Production: Model Development

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$ echo "Data Science Institute"
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Agenda: 5.1 Model Development and Offline Evaluation

- Model Development and Training
- Ensembles
- Experiment Tracking and Versioning
- Distributed Training
- AutoML
- Model Offline Evaluation

Agenda: 5.2 Experiment Tracking

- Observability and telemetry
- Docker and Portability
- Experiment Tracking in Python
- Experiment Components

About

- These notes are based on Chapter 6 of *Designing Machine Learning Systems*, by Chip Huyen.

Our Reference Architecture

The Flock Reference Architecture

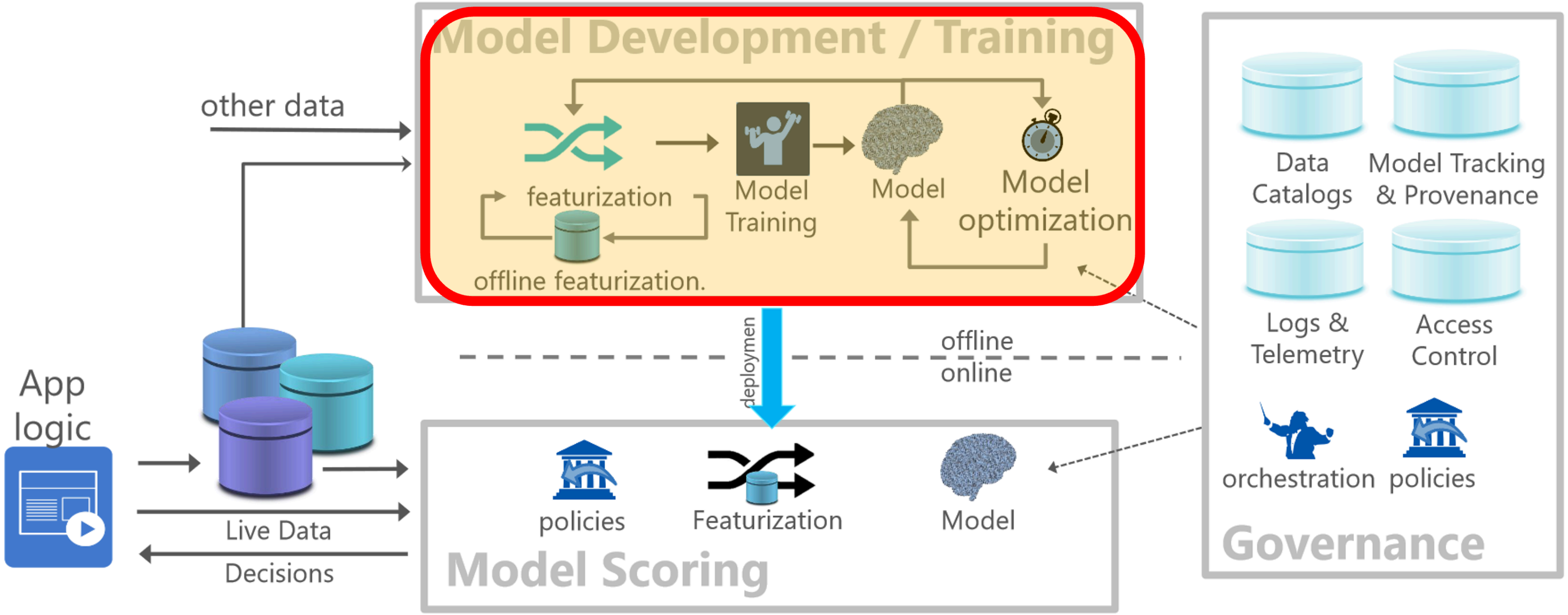


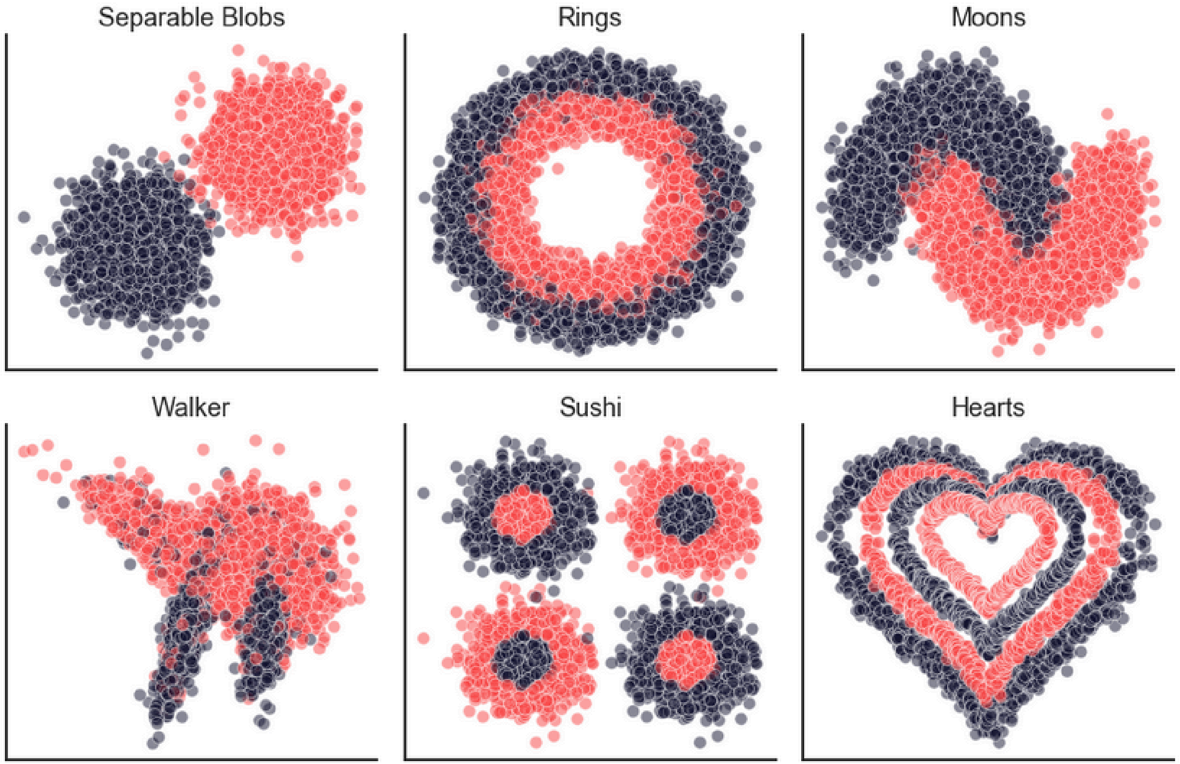
Figure 1: Flock reference architecture for a canonical data science lifecycle.

Agrawal et al (2019)

Exploring the Hypothesis Space

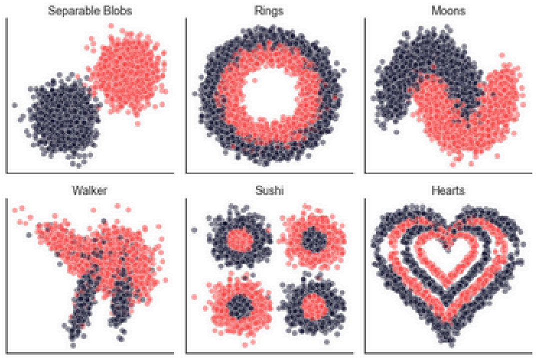
> “A classifier must be represented in some formal language that the computer can handle. Conversely, choosing a representation for a learner is tantamount to choosing the set of classifiers that it can possibly learn. This set is called the hypothesis space of the learner. If a classifier is not in the hypothesis space, it cannot be learned.” (Domingos, 2012)

Data Set Description

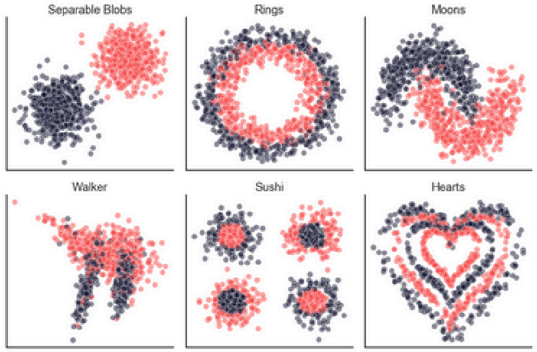


Data Set (5,000 observations)

Training
Data Set
(4,000 cases)



Test
Data Set
(1,000 cases)

