Wine Quality Classification: Logistic Regression and SVM with Kernel Extensions

October 17, 2025

Abstract

I predicted wine quality (binary: good if quality ≥ 6) on the combined red+white UCI Wine Quality data. All models are implemented **from scratch** (no scikit-learn estimators) and evaluated under a leakage-safe protocol: deduplication, Z-Score diagnostics with IQR winsorization (fit on train only), training-only standardization, stratified train/test split, and 5-fold cross-validation for hyperparameter tuning. On the holdout test set, **Kernel Logistic Regression (RBF)** achieves the best F1 (**0.807**) with Accuracy 0.748, Precision 0.783, Recall 0.833, closely followed by a strong **Logistic Regression** baseline (F1 = 0.800). The **SVM-RBF** model attains very high recall (0.954) with lower precision, representing a different operating point that may be preferable if recall is prioritized.

1 Introduction and Objectives

The goal is to compare **Logistic Regression (LR)** and **Support Vector Machines (SVM)**—both linear and kernelized—for predicting wine quality. I emphasized a **sound methodology**: (i) prevent test-set leakage, (ii) use cross-validation for hyperparameter tuning, (iii) handle outliers robustly without discarding data, and (iv) **exclude the `type` (red/white) variable from modeling** to avoid shortcut learning (kept for EDA only).

2 Dataset and Target Definition

I merged the red and white wine datasets into a single frame of **6,497 rows** and **14 columns**: `[fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality, type, target]`. The binary target is **1** for quality ≥ 6 and **0** otherwise. There were **no missing values** and **1,177 exact duplicates**, which I dropped prior to splitting. Class balance and wine-type counts are shown in Fig. 1 and Fig. 2.

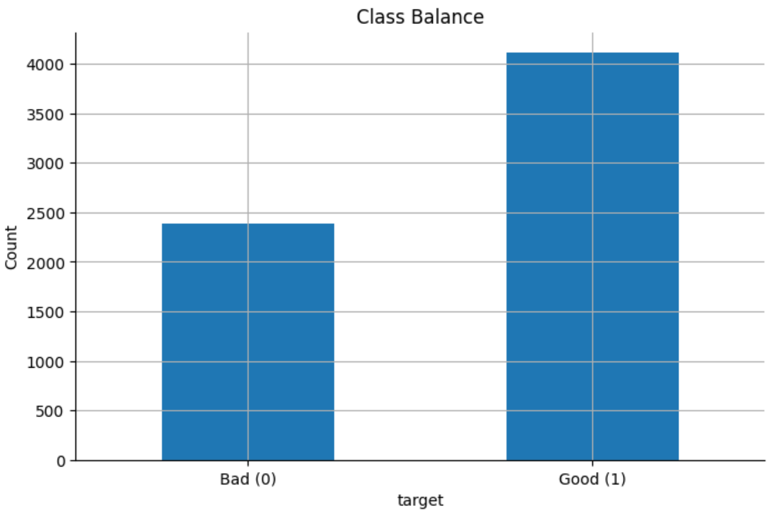


Figure 1: Class balance on the combined dataset (Bad vs Good).

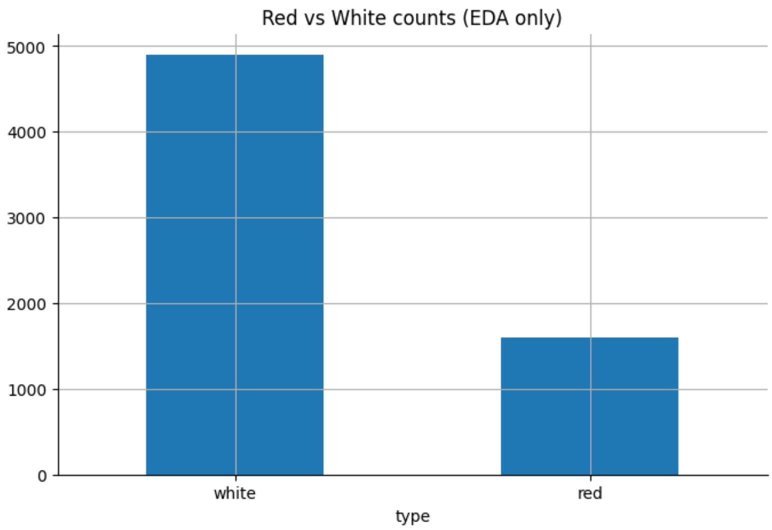


Figure 2: Counts of white vs. red wines (EDA only; `type` is excluded from modeling).

To understand marginal distributions and dependencies, Fig. 3 shows feature histograms and Fig. 4 shows the correlation heatmap. Note: alcohol positively correlates with `quality`; volatile acidity correlates negatively—consistent with oenological expectations.

