

Wine Quality Classification: Logistic Regression and SVM with Kernel Extensions

January 27, 2026

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.

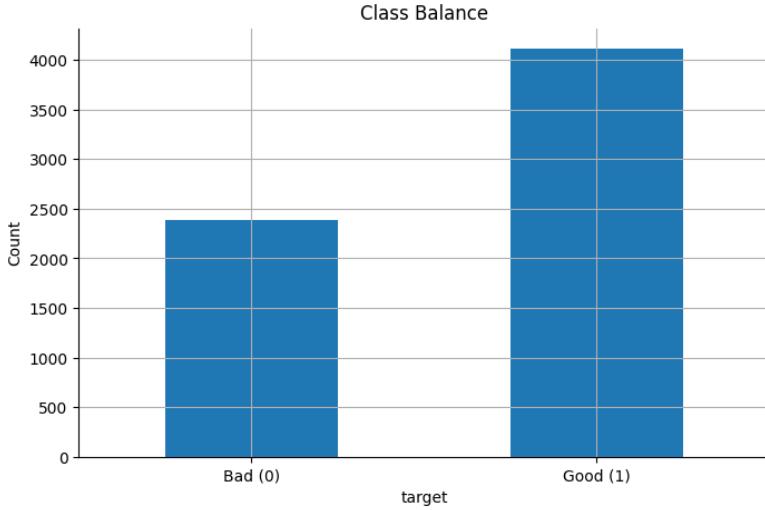


Figure 1: Class balance on the combined dataset (Bad vs Good).

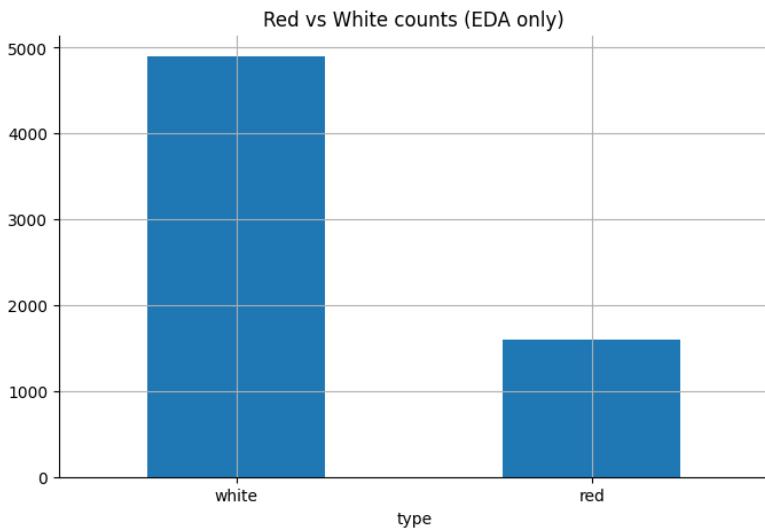


Figure 2: Counts of white vs. red wines (EDA only; type is excluded from modeling).

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.

Feature Histograms (combined red+white)

