Complete Machine Learning Algorithms & Libraries Cheat Sheet

Table of Contents

- 1. Core ML Libraries & Frameworks
- 2. <u>Supervised Learning Algorithms</u>
- 3. <u>Unsupervised Learning Algorithms</u>
- 4. <u>Deep Learning Architectures</u>
- 5. Reinforcement Learning
- 6. Ensemble Methods
- 7. <u>Dimensionality Reduction</u>
- 8. Evaluation Metrics
- 9. Feature Engineering & Selection
- 10. Model Optimization Techniques

1. Core ML Libraries & Frameworks {#core-libraries}

Python Libraries

Scikit-learn

- **Purpose**: General-purpose ML library
- **Key Features**: Classification, regression, clustering, dimensionality reduction
- Common Classes:

```
python
```

```
from sklearn.model_selection import train_test_split, cross_val_score, GridSearchCV from sklearn.preprocessing import StandardScaler, MinMaxScaler, LabelEncoder from sklearn.metrics import accuracy score, precision score, recall score
```

TensorFlow/Keras

- **Purpose**: Deep learning framework
- Architecture Types: Sequential, Functional API, Subclassing
- Key Components:
 - Layers: Dense, Conv2D, LSTM, GRU, Dropout, BatchNormalization
 - Optimizers: Adam, SGD, RMSprop, Adagrad
 - Loss Functions: MSE, CrossEntropy, Huber, Custom losses

PyTorch

- Purpose: Dynamic deep learning framework
- **Key Features**: Autograd, dynamic computation graphs
- Core Components:
 - torch.nn: Neural network modules
 - torch.optim: Optimization algorithms
 - torch.utils.data: DataLoader, Dataset classes

XGBoost/LightGBM/CatBoost

- Purpose: Gradient boosting frameworks
- Key Parameters:
 - learning_rate: Step size shrinkage
 - max_depth: Maximum tree depth
 - n_estimators: Number of boosting rounds
 - subsample: Fraction of samples per tree

2. Supervised Learning Algorithms {#supervised-learning}

Linear Models

Linear Regression

- **Equation**: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_n x_n + \epsilon$
- **Objective**: Minimize MSE = $\Sigma (y_i \hat{y}_i)^2/n$
- Methods:
 - Ordinary Least Squares (OLS): $\beta = (X'X)^{-1}X'y$
 - Gradient Descent: $\theta = \theta \alpha \nabla J(\theta)$
- Assumptions: Linearity, independence, homoscedasticity, normality
- Regularization:
 - **Ridge (L2)**: $J(\theta) = MSE + \lambda \Sigma \theta_i^2$
 - Lasso (L1): $J(\theta) = MSE + \lambda \Sigma |\theta_i|$
 - Elastic Net: $J(\theta) = MSE + \lambda_1 \Sigma |\theta_i| + \lambda_2 \Sigma \theta_i^2$

Logistic Regression

- Function: $p(y=1|x) = 1/(1 + e^{-(-z)})$, where $z = \beta_0 + \beta_1 x_1 + ... + \beta_n x_n$
- Loss Function: Binary Cross-Entropy = $-\Sigma[y_i\log(p_i) + (1-y_i)\log(1-p_i)]$

- Optimization: Maximum Likelihood Estimation via gradient descent
- Multiclass Extensions:
 - One-vs-Rest (OvR): Train k binary classifiers
 - Softmax Regression: $p(y=k|x) = e^{(z_k)}/\Sigma e^{(z_i)}$

Tree-Based Models

Decision Trees

- Splitting Criteria:
 - Gini Impurity: $G = 1 \Sigma p_i^2$
 - **Entropy**: $H = -\Sigma p_i \log_2(p_i)$
 - Information Gain: $IG = H(parent) \Sigma(n_i/n)H(child_i)$
- Algorithms:
 - CART: Binary splits, supports regression
 - **ID3**: Uses entropy and information gain
 - **C4.5**: Handles continuous attributes, missing values
- Pruning Methods:
 - **Pre-pruning**: Stop growing based on criteria
 - **Post-pruning**: Remove branches that don't improve validation performance

