Wine Quality Prediction

4조

독하게 데이터 사이언스

김태영 류채환 박준영 신해솔 홍성희

Introduction

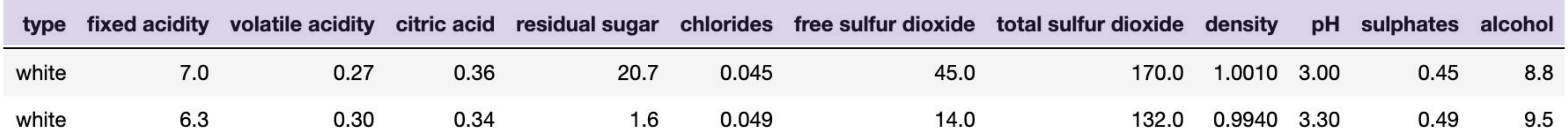
Data and Purpose

Problems of Prior Research

Our Improvement

분석 수행 목적: y = f(X)

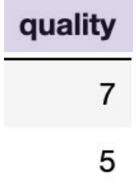
X : 와인의 화학적 성분 데이터로



type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
white	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8
white	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5

타입, 알코올, 밀도, pH, 산도, 구연산, 잔류 설탕, 염화물, 이산화황, …

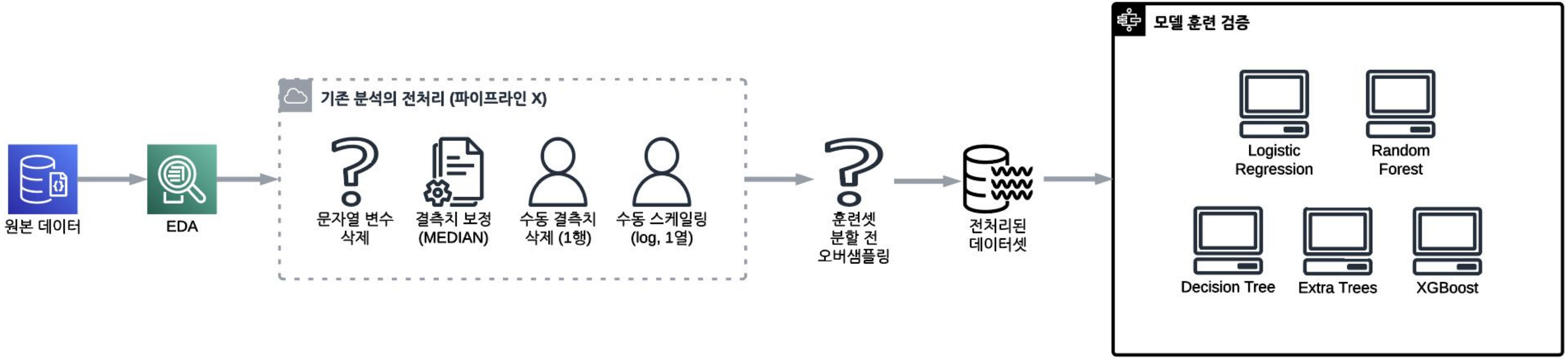
y : 와인의 품질 등급 맞추기



quality
7
5

품질(0~10점) → 실질적으로는 3~9의 값

선행 연구 Workflow

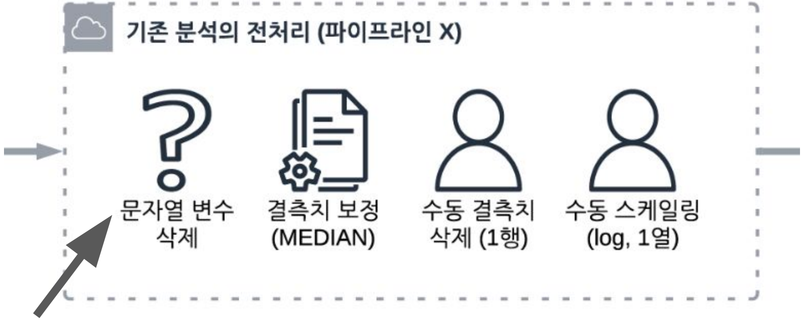


모델 평가 결과

최종모델선택: Extra Trees

Accuracy: 89.9

선행 연구의 문제점 1: 불완전한 전처리



기존 분석의 전처리 (파이프라인 X)

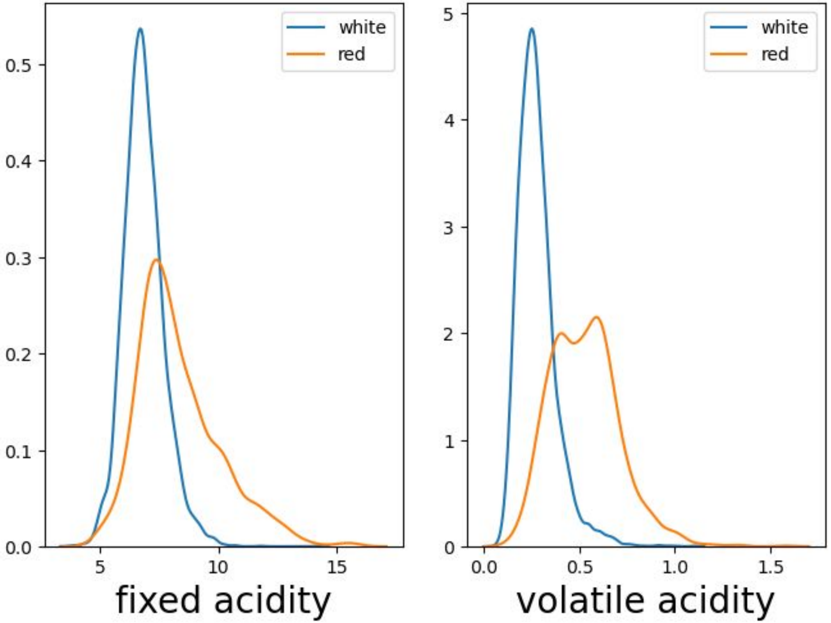
문자열 변수 삭제

결측치 보정 (MEDIAN)

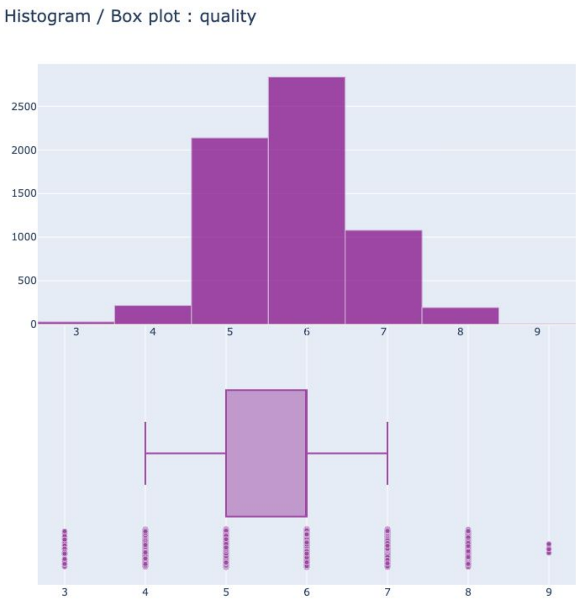
수동 결측치 삭제 (1행)

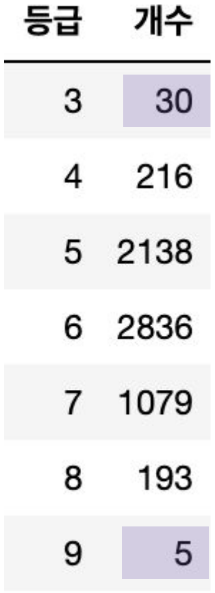
수동 스케일링 (log, 1열)

type (white, red)



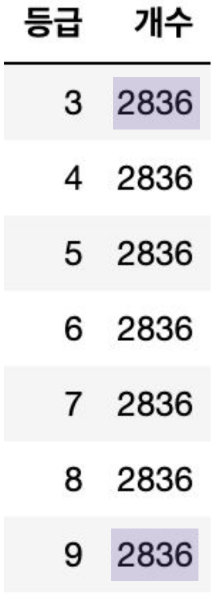
선행 연구의 문제점 2: 비합리적 오버샘플링





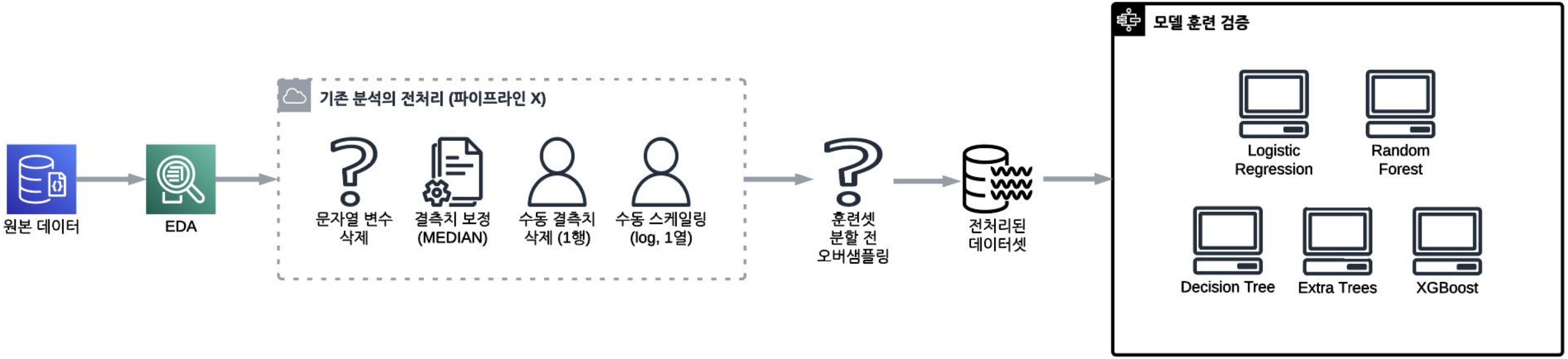
등급	개수
3	30
4	216
5	2138
6	2836
7	1079
8	193
9	5

훈련셋 분할 전 오버샘플링



등급	개수
3	2836
4	2836
5	2836
6	2836
7	2836
8	2836
9	2836

선행 연구 재평가



잘못된 선행 연구 평가 결과

최종모델선택: Extra Trees

Accuracy: 89.9

F1: 89.2

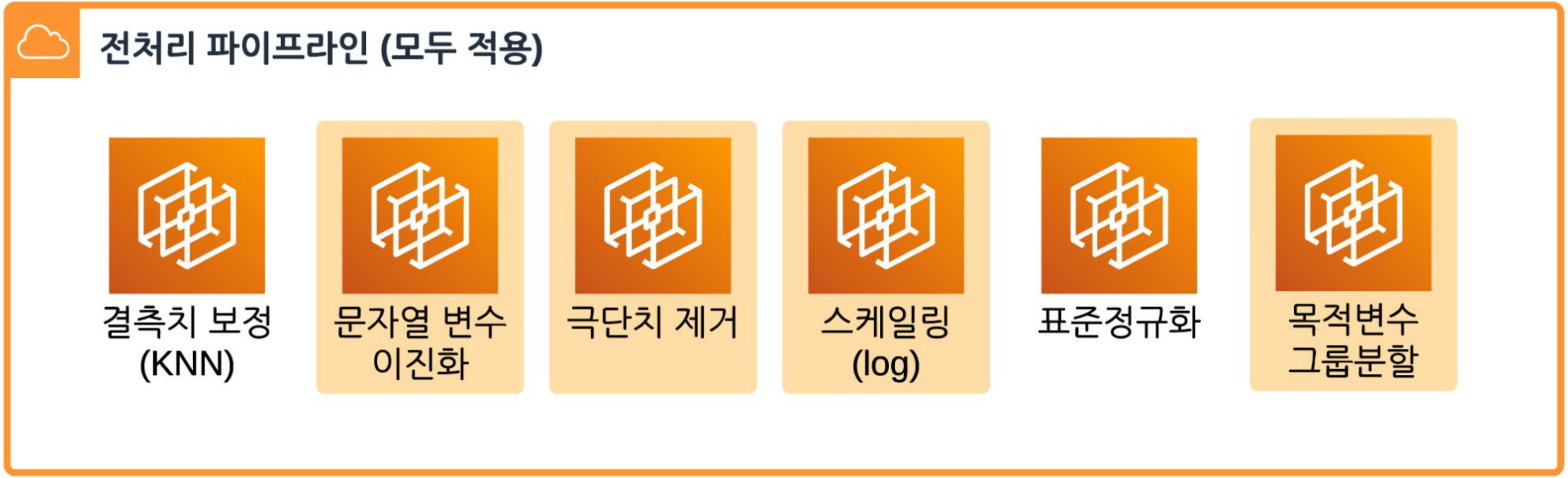
비합리적 가정 제거 후 선행 연구 평가 결과

최종모델선택: Extra Trees

Accuracy: 67.5

F1: 66.9

선행 연구 개선 1: 전처리



전처리 파이프라인 (모두 적용)

결측치 보정 (KNN)