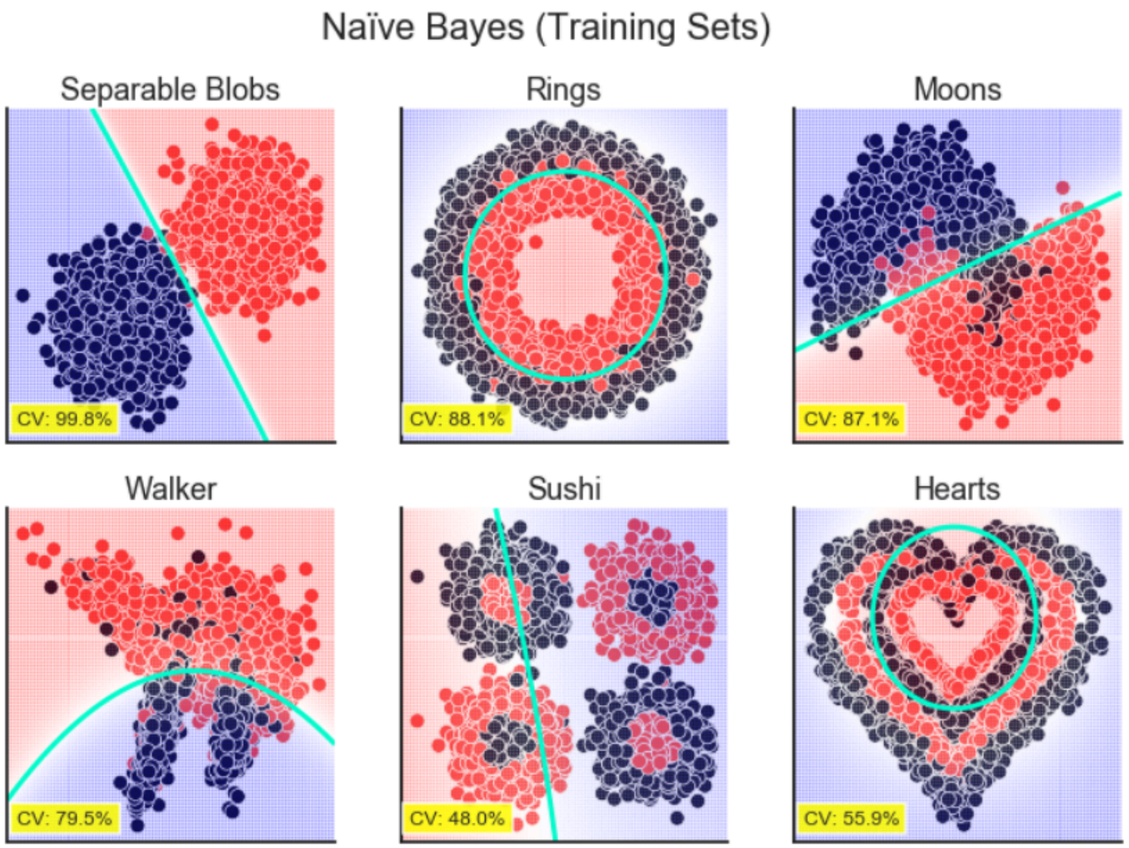


Naïve Bayes

- Conditional probability using Bayes' Theorem.
- Assume conditional independence

$$P(C|x_1, x_2) = \frac{P(x_1, x_2|C) \cdot P(C)}{P(x_1, x_2)}$$

$$\approx \frac{P(x_1|C) \cdot P(x_2|C) \cdot P(C)}{P(x_1, x_2)}$$



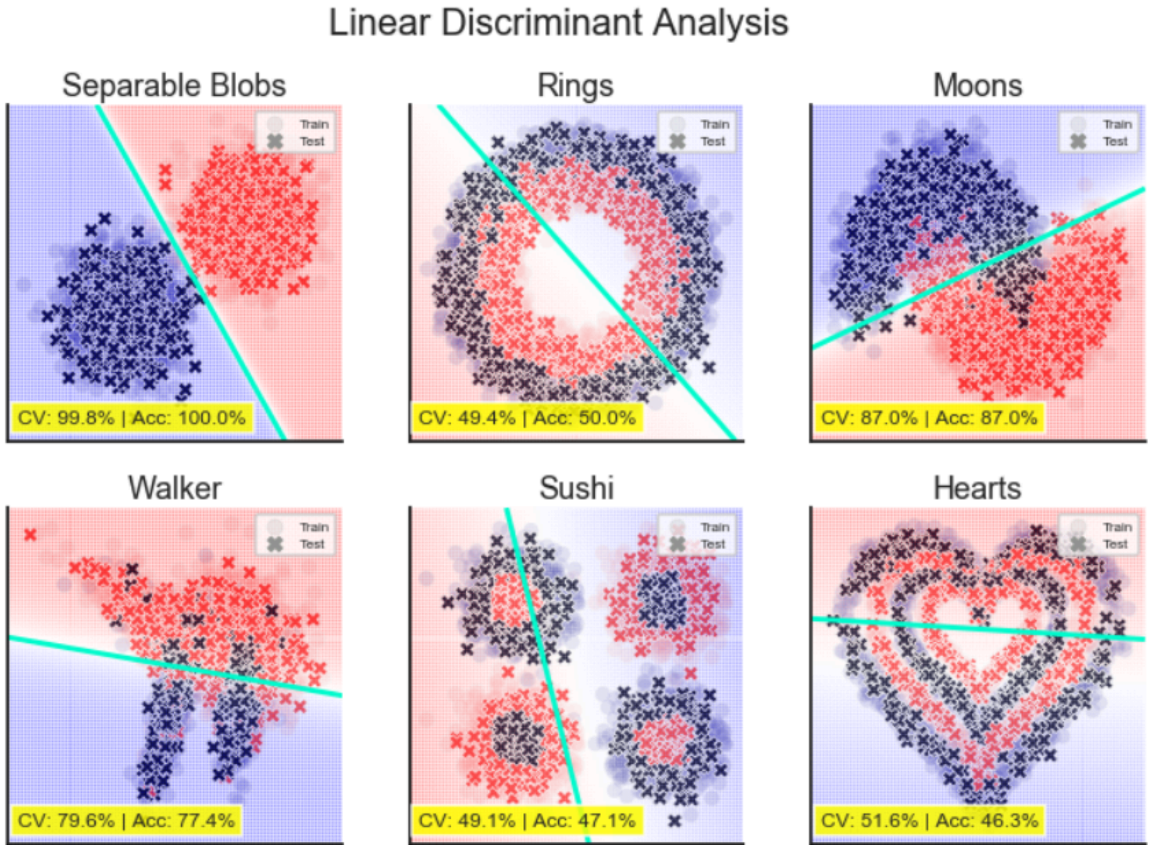
Discriminant Analysis

Discriminant Analysis methods find regions in feature space that:

- Minimize the distance within groups.
- Maximizes the distance between groups.

Linear Discriminant Analysis (LDA):

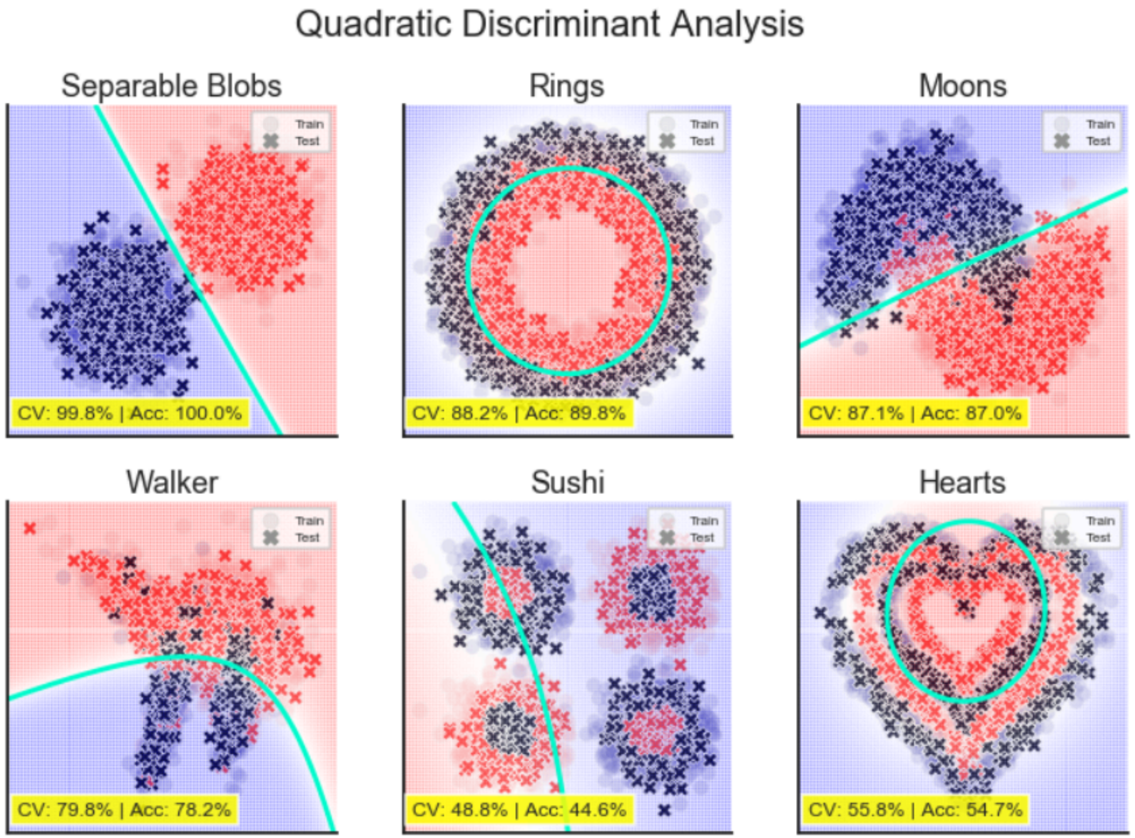
- Assumes attributes are normally distributed.
- Classes share covariance matrix.



