

LINEAR REGRESSION

Linear regression needs clean, well-preprocessed data, a suitable loss (cost) function such as Mean Squared Error, is commonly trained with Gradient Descent, and evaluated using metrics like MSE, RMSE, MAE, and R^2 , each with standard formulas.

Preprocessing for linear regression

Typical preprocessing steps for linear regression include:

Handle missing values (drop rows/columns or impute with mean/median, etc.).

- Treat outliers (remove, cap, or transform if they distort the fit).
- Encode categorical features (one-hot/dummy encoding).
- Scale/standardize features if magnitudes differ greatly (e.g., z-score standardization).
- Remove perfectly collinear or near-constant features to avoid multicollinearity issues.

Loss function (cost) for linear regression

For a dataset $\{(x_i, y_i)\}_{i=1}^n$ and a linear model $\hat{y}_i = w^\top x_i + b$, the standard **loss (cost) function** is Mean Squared Error (MSE):

$$\mathbf{MSE}(\mathbf{w}, \mathbf{b}) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Sometimes the cost uses $\frac{1}{2n}$ for convenience in derivatives:

$$J(\mathbf{w}, \mathbf{b}) = \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Other common regression losses:

- Mean Absolute Error (MAE):

$$\mathbf{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

- Huber loss (quadratic near zero, linear for large errors).

Gradient Descent for linear regression

Goal: minimize the cost $J(w, b)$ by iteratively updating parameters in the negative gradient direction.^{[11][6]}

For MSE cost $J(w, b) = \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$:

- Prediction: $\hat{y}_i = w^\top x_i + b$.
- Gradients:

$$\frac{\partial J}{\partial w} = -\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i) x_i$$

$$\frac{\partial J}{\partial b} = -\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)$$

- Gradient Descent updates with learning rate α :

$$w := w - \alpha \frac{\partial J}{\partial w}$$

$$b := b - \alpha \frac{\partial J}{\partial b}$$

Variants include batch GD, stochastic GD (update per sample), and mini-batch GD.^[6]

Evaluation metrics with formulas

For true values y_i and predictions $\hat{y}_i, i = 1, \dots, n$:

- **Mean Squared Error (MSE):**

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

- **Root Mean Squared Error (RMSE):**

$$\text{RMSE} = \sqrt{\text{MSE}} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

- **Mean Absolute Error (MAE):**

$$\mathbf{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

- **Coefficient of Determination R^2 :**

Let $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$. Then:

$$\mathbf{SSE} = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

$$\mathbf{SST} = \sum_{i=1}^n (y_i - \bar{y})^2$$

$$\mathbf{R^2} = 1 - \frac{\mathbf{SSE}}{\mathbf{SST}}$$

Logistic Regression

Logistic Regression, Preprocessing Is Similar To Linear Regression, The Loss Is Usually Binary Cross-Entropy (Log Loss), Optimization Commonly Uses Gradient Descent, And Evaluation Relies On Classification Metrics Such As Accuracy, Precision, Recall, F1, ROC-AUC, With Standard Formulas.

Preprocessing for logistic regression

Core preprocessing steps for logistic regression:

- Handle missing values (drop or impute with mean/median/mode as suitable).
- Detect and treat outliers that can distort the decision boundary.
- Encode categorical variables (one-hot/dummy encoding for non-ordinal categories).
- Optionally scale/standardize numeric features, especially when using regularization or gradient-based solvers.
- Remove highly collinear features and ensure the target is binary (0/1) for standard binary logistic regression.

Logistic model and prediction

For input $x_i \in \mathbb{R}^d$, parameters w, b , the logistic regression model predicts a probability of class 1:

$$z_i = w^\top x_i + b$$
$$\hat{p}_i = \sigma(z_i) = \frac{1}{1 + e^{-z_i}}$$

To convert probability to a class label (binary case):

$$\hat{y}_i = \begin{cases} 1 & \text{if } \hat{p}_i \geq \tau \\ 0 & \text{if } \hat{p}_i < \tau \end{cases}$$

where τ is a threshold, often 0.5.