문자열 변수 이진화

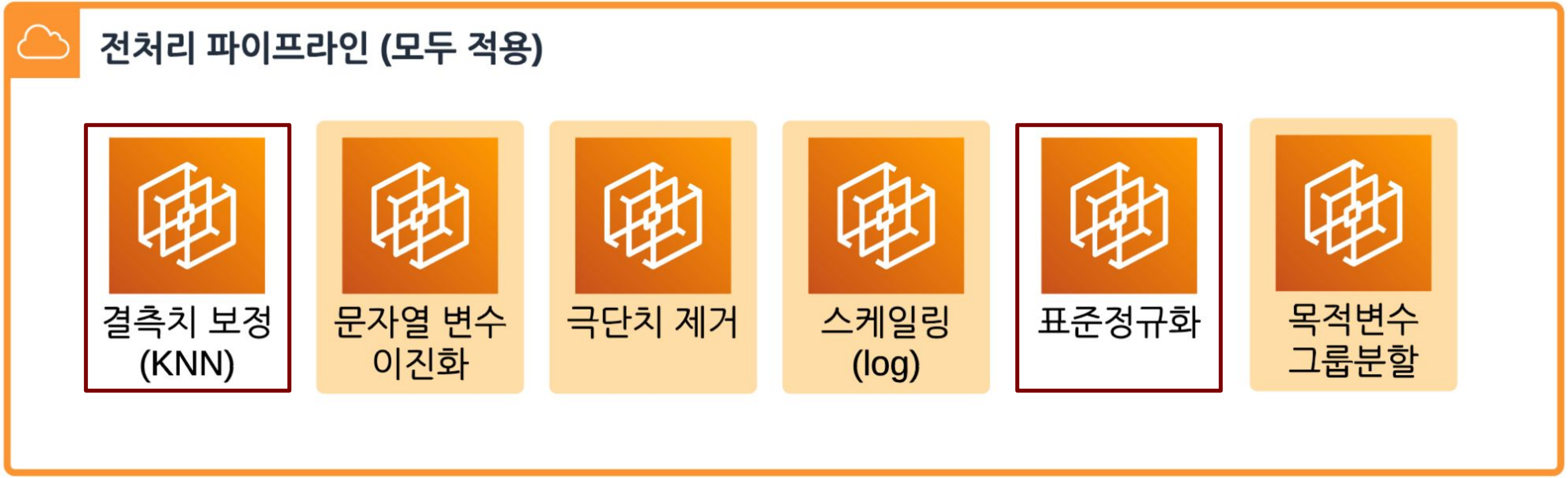
극단치 제거

스케일링 (log)

표준정규화

목적변수 그룹분할

선행 연구 개선 1: 전처리



전처리 파이프라인 (모두 적용)

결측치 보정 (KNN)

문자열 변수 이진화

극단치 제거

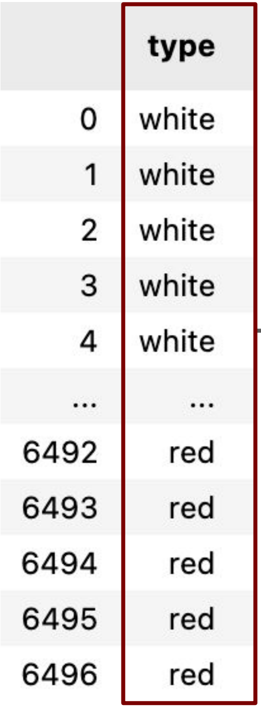
스케일링 (log)

표준정규화

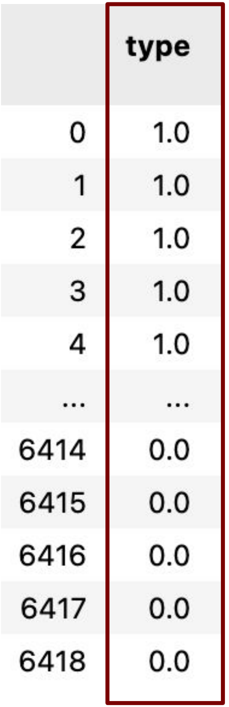
목적변수 그룹분할

선행 연구 개선 1: 전처리

문자열 변수 이진화



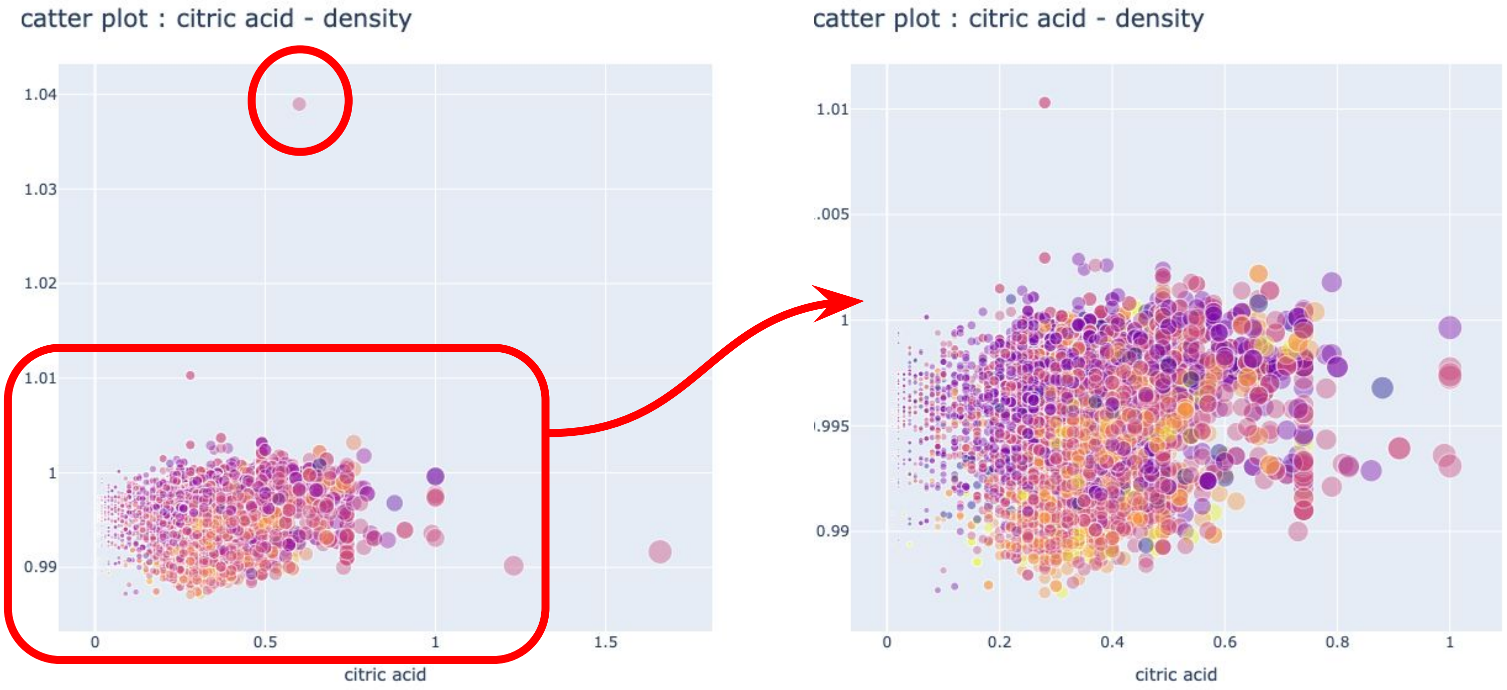
	type
0	white
1	white
2	white
3	white
4	white
...	...
6492	red
6493	red
6494	red
6495	red
6496	red



	type
0	1.0
1	1.0
2	1.0
3	1.0
4	1.0
...	...
6414	0.0
6415	0.0
6416	0.0
6417	0.0
6418	0.0

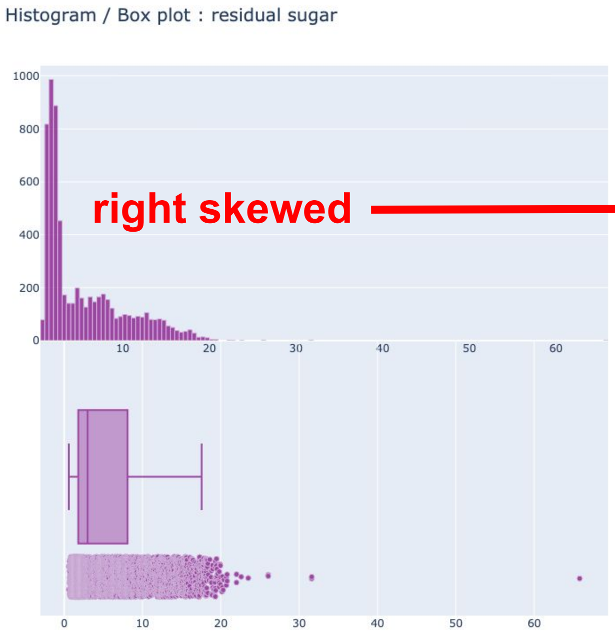
선행 연구 개선 1: 전처리

극단치 제거

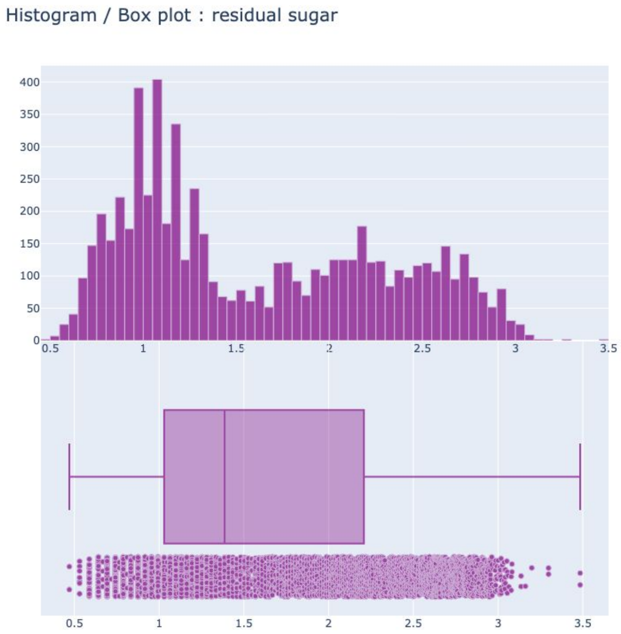


선행 연구 개선 1: 전처리

스케일링 (log)