Random Forests

- **Concept**: Ensemble of decision trees with bagging
- Key Features:
 - Bootstrap sampling for each tree
 - Random feature selection at each split
 - Out-of-bag (OOB) error estimation
- Hyperparameters:
 - n_estimators: Number of trees
 - max_features: Features to consider at each split
 - min_samples_split: Minimum samples to split node

Support Vector Machines (SVM)

Linear SVM

- **Objective**: Maximize margin = 2/||w||
- Constraints: $y_i(w \cdot x_i + b) \ge 1$ for all i

• **Soft Margin**: Allows misclassification with penalty C

• **Dual Form**: Optimize α subject to $\Sigma \alpha_i y_i = 0$

Kernel SVM

• **Kernel Trick**: $K(x,y) = \phi(x) \cdot \phi(y)$

• Common Kernels:

• **RBF**: $K(x,y) = \exp(-\gamma ||x-y||^2)$

• **Polynomial**: $K(x,y) = (\gamma x \cdot y + r)^d$

• **Sigmoid**: $K(x,y) = tanh(\gamma x \cdot y + r)$

Naive Bayes

Gaussian Naive Bayes

• Assumption: Features follow Gaussian distribution

• **Likelihood**: $P(x_i|y) = (1/\sqrt{(2\pi\sigma^2_y)}) \exp(-(x_i-\mu_y)^2/2\sigma^2_y)$

Multinomial Naive Bayes

• Use Case: Text classification, discrete features

• Likelihood: $P(x_i|y) = (N_{y_i} + \alpha)/(N_y + \alpha|V|)$

• **Smoothing**: Laplace smoothing with parameter α

k-Nearest Neighbors (k-NN)

• Algorithm: Find k nearest points, vote/average

• Distance Metrics:

• **Euclidean**: $d = \sqrt{\Sigma(x_i - y_i)^2}$

• Manhattan: $d = \Sigma |x_i - y_i|$

• Minkowski: $d = (\Sigma |x_i - y_i|^p)^{(1/p)}$

• Weighting Schemes:

• Uniform: Equal weights

• Distance: Weight = 1/distance

3. Unsupervised Learning Algorithms {#unsupervised-learning}

Clustering Algorithms

K-Means

• **Objective**: Minimize within-cluster sum of squares (WCSS)

• Algorithm:

- 1. Initialize k centroids randomly
- 2. Assign points to nearest centroid
- 3. Update centroids as mean of assigned points
- 4. Repeat until convergence

• Variants:

- K-Means++: Smart initialization
- Mini-Batch K-Means: Subsample for efficiency

Hierarchical Clustering

- Types:
 - Agglomerative: Bottom-up approach
 - **Divisive**: Top-down approach
- Linkage Criteria:
 - **Single**: $min\{d(a,b): a \in A, b \in B\}$
 - **Complete**: max{d(a,b): a∈A, b∈B}
 - Average: Σd(a,b)/(|A||B|)
 - Ward: Minimize within-cluster variance

DBSCAN

- Parameters:
 - eps: Maximum distance between points
 - min_samples: Minimum points to form dense region
- Concepts:
 - Core points: Have min_samples within eps
 - Border points: Within eps of core point
 - Noise points: Neither core nor border

Gaussian Mixture Models (GMM)

- **Model**: $p(x) = \Sigma \pi_k \mathcal{N}(x|\mu_{kr}\Sigma_k)$
- EM Algorithm:
 - E-step: Calculate responsibilities
 - M-step: Update parameters π, μ, Σ
- Covariance Types: Full, diagonal, spherical, tied

Association Rules

Apriori Algorithm

- Metrics:
 - **Support**: $supp(X) = |t \in T: X \subseteq t|/|T|$
 - Confidence: $conf(X \rightarrow Y) = supp(X \cup Y)/supp(X)$
 - **Lift**: $lift(X \rightarrow Y) = supp(X \cup Y)/(supp(X) \times supp(Y))$

4. Deep Learning Architectures {#deep-learning}

Feedforward Neural Networks

Multi-Layer Perceptron (MLP)