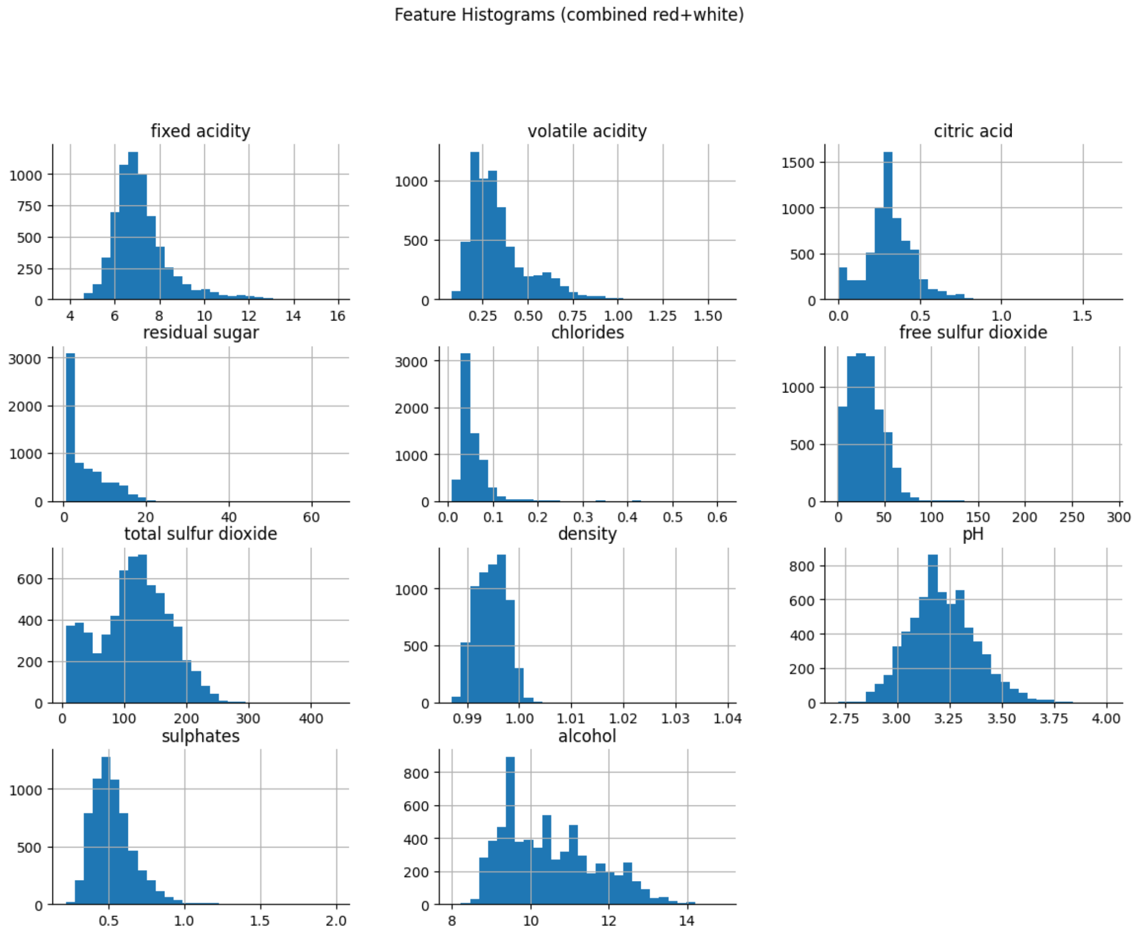


Figure 3: Feature histograms (combined red+white). Heavy tails in several variables motivate winsorization.

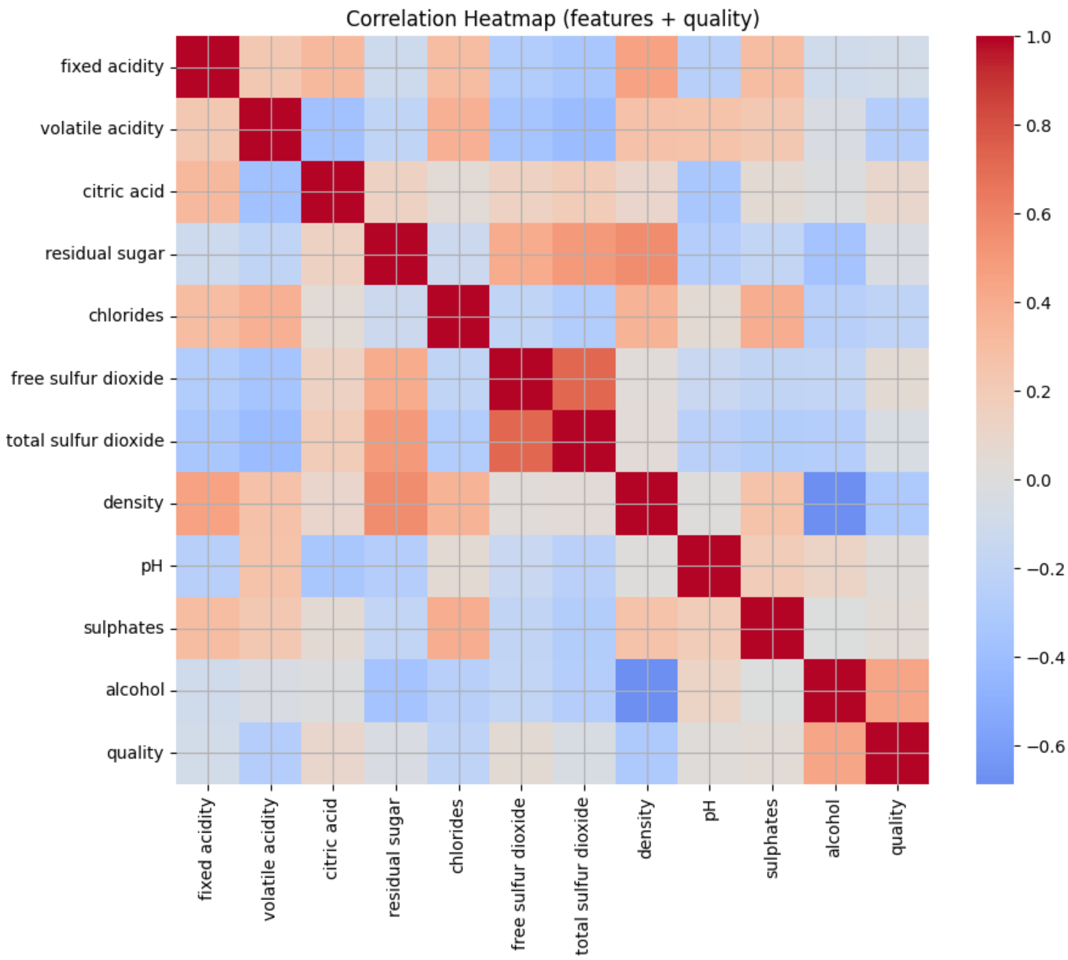


Figure 4: Correlation heatmap (features + quality). Alcohol correlates positively with quality; volatile acidity is negatively associated.