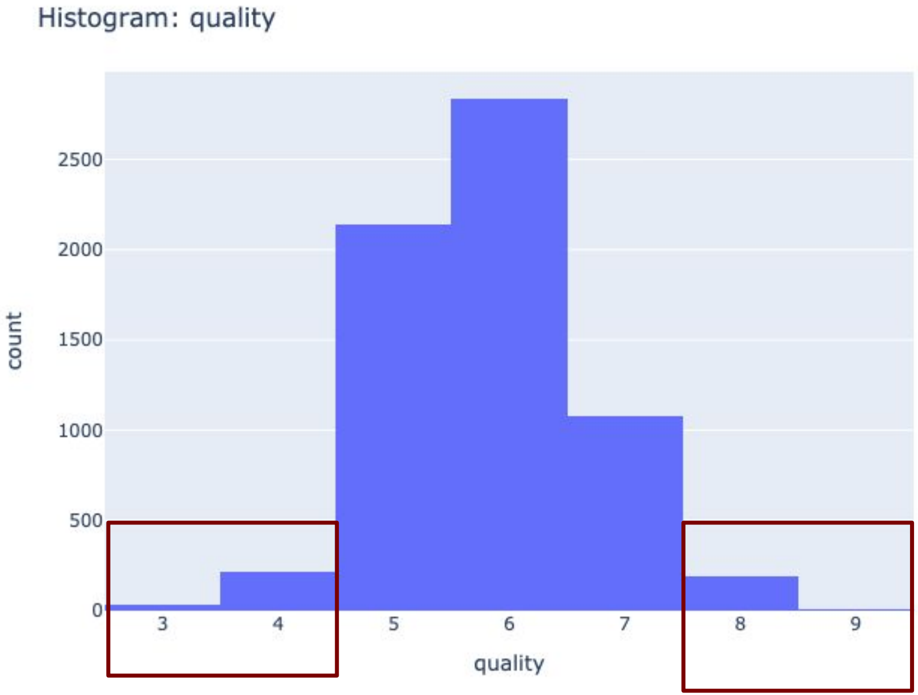


right skewed



선행 연구 개선 1: 전처리

목적변수
그룹분할

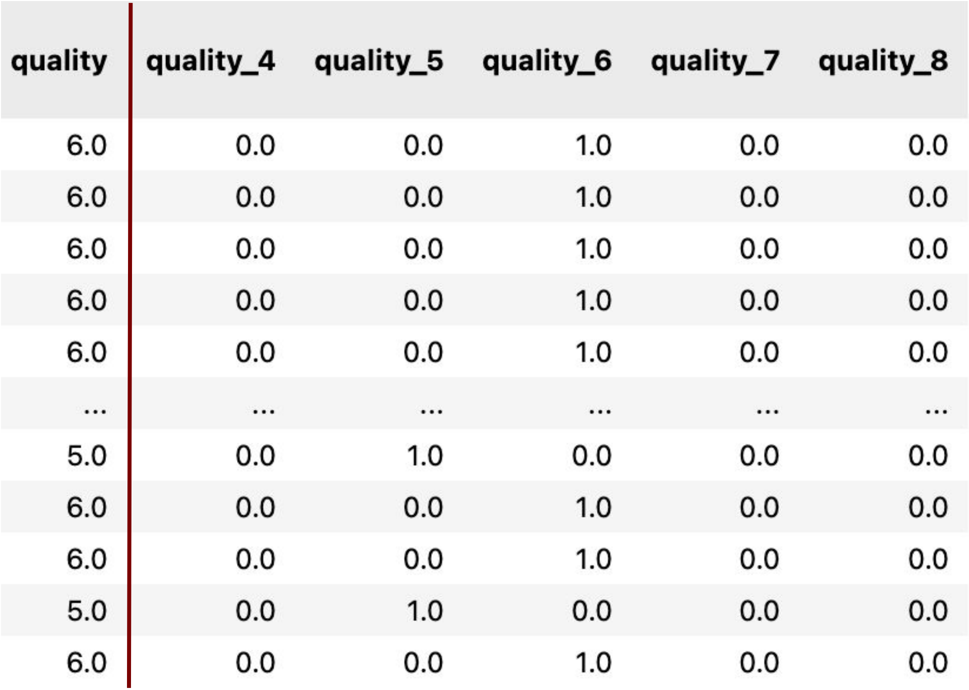


quality 3, 4
→ **quality 4**

quality 8, 9
→ **quality 8**

선행 연구 개선 1: 전처리

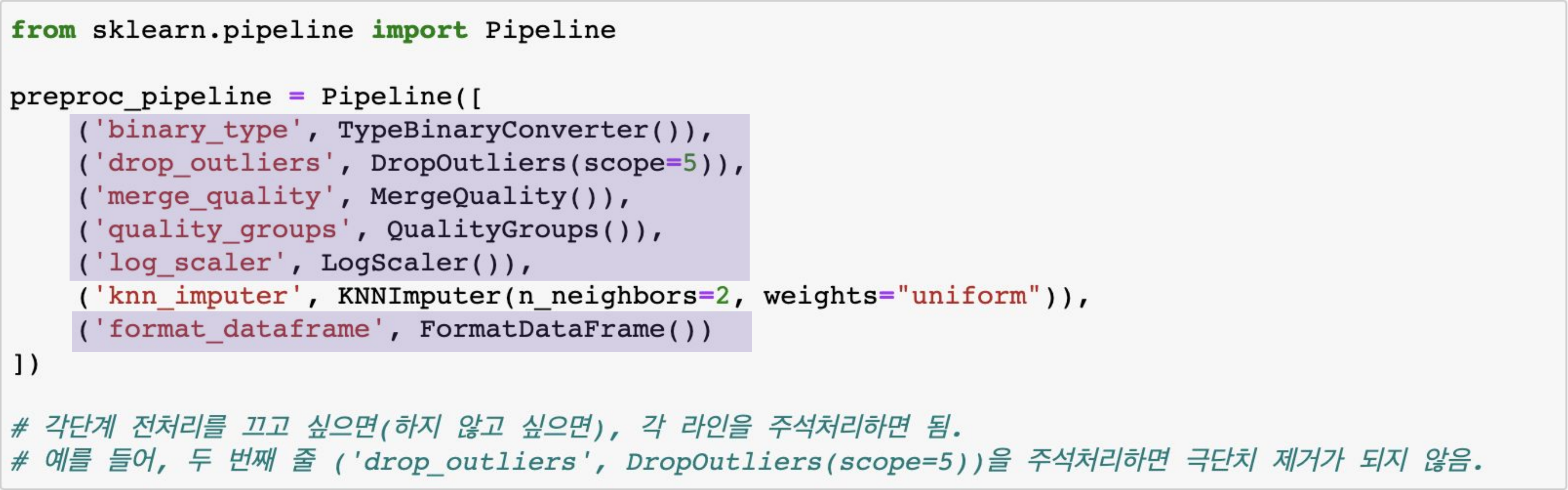
목적변수 그룹분할



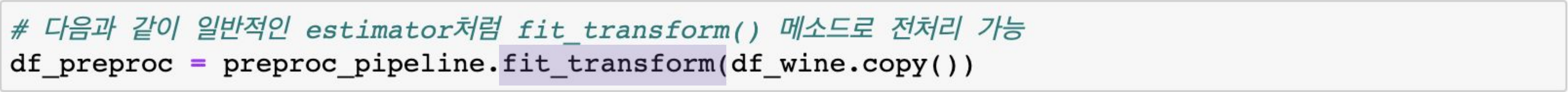
quality	quality_4	quality_5	quality_6	quality_7	quality_8
6.0	0.0	0.0	1.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
...	...	...	...	...	...
5.0	0.0	1.0	0.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0
5.0	0.0	1.0	0.0	0.0	0.0
6.0	0.0	0.0	1.0	0.0	0.0

quality 이진 처리

전처리기: scikit-learn 방식 구현



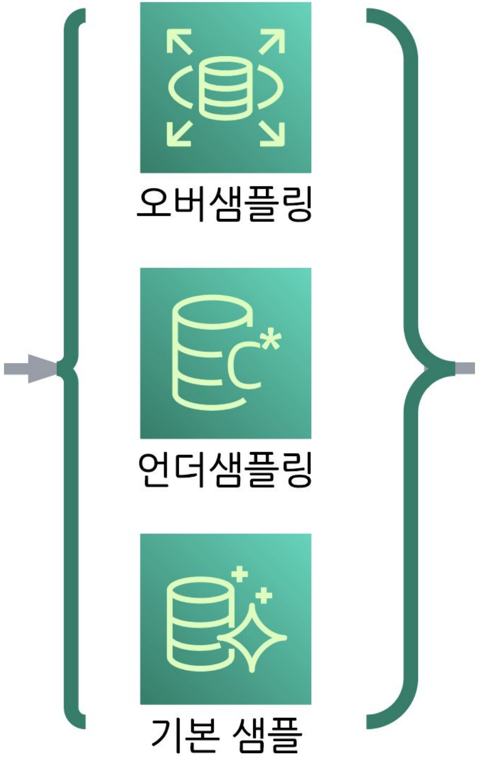
```python
from sklearn.pipeline import Pipeline

preproc_pipeline = Pipeline([
    ('binary_type', TypeBinaryConverter()),
    ('drop_outliers', DropOutliers(scope=5)),
    ('merge_quality', MergeQuality()),
    ('quality_groups', QualityGroups()),
    ('log_scaler', LogScaler()),
    ('knn_imputer', KNNImputer(n_neighbors=2, weights="uniform")),
    ('format_dataframe', FormatDataFrame())
])

# 각단계 전처리를 끄고 싶으면(하지 않고 싶으면), 각 라인을 주석처리하면 됨.
# 예를 들어, 두 번째 줄 ('drop_outliers', DropOutliers(scope=5))을 주석처리하면 극단치 제거가 되지 않음.
```



```python
# 다음과 같이 일반적인 estimator처럼 fit_transform() 메소드로 전처리 가능
df_preproc = preproc_pipeline.fit_transform(df_wine.copy())
```

ref) 오렐리앙 제롱, 핸즈온머신러닝 2판 "2.5.3 나만의 변환기" p106

선행 연구 개선 2: 오버샘플링

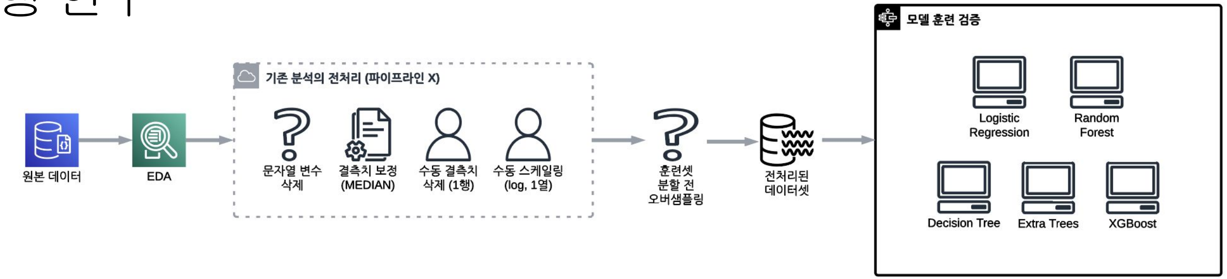


1. Train set 분할 후
   Train set에 대해서만 오버샘플링

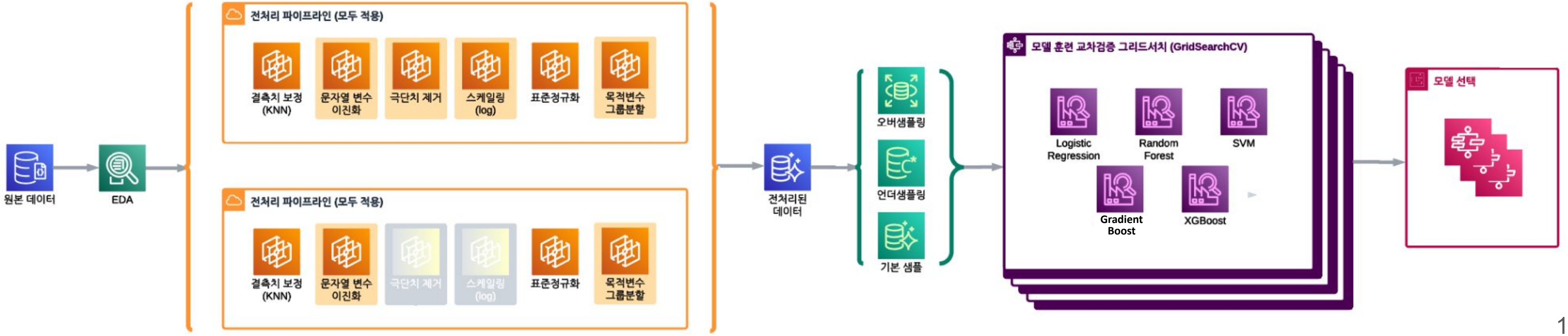
2. 오버샘플링/언더샘플링/기본샘플
   모델 분석 x3 수행
   (샘플링 방식에 따른 모델 학습 편향 방지)

선행 연구와의 비교: Workflow Diagram

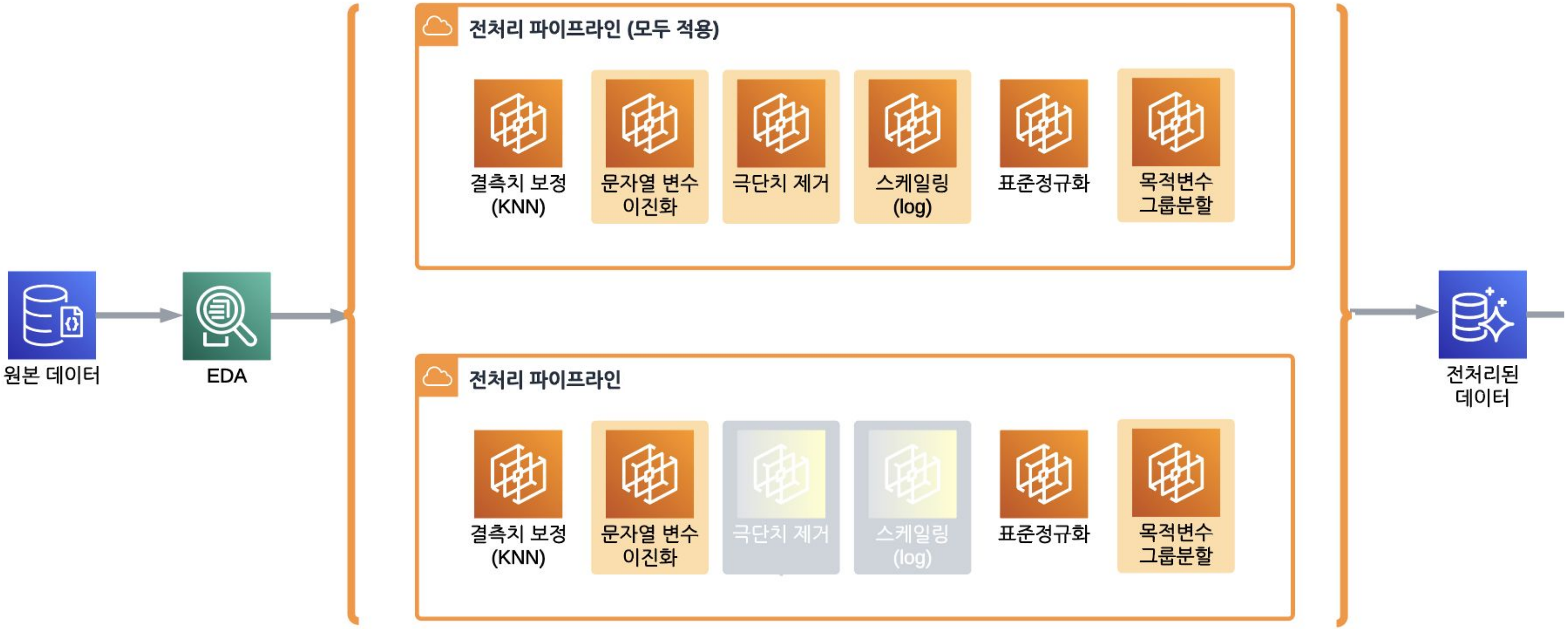
선행 연구



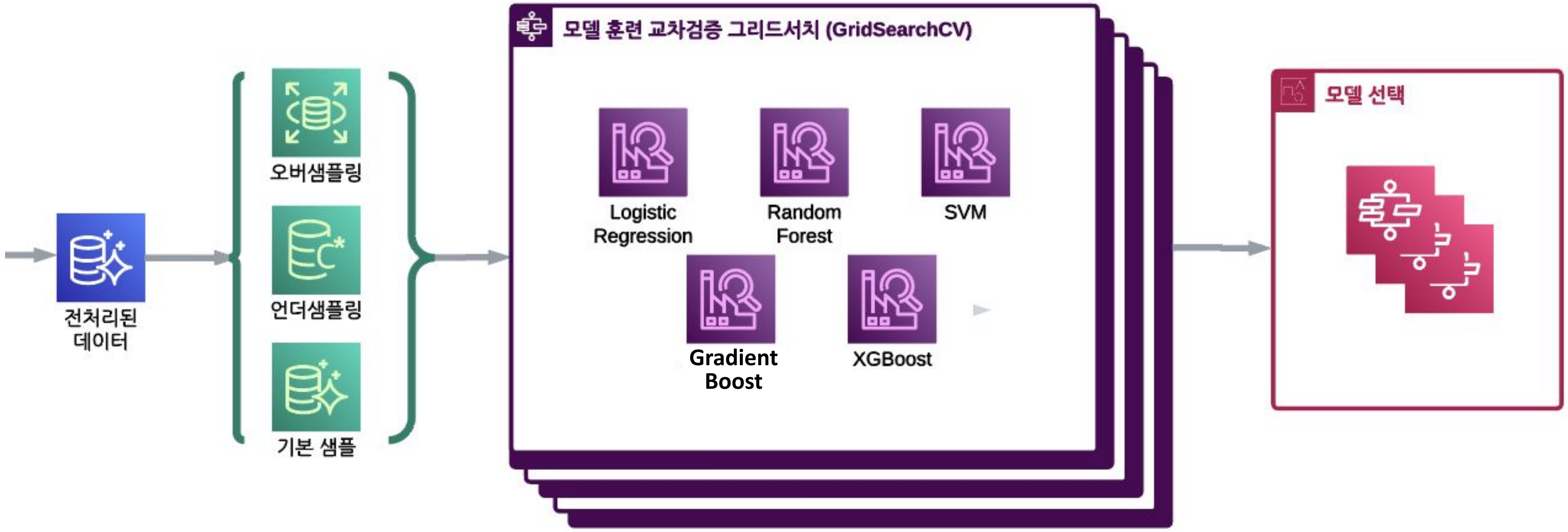
수행한 연구



수행한 분석 Workflow (1/2)



수행한 분석 Workflow (2/2)



Models
(Supervised Machine Learning)