Discriminant Analysis

Quadratic Discriminant Analysis (QDA):

- Classes do not share covariance matrix.



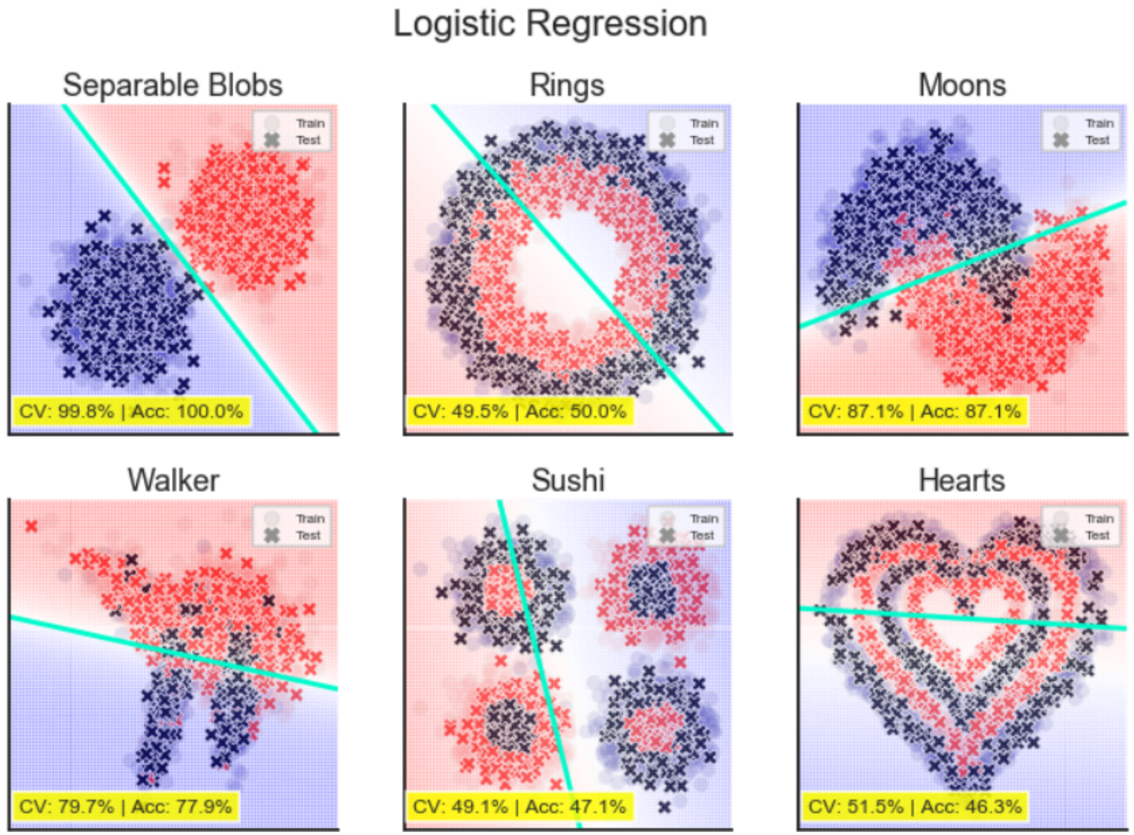
Logistic Regression

- Builds a linear model based on

$$log\left(\frac{P(C|x_1,x_2)}{1-P(C|x_1,x_2)}\right)$$

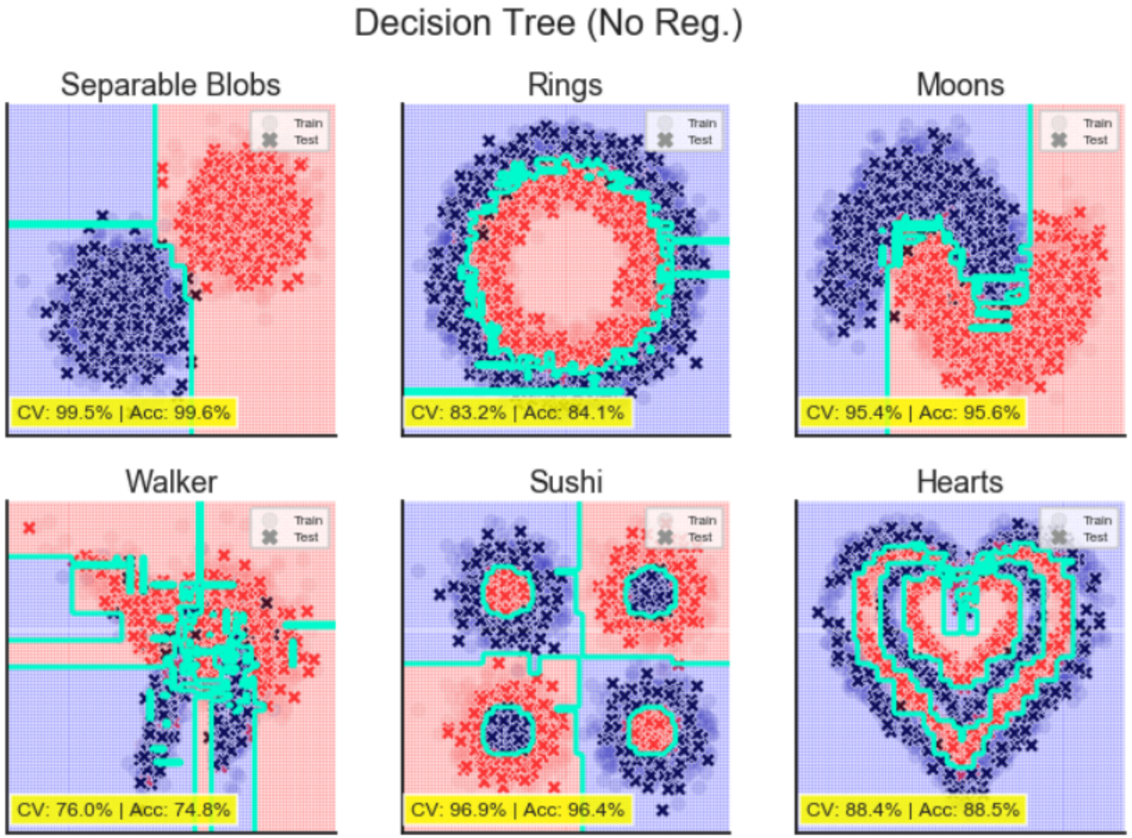
- The resulting model has the form:

$$P(C|x_1,x_2)=\frac{1}{1+exp(-w_0-w_1x_1-w_2x_2)}$$



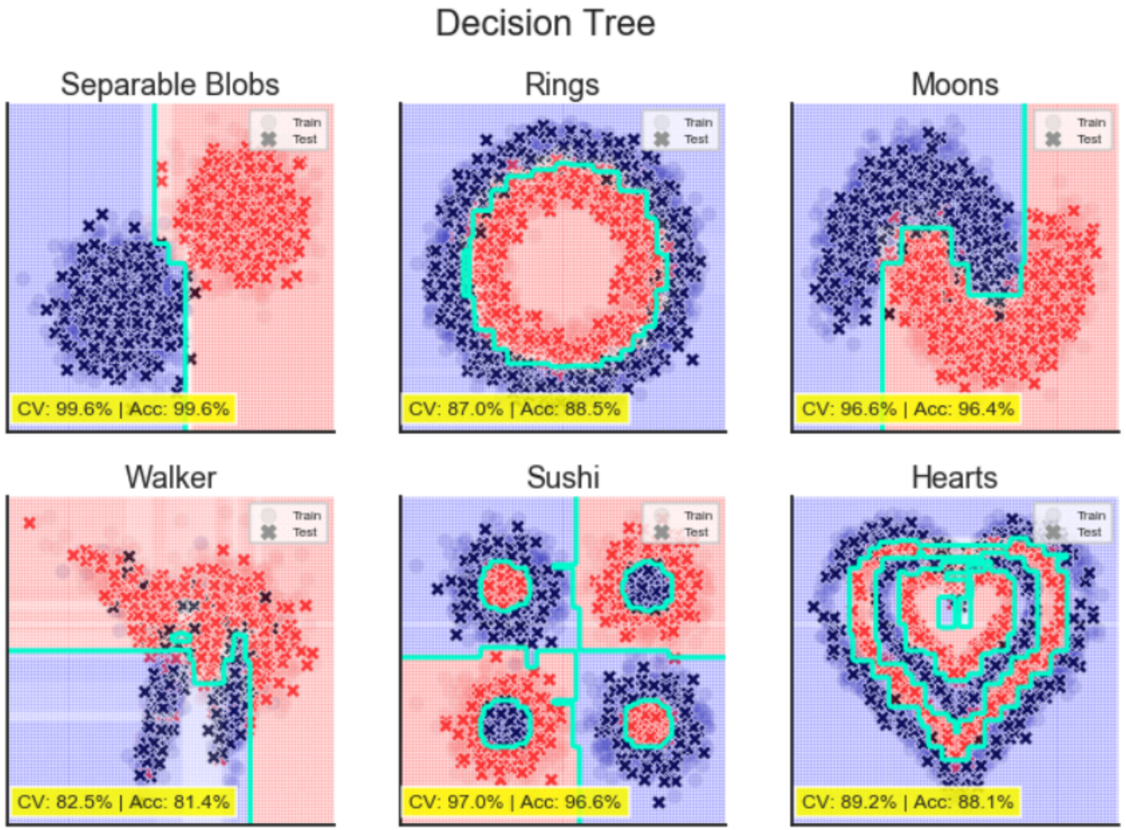
Unregularized Decision Trees

- Divide-and-conquer strategy: segment data based on an attribute such that information gain is maximized.
- Information can be measured with Gini coefficient or entropy.
- Fully expanded decision trees often contain unnecessary structure.