For completeness, Fig. 5 visualizes feature distributions by `type`. This is *EDA only*; `type` is not used in any model.

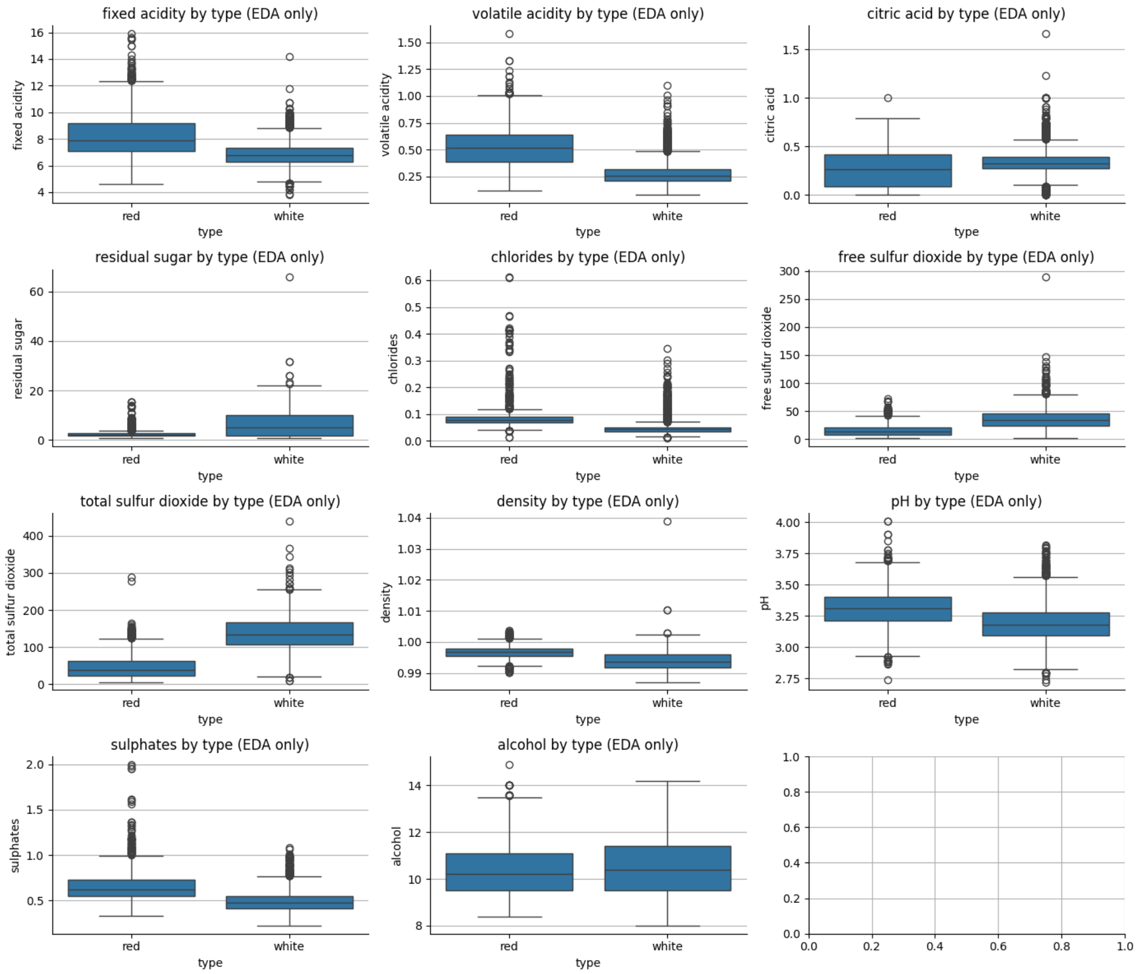


Figure 5: Feature distributions by `type` (EDA only).

3 Preprocessing and Leakage Control

3.1 Why Winsorization (and not deletion)?

Z-Score screening shows non-negligible tails (e.g., fixed acidity $\sim$1.97% with $|Z| > 3$). Deleting outliers would reduce data and distort distributions. I instead perform **IQR winsorization**, capping values outside $[Q1 - 1.5 \cdot IQR, Q3 + 1.5 \cdot IQR]$. Caps are **learned on the training set only** and then applied to validation/test, preventing leakage. Fig. 6 and Fig. 7 show the effect.