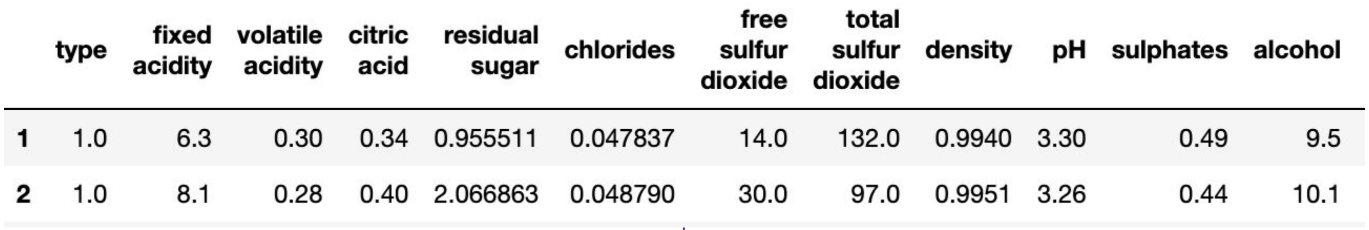
Logistic Regression | Random Forest

SVM | Gradient Boost | XGBoost

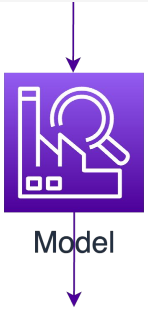
Trial 1.
Multi Classification

Multi Classification

X: Wine Features



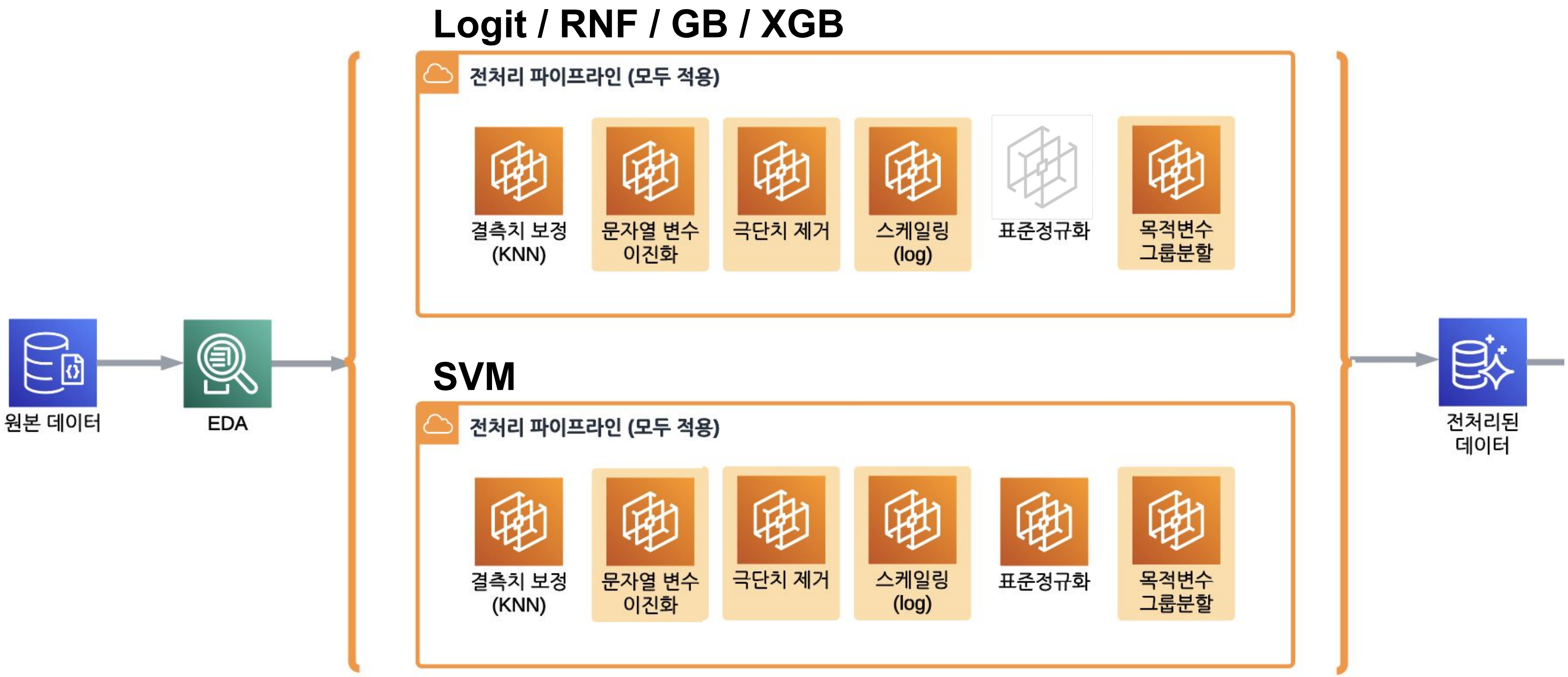
	type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
1	1.0	6.3	0.30	0.34	0.955511	0.047837	14.0	132.0	0.9940	3.30	0.49	9.5
2	1.0	8.1	0.28	0.40	2.066863	0.048790	30.0	97.0	0.9951	3.26	0.44	10.1



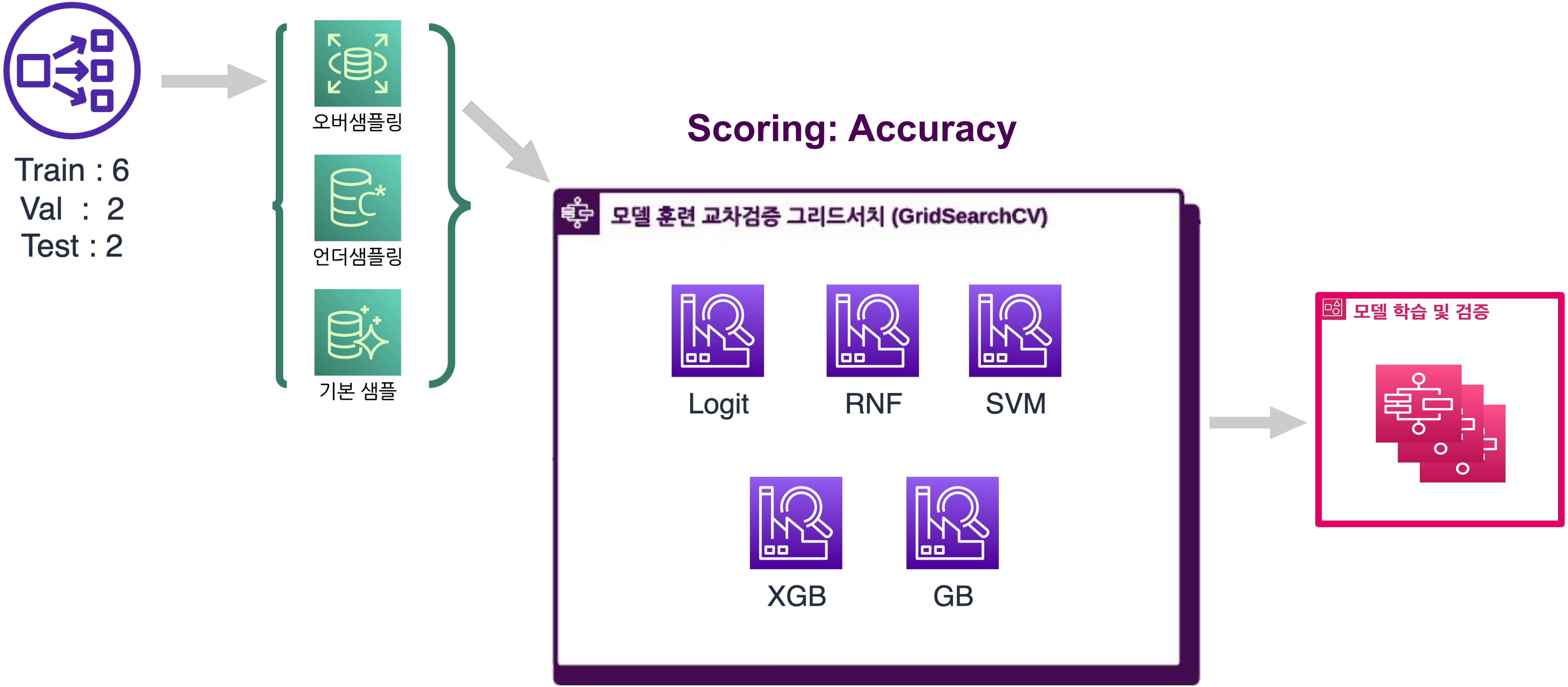
Y: Wine Quality

4 | 5 | 6 | 7 | 8

Multi Classification Workflow



Multi Classification Workflow



Train : 6
Val : 2
Test : 2

오버샘플링

언더샘플링

기본 샘플

Scoring: Accuracy

모델 훈련 교차검증 그리드서치 (GridSearchCV)

Logit

RNF

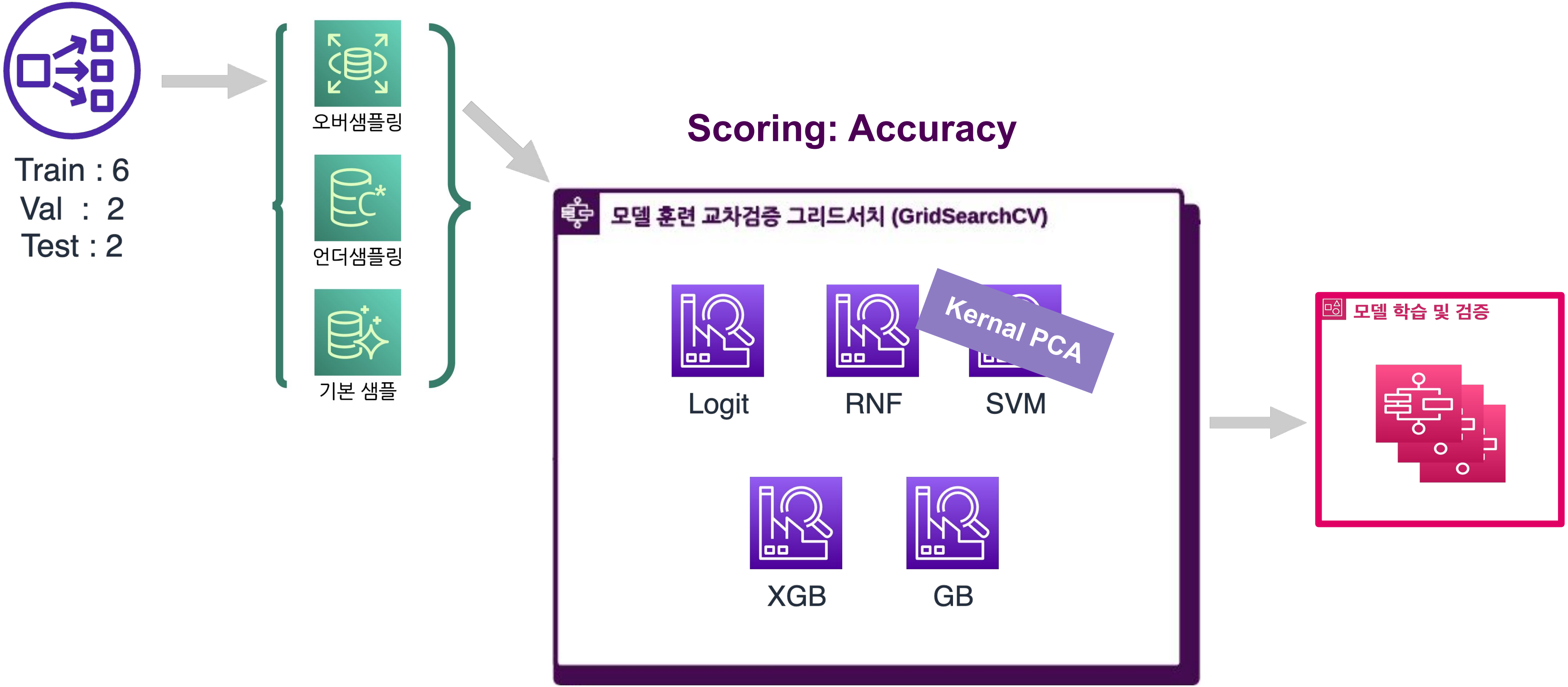
SVM

XGB

GB

모델 학습 및 검증

Multi Classification Workflow



Train : 6
Val : 2
Test : 2

오버샘플링

언더샘플링

기본 샘플

Scoring: Accuracy

모델 훈련 교차검증 그리드서치 (GridSearchCV)

Logit

RNF

SVM

Kernal PCA

XGB

GB

모델 학습 및 검증

Logistic Regression (oversampling)

Confusion Matrix:

```
                 pred
     [  26   15    0    3    5 ]
     [  94  174   38   30   63 ]
real [  63  141   69  157  134]
     [  14   23   16   96   79 ]
     [   3    4    2   19   16 ]
```

Total Accuracy:
0.2967

Class 4
Accuracy: 0.5306
Precision: 0.13
Recall: 0.5306
f1: 0.2088

Class 5
Accuracy: 0.436
Precision: 0.4873
Recall: 0.436
f1: 0.4603

Class 6
Accuracy: 0.1223
Precision: 0.552
Recall: 0.1223
f1: 0.2002

Class 7
Accuracy: 0.421
Precision: 0.3147
Recall: 0.4210
f1: 0.3602

Class 8
Accuracy: 0.3636
Precision: 0.0538
Recall: 0.3636
f1: 0.0938

Random Forest (oversampling)

Confusion Matrix:

```
               pred
     [ 8    20    17    3    0 ]
     [ 6   296   104    9    0 ]
real [ 3   108   383   85    5 ]
     [ 0    10    82  119    3 ]
     [ 0     0     9   17   12 ]
```

Total Accuracy:
0.6297

Class 5
Accuracy: 0.7132
Precision: 0.6833
Recall: 0.7518
f1: 0.7159

Class 7
Accuracy: 0.556
Precision: 0.6414
Recall: 0.5570
f1: 0.5962

Class 4
Accuracy: 0.1666
Precision: 0.4444
Recall: 0.1632
f1: 0.2388

Class 6
Accuracy: 0.6558
Precision: 0.6557
Recall: 0.7092
f1: 0.6814

Class 8
Accuracy: 0.3157
Precision: 0.7894
Recall: 0.3409
f1: 0.4761

Gradient Boost (oversampling)