Regularized Decision Trees

- Pre-pruning: during training, decide which branches to stop developing.
- Post-pruning: subtree replacement involves training a full tree, then decide if a branch can be substituted by a leaf node.
- Constrain tree depth or number of examples in leaf nodes (hyperparameters).



Ensemble Methods: Bagging

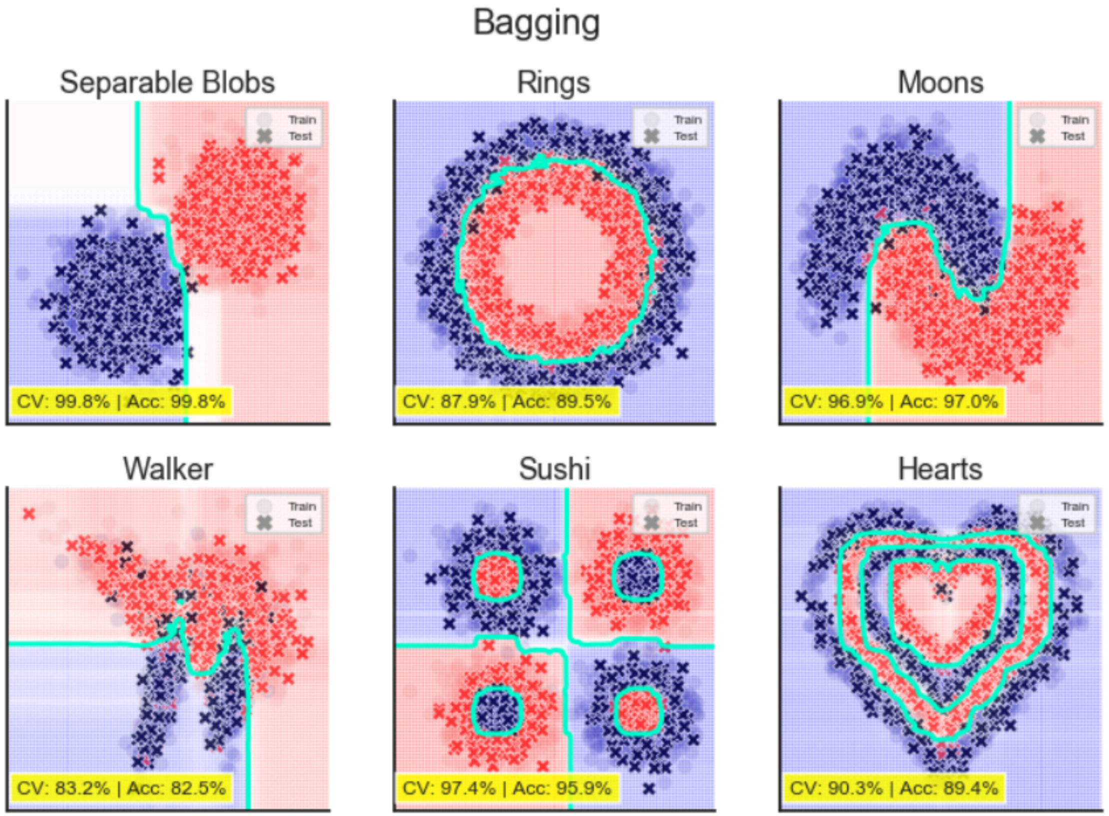
- Bagging = Bootstrap + Aggregation

Bootstrap

- Create subsets of data by sampling with replacement; train decision trees on each subset.

Aggregation

- Average predictions (regression) or add votes (classification).



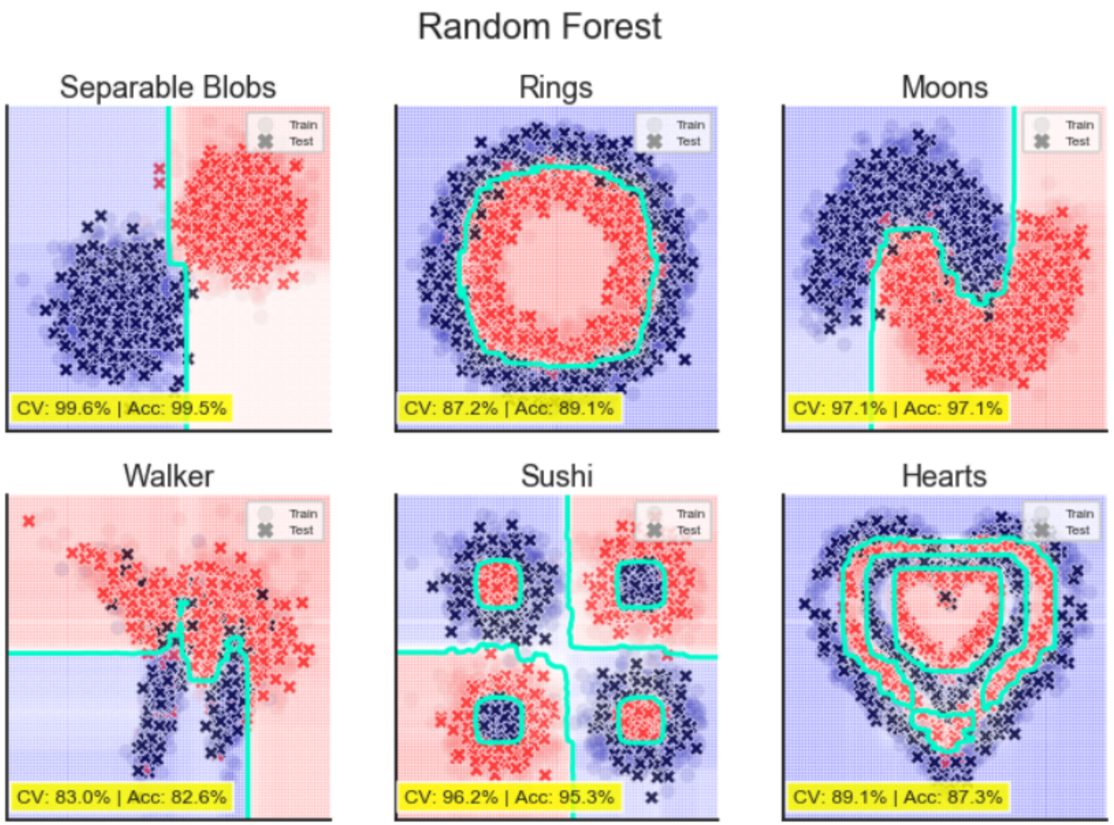
Ensemble Methods: Random Forest

Bootstrap

- Create subsets of data by sampling with replacement.
- Create subsets of features.
- Train Decision Tree Model (weak learner) on each subset.