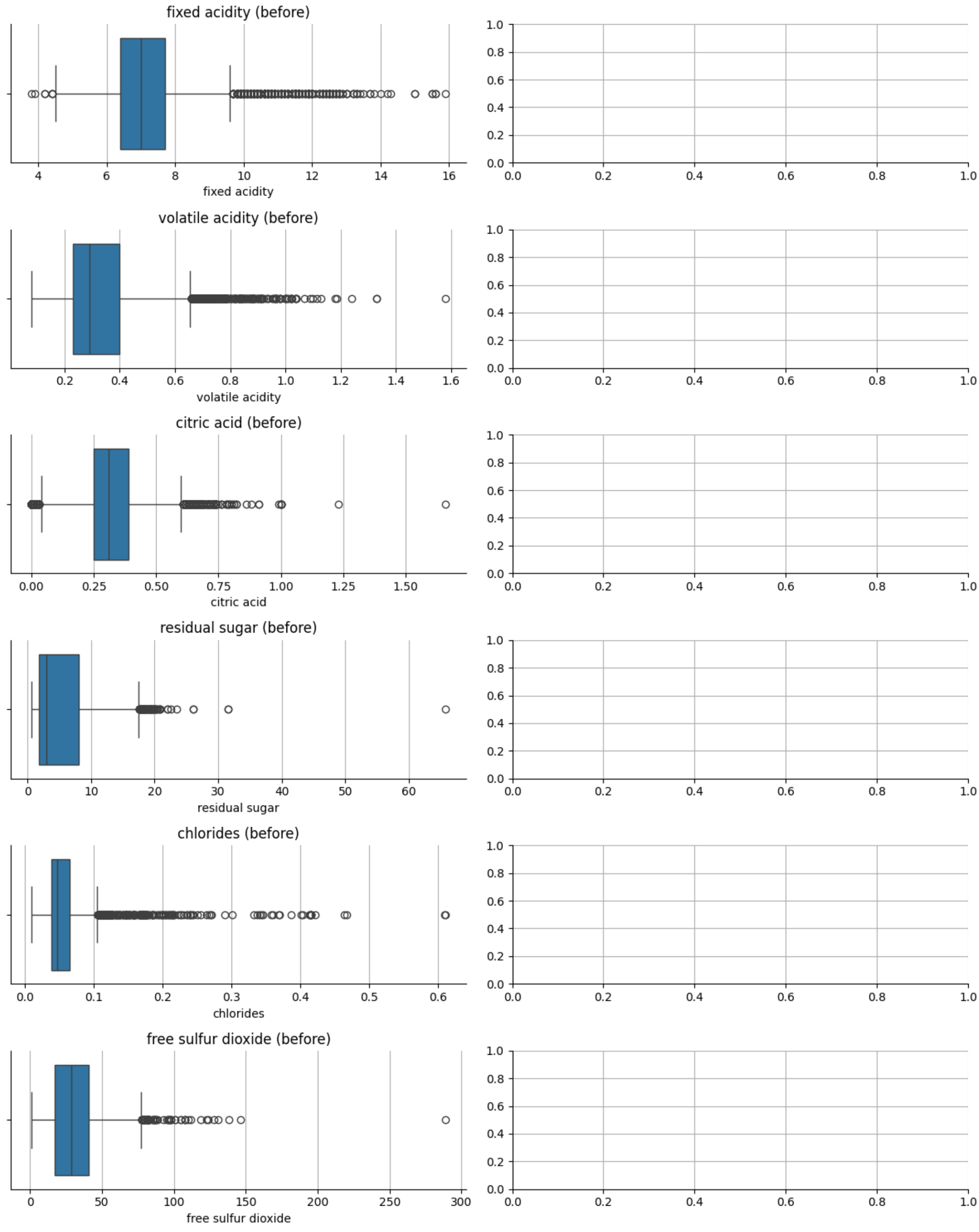


Figure 6: Diagnostic boxplots *before* IQR winsorization. Multiple features exhibit long right tails.