Confusion Matrix:

```
                pred
     [  8    20    10    0    0  ]
     [ 10   292   128    3    1  ]
real [  4   109   437   25    1  ]
     [  0     4    98  107    0  ]
     [  0     0    14   13    9  ]
```

Total Accuracy:
0.6597

Class 4
Accuracy: 0.2105
Precision: 0.3636
Recall: 0.2105
f1: 0.2666

Class 5
Accuracy: 0.6728
Precision: 0.6870
Recall: 0.6728
f1: 0.6798

Class 6
Accuracy: 0.7586
Precision: 0.6360
Recall: 0.7586
f1: 0.6920

Class 7
Accuracy: 0.5119
Precision: 0.7229
Recall: 0.5119
f1: 0.5994

Class 8
Accuracy: 0.25
Precision: 0.8181
Recall: 0.25
f1: 0.3829

XGBoost (orign)

Confusion Matrix:

```
                pred
       [ 1    31    17    0    0 ]
       [ 2   274   121    2    0 ]
real   [ 0    96   439   29    0 ]
       [ 0     9   117  102    0 ]
       [ 0     2    20    8   14 ]
```

Total Accuracy:
0.6464

Class 5
Accuracy: 0.6867
Precision: 0.6650
Recall: 0.6867
f1: 0.6757

Class 7
Accuracy: 0.4473
Precision: 0.7234
Recall: 0.4473
f1: 0.5528

Class 4
Accuracy: 0.0204
Precision: 0.3333
Recall: 0.0204
f1: 0.0384

Class 6
Accuracy: 0.7783
Precision: 0.6148
Recall: 0.7783
f1: 0.6870

Class 8
Accuracy: 0.3181
Precision: 1.0
Recall: 0.3181
f1: 0.4827

KPCA_SVC (orign)

Confusion Matrix:

```
              pred
     [  3    1    44    0    0 ]
     [  0  129   286    0    0 ]
real [  0   16   567    1    0 ]
     [  0    1   149   64    0 ]
     [  0    0    25    1   12 ]
```

Total Accuracy:
0.5966

Class 4
Accuracy: 0.0625
Precision: 1.0
Recall: 0.0625
f1: 0.1176

Class 5
Accuracy: 0.3108
Precision: 0.8775
Recall: 0.3108
f1: 0.4590

Class 6
Accuracy: 0.9708
Precision: 0.5294
Recall: 0.9708
f1: 0.6851

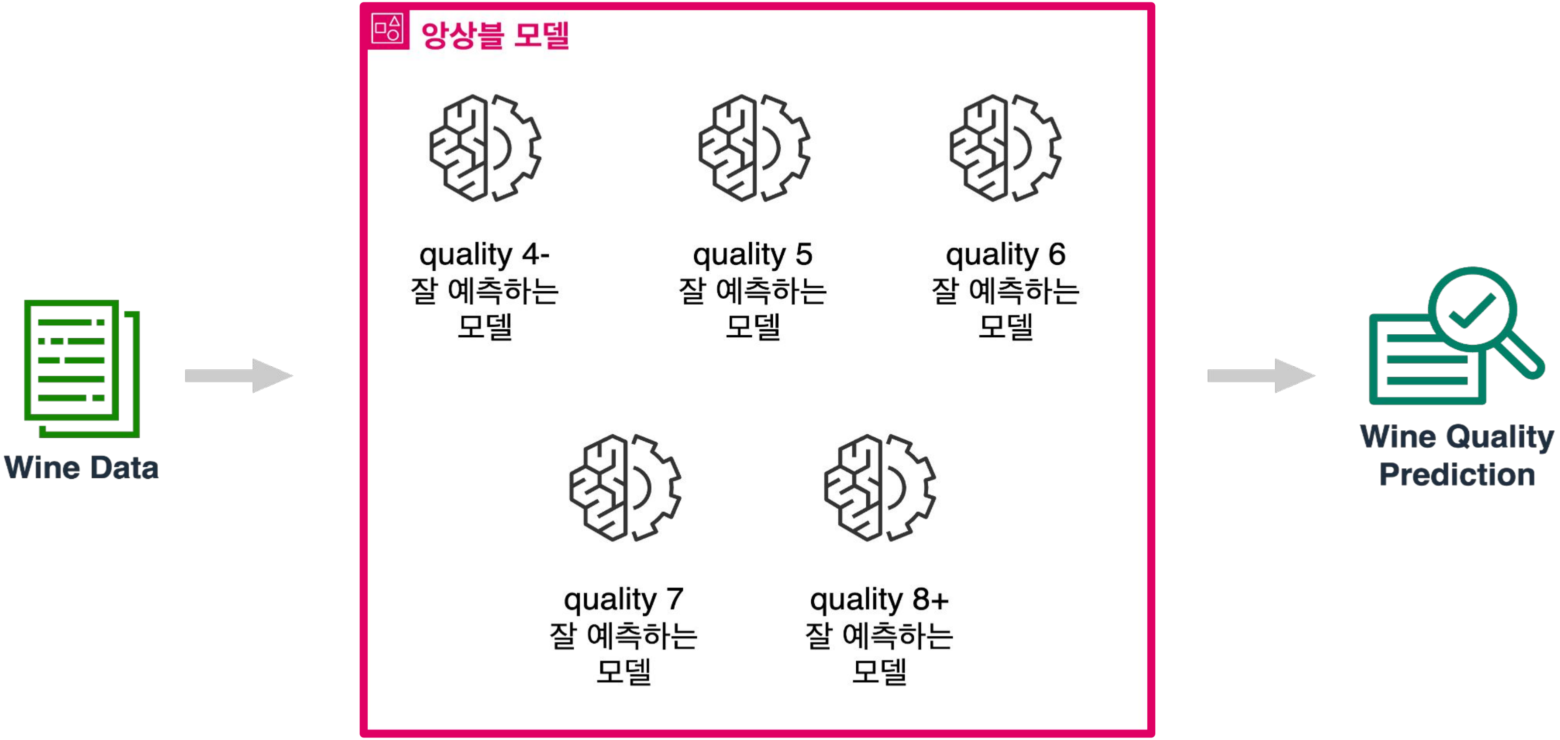
Class 7
Accuracy: 0.2990
Precision: 0.9696
Recall: 0.2990
f1: 0.4571

Class 8
Accuracy: 0.3157
Precision: 1.0
Recall: 0.3157
f1: 0.4799

모델 성능 비교 (Accuracy)

	Logistic Regression (over)	Random Forest (over)	Gradient Boost (over)	XGBoost (orign)	KPCA-SVM (orign)
Total	0.2967	0.6297	0.6597	0.6464	0.5966
quality 4 -	0.5306	0.1666	0.2105	0.0204	0.0625
quality 5	0.436	0.7132	0.6728	0.6867	0.3108
quality 6	0.1223	0.6558	0.7586	0.7783	0.9708
quality 7	0.421	0.556	0.5119	0.4473	0.2990
quality 8 +	0.3636	0.3157	0.25	0.3181	0.3157

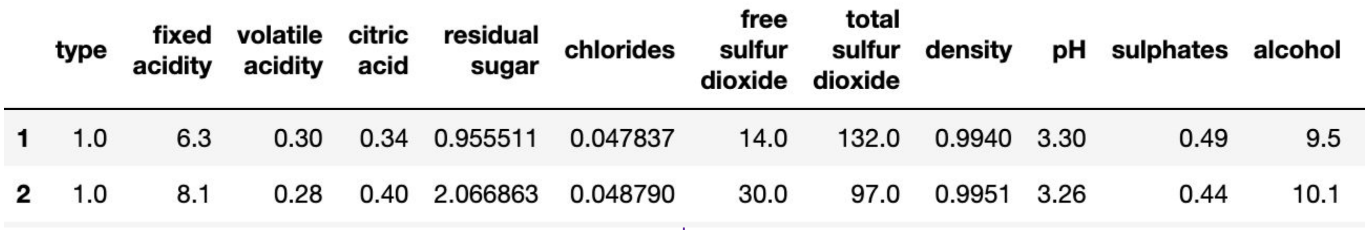
Model Essemble



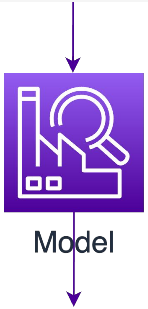
Trial 2.
Binary classification

Binary Classification

X: Wine Features



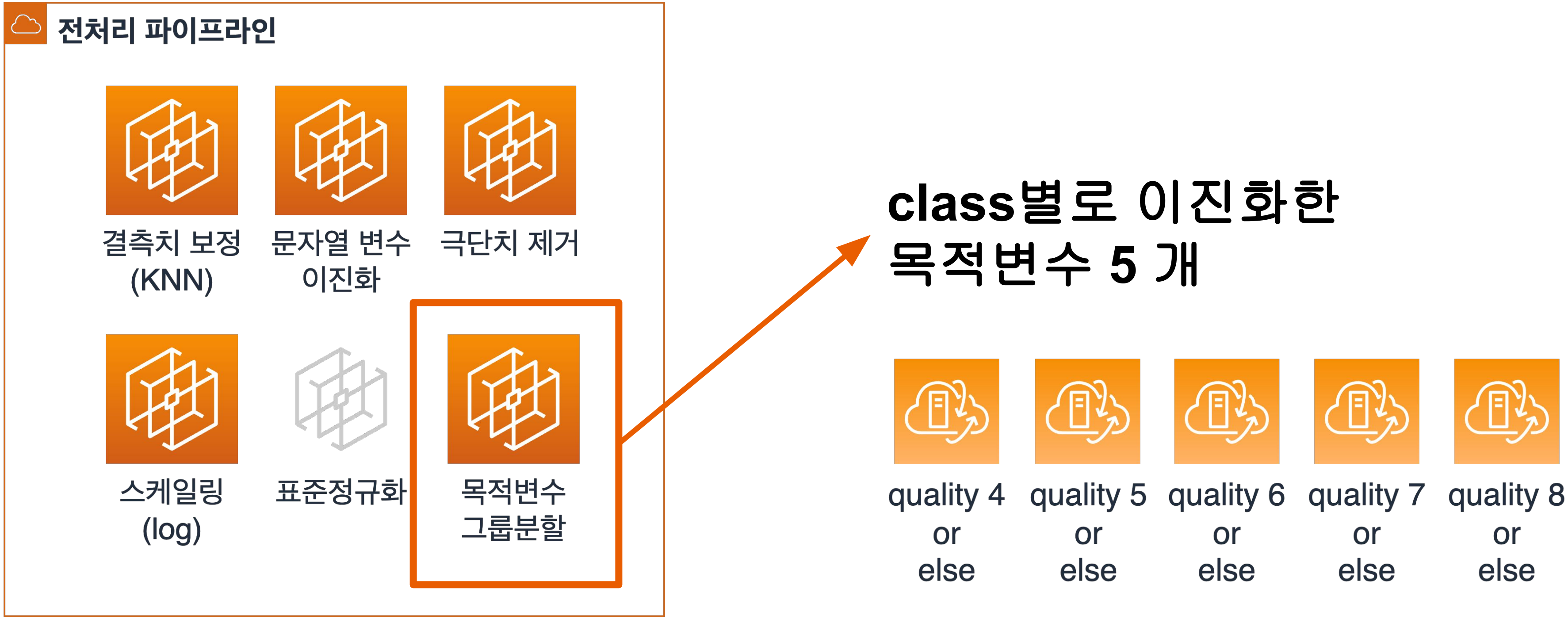
	type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
1	1.0	6.3	0.30	0.34	0.955511	0.047837	14.0	132.0	0.9940	3.30	0.49	9.5
2	1.0	8.1	0.28	0.40	2.066863	0.048790	30.0	97.0	0.9951	3.26	0.44	10.1



Y_4: Wine Quality

4 or else

Binary Classification Workflow



전처리 파이프라인

결측치 보정 (KNN)

문자열 변수 이진화

극단치 제거

스케일링 (log)

표준정규화

목적변수 그룹분할

class별로 이진화한 목적변수 5 개

quality 4 or else

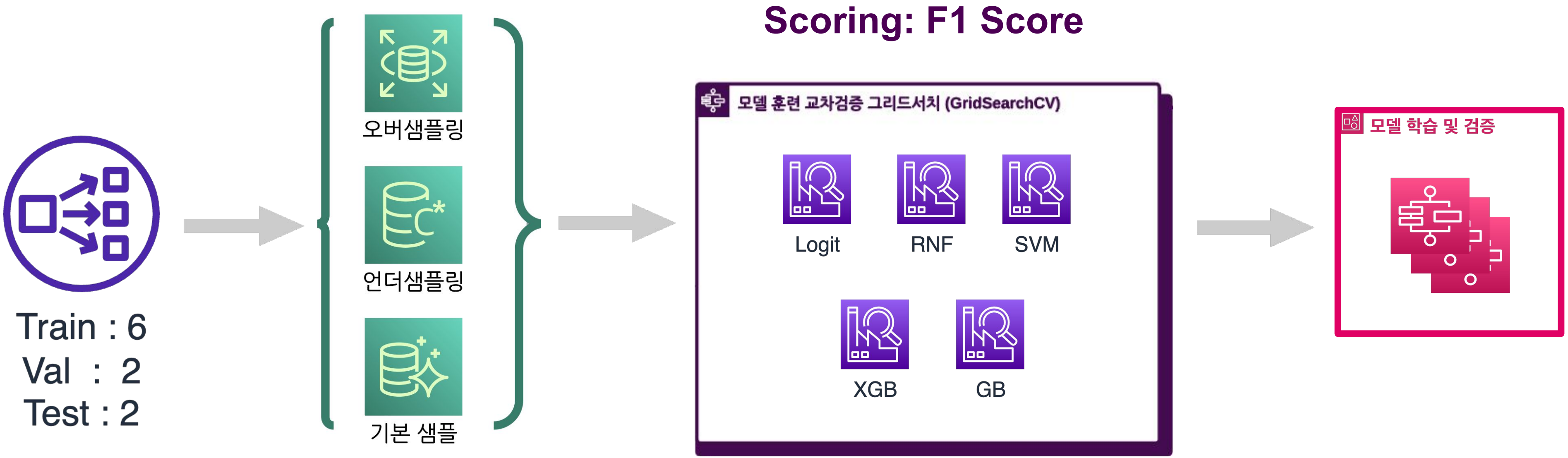
quality 5 or else

quality 6 or else

quality 7 or else

quality 8 or else

Binary Classification Workflow



Train : 6
Val : 2
Test : 2

오버샘플링

언더샘플링

기본 샘플

Scoring: F1 Score

모델 훈련 교차검증 그리드서치 (GridSearchCV)