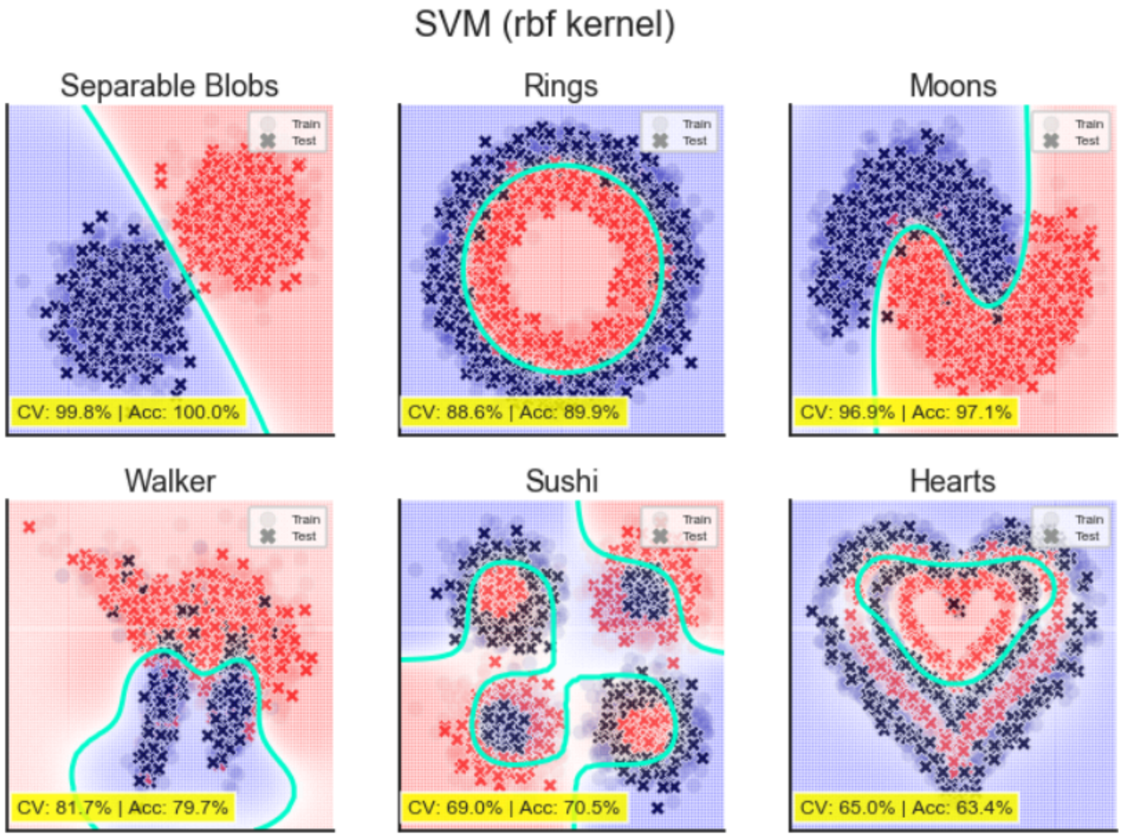
Aggregation

- Average predictions or vote.



Support Vector Machines (1/2)

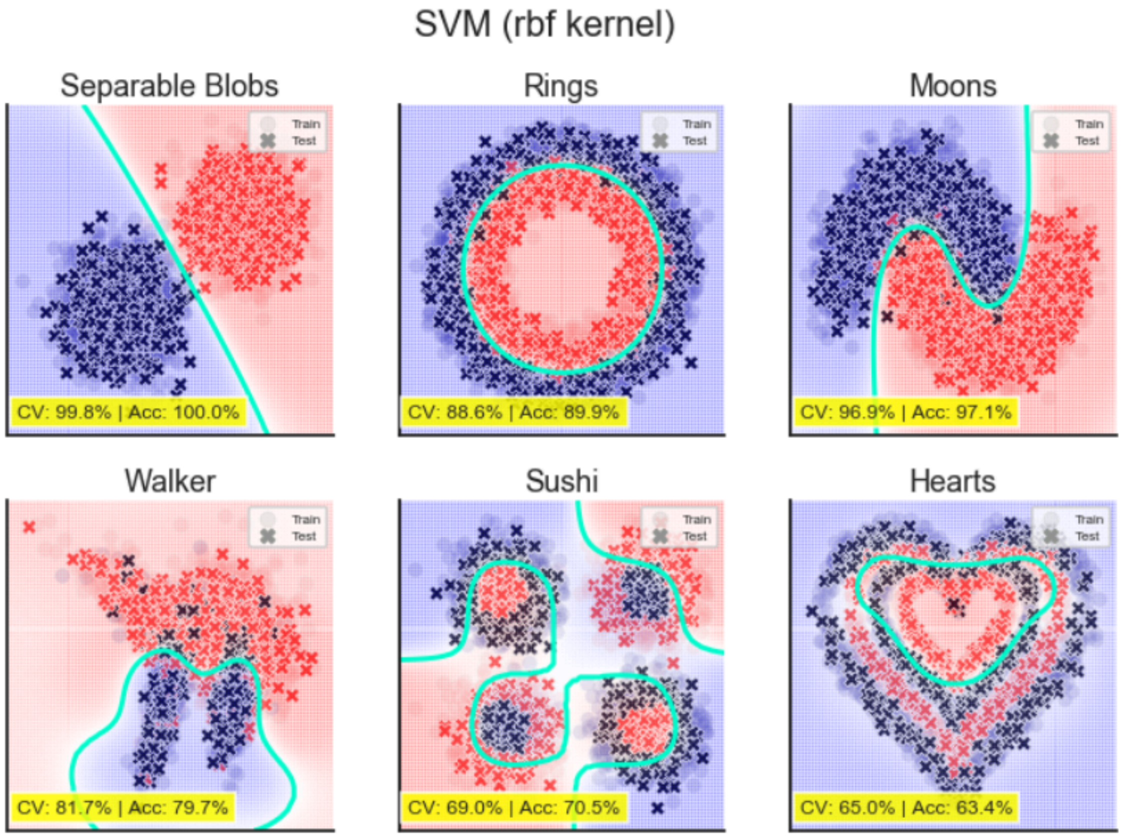
- Support vectors: The model selects a small number of critical boundary instances from each class.
- Builds a linear discriminant function that separates classes with a margin that is as wide as possible, the maximum margin hyperplane.



Support Vector Machines (2/2)

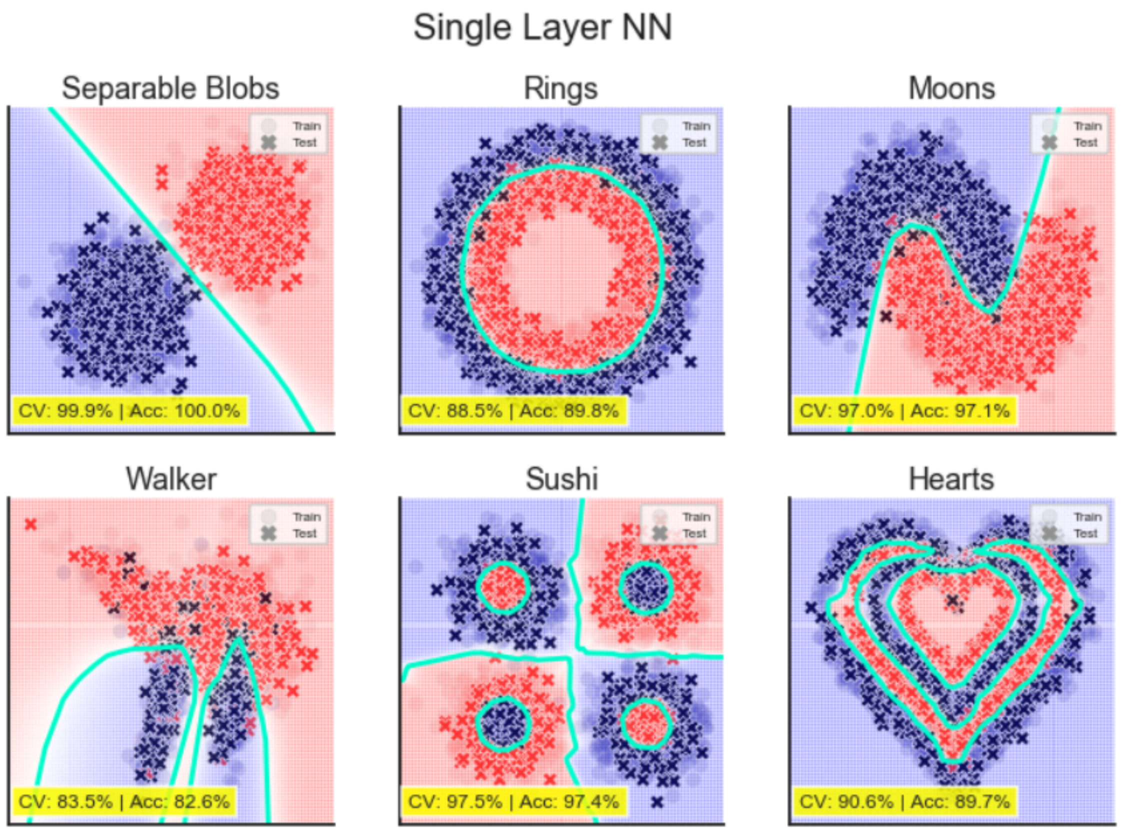
SVM use linear models to implement non-linear boundaries by performing a non-linear mapping of inputs:

- Polynomial
- Radial Basis Function
- Sigmoid



Neural Net

- Combine simple perceptron-like models in a hierarchical structure.
- Use (mostly) differentiable activation functions such as sigmoid or ReLU, such that gradient-based optimization can be applied.