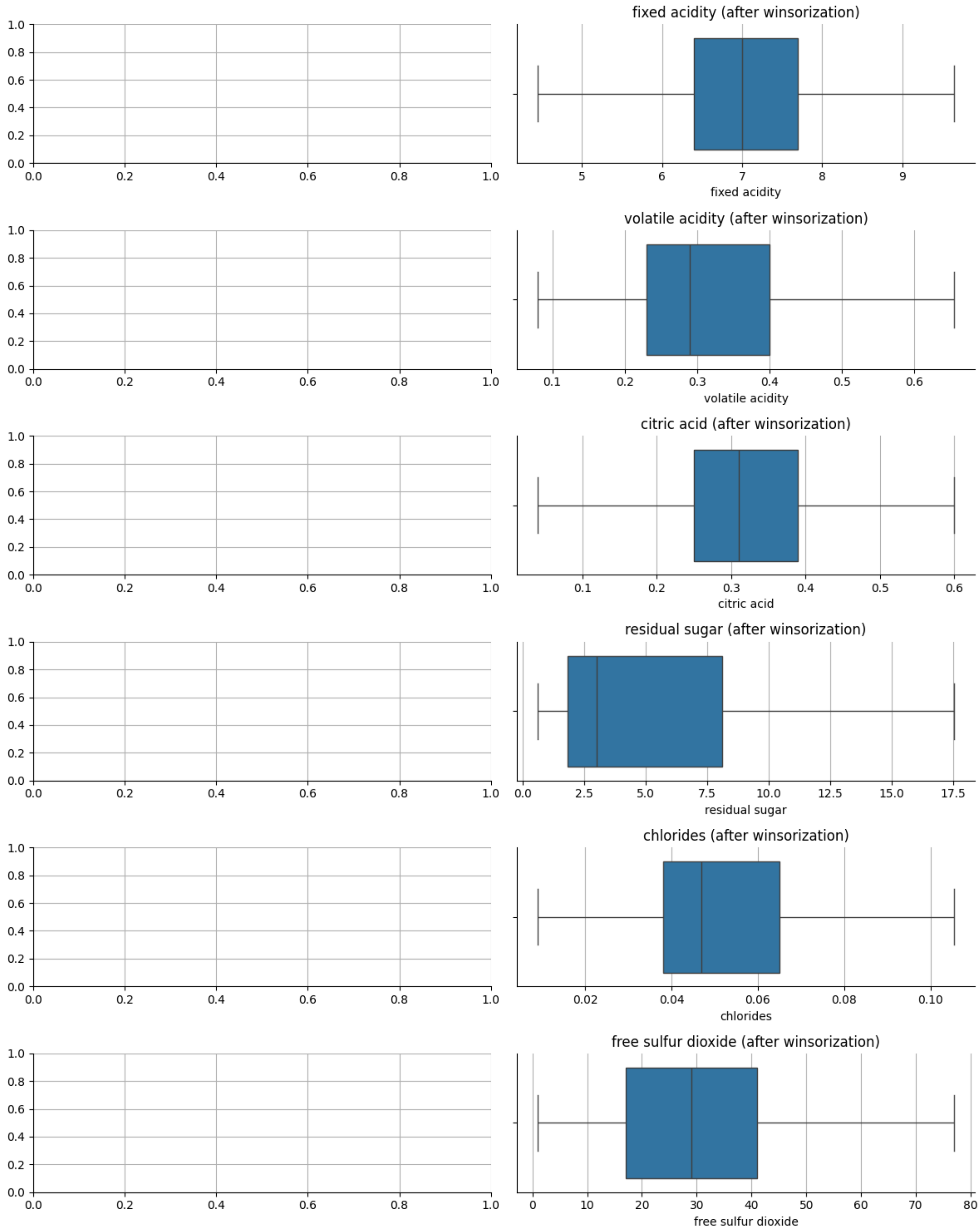


Figure 7: Boxplots *after* winsorization. Caps mitigate leverage of extreme values while preserving samples.

3.2 Standardization and Split Strategy

I **standardized** each feature using mean/SD from the **training data** only; the same transform is applied to CV folds and test data. I performed a **stratified** train/test split to preserve the class ratio. All cross-validation is done within the training split.

4 Models Implemented from Scratch

4.1 Logistic Regression (Linear)

I minimize the L2-regularized logistic loss in the *primal*, trained via (stochastic) gradient descent with a step-decay schedule. Prediction: $\hat{p}(x) = \sigma(w^\top x + b)$; by default used a 0.5 threshold.

4.2 Kernel Logistic Regression (KLR)

I use a **dual** representation with coefficients α and kernel matrix $K(X, X)$: $\hat{p}(x) = \sigma(\sum_i \alpha_i K(x, X_i))$, with L2 regularization on α. I considered two kernels: (i) **RBF** $K(x, z) = \exp(-\gamma\|x - z\|^2)$ capturing smooth local structure; (ii) **Polynomial** (degree 2) $K(x, z) = (\alpha\, x^\top z + c)^2$ capturing pairwise interactions. I center/normalize K for numerical stability in the polynomial case.

4.3 Support Vector Machines

Linear SVM is trained via **Pegasos** (stochastic subgradient on hinge loss with L2 penalty λ). Kernel SVM applies the kernel trick in dual form with the same kernels as KLR. Predictions are $\mathrm{sign}\big(\sum_i \beta_i K(x, X_i) + b\big)$.

5 Model Selection and Metrics

5.1 Cross-Validation and Grids

I use **5-fold stratified CV** on the training split and select hyperparameters by **F1**, more informative under moderate imbalance. Illustrative grids:

- **LR:** $lr \in \{0.005, 0.01, 0.1\}$; $n\_epochs \in \{400, 600, 800\}$; $reg \in \{10^{-3}, 10^{-2}, 10^{-1}\}$.
- **KLR-Poly:** degree 2; $\alpha \approx 0.05$; $c = 1.0$; centered/normalized; $reg \in \{0.001, 0.01, 0.1\}$; $lr \in \{0.005, 0.01\}$; epochs $\in \{400, 800\}$.
- **KLR-RBF:** γ tuned; $reg/lr/epochs$ as above.
- **SVM-Linear:** $\lambda \in [10^{-4}, \dots]$; epochs/mini-batch sizes tuned.
- **SVM-Kernels:** analogous to KLR for γ (RBF) or (α, c) (Poly); λ tuned.

5.2 Why These Metrics?

Accuracy can be misleading with imbalance; **Precision** (purity of predicted positives) and **Recall** (coverage of true positives) provide complementary views; their harmonic mean **F1** summarizes the trade-off. **ROC AUC** measures ranking quality independent of threshold. I reported all four on the holdout test set; ROC curves appear in Fig. 8.

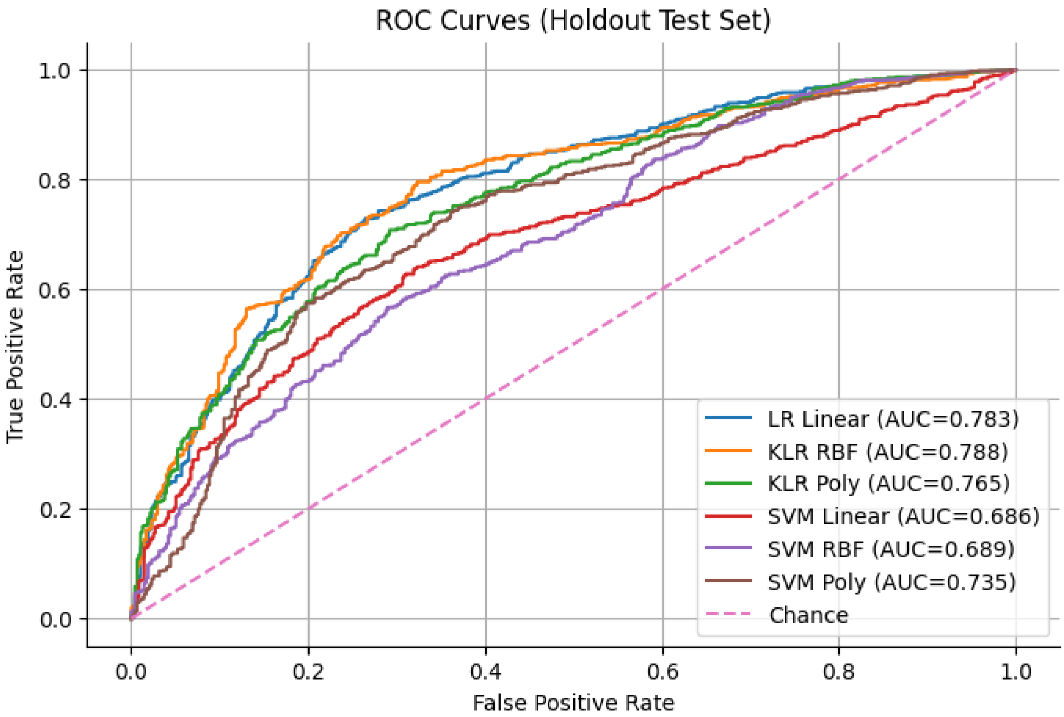
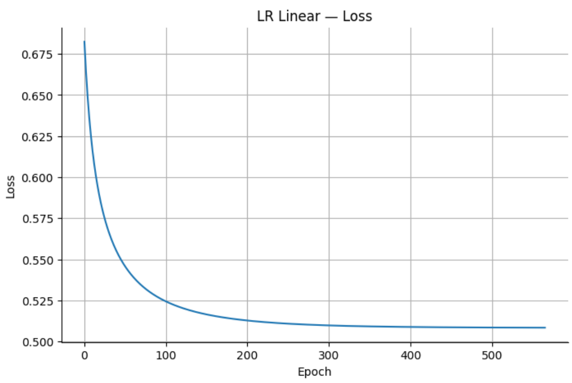