Logit

RNF

SVM

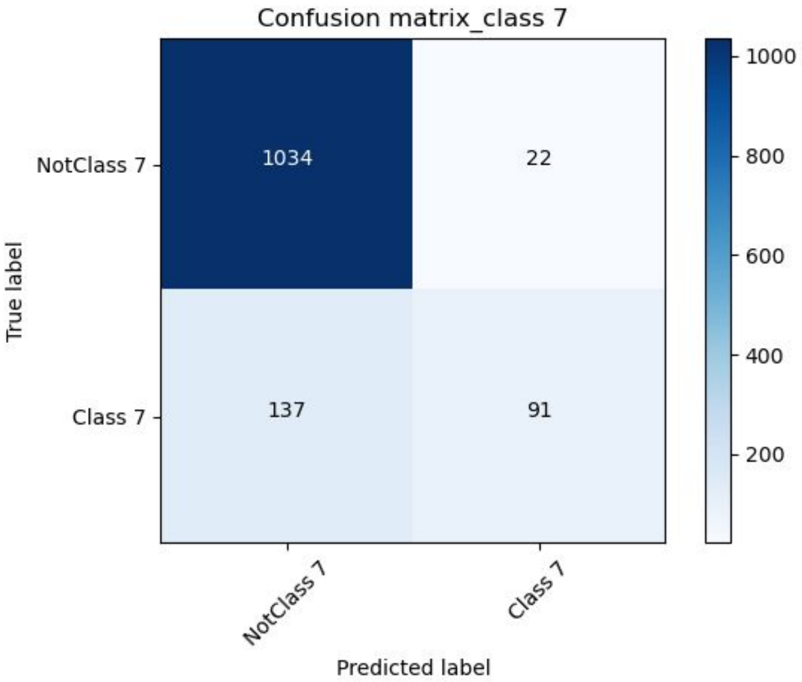
XGB

GB

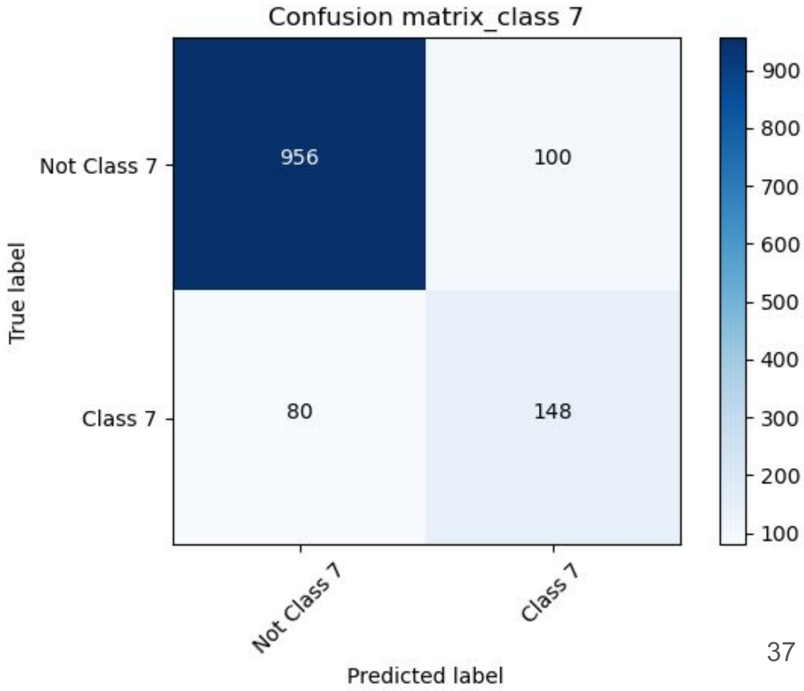
모델 학습 및 검증

Random Forest (class 7)

Scoring: Accuracy

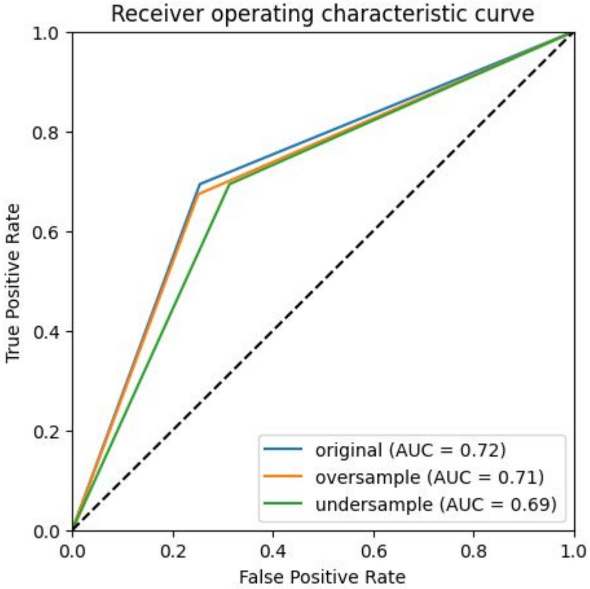


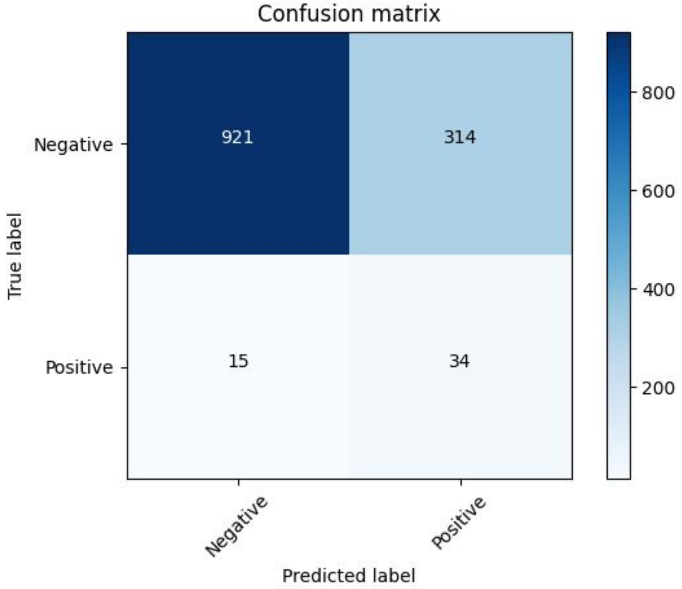
Scoring: F1



Logistic Regression (class 4)

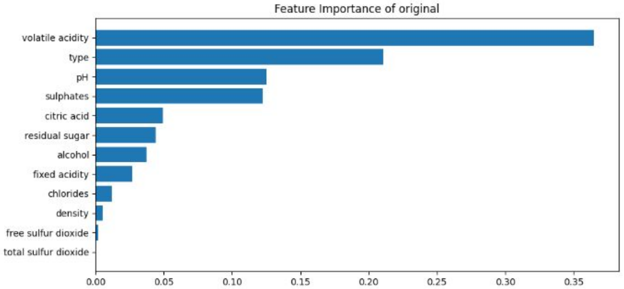
	Accuracy	Precision	Recall	F1-score	AUC
original	0.7438	0.0977	0.6939	0.1713	0.7198
oversample	0.7461	0.0962	0.6735	0.1684	0.7112
undersample	0.6869	0.0808	0.6939	0.1447	0.6903

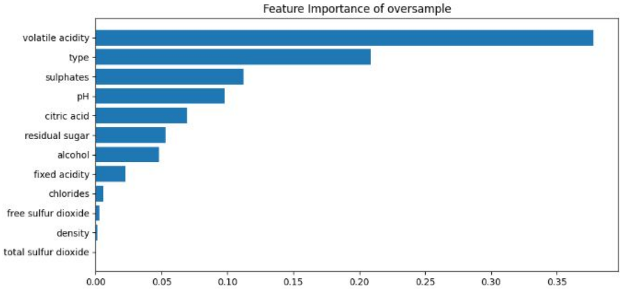


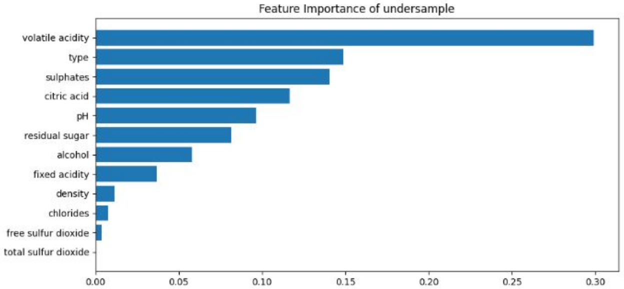


Logistic Regression (class 4)

	Accuracy	Precision	Recall	F1-score	AUC
original	0.7438	0.0977	0.6939	0.1713	0.7198
oversample	0.7461	0.0962	0.6735	0.1684	0.7112
undersample	0.6869	0.0808	0.6939	0.1447	0.6903

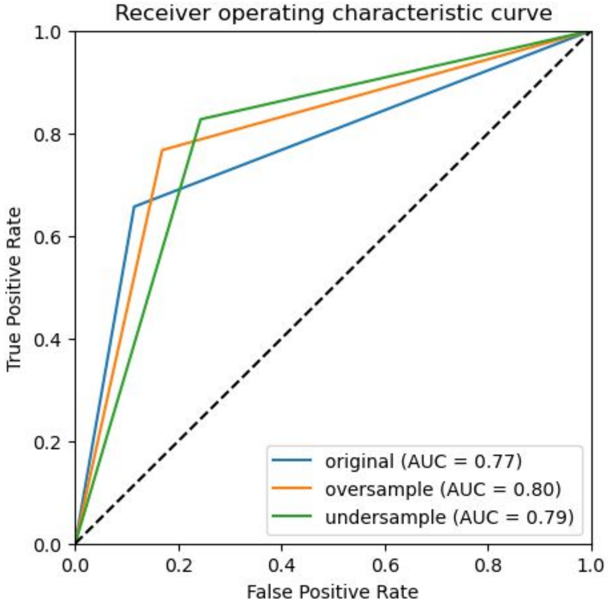

Feature Importance of original

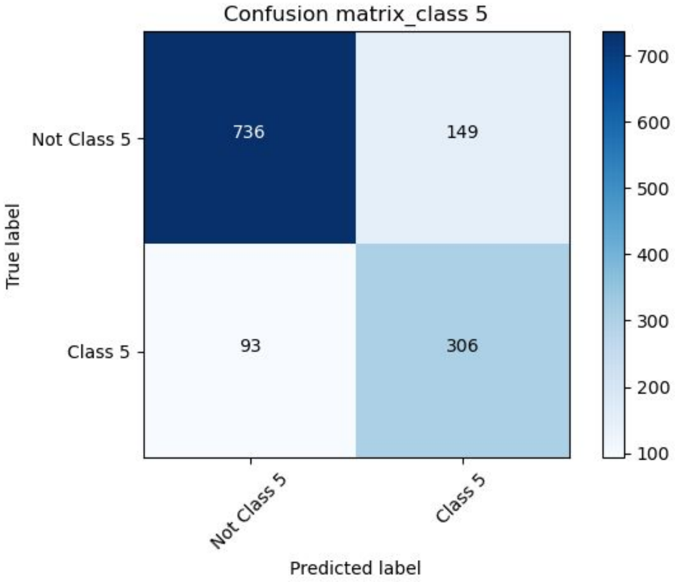

Feature Importance of oversample


Feature Importance of undersample

Random Forest (class 5)

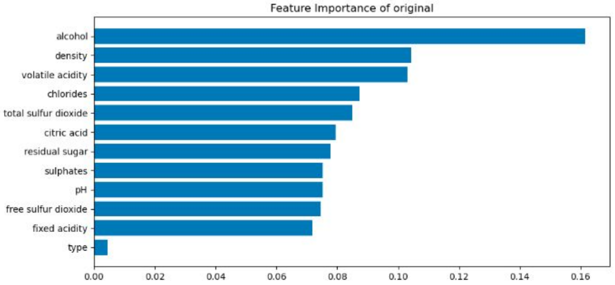
	Accuracy	Precision	Recall	F1-score	AUC
original	0.8146	0.7218	0.6566	0.6877	0.7713
oversample	0.8115	0.6725	0.7669	0.7166	0.7993
undersample	0.7788	0.6055	0.8271	0.6992	0.7921

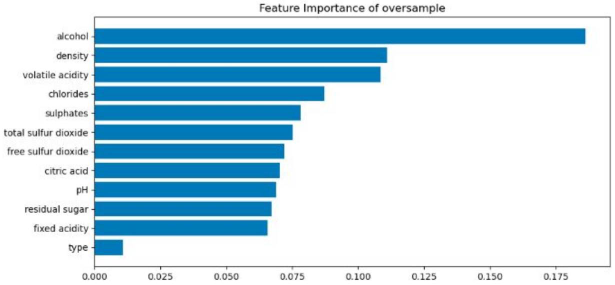


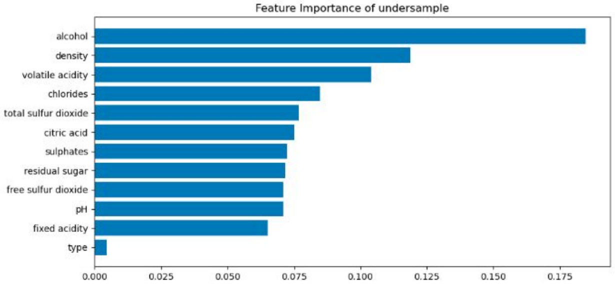


Random Forest (class 5)

	Accuracy	Precision	Recall	F1-score	AUC
original	0.8146	0.7218	0.6566	0.6877	0.7713
oversample	0.8115	0.6725	0.7669	0.7166	0.7993
undersample	0.7788	0.6055	0.8271	0.6992	0.7921