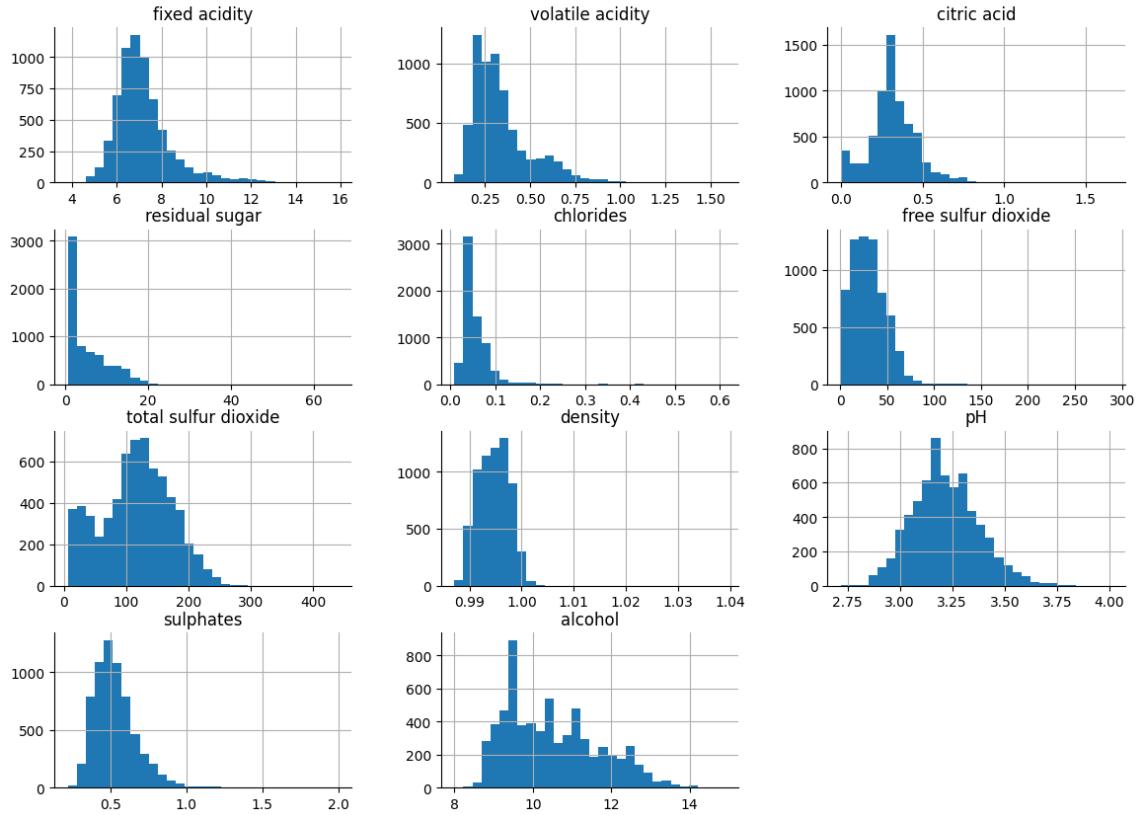


Figure 3: Feature histograms (combined red+white). Heavy tails in several variables motivate winsorization.

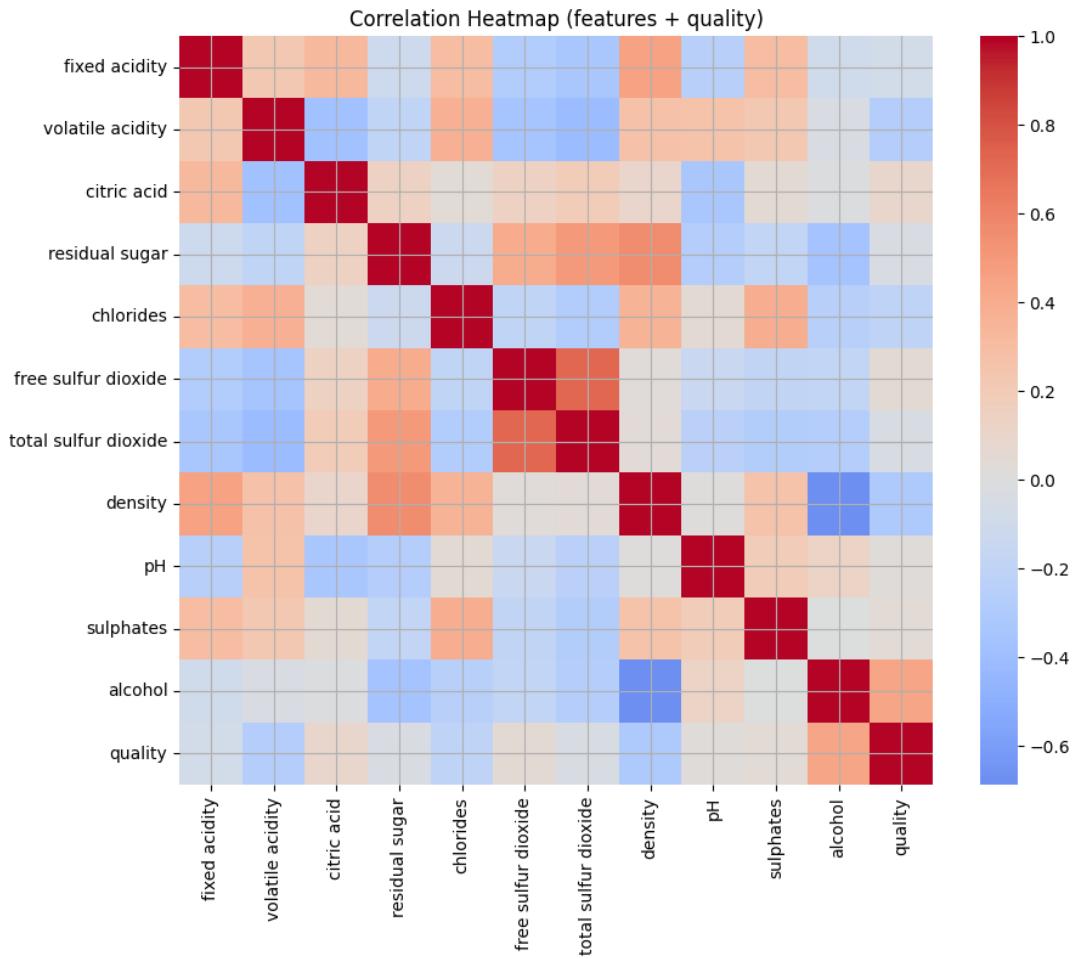


Figure 4: Correlation heatmap (features + quality). Alcohol correlates positively with quality; volatile acidity is negatively associated.