Model Development and Training

Evaluating ML Models

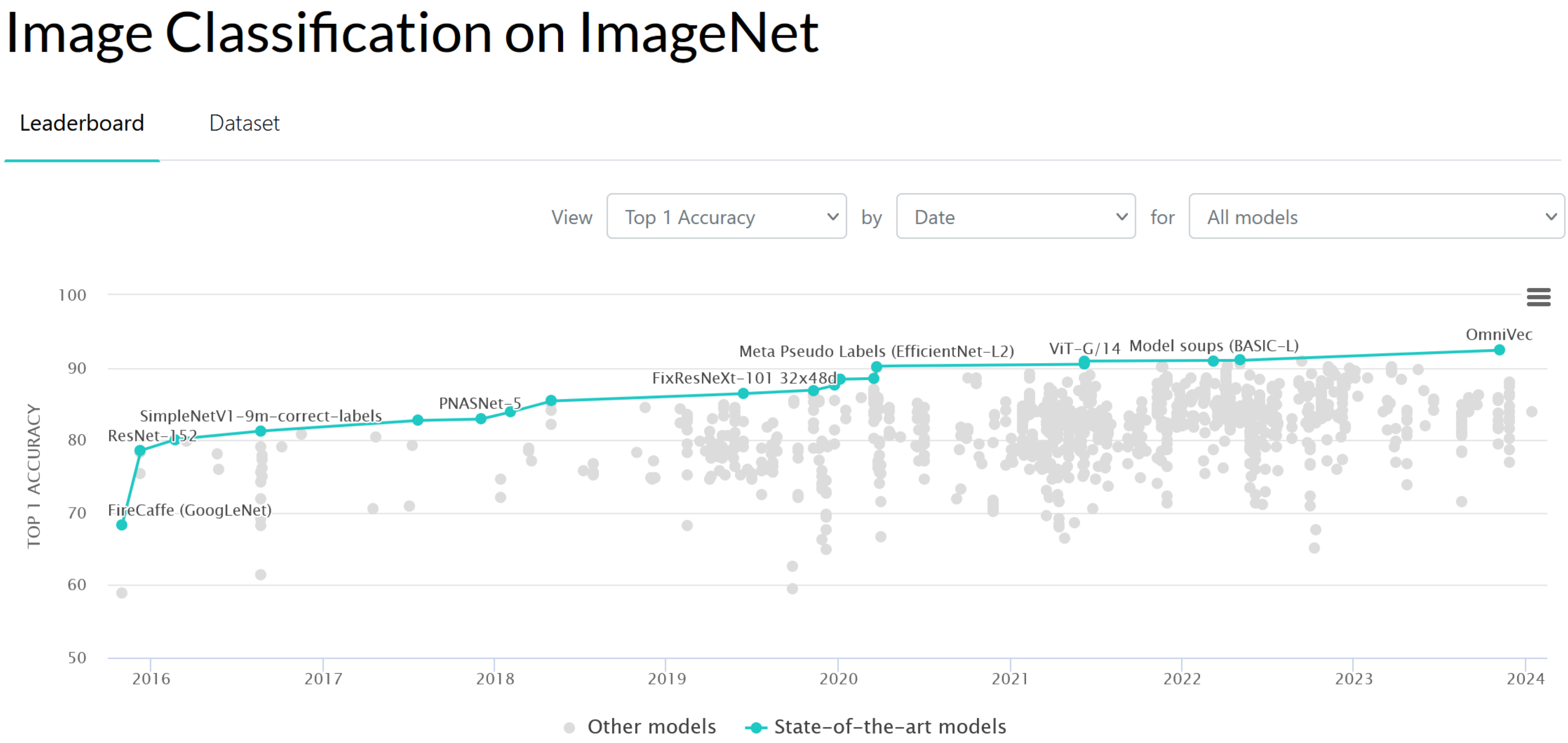
- Evaluating ML models in production is a multidimensional problem.
- Model performance (of course) is important, but so are how long it takes to train, latency at inference, (cost of) compute requirements, and explainability.
- Different types of algorithms require different numbers of labels as well as different amounts of computing power.
- Some take longer to train than others, whereas some take longer to make predictions.

Guidance for Model Selection (1/3)

Avoid the state-of-the-art trap

- Researchers evaluate models in academic settings: if a model is state-of-the-art, it performs better than existing models on some static dataset.
- It is essential to remain up to date but solve the problem first.
- Start with the simplest models
- Simple is better than complex: easier to deploy, easier to understand, and serve as a baseline.
- Easier to deploy: speeds up the experimentation cycle.
- Easier to understand: adds complexity as needed.
- Baseline: simple models serve as a starting comparison point for model development.

Guidance for Model Selection (1/3)

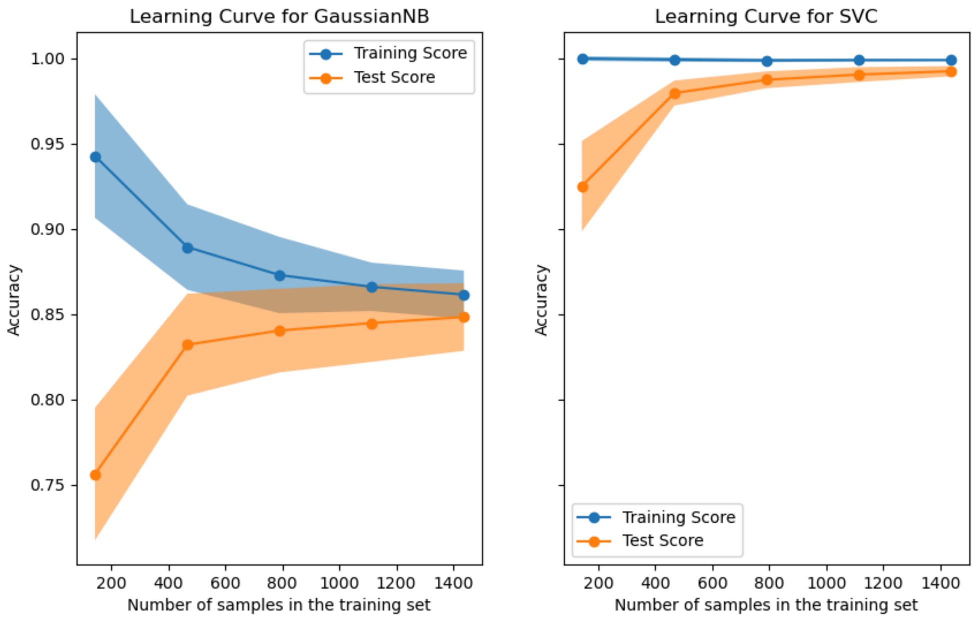


State of the Art Model Performance on ImageNet c.2023 (paperswithcode.com)

Guidance for Model Selection (2/3)

Avoid human biases in selecting models

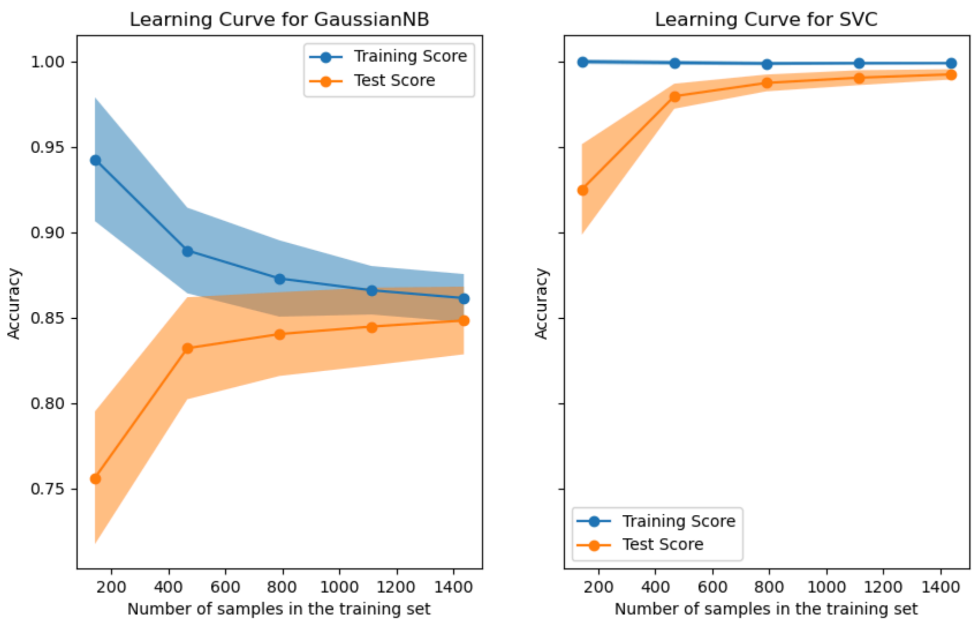
- Human biases can be introduced throughout the model development process.
- Experiment methodically and store results.
- Any model has three components: algorithmic logic, code, and data.



Guidance for Model Selection (2/3)

Evaluate good performance now versus good performance later

- Using learning curves is a simple way to estimate how your model's performance might change with more data.
- While evaluating models, consider their potential for improvement and how easy/difficult it is to achieve.



Guidance for Model Selection (3/3)

Evaluate trade-offs

- False positives vs false negatives: reducing false positives may increase false negatives and vice versa.
- Compute requirement and model performance: a more complex model may deliver better performance, but at what cost?