Loss (cost) function for logistic regression

For binary logistic regression with true labels $y_i \in \{0,1\}$ and predicted probabilities \hat{p}_i , the usual loss is binary cross-entropy (log loss):

Single sample loss:

$$\ell(y_i, \hat{p}_i) = -[y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)]$$

For a dataset of size n , cost function:

$$J(w, b) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \hat{p}_i) = -\frac{1}{n} \sum_{i=1}^n [y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)]$$

This cost is convex in w, b for logistic regression.

Gradient Descent for logistic regression

Using the cost $J(w, b)$ above, with $\hat{p}_i = \sigma(w^\top x_i + b)$, the partial derivatives are:

$$\frac{\partial J}{\partial w} = \frac{1}{n} \sum_{i=1}^n (\hat{p}_i - y_i) x_i$$
$$\frac{\partial J}{\partial b} = \frac{1}{n} \sum_{i=1}^n (\hat{p}_i - y_i)$$

Gradient Descent updates (learning rate α):

$$w := w - \alpha \frac{\partial J}{\partial w}$$
$$b := b - \alpha \frac{\partial J}{\partial b}$$

Again, there are batch, stochastic, and mini-batch variants.

Evaluation metrics and formulas

Assume binary classes 0 (negative) and 1 (positive), with:

- True Positives (TP)
- True Negatives (TN)
- False Positives (FP)

- False Negatives (FN)

Key metrics:

- Accuracy

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

- Precision (Positive Predictive Value)

$$\text{Precision} = \frac{TP}{TP + FP}$$

- Recall (Sensitivity, True Positive Rate)

$$\text{Recall} = \frac{TP}{TP + FN}$$

- F1-score (harmonic mean of precision and recall)

$$F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

- Specificity (True Negative Rate)

$$\text{Specificity} = \frac{TN}{TN + FP}$$

From these, the ROC curve plots True Positive Rate vs False Positive Rate, where:

$$\text{FPR} = \frac{FP}{FP + TN}$$

ROC-AUC is the area under this curve; PR-AUC is area under the Precision-Recall curve.

Decision trees

Decision trees need basic preprocessing (clean labels, handle missing values, encode categories if required) but usually do not need feature scaling; they choose splits using impurity/loss measures such as Gini or entropy and are evaluated with the same classification metrics used for logistic regression (accuracy, precision, recall, F1, ROC-AUC, etc.).

Preprocessing for decision trees

Compared to linear/logistic models, decision trees are less sensitive to monotonic transformations and scaling of features.

- Handle missing values (impute or drop; some libraries can handle a limited amount directly).
- Encode categorical features (label or one-hot encoding depending on implementation; many tree algorithms can work directly with categories).
- Detect extreme outliers if they are data errors; trees are relatively robust but bad data can still hurt.
- No strict need to normalize/standardize features, but cleaning data and removing obvious data-quality issues remains important.

Tree prediction

For classification trees, each leaf holds a class distribution; prediction is commonly the majority class.

- For an input x , the tree routes down internal nodes via tests like “feature $j \leq t$?” until reaching a leaf.
- Let p_k be the proportion of class k among training samples in the leaf; predicted class is $\arg \max_k p_k$.

For regression trees, the prediction is typically the mean of the target values in the leaf.

Split “loss” functions (impurity)

At each node, the tree chooses the split that maximizes impurity reduction (information gain).

Assume a node has class proportions p_1, \dots, p_K . Common impurities:

- **Gini impurity**

Gini Impurity checks how often a randomly selected sample would be mislabeled if assigned by class probability. It is computationally simple and used in tree-based classifiers.

$$G = 1 - \sum_{k=1}^K p_k^2$$

Where p_k is the probability of class k .

- **Entropy**

Entropy measures uncertainty in a node’s class distribution and originates from information theory. Higher entropy indicates greater disorder among class labels.

$$H = - \sum_{k=1}^K p_k \log_2 p_k$$

Where p_k represents the proportion of class k in the node

Given a parent node P split into children C_1, \dots, C_m with N_P total samples and N_j samples in child C_j , the information gain (using entropy) is:

$$\text{Gain} = H(P) - \sum_{j=1}^m \frac{N_j}{N_P} H(C_j)$$

Analogously, Gini-based trees minimize weighted child Gini. For regression trees, a common “loss” at a node is variance or MSE:

$$\text{Var}(P) = \frac{1}{N_P} \sum_{i \in P} (y_i - \bar{y}_P)^2$$

and splits are chosen to minimize weighted child variance.