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

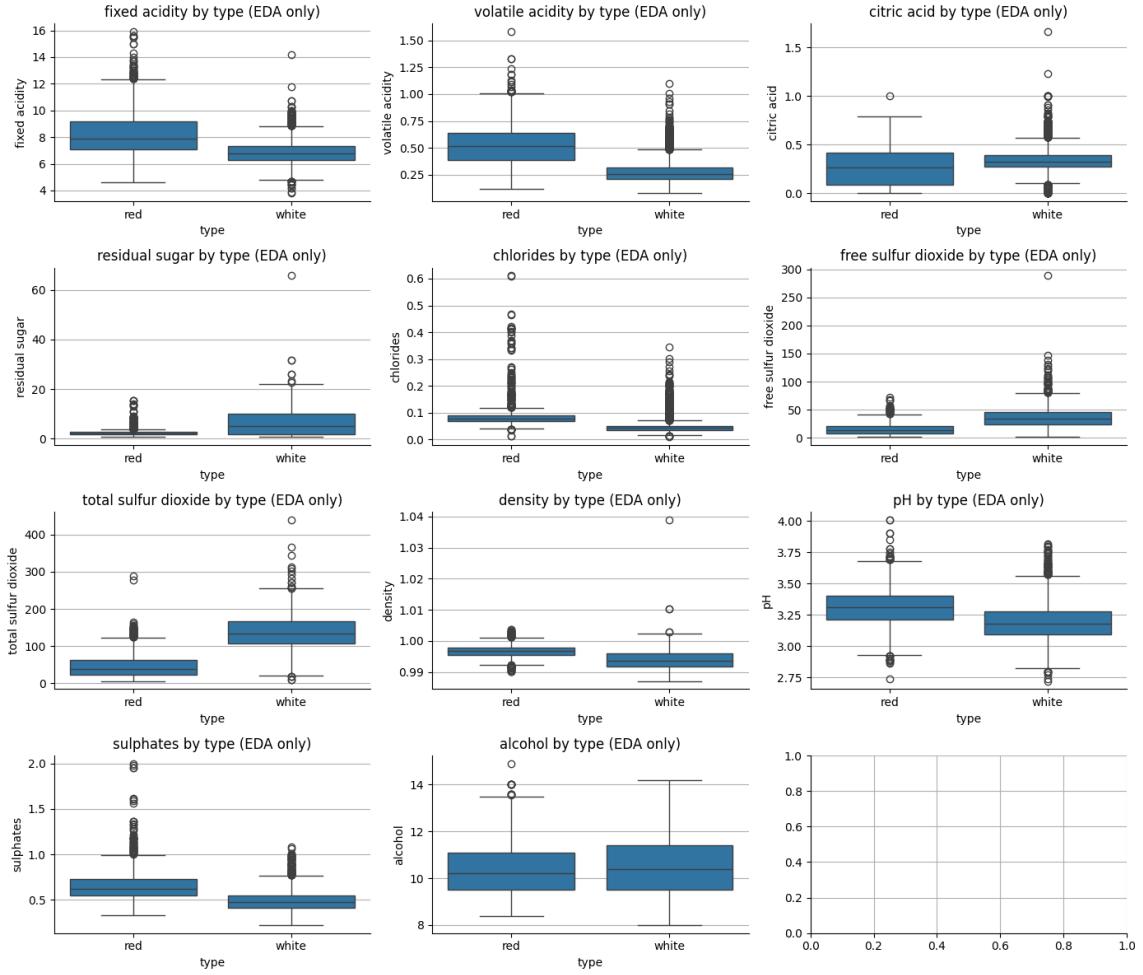


Figure 5: Feature distributions by type (EDA only).

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 $[Q_1 - 1.5 \cdot IQR, Q_3 + 1.5 \cdot IQR]$. Caps are **learned on the training set only** and then applied to validation/test, preventing leakage. Fig. 6 and Fig. 7 show the effect.

