





Quality





Quality

this model is highly accurate on training data



Quality

■ too-precise fits to original data without generalization is called **overfitting**



underfitting



model is unable to capture relationship between variables











underfitting









overfitting frequently takes place when the degree of a regression model is set too high

How do we address under/overfitting?



training data

training data



validation data

test data



we use validation and test sets, small subsets of data the model hasn't seen before,

Model Has Seen

training data



Model Hasn't Seen

test data



wait but what's the difference?





test sets are, unlike validation sets, usually set by the data creator as common, unseen benchmark data.

overfitting can be dangerous data ethics

data ethics





which one has pneumonia?

data ethics



models, when not controlled for external factors, often overfit on easy targets

Feature selection & Feature engineering



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Motivation

- the target variable.
- Overfitting for tasks with a smaller # of samples
- A large number of variables can be computationally expensive

Performance could degrade when including input variables that are not relevant to



Typical techniques

- Remove features with low variance (e.g., zero variance)
- Remove features with low correlation based on statistical tests
- Sequential feature selection
 - Forward: iteratively add the best new features \succ
 - Backward: iteratively remove the least useful feature \blacktriangleright
- https://scikit-learn.org/stable/modules/feature_selection.html



Feature Engineering

- Different from feature selection
- Example: predict time-to-sell of a house
- price
- Engineered features could include
 - Cost per sq. ft \succ
 - House age \succ
 - Zip code \succ
 - School rating \succ
- considered as feature engineering

Input (features and label): square footage, lot size, transaction date, built date, and

Data preprocessing (e.g., normalization, missing data) sometimes are also



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Typical process

- Brainstorming features
- Deciding what features to create
- Creating features
- Testing the impact of the identified features on the task
- Improving your features if needed
- Repeat



Features

- Feature selection
- Feature engineering
- PCA
- Differences





Debugging a learning algorithm

- A dataset
- Applied a machine learning algorithm
- Got a result, e.g., error rate 11%
- Is this a good result?

Credit: Advanced Machine learning, Andrew Ng, Coursera, for the debugging discussion .

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Establish a baseline

- What is a reasonable level of error we can hope for?
 - Human level performance \succ
 - Competing/existing algorithms \succ
 - Educated guess based on experience \succ
- Additional baselines
 - Random guess \succ
 - Simple heuristics \succ



Bias/variance

Case 1

Baseline	10.6%
(e.g., human)	
Training error	11%
Validation error	16%

Case 2	Case 3
10.6%	10.6%
15.5%	11%
16%	12%



Improving Outcome Debugging

- Bias: error from algorithm.
- Variance: error training set.
- Q: how do they manifest?

- Bias: error from erroneous assumptions in the learning
- Variance: error from sensitivity to small fluctuations in the



Debugging

- High bias: training error high
- High variance: validation error high



Model Complexity



Debugging

- High bias: training error high
- High variance: validation error high
- What can we do?



Debugging

- High bias: training error high High variance: validation error high
- Try getting additional features
- Try adding polynomial features
- Try decreasing regularization or use larger models
- Get more training samples
- Try smaller set of features
- Try increasing regularization or use smaller models



Debugging

- Try getting additional features (high bias)
- Try adding polynomial features (high bias)
- Get more training samples (fixes high variance)
- Try smaller set of features (high variance)

Try decreasing regularization or use larger models (high bias)

Try increasing regularization or use smaller models (high variance)



Error analysis

- Examine where the model went wrong
- Categorize the errors
- Focus on how to fix these errors (or most of them)



Example

- Food spoilage prediction
- Categorize them based on common traits
- Southern CA: 21
- Valley: 10
- Raining weather: 50
- Packaging: 5
- More data and features for SoCal and raining days

Manually examine 100 examples where our model got wrong



A Real Example

Gait analysis to classify stroke patient in recovery vs. control

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When to Use Which Algorithm?

- Start simple
- Try the typical ones
- Sklearn guideline



Potential Pitfalls



Potential Pitfalls

Things that can go wrong

- Inconsistent preprocessing
- Data leakage
- Model is used on test data that has changed
- Selecting appropriate metrics
- Hidden confounders
- Spurious correlations
- Performance on subgroups may be missing
- Data biases





Potential Pitfalls

Things that can go wrong

- Inconsistent preprocessing (e.g., different scaling/normalization) Data leakage (e.g., temporal or mixing subjects)
- Model is used on test data that has changed
- Selecting appropriate metrics (e.g., is 99% accuracy good enough?)
- Hidden confounders (e.g., golf is correlated with heart attacks)
- Spurious correlations (e.g., hospital ID on images)
- Performance on subgroups may be missing
- Data biases (e.g., AI recruiter)







Be Cautious

- AI/ML is not a cure-all
- "All models are wrong, some are useful." –George Box
- Is AI a hype or a GE?

Understand your models, know the assumptions and limitations of the models

Typical steps to apply ML

- Data preprocessing
- Trying different ML algorithms
 - Training set, validation set, test set \blacktriangleright
- Diagnostics
 - More training samples \succ
 - Increase/decrease feature set
 - Increase/decrease regularization \succ
- Loop back



A ML Project

- Why ML is a suitable approach
 - Do not use ML for the purpose of using ML \succ
 - Evaluate existing approaches and room for improvement \succ
- Problem abstraction and formulation
 - Set appropriate goals
 - Model complexity, data availability, evaluation
 - Domain knowledge critical \succ
- Data collection and data cleaning
 - > What, where, and how
- ML algorithms
 - This is often the "easy" part
- Evaluation, sanity check, interpretation
- Iterate the process

Characteristics of Good Problems

- Existing solutions not satisfactory
 - Automate the process \succ
 - Improve performance \succ
- Data availability: suitable data available or obtainable
- Data quality and quantity
- Can evaluate proposed approaches
- Large complex problem beyond white-box modeling
- Understanding complex venue and large data

Project Examples

- Sanitation classification
- Tomato processing loss prediction
- Dietary recommendation
- Help breeders to run more efficient and targeted breeding programs
- Gait analysis
- **Biomarker identification**
- Disease outbreak prediction
- Weather outbreak spatial temporal analysis
- Network traffic scheduling
- Encrypted traffic classification
- Traveling salesman