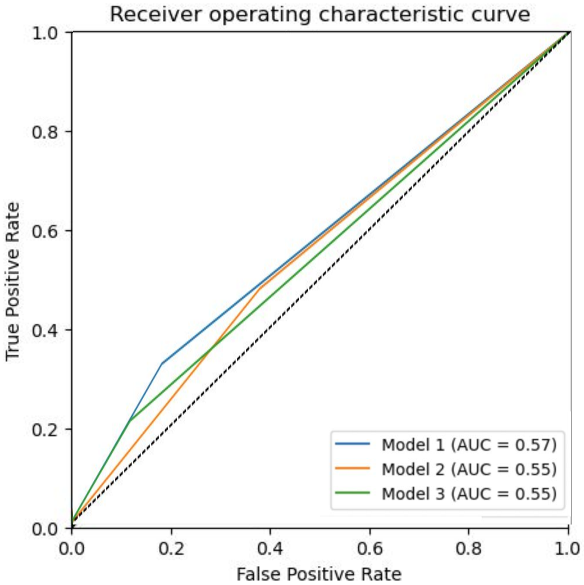


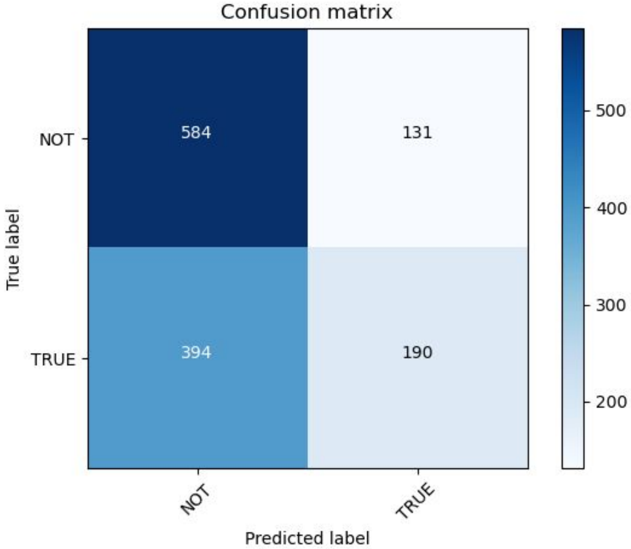




KPCA-SVC (class 6)

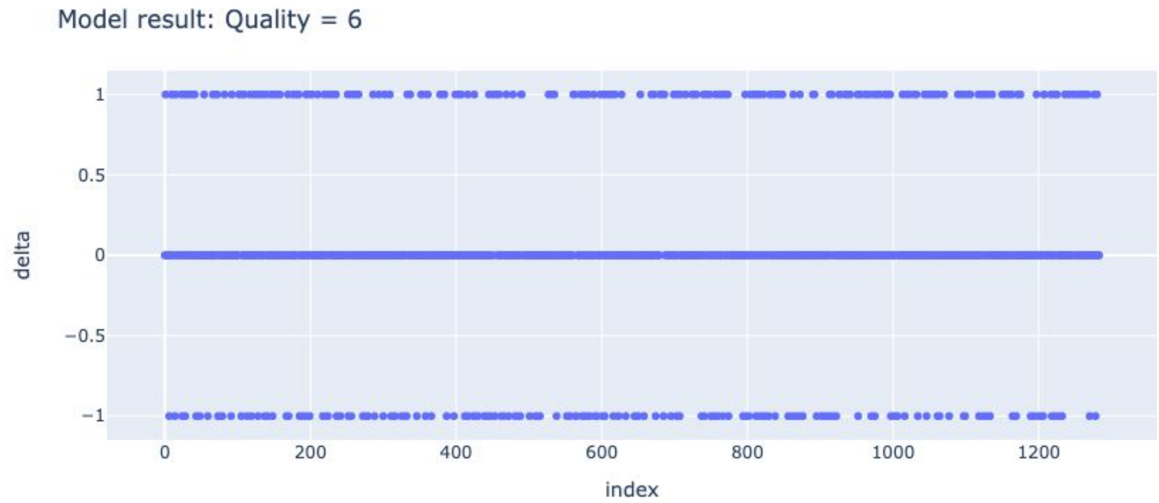
	Accuracy	Precision	Recall	F1-score	AUC
original	0.5958	0.5919	0.3253	0.4199	0.5711
oversample	0.5566	0.5073	0.4777	0.4921	0.5494
undersample	0.5789	0.5885	0.2106	0.3102	0.5452





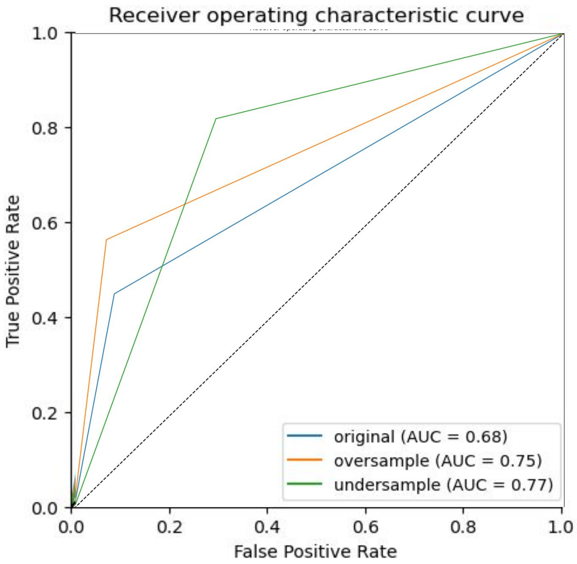
KPCA-SVC (class 6)

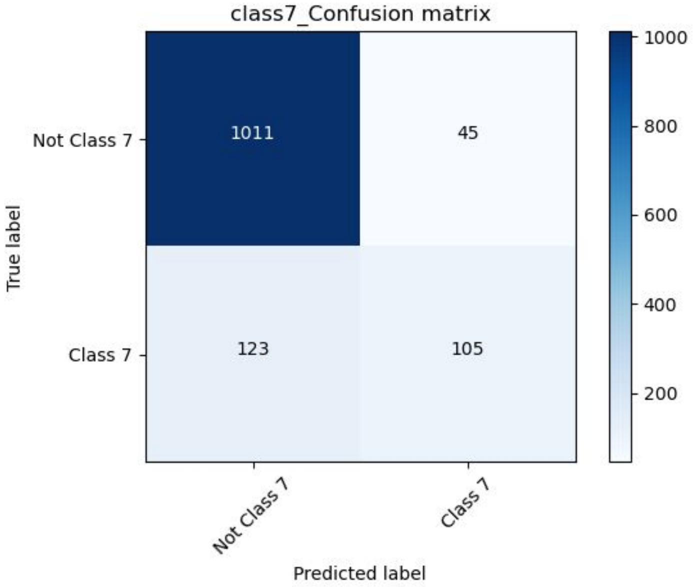
	Accuracy	Precision	Recall	F1-score	AUC
original	0.5958	0.5919	0.3253	0.4199	0.5711
oversample	0.5566	0.5073	0.4777	0.4921	0.5494
undersample	0.5789	0.5885	0.2106	0.3102	0.5452



Gradient Boost (class 7)

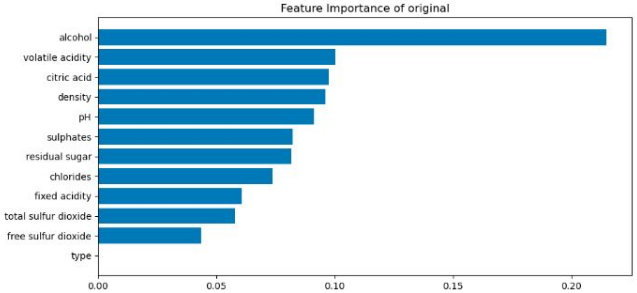
	Accuracy	Precision	Recall	F1-score	AUC
original	0.8692	0.7000	0.4605	0.5556	0.7090
oversample	0.8575	0.6154	0.5263	0.5674	0.7276
undersample	0.7360	0.3856	0.8202	0.5245	0.7690

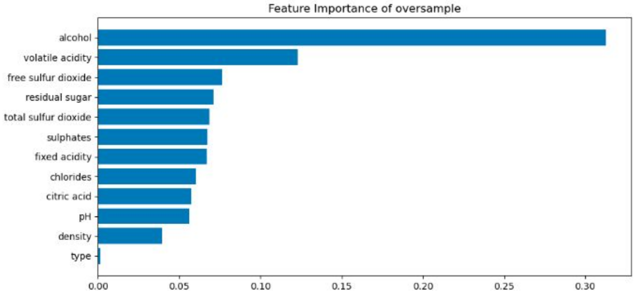


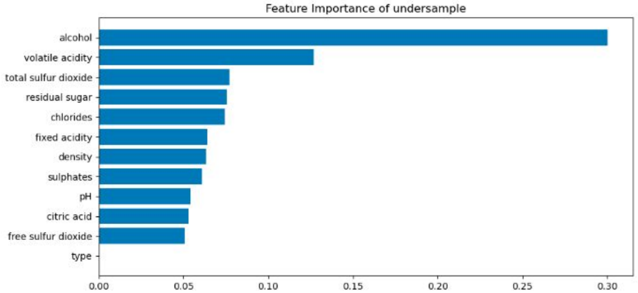


Gradient Boost (class 7)

	Accuracy	Precision	Recall	F1-score	AUC
original	0.8692	0.7000	0.4605	0.5556	0.7090
oversample	0.8575	0.6154	0.5263	0.5674	0.7276
undersample	0.7360	0.3856	0.8202	0.5245	0.7690

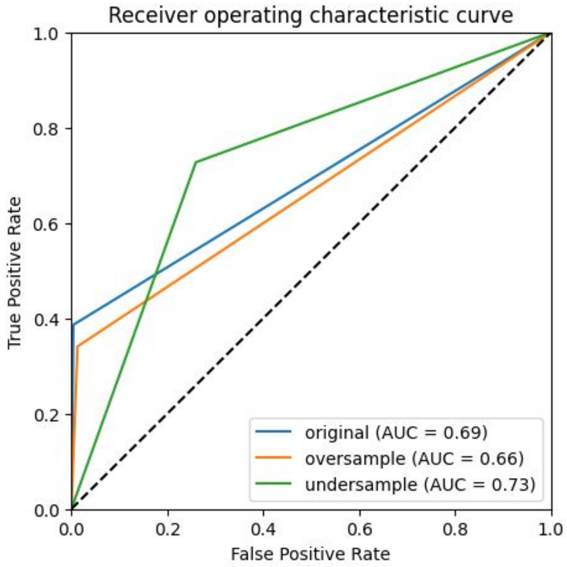


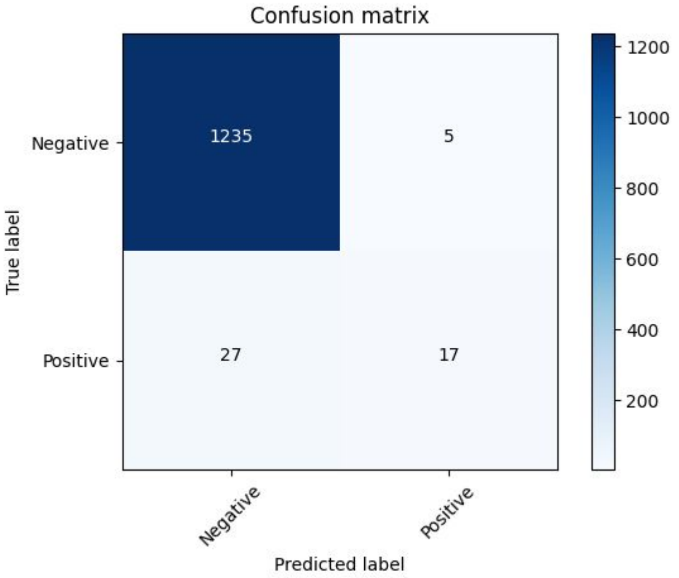




XGBoost (class 8)

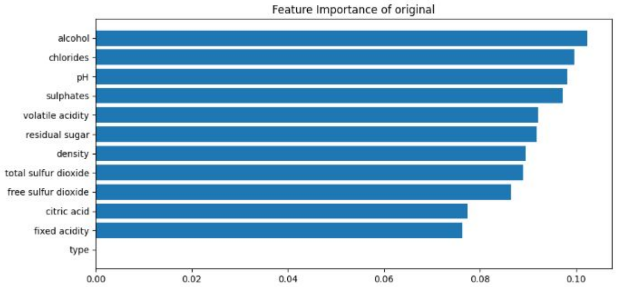
	Accuracy	Precision	Recall	F1-score	AUC
original	0.9751	0.7727	0.3864	0.5152	0.6912
oversample	0.965	0.4839	0.3409	0.4	0.664
undersample	0.7399	0.0904	0.7273	0.1608	0.7338

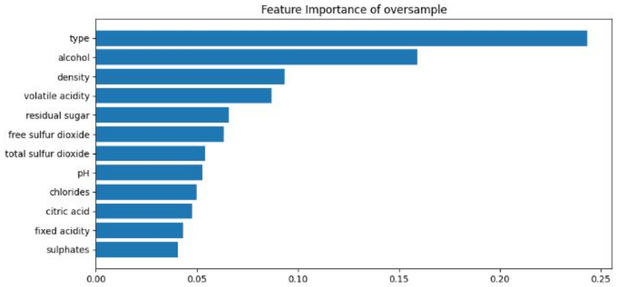


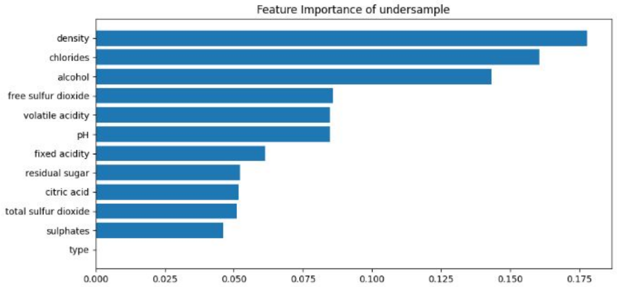


XGBoost (class 8)

	Accuracy	Precision	Recall	F1-score	AUC
original	0.9751	0.7727	0.3864	0.5152	0.6912
oversample	0.965	0.4839	0.3409	0.4	0.664
undersample	0.7399	0.0904	0.7273	0.1608	0.7338





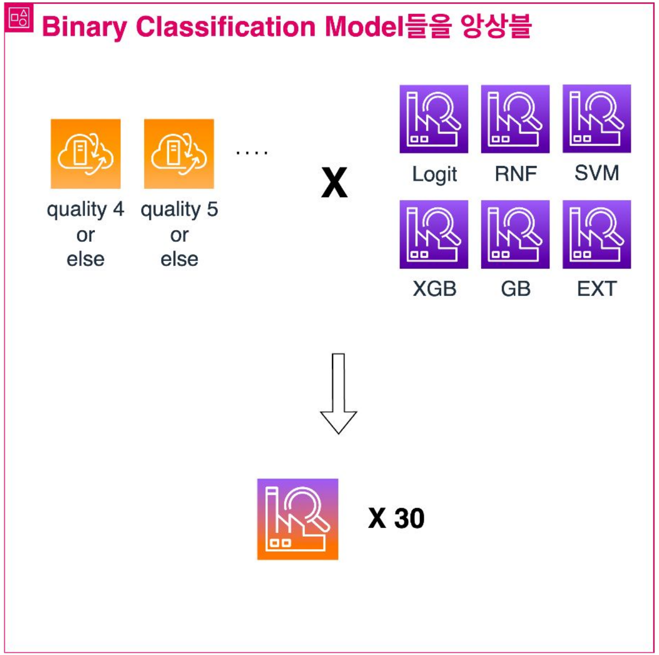


Ensemble Model

VotingClassifier | StackingClassifier

Model Ensemble

Trial 2


Binary Classification Model들을 앙상블

quality 4 or else

quality 5 or else

....