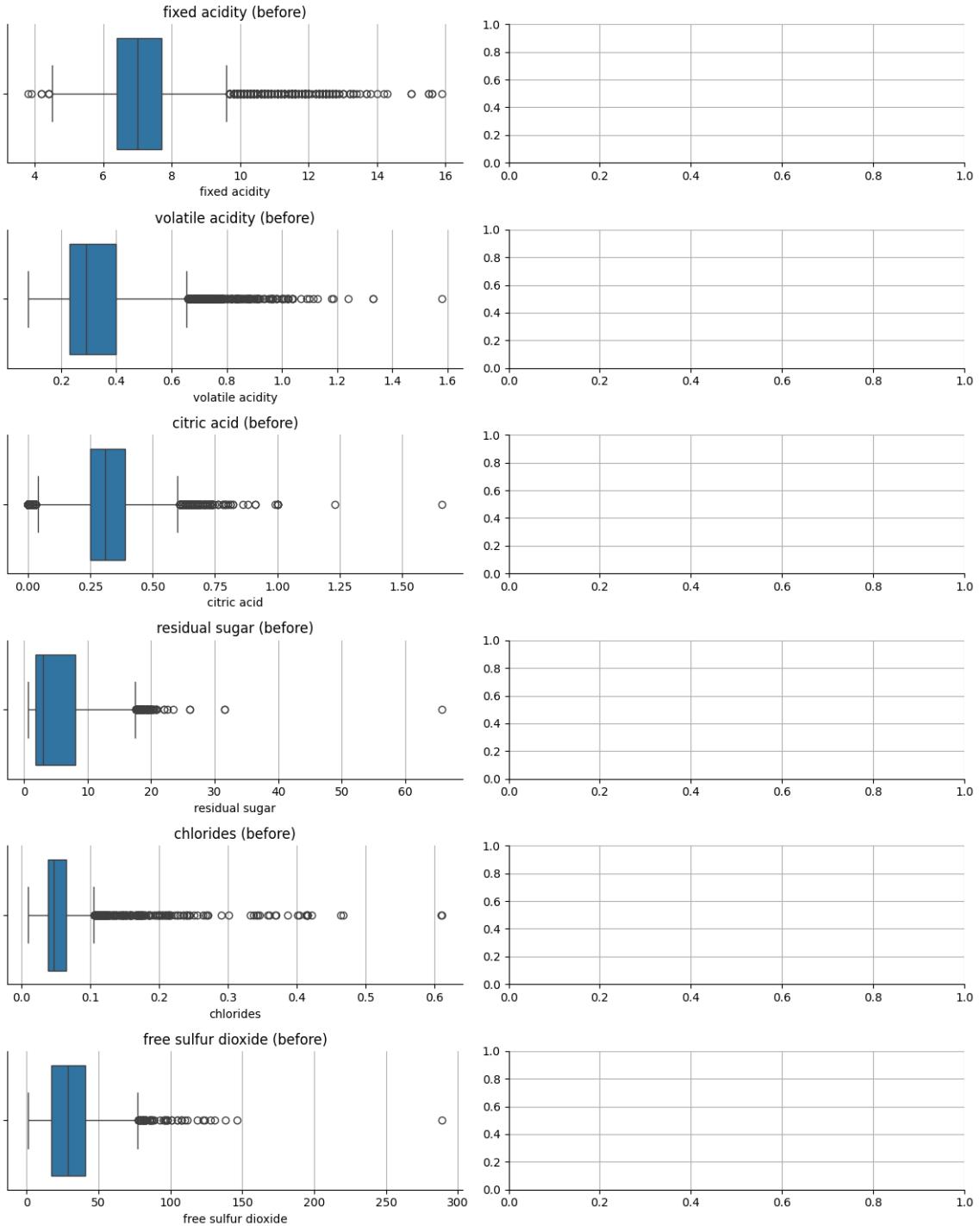


Figure 6: Diagnostic boxplots *before* IQR winsorization. Multiple features exhibit long right tails.

