The LD1 score distributions for both classes are clearly separated with only a narrow overlap (Fig. 8 a), consistent with the near-perfect AUC. The confusion matrix on test data (TN= 184, FP= 5, FN= 16, TP= 54; Fig. 8 b) indicates very high specificity for the majority class and competitive recall for the minority class; the precision–recall trade-off at the default threshold is therefore reasonable. If fairness identification (True) must be prioritized, the operating point can be shifted to increase sensitivity with limited loss in overall accuracy.

Overall, LDA with shrinkage produced a parsimonious, interpretable boundary, strong generalization (cross-validated accuracy ≈ 0.93), and coherent variable importance (Fig. 9) highlighting performance and carbon-cost factors as the dominant discriminants. These outcomes justify LDA as a robust linear baseline; more complex models (e.g., QDA or non-linear kernels) would only be warranted if heteroscedasticity or curvature were demonstrably exploitable for additional gains.

IV. Conclusions

References

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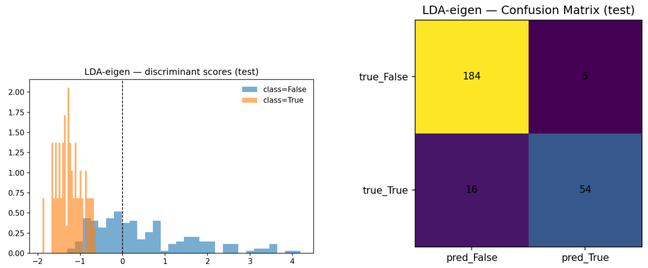

(a) LD1 scores (test).

(b) Confusion matrix (test).

Fig. 8: Geometric separation and error structure. The dashed line in a marks the default decision boundary.

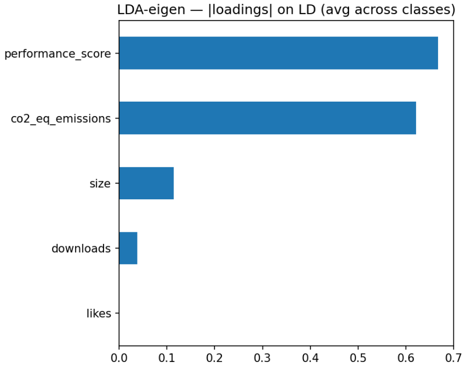

Fig. 9: Absolute loadings on LD1 (averaged across classes). Performance and CO_2 dominate; size and downloads are secondary; likes is negligible.