Guidance for Model Selection (3/3)

Understand your model's assumptions

- Every model comes with its assumptions.
- Prediction assumption: every model that aims to predict an output Y from an input X assumes that it is possible to predict Y based on X.
- Independent and Identically Distributed: neural nets assume that examples are independent and identically distributed.
- Smoothness: supervised learning models assume that a set of functions can transform inputs into outputs such that similar inputs are transformed into similar outputs. If an input X produces Y, then an input close to X would produce an output proportionally close to Y.
- Linear boundaries, conditional independence, normally distributed, and so on.

Ensembles

The Wisdom of the Crowds

> “Aggregating the judgment of many consistently beats the accuracy of the average member of the group, and is often as startlingly accurate […] In fact, in any group there are likely to be individuals who beat the group. But those bull’s-eye guesses typically say more about the power of luck […] than about the skill of the guesser. That becomes clear when the exercise is repeated many times.”

> (Tetlock and Gardner, 2015)

Ensembles

- Ensemble methods are less favoured in production because ensembles are more complex to deploy and harder to maintain.
- Common in tasks where small performance boosts can lead to substantial financial gains, such as predicting the click-through rate for ads.
- Ensembles perform better when underlying classifiers are uncorrelated.

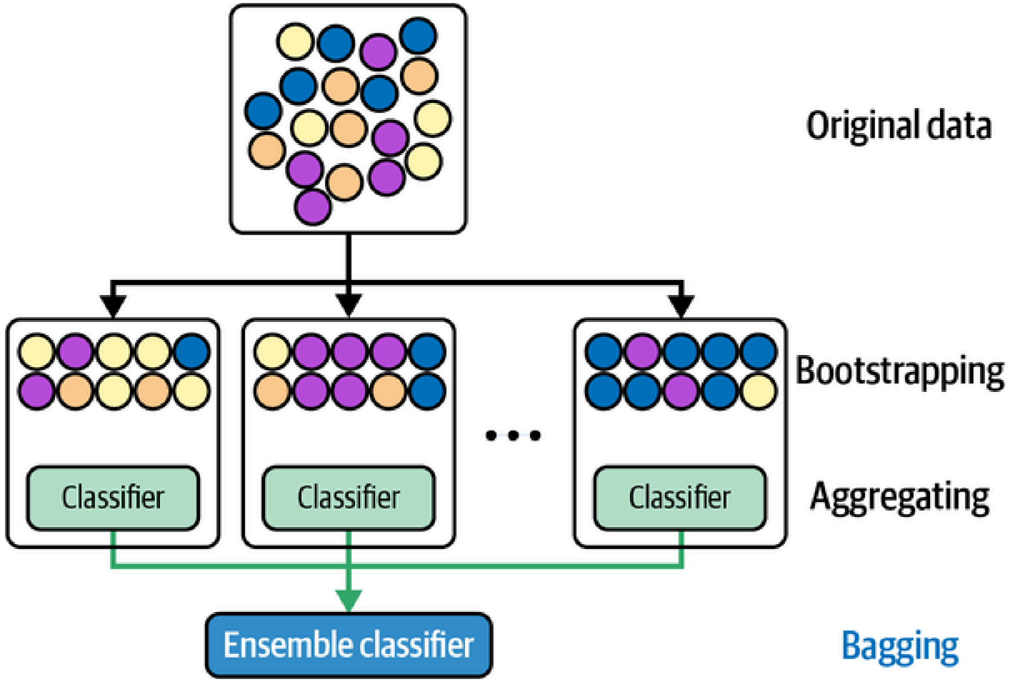
Leaderboard

SQuAD2.0 tests the ability of a system to not only answer reading comprehension questions, but also abstain when presented with a question that cannot be answered based on the provided paragraph.

Rank	Model	EM	F1
	Human Performance *Stanford University* (Rajpurkar & Jia et al. '18)	86.831	89.452
1 Jun 04, 2021	IE-Net (ensemble) *RICOH_SRCB_DML*	**90.939**	**93.214**
2 Feb 21, 2021	FPNet (ensemble) *Ant Service Intelligence Team*	90.871	93.183
3 May 16, 2021	IE-NetV2 (ensemble) *RICOH_SRCB_DML*	90.860	93.100
4 Apr 06, 2020	SA-Net on Albert (ensemble) *QIANXIN*	90.724	93.011
5 May 05, 2020	SA-Net-V2 (ensemble) *QIANXIN*	90.679	92.948
5 Apr 05, 2020	Retro-Reader (ensemble) *Shanghai Jiao Tong University* http://arxiv.org/abs/2001.09694	90.578	92.978
5 Feb 05, 2021	FPNet (ensemble) *YuYang*	90.600	92.899

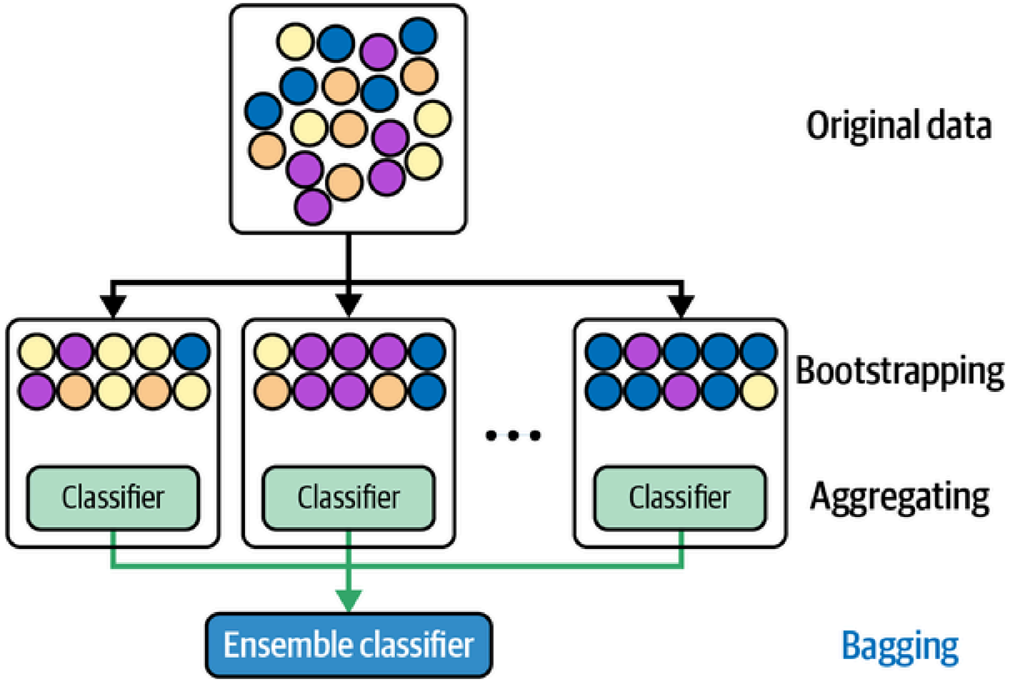
Possible Outcomes

Outputs of three models	Probability	Ensemble's output
All three are correct	0.7 * 0.7 * 0.7 = 0.343	Correct
Only two are correct	(0.7 * 0.7 * 0.3) * 3 = 0.441	Correct
Only one is correct	(0.3 * 0.3 * 0.7) * 3 = 0.189	Wrong
None are correct	0.3 * 0.3 * 0.3 = 0.027	Wrong



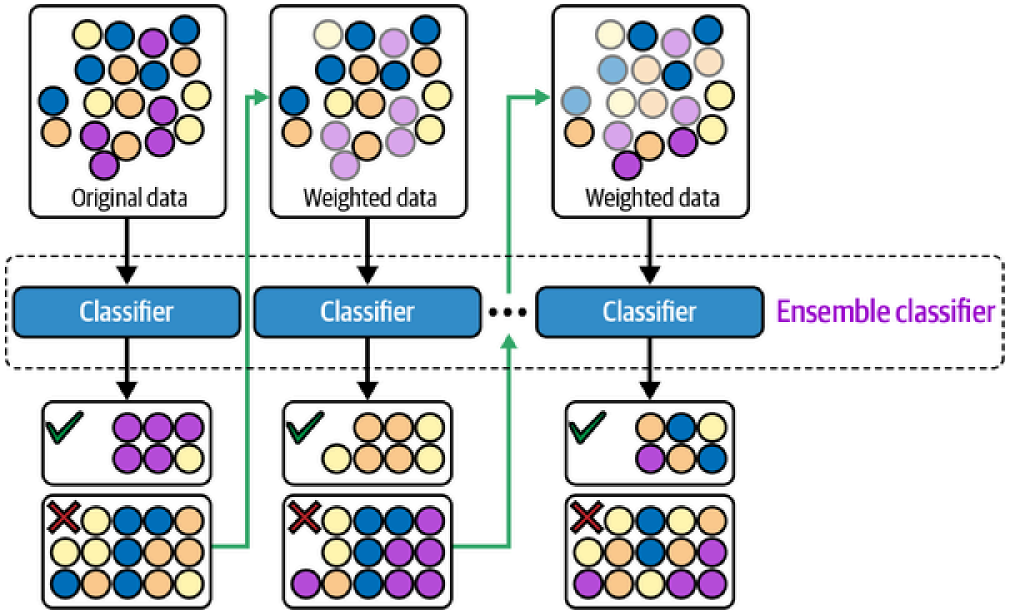
Bagging

- Bagging (bootstrap aggregating) is designed to improve ML algorithms' training stability and accuracy.
- Reduces variance and helps avoid overfitting; it improves unstable methods (e.g., tree-based methods)
- Sampling with replacement ensures that each bootstrap is created independently from its peers.