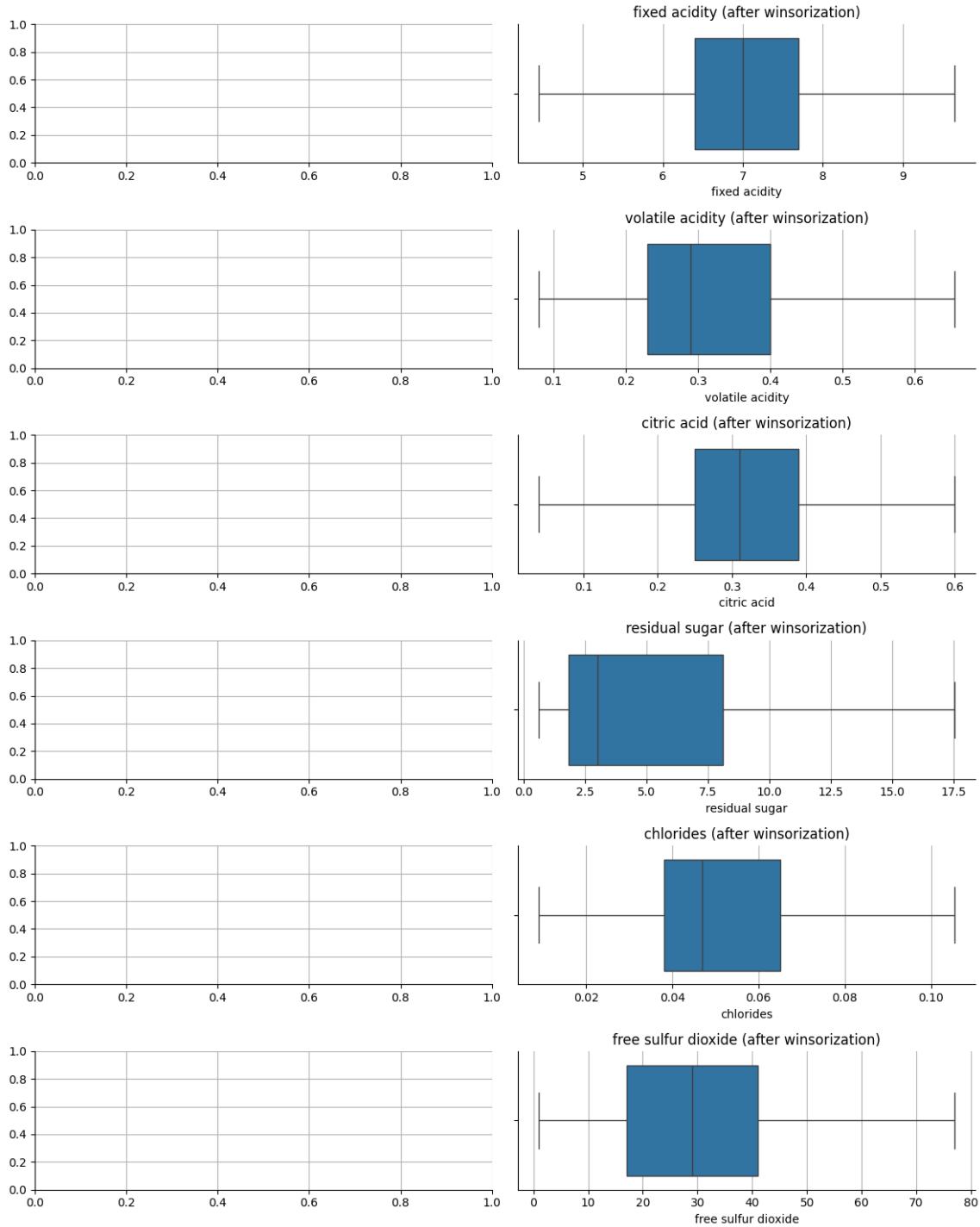


Figure 7: Boxplots *after* winsorization. Caps mitigate leverage of extreme values while preserving samples.

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.

3.3 Detailed Stratified Cross-Validation Strategy

To rigorously evaluate model performance while handling the class imbalance, I implemented a **Stratified K-Fold Cross-Validation** procedure from scratch. Unlike standard random splitting, stratification guarantees that the proportion of samples for each class is preserved in every fold. The procedure is as follows:

1. **Index Separation:** I separate the dataset indices into two distinct pools: I_{pos} (where target=1) and I_{neg} (where target=0).
2. **Shuffling:** To eliminate ordering bias, I randomly shuffle both I_{pos} and I_{neg} independently using a fixed random seed.
3. **Partitioning:** I split the shuffled I_{pos} array into $K = 5$ equal-sized chunks. Similarly, I split the I_{neg} array into $K = 5$ equal chunks.
4. **Fold Assembly:** For each round k (from 1 to 5):
 - **Validation Set:** Constructed by concatenating the k -th chunk of positive indices with the k -th chunk of negative indices.
 - **Training Set:** Constructed by aggregating the remaining $K - 1$ chunks from both classes.
5. **Execution:** The model is trained on the Training Set (standardized using statistics derived *only* from that training fold) and evaluated on the Validation Set. The resulting metrics are averaged to estimate generalization performance.

4 Models Implemented from Scratch

4.1 Logistic Regression (Linear) and SGD

I minimize the L2-regularized binary cross-entropy loss (Log-Loss). The optimization is performed via **Stochastic Gradient Descent (SGD)**. Rather than summing the gradient over the entire dataset, we update weights iteratively using small batches. For a single training example (x_i, y_i) , the update proceeds as follows:

1. **Forward Pass:** Compute the predicted probability via the sigmoid function:

$$\hat{y}_i = \sigma(w^T x_i + b) = \frac{1}{1 + e^{-(w^T x_i + b)}} \quad (1)$$

2. **Gradient Calculation:** Compute the gradient of the loss w.r.t. weights w . For log-loss, this simplifies to the error times the input feature, plus the L2 penalty:

$$\nabla L_w = (\hat{y}_i - y_i) \cdot x_i + \lambda w \quad (2)$$

3. **Weight Update:** Adjust weights in the opposite direction of the gradient, scaled by learning rate η :

$$w_{new} = w_{old} - \eta \cdot \nabla L_w \quad (3)$$

By default, I used a prediction threshold of 0.5.

4.2 Kernel Logistic Regression (KLR)

To capture non-linear relationships, I formulated Logistic Regression in its **dual form** using the kernel trick. By the Representer Theorem, the weight vector w is a linear combination of the training samples in feature space: $w = \sum_{i=1}^m \alpha_i \phi(x_i)$.

Step-by-Step Implementation:

- Kernel Matrix Computation:** I pre-compute the Gram matrix $K \in \mathbb{R}^{m \times m}$ where $K_{ij} = k(x_i, x_j)$.

- For **RBF**: $K_{ij} = \exp(-\gamma \|x_i - x_j\|^2)$.
- For **Poly**: $K_{ij} = (\alpha x_i^T x_j + c)^d$.