Training / “gradient” intuition

Standard decision trees do not use Gradient Descent; training is a greedy, top-down search for the best split at each node.

- Start at root with all data.
- For each candidate feature/threshold, compute impurity before/after split and pick the best.
- Recurse on each child until stopping criteria (max depth, min samples, no gain, etc.) are met.

Evaluation metrics and formulas

For classification trees, metrics are the same as for logistic regression.

Let TP, TN, FP, FN be counts from the confusion matrix:

- Accuracy: $\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$
- Precision: $\text{Precision} = \frac{TP}{TP+FP}$
- Recall (TPR): $\text{Recall} = \frac{TP}{TP+FN}$
- F1-score: $F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

ROC-AUC, PR-AUC and other metrics are defined exactly as for logistic regression, using the tree’s class probabilities (or scores) across thresholds.

For regression trees, use MSE, RMSE, MAE, and R^2 with the same formulas as in linear regression.

Random Forests

Random Forests use similar basic preprocessing to decision trees, train many trees on bootstrapped and feature-sampled data, aggregate predictions by averaging (regression) or majority vote (classification), and are typically evaluated with regression or classification metrics depending on the task.

Preprocessing for Random Forests

For tabular data, Random Forests are quite robust and do not need feature scaling.

- Handle missing values: use imputers such as KNN Imputer or simple mean/median; some implementations can handle limited missingness.
- Encode categorical features (label or one-hot encoding) before fitting in libraries like scikit-learn.
- Clean obvious data errors and consider handling severe class imbalance (class weights, resampling) for classification tasks.

Model, training, and “loss”

Random Forests are ensembles of decision trees, trained with randomness in both data and features.

- Bootstrap sampling: each tree is trained on a bootstrap sample (sampling rows with replacement) from the original dataset.
- Feature sampling: at each split, a random subset of features is considered, promoting diversity among trees.
- Tree-level split criteria:
 - Classification: use Gini impurity or entropy, as in standard decision trees.
 - Regression: minimize MSE / variance within nodes.

For regression, tree t outputs prediction $\hat{y}^{(t)}(x)$; Random Forest prediction is:

$$\hat{y}(x) = \frac{1}{T} \sum_{t=1}^T \hat{y}^{(t)}(x)$$

For classification with K classes, if tree t predicts class $\hat{c}^{(t)}(x)$, the forest prediction is the majority vote:

$$\hat{c}(x) = \arg \max_{k \in \{1, \dots, K\}} \sum_{t=1}^T \mathbf{1}\{\hat{c}^{(t)}(x) = k\}$$

No Gradient Descent is used; training is greedy at each tree, like decision trees.

Out-of-bag (OOB) estimate

Because each tree sees only a bootstrap sample, some rows are left out (OOB samples) for that tree.

- For each data point, aggregate predictions from trees where it was OOB.
- Compute an OOB performance metric (e.g., R^2 for regression, accuracy for classification).

This gives an internal validation estimate without a separate validation set.

Evaluation metrics (regression forests)

For Random Forest regression, use the same metrics as linear regression.

Let true values y_i and predictions \hat{y}_i , $i = 1, \dots, n$:

- MSE: $\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
- RMSE: $\text{RMSE} = \sqrt{\text{MSE}}$
- MAE: $\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$
- R^2 : with $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$,

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

KNN model

KNN “trains” by storing the labeled training data.

Given a query point x :

1. Compute distance from x to every training point x_i , often Euclidean:

$$d(x, x_i) = \sqrt{\sum_{j=1}^d (x_j - x_{ij})^2}$$

2. Select the k nearest neighbors $\mathcal{N}_k(x)$ with smallest distances.
- Classification: majority vote among neighbors' labels y_i :

$$\hat{y} = \arg \max_c \sum_{i \in \mathcal{N}_k(x)} \mathbf{1}\{y_i = c\}$$

Optionally weight votes by inverse distance.