- **Architecture**: Input → Hidden layers → Output
- Forward Pass: z = Wx + b, a = q(z)
- Activation Functions:
 - **ReLU**: f(x) = max(0,x)
 - **Sigmoid**: $f(x) = 1/(1+e^{(-x)})$
 - Tanh: $f(x) = (e^x-e^(-x))/(e^x+e^(-x))$
 - Leaky ReLU: $f(x) = max(\alpha x, x)$
 - **GELU**: $f(x) = x \cdot \Phi(x)$

Convolutional Neural Networks (CNN)

Core Components

- Convolution Layer:
 - Operation: $(f^*g)(t) = \Sigma f(\tau)g(t-\tau)$
 - Parameters: filters, kernel_size, stride, padding
- Pooling Layers:
 - Max Pooling: Select maximum value
 - Average Pooling: Calculate mean
 - Global Pooling: Reduce to single value per channel

Popular Architectures

- LeNet-5: Early CNN for digit recognition
- AlexNet: Deep CNN with ReLU, dropout
- VGGNet: Small filters, deep architecture

• **ResNet**: Skip connections, residual blocks

• **Inception**: Multiple filter sizes in parallel

• **EfficientNet**: Compound scaling of depth/width/resolution

Recurrent Neural Networks (RNN)

Vanilla RNN

• Hidden State: $h_t = tanh(W_{hh}h_{t-1} + W_{xh}x_t + b)$

• Output: $y_t = W_{hy}h_t + b_y$

• **Problem**: Vanishing/exploding gradients

Long Short-Term Memory (LSTM)

• Gates:

• Forget Gate: $f_t = \sigma(Wf[h_{t-1}, x_t] + bf)$

• Input Gate: $i_t = \sigma(Wi[h_{t-1}, x_t] + bi)$

• Output Gate: $o_t = \sigma(Wo[h_{t-1}, x_t] + bo)$

• Cell State: $C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$

Gated Recurrent Unit (GRU)

• Gates:

• Reset Gate: $r_t = \sigma(Wr[h_{t-1}, x_t])$

• Update Gate: $z_t = \sigma(Wz[h_{t-1}, x_t])$

• Hidden State: $h_t = (1-z_t) \odot h_{t-1} + z_t \odot \tilde{h}_t$

Transformer Architecture

Self-Attention Mechanism

• Query, Key, Value: $Q = XW^{\phi}$, $K = XW_k$, $V = XW_v$

• **Attention**: Attention(Q,K,V) = softmax(QK'/ $\sqrt{d_k}$)V

Multi-Head: Concat(head₁,...,head_h)W_o

Positional Encoding

• **Sinusoidal**: PE(pos,2i) = sin(pos/10000^(2i/d))

• **Learned**: Trainable embedding vectors

Autoencoders

Types

- Vanilla Autoencoder: Encoder → Bottleneck → Decoder
- Variational Autoencoder (VAE):
 - Encoder outputs μ and σ
 - Sample z ~ $N(\mu, \sigma^2)$
 - Loss = Reconstruction + KL divergence
- Denoising Autoencoder: Input corrupted data, reconstruct clean

Generative Adversarial Networks (GAN)

Architecture

• **Generator**: G(z) generates fake samples from noise z

• **Discriminator**: D(x) classifies real vs fake

Objective: min_G max_D V(D,G) = E[log D(x)] + E[log(1-D(G(z)))]

Variants

DCGAN: Convolutional architecture

• WGAN: Wasserstein distance loss

• CycleGAN: Unpaired image translation

• **StyleGAN**: Style-based generation

5. Reinforcement Learning {#reinforcement-learning}

Core Concepts

Markov Decision Process (MDP)

• Components: (S, A, P, R, γ)

• S: State space

• A: Action space

• P: Transition probability

• R: Reward function

γ: Discount factor

Value Functions

• **State Value**: $V^{\pi}(s) = E[\Sigma \gamma^t r_t | s_0 = s]$

• Action Value: $Q^{\pi}(s,a) = E[\Sigma \gamma^t r_t | s_0 = s, a_0 = a]$

• Bellman Equations:

• $V^{\pi}(s) = \Sigma_a \pi(a|s)\Sigma_s' P(s'|s,a)[R(s,a,s') + \gamma V^{\pi}(s')]$