- Prediction:** The probability for a sample x is computed using the dual coefficients α :

$$P(y = 1|x) = \sigma \left(\sum_{j=1}^m \alpha_j K(x_j, x) + b \right) \quad (4)$$

- Optimization:** We minimize the regularized log-loss with respect to α using gradient descent.

- Calculate predictions: $\hat{p} = \sigma(K\alpha)$.
- Compute Gradient: $\nabla_\alpha L = K^T(\hat{p} - y) + \lambda K\alpha$.
- Update Rule: $\alpha_{new} = \alpha_{old} - \eta \nabla_\alpha L$.

4.3 Support Vector Machines and Pegasos

I trained the Linear SVM using the **Pegasos algorithm** (Primal Estimated sub-GrAdient SOlver). This is a stochastic method designed directly for the SVM objective (Hinge Loss + L2 Regularization). The objective is:

$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{m} \sum_{i=1}^m \max(0, 1 - y_i(w^T x_i)) \quad (5)$$

Step-by-Step Execution:

- Iteration:** At step t , select a random sample (x_i, y_i) .
- Margin Check:** Calculate the decision score $z = y_i(w^T x_i)$. Check if the sample violates the margin ($z < 1$).
- Update Rule:**

- If $y_i(w^T x_i) < 1$ (**Violation/Misclassification**): The weights are updated to minimize error and apply regularization:

$$w_{t+1} = (1 - \eta_t \lambda) w_t + \eta_t y_i x_i \quad (6)$$

- If $y_i(w^T x_i) \geq 1$ (**Correct**): Only regularization (weight decay) is applied:

$$w_{t+1} = (1 - \eta_t \lambda) w_t \quad (7)$$

- Learning Rate:** The step size decays as $\eta_t = \frac{1}{\lambda t}$.

5 Model Selection and Metrics

5.1 Systematic Hyperparameter Grid Search

To ensure the selected models are optimal, I implemented an automated grid search framework. The step-by-step procedure is as follows:

1. **Grid Definition:** For each model architecture, I defined a dictionary of hyperparameters (e.g., Learning Rate $\in \{0.01, 0.005\}$, Regularization $\lambda \in \{0.1, 0.01, 0.001\}$).
2. **Combination Generation:** I generated the Cartesian product of all parameters to create a list of all possible candidate configurations.
3. **Candidate Evaluation (Inner Loop):**
 - For each candidate configuration θ :
 - Iterate through the 5 folds defined in Section 3.3.
 - Train a fresh model with parameters θ on the Training Fold.
 - Evaluate on the Validation Fold and store the F1 score.
 - Compute the average F1 score across all 5 folds.
4. **Selection:** The configuration θ^* with the highest average F1 score is selected as the best model.
5. **Final Retraining:** A final model is instantiated with θ^* and trained on the *entire* training dataset (Train + Validation) before final evaluation on the Holdout Test Set.

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.

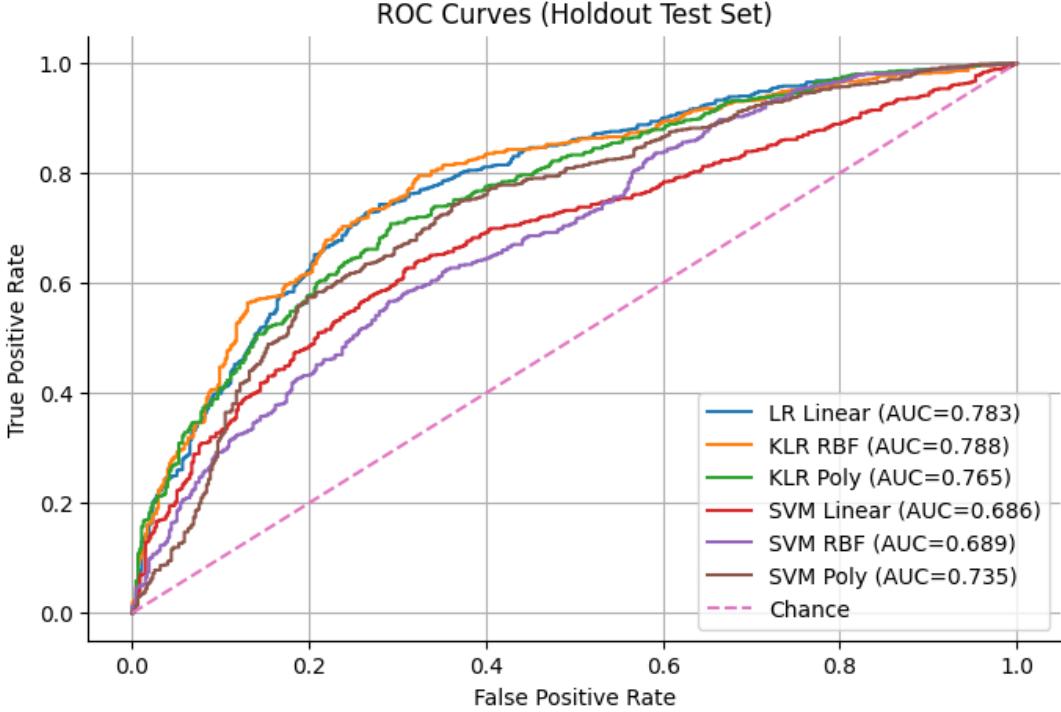


Figure 8: ROC curves on the holdout test set. KLR-RBF and LR are the top two by AUC.