Figure 8: ROC curves on the holdout test set. KLR-RBF and LR are the top two by AUC.

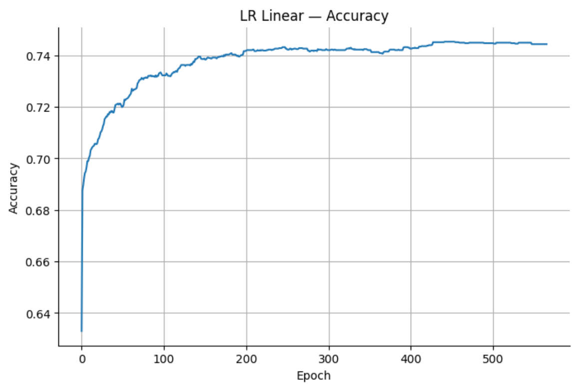
6 Results

6.1 Training Dynamics

Fig. 9 shows LR loss/accuracy converging smoothly, indicating stable optimization; Fig. 10 shows linear SVM margin/accuracy across epochs under Pegasos.

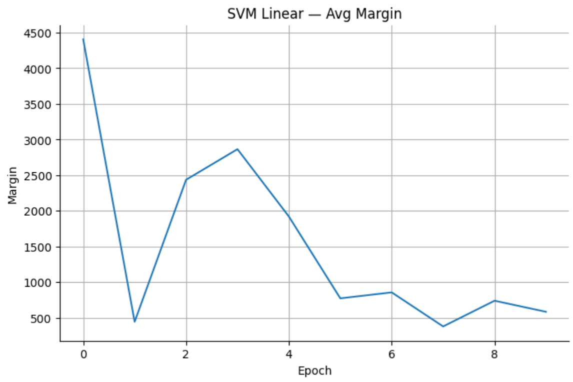


(a) LR loss vs. epochs

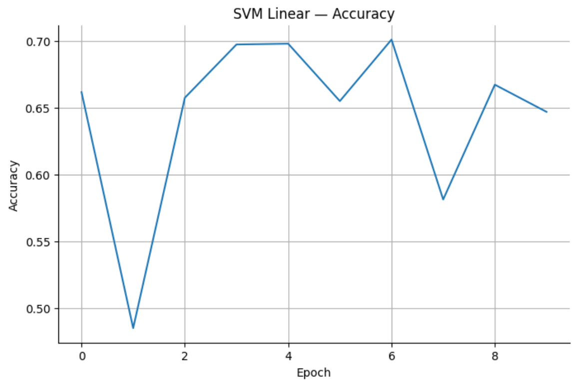


(b) LR accuracy vs. epochs

Figure 9: Convergence of Logistic Regression.



(a) Avg margin vs. epochs



(b) Accuracy vs. epochs

Figure 10: Dynamics of Linear SVM (Pegasos).

Learning Dynamics (per plot)

LR Loss vs Epochs.

- A steady, monotonic decrease indicates consistent progress minimizing the logistic objective.
- Typical shape: steep early drop (large gradients), then a shallow tail as the model approaches a minimum.
- Small oscillations with stochastic updates are fine as long as the overall trend decreases.
- If the curve plateaus high, learning rate may be too small or L2 too strong; divergence suggests learning rate too large.
- Continued loss decrease after accuracy plateaus often reflects improved probability calibration rather than better classification.

LR Accuracy vs Epochs.

- Accuracy should rise rapidly then saturate as the decision boundary stabilizes.
- If accuracy peaks then declines while training loss still falls, that's overfitting—increase regularization or use early stopping.
- High jitter suggests tiny batches or an aggressive step size; smooth via larger batches or decays.
- A flat curve from the start implies underfitting (too much regularization, too few epochs, or missing features).

Linear SVM (Pegasos) — Average Margin vs Epochs.

- Pegasos seeks a max-margin separator with step size $1/(\lambda t)$; an increasing then stabilizing margin indicates convergence.
- Early fluctuations are expected as support vectors settle; persistent oscillations may mean step size too large or λ too small.
- A late falling margin can indicate an over-aggressive step or ill-scaled features—standardization mitigates this.

- Larger margins tend to generalize better, but margin alone does not guarantee optimal Precision/Recall at a fixed threshold.

Linear SVM (Pegasos) — Accuracy vs Epochs.