- Regression: average neighbors' targets y_i :

$$\hat{y} = \frac{1}{k} \sum_{i \in \mathcal{N}_k(x)} y_i$$

or a distance-weighted average.

“Loss” / optimization perspective

KNN does not learn parameters with Gradient Descent; there is no global cost function being minimized during training.

- The main “hyperparameters” are k , distance metric (Euclidean, Manhattan, etc.), and weighting scheme.
- k is usually chosen via validation or cross-validation to balance overfitting (small k) vs underfitting (large k).

Evaluation metrics for KNN classification

Use the same metrics as logistic regression / decision tree / Random Forest classification.

With TP, TN, FP, FN:

- Accuracy: $\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$
- Precision: $\text{Precision} = \frac{TP}{TP+FP}$
- Recall: $\text{Recall} = \frac{TP}{TP+FN}$
- F1-score: $F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

Using predicted class probabilities (fraction of neighbors in each class) across thresholds, compute ROC-AUC and PR-AUC as usual.

Evaluation metrics for KNN regression

For regression KNN, use the same regression metrics as linear regression / Random Forest regression.

With true targets y_i , predictions \hat{y}_i :

- MSE: $\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
- RMSE: $\text{RMSE} = \sqrt{\text{MSE}}$
- MAE: $\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$

- R^2 : $R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$, with \bar{y} the mean of y_i .

Evaluation metrics (classification forests)

For Random Forest classification, use the same metrics as logistic regression and decision trees.

With TP, TN, FP, FN:

- Accuracy: $\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$
- Precision: $\text{Precision} = \frac{TP}{TP+FP}$
- Recall: $\text{Recall} = \frac{TP}{TP+FN}$
- F1-score: $F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

Using predicted class probabilities across thresholds, ROC-AUC and PR-AUC are defined as for any classifier.

Gradient Boosting

Gradient Boosting builds an ensemble of weak learners (usually shallow trees) sequentially, each new model fitting the negative gradient of a chosen loss (e.g., MSE for regression, log-loss for classification) and is evaluated with the usual regression or classification metrics.

Preprocessing for Gradient Boosting

Gradient Boosted Trees (GBMs like XGBoost, LightGBM) have similar preprocessing needs to decision trees and Random Forests.

- Handle missing values; many implementations can natively route missing values but basic cleaning is still recommended.
- Encode categorical variables when required (some libraries need one-hot; others like CatBoost handle categories directly).
- Feature scaling is usually not required for tree-based GBMs, though it can help if using non-tree base learners.
- Remove obvious data errors and consider strategies for imbalance (class weights, sampling) for classification.

Model and prediction

Gradient Boosting builds a strong model $F_M(x)$ as a sum of M weak learners $h_m(x)$, often small decision trees.

- Start with an initial model, e.g.

$$F_0(x) = \arg \min_{\gamma} \sum_i L(y_i, \gamma)$$

- At each iteration $m = 1, \dots, M$:
 - Compute pseudo-residuals (negative gradient of the loss):

$$r_{im} = - \left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)}$$

- Fit a weak learner $h_m(x)$ to r_{im} .
- Find optimal step size ρ_m (line search).
- Update model:

$$F_m(x) = F_{m-1}(x) + \nu \rho_m h_m(x)$$

text

where ν is the learning rate (shrinkage).

- Regression prediction: $\hat{y}(x) = F_M(x)$.
- Classification prediction: use $F_M(x)$ as a score or log-odds, convert to probability via a link function (e.g., logistic), then apply a threshold.

Loss functions (“cost”)

The key idea is: each new tree fits the negative gradient of the chosen differentiable loss function.

Common choices:

- Regression:
 - Squared error (MSE):

$$L(y, F(x)) = \frac{1}{2} (y - F(x))^2$$

- Absolute error (MAE) or Huber loss for robustness to outliers.
- Binary classification:
 - Logistic (cross-entropy) loss:

$$L(y, F(x)) = \log(1 + e^{-yF(x)}), y \in \{-1, +1\}$$

Multiclass classification:

- Multinomial log-loss (softmax cross-entropy).