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.

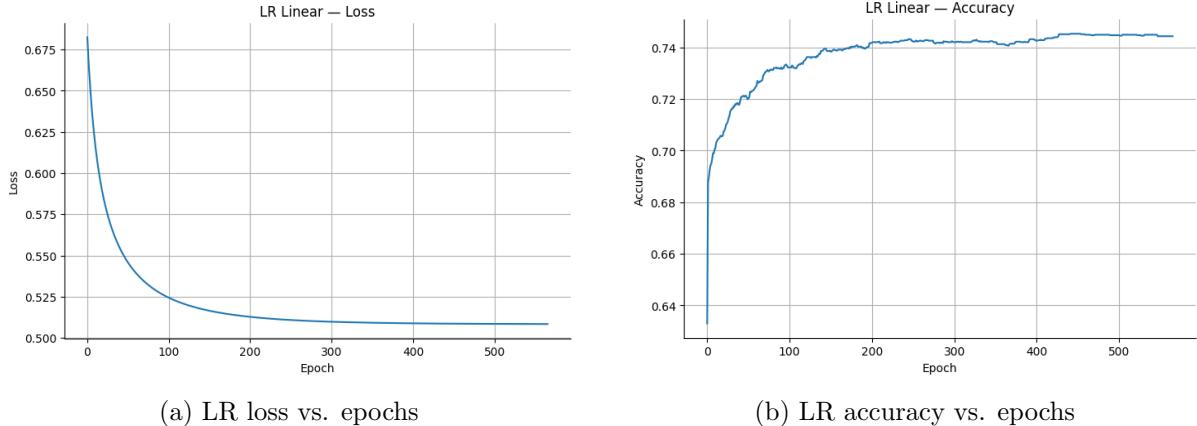


Figure 9: Convergence of Logistic Regression.

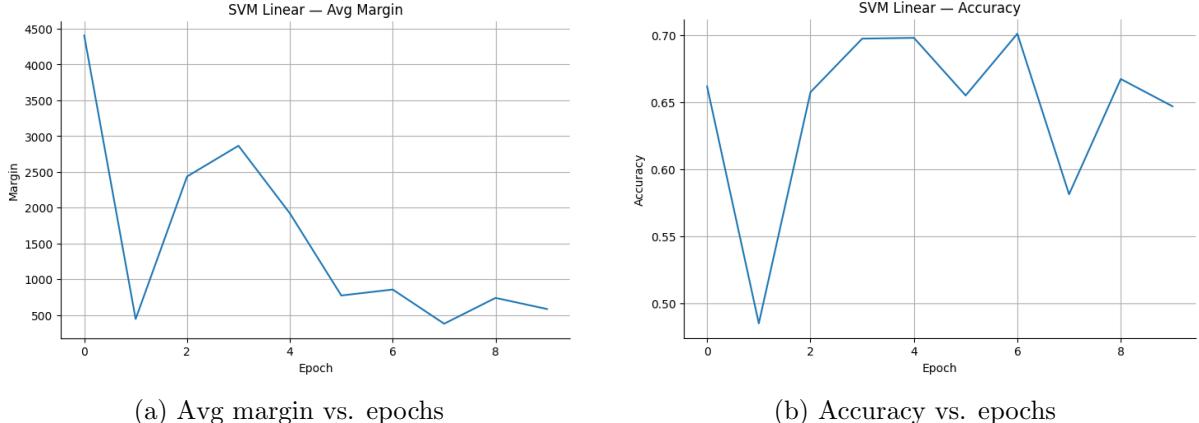


Figure 10: Dynamics of Linear SVM (Pegasos).

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.