- Training accuracy improves with the margin, then plateaus as the margin stabilizes.
- Spikes/dips occur when batches contain many (near-)support vectors; decaying steps reduce this with time.
- If accuracy degrades after a peak, try increasing λ or reducing the step size.
- A low, flat curve points to underfitting; try more epochs, a smaller λ, or a kernel if the boundary is non-linear.

6.2 Holdout Metrics

Table 1: Holdout test performance. Best F1 in **bold**.

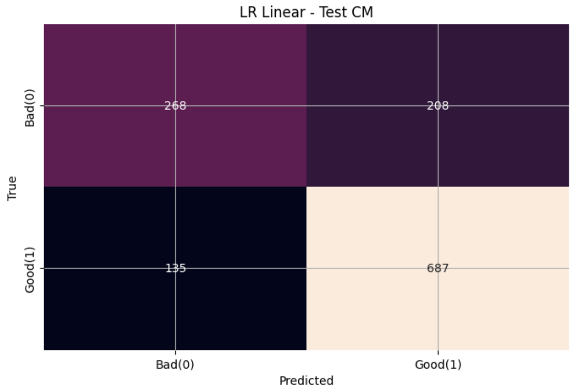
Model	Accuracy	Precision	Recall	F1
KLR RBF	0.748	0.783	0.833	**0.807**
LR Linear	0.736	0.768	**0.836**	0.800
SVM RBF	0.693	0.685	0.954	0.798
SVM Poly	0.697	0.746	0.791	0.768
KLR Poly	0.686	0.814	0.655	0.726
SVM Linear	0.652	0.754	0.668	0.708

Table 2: ROC AUC on the test set.

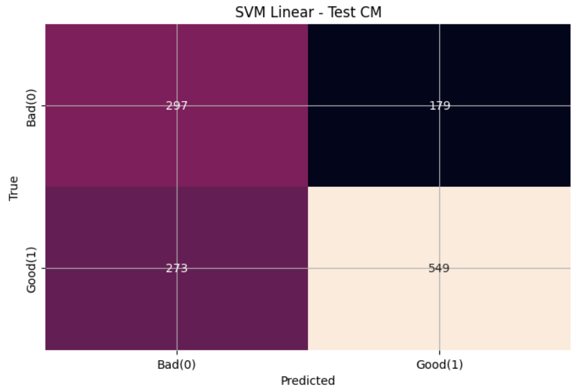
Model	AUC
KLR RBF	0.788
LR Linear	0.783
KLR Poly	0.765
SVM Poly	0.735
SVM RBF	0.689
SVM Linear	0.686

6.3 Confusion Matrices & Operating Points

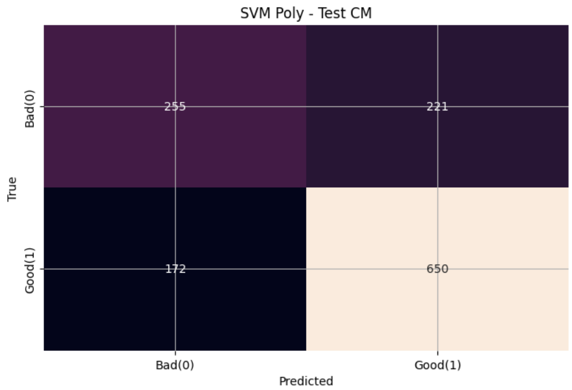
Fig. 11–12 show confusion matrices. Notably, **SVM-RBF** achieves very high **recall** (few false negatives) at the expense of more false positives, while **KLR-RBF** and **LR** strike a more balanced trade-off.



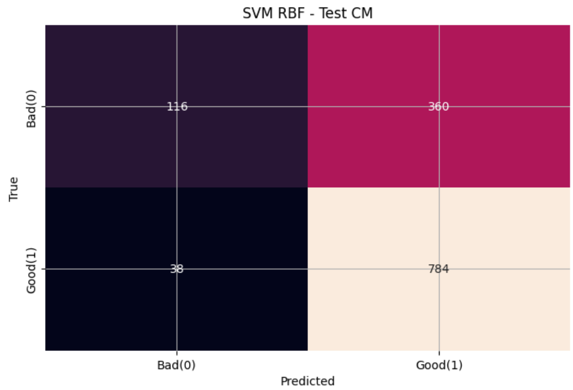
(a) LR (Linear)



(b) SVM Linear

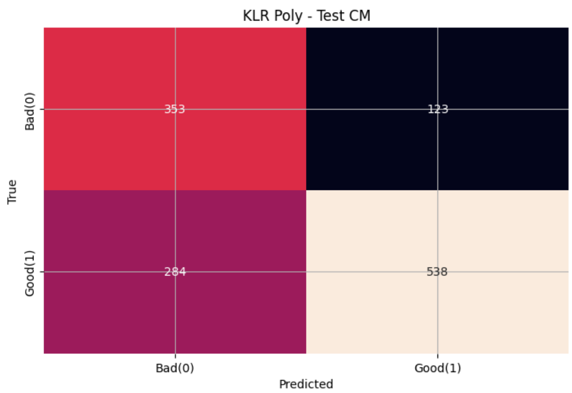


(c) SVM Poly

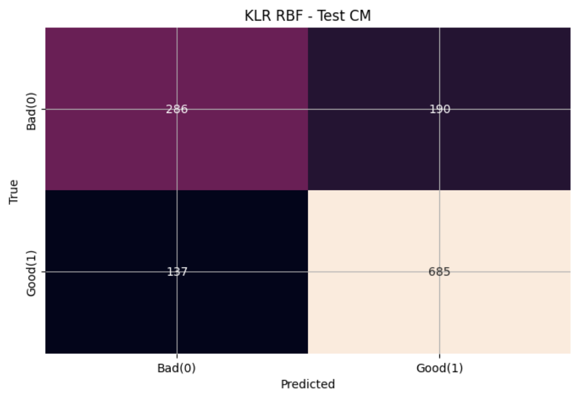


(d) SVM RBF

Figure 11: Confusion matrices (part 1).