Algorithms

Dynamic Programming

- **Policy Iteration**: Evaluate → Improve → Repeat
- Value Iteration: $V(s) = \max_a \Sigma_s' P(s'|s,a)[R + \gamma V(s')]$

Monte Carlo Methods

- First-Visit MC: Average returns from first visit
- Every-Visit MC: Average all returns
- MC Control: Use ε-greedy for exploration

Temporal Difference Learning

- **TD(0)**: $V(s) \leftarrow V(s) + \alpha[r + \gamma V(s') V(s)]$
- **SARSA**: $Q(s,a) \leftarrow Q(s,a) + \alpha[r + \gamma Q(s',a') Q(s,a)]$
- **Q-Learning**: $Q(s,a) \leftarrow Q(s,a) + \alpha[r + \gamma max_a'Q(s',a') Q(s,a)]$

Deep RL

- **DQN**: Neural network approximates Q-function
 - Experience replay buffer
 - Target network for stability
- Policy Gradient:
 - **REINFORCE**: $\nabla J(\theta) = E[\nabla \log \pi(a|s)G]$
 - Actor-Critic: Separate value and policy networks
- PPO: Proximal Policy Optimization with clipped objective
- A3C: Asynchronous Advantage Actor-Critic

6. Ensemble Methods {#ensemble-methods}

Bagging (Bootstrap Aggregating)

Random Forest (covered above)

Extra Trees

- **Difference from RF**: Random thresholds for splitting
- Advantages: Faster training, more randomness

Boosting

AdaBoost

- Weight Update: $w_i = w_i \times exp(\alpha_t \times I(y_i \neq h_t(x_i)))$
- Classifier Weight: $\alpha_t = 0.5 \times \log((1-\epsilon_t)/\epsilon_t)$
- Final Prediction: $H(x) = sign(\Sigma \alpha_t h_t(x))$

Gradient Boosting

- Algorithm:
 - 1. Initialize with constant prediction
 - 2. For m = 1 to M:
 - Compute residuals r_i = y_i F_{_{}{m-1}(x_i)
 - Fit tree h_m to residuals
 - Update $F_m = F_{m-1} + vh_m$
- Loss Functions: MSE, MAE, Huber, Quantile

XGBoost

- **Objective**: Obj = $\Sigma I(y_i, \hat{y_i}) + \Sigma \Omega(f_k)$
- Regularization: $\Omega(f) = \gamma T + 0.5 \lambda \Sigma w_i^2$
- Features:
 - Parallel tree construction
 - Built-in cross-validation
 - Missing value handling

Stacking

- Level-0 Models: Base learners (diverse algorithms)
- Level-1 Model: Meta-learner combines base predictions
- Cross-Validation: Avoid overfitting with CV predictions

7. Dimensionality Reduction {#dimensionality-reduction}

Linear Methods

Principal Component Analysis (PCA)

- **Objective**: Find directions of maximum variance
- Algorithm:
 - 1. Standardize data
 - 2. Compute covariance matrix C

- 3. Find eigenvectors/eigenvalues of C
- 4. Select top k components
- **Transformation**: Z = XW, where W contains eigenvectors

Linear Discriminant Analysis (LDA)

- Goal: Maximize between-class/within-class variance ratio
- Steps:
 - 1. Compute class means and scatter matrices
 - 2. Solve generalized eigenvalue problem
 - 3. Project data onto discriminant vectors

Independent Component Analysis (ICA)

- Assumption: Sources are statistically independent
- Methods: FastICA, Infomax, JADE
- **Applications**: Blind source separation

Non-Linear Methods

t-SNE

- Objective: Preserve local neighborhoods
- **Perplexity**: Controls effective number of neighbors
- Algorithm:
 - 1. Compute pairwise similarities in high-D
 - 2. Initialize low-D representation
 - 3. Minimize KL divergence between distributions

UMAP

- Advantages over t-SNE: Preserves global structure, faster
- **Parameters**: n_neighbors, min_dist
- **Theory**: Based on Riemannian geometry

Autoencoders (covered above)

Matrix Factorization

Non-negative Matrix Factorization (NMF)