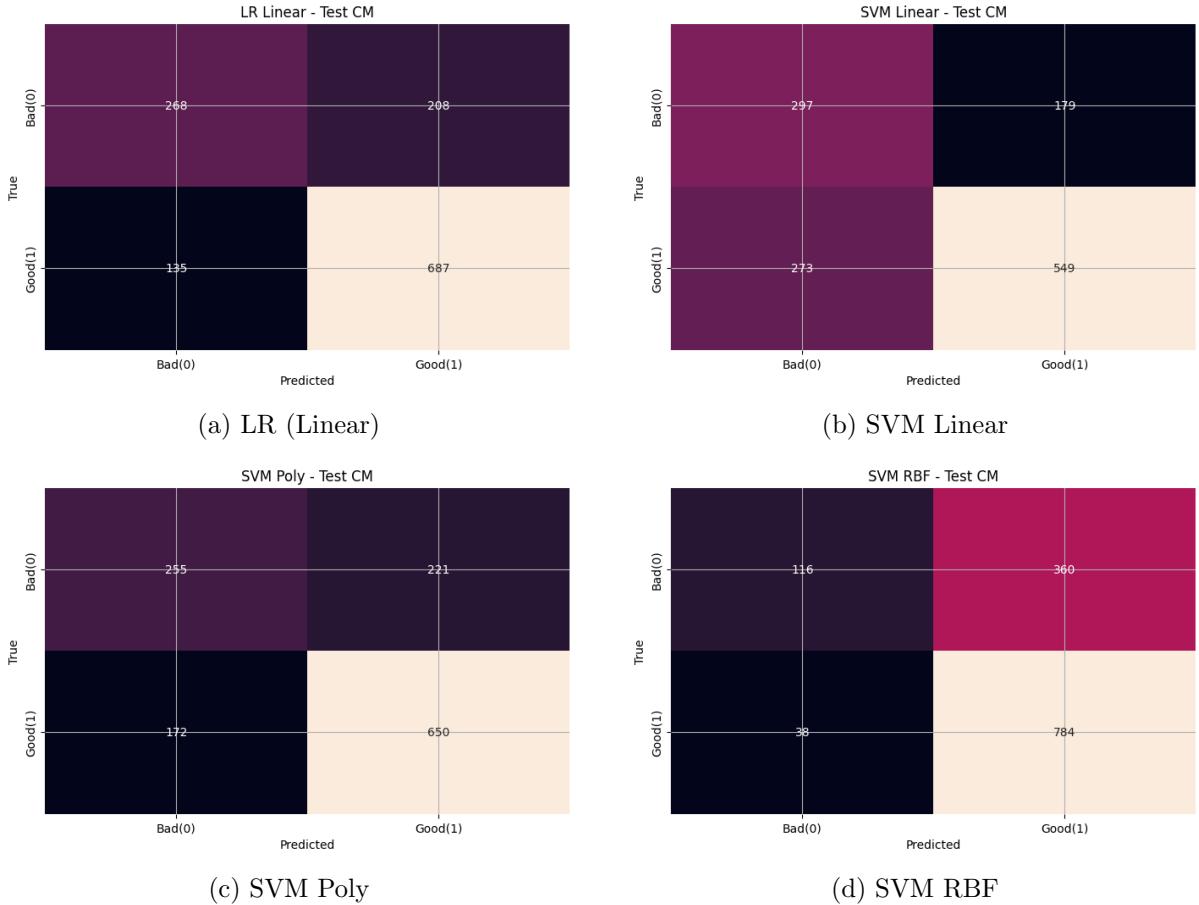


Figure 11: Confusion matrices (part 1).

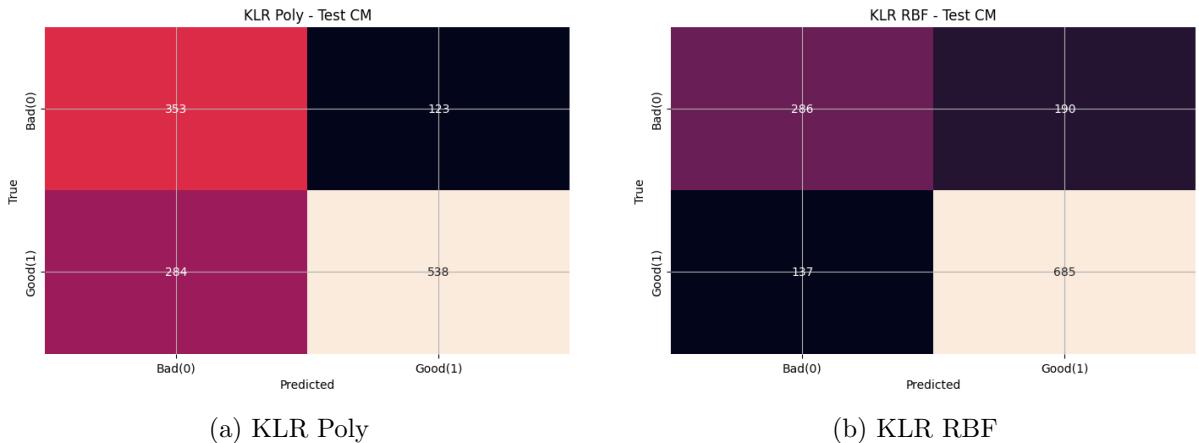


Figure 12: Confusion matrices (part 2).

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 $\approx 11.4\text{--}12.0$, moderate sulphates, low residual sugar/chlorides; true class = 0 but predicted = 1 with confidence $\sim 0.38\text{--}0.45$. 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., $2.5 \times \text{IQR}$ vs $1.5 \times \text{IQR}$). **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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