The algorithm is effectively doing Gradient Descent in function space on these losses.

Evaluation metrics (regression GBM)

For gradient boosting regression, use the standard regression metrics as before.

Given true targets y_i and predictions \hat{y}_i :

- MSE: $\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
- RMSE: $\text{RMSE} = \sqrt{\text{MSE}}$
- MAE: $\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$
- R^2 : $R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$

Some libraries also report “training deviance”, which is essentially the average loss.

Evaluation metrics (classification GBM)

For gradient boosting classification, use the same metrics as logistic regression / Random Forest classification.

With TP, TN, FP, FN:

- Accuracy: $\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$
- Precision: $\text{Precision} = \frac{TP}{TP+FP}$
- Recall: $\text{Recall} = \frac{TP}{TP+FN}$
- F1-score: $F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

From predicted probabilities, compute ROC-AUC and PR-AUC over thresholds. Many GBM frameworks also report log-loss directly, since that is the optimized objective in classification.

Naive Bayes

Naive Bayes is a probabilistic classifier that assumes features are conditionally independent given the class; it needs relatively light preprocessing, uses Bayes' theorem to compute posterior probabilities, and is evaluated with the same classification metrics as other classifiers (accuracy, precision, recall, F1, etc.).

Preprocessing for Naive Bayes

Preprocessing depends on data type (numeric vs text) and variant (Gaussian, Multinomial, Bernoulli).

- Handle missing values (impute or drop), since probability estimates require complete features.
- For numeric features (Gaussian NB), optional scaling/standardization can help but is not strictly required.
- For categorical/text features (Multinomial/Bernoulli NB):
 - Clean text (lowercasing, removing punctuation, tokenization).
 - Convert to counts or binary indicators (e.g., bag-of-words, TF-IDF).
- Remove or merge highly correlated / duplicate features when possible, since these violate independence and can distort probabilities.

Naive Bayes model and formula

Naive Bayes applies Bayes' theorem with the naive independence assumption.

Bayes' theorem for class y and features $x = (x_1, \dots, x_n)$:

$$P(y | x) = \frac{P(y) P(x | y)}{P(x)}$$

With conditional independence:

$$P(x | y) = \prod_{i=1}^n P(x_i | y)$$

So, up to a normalization constant:

$$P(y | x) \propto P(y) \prod_{i=1}^n P(x_i | y)$$

Classifier prediction is:

$$\hat{y} = \arg \max_y P(y) \prod_{i=1}^n P(x_i | y)$$

In practice, log-probabilities are used to avoid underflow:

$$\hat{y} = \arg \max_y \left[\log P(y) + \sum_{i=1}^n \log P(x_i | y) \right]$$

Different variants model $P(x_i | y)$ differently (Gaussian for continuous, Multinomial for counts, Bernoulli for binary).

“Loss” / optimization view

Naive Bayes typically does not use Gradient Descent; parameters are estimated by maximum likelihood via simple counting/averaging.

- Class prior:

$$P(y = c) = \frac{\text{number of samples with class } c}{\text{total samples}}$$

- Conditional probabilities:
 - Categorical/count features: smoothed relative frequencies (e.g., Laplace/add-one smoothing).
 - Gaussian: estimate mean $\mu_{c,i}$ and variance $\sigma_{c,i}^2$ of feature i within class c , then use a normal density.

The implicit loss minimized by the maximum likelihood estimate under the model corresponds to the negative log-likelihood (cross-entropy) of the training data, but this is solved in closed form rather than with iterative gradient updates.

Evaluation metrics and formulas

Naive Bayes is almost always used for classification, so the standard classification metrics apply.

With:

- TP: true positives
- TN: true negatives
- FP: false positives
- FN: false negatives

Key metrics:

- Accuracy

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

- Precision

$$\text{Precision} = \frac{TP}{TP + FP}$$

- Recall (Sensitivity, True Positive Rate)

$$\text{Recall} = \frac{TP}{TP + FN}$$

- F1-score (harmonic mean of precision and recall)

$$F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

For probabilistic outputs from Naive Bayes, ROC-AUC and PR-AUC are computed over varying decision thresholds exactly as for logistic regression or other classifiers