Constraint: All values ≥ 0

• **Objective**: $||X - WH||^2$ subject to W,H ≥ 0

• Applications: Topic modeling, image analysis

Singular Value Decomposition (SVD)

Decomposition: X = UΣV'

• Truncated SVD: Keep top k singular values

• Applications: Recommender systems, LSA

8. Evaluation Metrics {#evaluation-metrics}

Classification Metrics

Binary Classification

• Accuracy: (TP + TN)/(TP + TN + FP + FN)

• **Precision**: TP/(TP + FP)

• **Recall/Sensitivity**: TP/(TP + FN)

• **F1-Score**: 2 × (Precision × Recall)/(Precision + Recall)

Specificity: TN/(TN + FP)

• AUC-ROC: Area under ROC curve

• AUC-PR: Area under Precision-Recall curve

Multi-class Classification

• Macro Average: Average metric across classes

Weighted Average: Weight by class frequency

• Cohen's Kappa: Agreement corrected for chance

• Matthews Correlation Coefficient: Balanced measure

Regression Metrics

• Mean Absolute Error (MAE): $\Sigma |y_i - \hat{y}_i|/n$

Mean Squared Error (MSE): Σ(y_i - ŷ_i)²/n

• Root Mean Squared Error (RMSE): √MSE

• **R² Score**: 1 - $\Sigma (y_i - \hat{y}_i)^2 / \Sigma (y_i - \bar{y})^2$

• Mean Absolute Percentage Error (MAPE): $\Sigma |y_i - \hat{y}_i|/|y_i| \times 100/n$

Clustering Metrics

• Silhouette Score: (b - a)/max(a, b)

- Davies-Bouldin Index: Average similarity ratio
- Calinski-Harabasz Index: Between/within cluster variance
- Adjusted Rand Index: Corrected for chance

Cross-Validation Strategies

- **k-Fold**: Split data into k equal parts
- Stratified k-Fold: Preserve class distribution
- **Leave-One-Out**: k = n samples
- Time Series Split: Respect temporal order

9. Feature Engineering & Selection {#feature-engineering}

Feature Creation

Numerical Features

- Binning: Discretize continuous values
- Polynomial Features: x_1^2 , x_1x_2 , etc.
- Log Transform: Handle skewed distributions
- Scaling Methods:
 - StandardScaler: (x μ)/σ
 - MinMaxScaler: (x min)/(max min)
 - RobustScaler: Use median and IOR

Categorical Features

- One-Hot Encoding: Binary columns for each category
- Label Encoding: Integer representation
- Target Encoding: Replace with target mean
- Ordinal Encoding: For ordered categories

Text Features

- Bag of Words: Word frequency vectors
- **TF-IDF**: Term frequency × inverse document frequency
- Word Embeddings: Word2Vec, GloVe, FastText
- **N-grams**: Sequences of n words

Feature Selection

Filter Methods

- Variance Threshold: Remove low-variance features
- Correlation: Remove highly correlated features
- Chi-Square Test: For categorical targets
- ANOVA F-test: For continuous targets
- Mutual Information: Non-linear relationships

Wrapper Methods

- Recursive Feature Elimination (RFE): Iteratively remove features
- Forward Selection: Start empty, add best
- Backward Elimination: Start full, remove worst

Embedded Methods

- L1 Regularization: Lasso induces sparsity
- Tree-based Importance: Gini/entropy reduction
- Permutation Importance: Shuffle and measure impact

10. Model Optimization Techniques {#optimization}

Hyperparameter Tuning

Grid Search

- **Method**: Exhaustive search over parameter grid
- Pros: Guaranteed to find best in grid
- **Cons**: Computationally expensive

Random Search

- Method: Sample random combinations
- **Pros**: More efficient than grid search
- Theory: Better coverage of important parameters

Bayesian Optimization

- Method: Build probabilistic model of objective
- Acquisition Functions:
 - Expected Improvement
 - Probability of Improvement

• Upper Confidence Bound

Genetic Algorithms

• Operations: Selection, crossover, mutation

• Applications: Complex search spaces

Gradient Descent Variants

Batch Gradient Descent

• **Update**: $\theta = \theta - \alpha \nabla J(\theta)$

• **Pros**: Stable convergence

• Cons: Slow for large datasets

Stochastic Gradient Descent (SGD)