(a) KLR Poly



(b) KLR RBF

Figure 12: Confusion matrices (part 2).

Confusion Matrices (per model)

How to read these matrices. Rows are the *true* class (`Bad`=0, `Good`=1) and columns are the *predicted* class. Top-left = TN, top-right = FP, bottom-left = FN, bottom-right = TP. Precision = $TP/(TP + FP)$ quantifies purity of predicted `Good`; Recall = $TP/(TP + FN)$ quantifies coverage of true `Good`.

Logistic Regression (Linear). Balanced trade-off with moderately low FP and FN, matching its test Precision 0.768 and Recall 0.836. Misclassifications cluster near the decision boundary. To tilt toward higher precision: raise the classification threshold above 0.5 or increase L2; to raise recall: lower the threshold or reduce L2 slightly.

SVM Linear. Lower Recall (0.668) implies *more FN* than LR—a conservative boundary typical for a linear margin on mildly non-linear data. Actions: reduce λ (weaker regularization), run more epochs, or switch to a kernel; optionally shift the decision threshold on the distance-to-hyperplane score.

SVM Polynomial (degree 2). Improves Recall (0.791) over SVM-Linear but introduces more FP (Precision 0.746), reflecting quadratic interactions. Tuning: adjust (α, c) to modulate feature scale/bias; increase λ to curb FP, or reduce λ to chase recall.

SVM RBF. Extremely high Recall (0.954) with lower Precision (0.685) means *many FP but very few FN*. Interpretation: small λ or large γ pushes the boundary outward. To rebalance: increase λ or decrease γ; or move the threshold away from 0 on the signed margin.

Kernel Logistic Regression (Polynomial, degree 2). High Precision (0.814) and lower Recall (0.655) indicate a *conservative positive rule* (many FN, few FP). This kernel captures some interactions but misses local structure; to boost Recall: reduce regularization, increase degree to 3, or alter (α, c) while keeping kernel centering/normalization.

Kernel Logistic Regression (RBF). Best overall F1: Precision 0.783, Recall 0.833. Matrix shows a balanced FP/FN profile; probabilistic training with a smooth kernel yields calibrated scores. To target a specific operating point, tune the probability threshold on validation (e.g., maximize F1 or business metric).

7 Interpretation and Insights

7.1 What the Metrics Tell Us

F1 balances Precision and Recall. Here, **KLR-RBF** is best by F1 and AUC, indicating strong overall ranking and a good operating point. **LR** remains competitive—evidence that much of the signal is approximately linear after preprocessing. **SVM-RBF**'s very high recall suggests a low effective margin or larger γ, aggressively labeling positives.

7.2 Feature-Level Intuition (from Linear Models)

Table 3 reports LR coefficients (standardized feature space). Alcohol and sulphates are positive; volatile acidity and density are negative—consistent with domain knowledge.

Table 3: Logistic Regression coefficients (standardized features). Signs align with oenological expectations.

Feature	Coefficient
alcohol	1.034
sulphates	0.328
free sulfur dioxide	0.268
residual sugar	0.431
fixed acidity	0.125
pH	0.111
citric acid	-0.091
chlorides	-0.026
density	-0.228
total sulfur dioxide	-0.375
volatile acidity	-0.707

7.3 Misclassification Analysis

The top "confidently wrong" KLR-RBF cases have borderline chemistry: alcohol $\approx$ 11.4–12.0, moderate sulphates, low residual sugar/chlorides; true class = 0 but predicted = 1 with confidence $\sim$ 0.38–0.45. These sit near the decision boundary or may reflect latent sensory attributes not captured by lab measures. This also explains why a simple degree-2 polynomial doesn't suffice, whereas RBF improves boundaries locally.

7.4 Over/Underfitting

CV and test scores are aligned; LR training curves are smooth (Fig. 9). SVM-RBF's pattern reflects a different operating point rather than classical overfit; adjusting λ or γ, or tuning the decision threshold, can rebalance precision/recall.

8 Design Choices Justified

- **Z-Score + IQR winsorization**: handles heavy tails without discarding data; crucial for stable optimization in from-scratch learners.
- **Standardization**: necessary for gradient descent and kernel scale interpretability.
- **Exclude `type` in modeling**: prevents shortcut learning and keeps the task focused on chemistry $\rightarrow$ quality.
- **RBF vs. Poly**: RBF captures smooth local structure; Poly-2 adds global pairwise interactions. Results show local smoothness matters more here.
- **F1-centric selection**: appropriate under moderate imbalance; complemented by Accuracy/Precision/Recall and AUC.

9 Recommendations and Next Steps

Operating point: If recall is paramount (screening), SVM-RBF is attractive; otherwise use KLR-RBF/LR and tune the threshold for desired Precision/Recall. **KLR-Poly improvements**: try degree 3 with stronger reg (0.03–0.3), larger c and smaller α, keep centering/normalization, and consider $\eta_t = \eta_0/\sqrt{t}$. **Robustness**: repeated CV (e.g., 3×5-fold) and sensitivity to winsor caps (e.g., 2.5×IQR vs 1.5×IQR). **Explainability**: report bootstrapped CIs for LR coefficients; consider classwise reliability diagrams for KLR probabilities.

10 Reproducibility Checklist

- Random seeds fixed for splits and initializations.
- All transforms fit on training data only (and within each CV fold).
- Hyperparameters selected by 5-fold CV; test used once for final reporting.
- Notebook: `Wine_Classification.ipynb`.

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Antonella Convertini