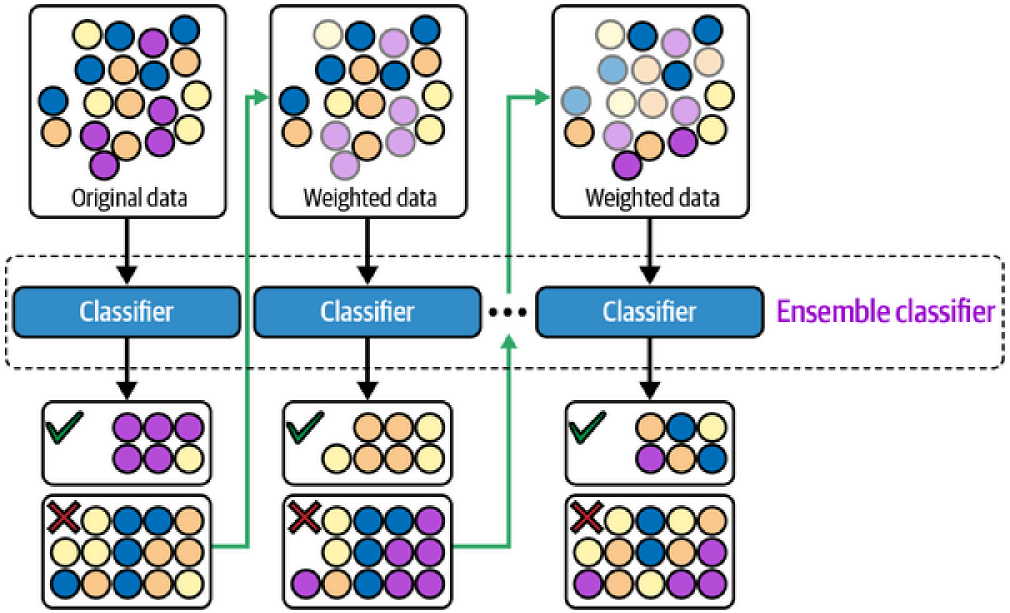
Bagging

- Given a data set, create n data sets by sampling with replacement (bootstrap).
- Train a classification or regression model on each bootstrap.
- If classification, decide by majority vote; if regression, use the mean result.



Boosting

- Family of iterative ensemble algorithms that convert weak learners to strong ones.
- Examples: Gradient Boosting Machine (GBM), XGBoost, and LightGBM.

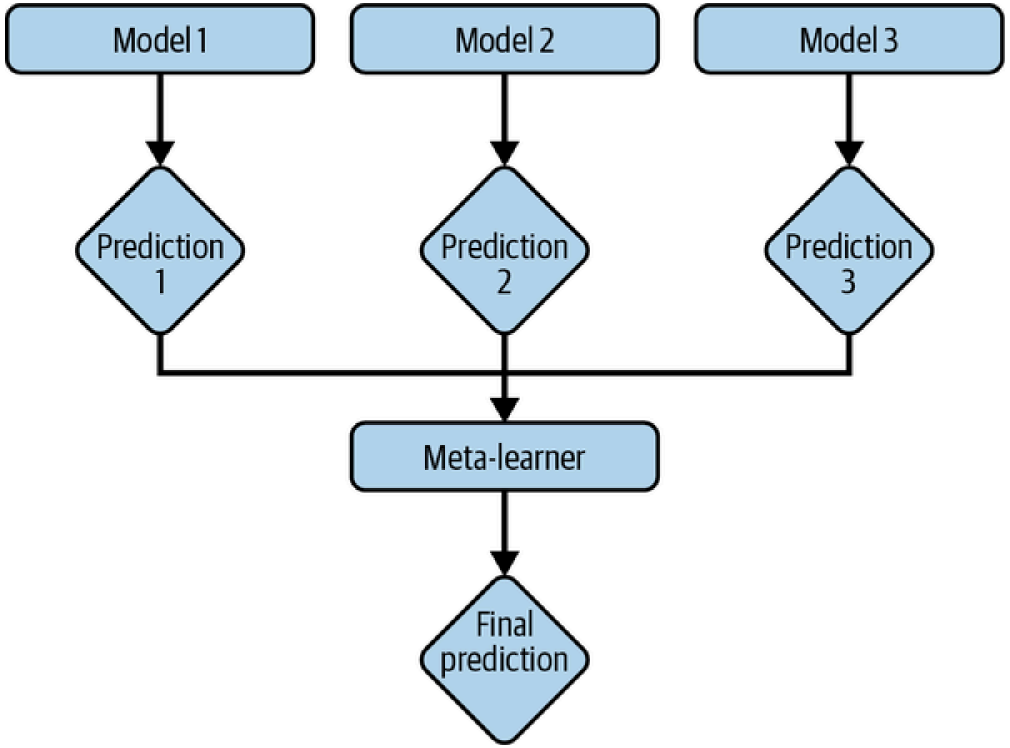


Boosting

- Each learner is trained on the same set of samples, but the samples are weighted differently in each iteration.
- Future weak learners focus more on the examples that previous weak learners misclassified.

Stacking

- Create base learners from the training data.
- Create a meta-learner that combines the outputs of the base learners to output predictions.



Experiment Tracking and Versioning

Experiment Tracking

- The process of tracking the progress and results of an experiment is called experiment tracking.
- ML Flow and Weights & Balances are experiment tracking tools.
- At a minimum, track performance (loss) and time (speed).
- Values over time of any parameter and hyperparameter whose changes can affect model performance.

Experiment Tracking

- Model performance metrics: on all nontest splits, like accuracy, F1, and perplexity.
- Loss curve: train split and each of the eval splits.
- Log of corresponding sample, prediction, and ground truth labels.
- Speed of the model: number of steps per second or tokens processed per second.
- System performance metrics: memory, CPU, GPU.

Versioning

- The process of logging an experiment's details to recreate it later or compare it with other experiments is called versioning.
- ML models in production are part code and part data.
- Code versioning has more or less become a standard in the industry.
- Data versioning is not standard.

Versioning

- Code versioning tools allow you to switch between versions of the codebase by keeping copies of all the old files. Data may be too large for duplication to be feasible.
- Code versioning tools allow several people to work on the same code simultaneously by replicating locally. Data may be too large, as well.
- What is a diff when versioning data? DVC, for example, only checks for changes in the checksum.
- Compliance with GDPR may also be problematic if the full history of data is kept.

Making Progress

Debugging: Why ML Models Fail

- Theoretical constraints: model assumptions are not met. For example, use a linear model when decision boundaries are not linear.
- Poor implementation: The model may be a good fit, but implementation has errors.
- Poor choice of hyperparameters: with the same model, one set of hyperparameters can give better results than others.

Debugging: Why ML Models Fail

- Data problems: noise and dirty data are everywhere. Additionally, poor implementation of data flows can lead to data problems.
- Poor choice of features: Too many features may cause overfitting or data leakage. Too few features might lack predictive power to allow for making good predictions.
- Some debugging approaches:
    - Start simple and gradually add more components.
    - Overfit a single batch.
    - Set a random seed.

AutoML

- AutoML is the automatic process of finding ML algorithms to solve real-world problems.
- The most popular form of AutoML is hyperparameter tuning.
- Searching the Hyperparameter space can be time-consuming and resource-intensive.

Model Offline Evaluation

- Measure model performance before and after deployment.
- Evaluation methods should be the same for models during development and production.
- Techniques for model offline evaluation:
    - Use baselines.
    - Tests: perturbation tests, invariance tests, directional expectation tests, model calibration, confidence measurement, slice-based evaluation.

Model Offline Evaluation: Baselines

- Random baseline: if the model predicts at random, how would it perform?
- Simple heuristic: how does the model perform vs a simple (non-ML) rule of thumb?
- Zero rule baseline: trivial prediction, always predicts the same thing.
- Human baseline: human-level performance may be the required baseline.
- Existing solutions.

Evaluation Methods in Production

- Perturbation tests: make changes to test splits, such as adding noise to input data. If a model is not robust to noise, it will be challenging to maintain.
- Invariance tests: specific input changes should not lead to output changes—for example, protected classes.
- Directional expectation tests.

Evaluation Methods in Production

Model calibration or conformal prediction methods

- Idea: If the forecast has a 70% chance of rain, then 70% of the time this forecast was made, it actually rained.
- Prediction scores are often normalized to values between 0 and 1. It is tempting to think of them as probabilities, but they are not necessarily so.
- Use conformal prediction methods to calibrate prediction scores.
- Confidence measurement: show only predictions where the model is confident.
- Slice-based evaluation: model performance is different in subsets of data.

References

References

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