• **Update**: $\theta = \theta - \alpha \nabla J(\theta; x_i, y_i)$

• Pros: Faster updates, can escape local minima

• Cons: Noisy updates

Mini-batch Gradient Descent

• **Balance**: Between batch and stochastic

• **Typical sizes**: 32, 64, 128, 256

Advanced Optimizers

Momentum

• **Update**: $v_t = \beta v_{t-1} + \alpha \nabla J(\theta)$

• θ Update: $\theta = \theta - v_t$

• Effect: Accelerates in consistent directions

RMSprop

• Accumulate: $E_t = \beta E_{t-1} + (1-\beta)(\nabla J)^2$

• **Update**: $\theta = \theta - \alpha \nabla J / \sqrt{(E_t + \epsilon)}$

Adam (Adaptive Moment Estimation)

• First moment: $m_t = \beta_1 m_{t-1} + (1-\beta_1) \nabla J$

• Second moment: $v_t = \beta_2 v_{t-1} + (1-\beta_2)(\nabla J)^2$

• Bias correction: $\hat{m}_t = m_t/(1-\beta_1{}^t), \ \hat{v}_t = v_t/(1-\beta_2{}^t)$

• **Update**: $\theta = \theta - \alpha \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$

AdamW

Modification: Decoupled weight decay

• **Update**: $\theta = \theta - \alpha(\hat{m}_t/(\sqrt{\hat{v}_t} + \epsilon) + \lambda\theta)$

Regularization Techniques

L1/L2 Regularization (covered above)

Dropout

• Training: Randomly zero out neurons with probability p

• Inference: Scale activations by (1-p)

• **Effect**: Ensemble of sub-networks

Batch Normalization

• Normalize: $\hat{x} = (x - \mu)/\sqrt{(\sigma^2 + \epsilon)}$

• Scale and Shift: $y = \gamma \hat{x} + \beta$

• Benefits: Faster training, higher learning rates

Early Stopping

• Monitor: Validation loss

Patience: Number of epochs without improvement

• Restore: Best weights when stopped

Data Augmentation

• Images: Rotation, flip, crop, color jitter

• **Text**: Synonym replacement, back-translation

• Time Series: Window slicing, noise injection

Advanced Techniques

Transfer Learning

Pre-trained Models: Use existing trained models

• Fine-tuning: Adapt to new task

Feature Extraction: Use as fixed feature extractor

Multi-task Learning

- **Shared Layers**: Common representations
- Task-specific Heads: Separate outputs
- Loss: Weighted sum of task losses

Meta-Learning

• Goal: Learn to learn

• Approaches: MAML, Prototypical Networks

• Applications: Few-shot learning

Federated Learning

• Concept: Train on distributed data

• Privacy: Data stays on device

• Aggregation: Average model updates

Quick Reference - Common Scikit-learn Code Patterns

```
python
# Data Preprocessing
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
# Model Training & Evaluation
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import classification_report, confusion_matrix
model = RandomForestClassifier(n_estimators=100, random_state=42)
model.fit(X_train_scaled, y_train)
y_pred = model.predict(X_test_scaled)
print(classification_report(y_test, y_pred))
# Hyperparameter Tuning
from sklearn.model_selection import GridSearchCV
param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [None, 10, 20, 30],
    'min_samples_split': [2, 5, 10]
grid_search = GridSearchCV(model, param_grid, cv=5, scoring='accuracy')
grid_search.fit(X_train_scaled, y_train)
best_model = grid_search.best_estimator_
# Pipeline
from sklearn.pipeline import Pipeline
from sklearn.decomposition import PCA
pipeline = Pipeline([
    ('scaler', StandardScaler()),
    ('pca', PCA(n_components=0.95)),
    ('classifier', RandomForestClassifier())
```

This cheat sheet provides a comprehensive overview of machine learning algorithms, libraries, and techniques. Each section includes the mathematical foundations, key parameters, and practical

1)

pipeline.fit(X_train, y_train)

considerations for implementation. Use this as a reference guide for understanding and implementing various ML approaches in your projects.