X

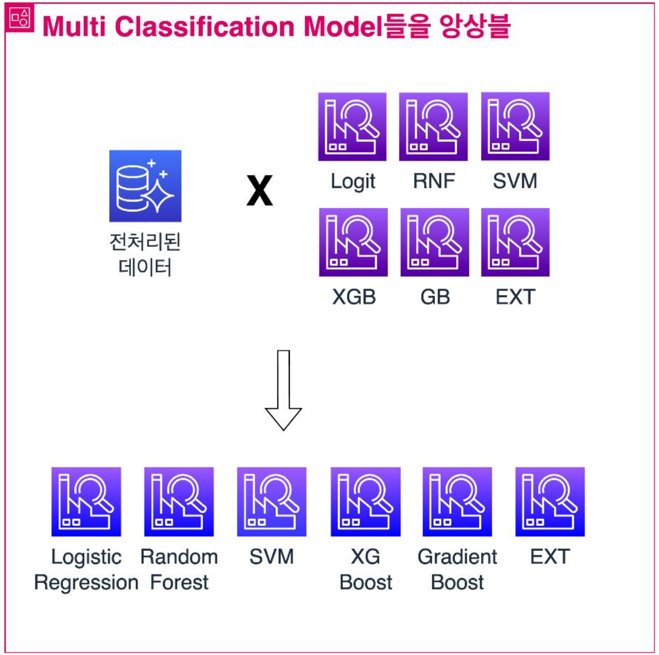
Logit RNF SVM

XGB GB EXT

X 30

VotingClassifier

Trial 1


Multi Classification Model들을 앙상블

전처리된 데이터

X

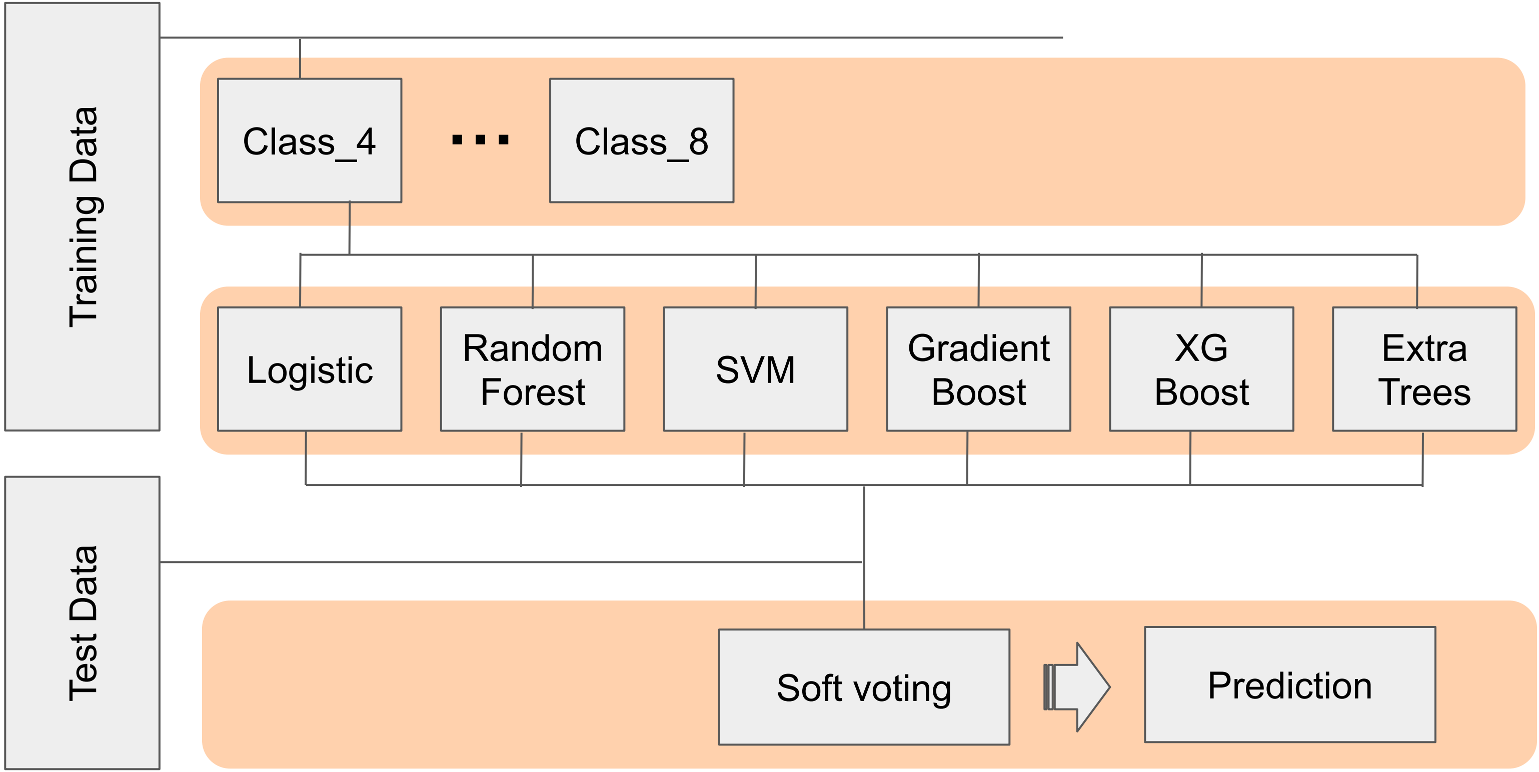
Logit RNF SVM

XGB GB EXT

Logistic Regression, Random Forest, SVM, XG Boost, Gradient Boost, EXT

StackingClassifier

VotingClassifier



Training Data

Class_4 ... Class_8

Logistic

Random Forest

SVM

Gradient Boost

XG Boost

Extra Trees

Test Data

Soft voting

Prediction

[scale]
ordinal
to
binary

[fitting]
original
over
under

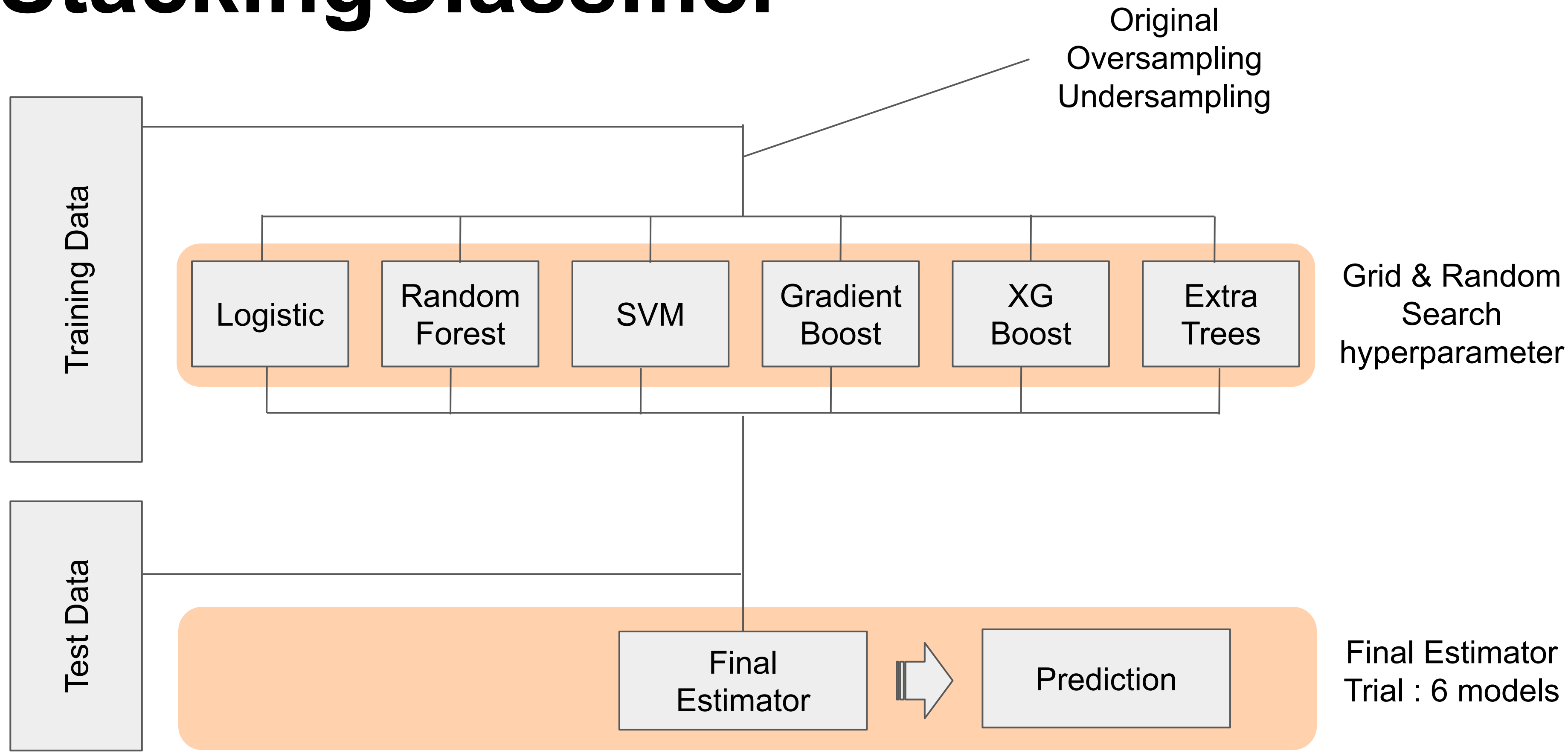
[weight]
uniformly
f1-score
precision
best

VotingClassifier

index weight	Accuracy	Precision	Recall	F1-score
uniformly	0.5522	0.5412	0.5522	0.5426
f1-score	0.5428	0.5473	0.5428	0.5361
precision	0.5405	0.5442	0.5405	0.5297
best	0.5506	0.5763	0.5506	0.5478

Poor prediction

StackingClassifier



StackingClassifier

		Accuracy	**Precision**	**Recall**	**F1-score**
log	orign	0.6838	0.6936	0.6838	0.6725
	over	0.6745	0.6761	0.6745	0.6678
	under	0.4455	0.5281	0.4455	0.4538
rnf	orign	0.6776	0.688	0.6776	0.6675
	over	0.6628	0.6728	0.6628	0.6487
	under	0.4587	0.549	0.4587	0.4755
svm	orign	0.6854	0.7239	0.6854	0.6678
	over	0.6783	0.6783	0.6783	0.6742
	under	0.4587	0.5283	0.4587	0.4635

StackingClassifier

		Accuracy	Precision	Recall	F1-score
xgb	orign	0.6745	0.6897	0.6745	0.6657
	over	0.655	0.6899	0.655	0.6362
	under	0.3894	0.5179	0.3894	0.4098
gdb	orign	0.6838	0.6994	0.6838	0.6766
	over	0.641	0.676	0.641	0.6259
	under	0.4073	0.5126	0.4073	0.4244
ext	orign	0.6822	0.6969	0.6822	0.6723
	over	0.6846	0.6933	0.6846	0.6752
	under	0.4478	0.5438	0.4478	0.4584

결론

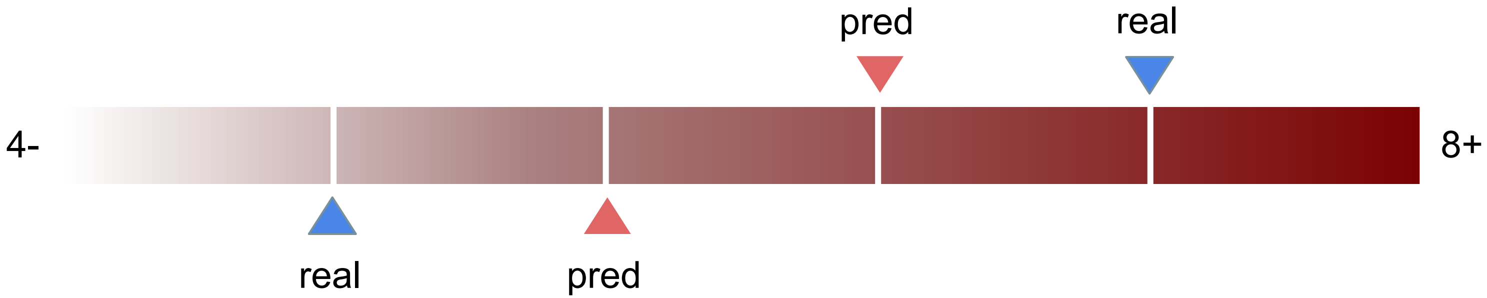
- Quality grade
- Result
- Unsupervised learning

Quality

PROBLEM β

예측등급 < 실제등급

- 적절한 가격산정 실패로 인한 판매손실 가능성



PROBLEM α

예측등급 > 실제등급

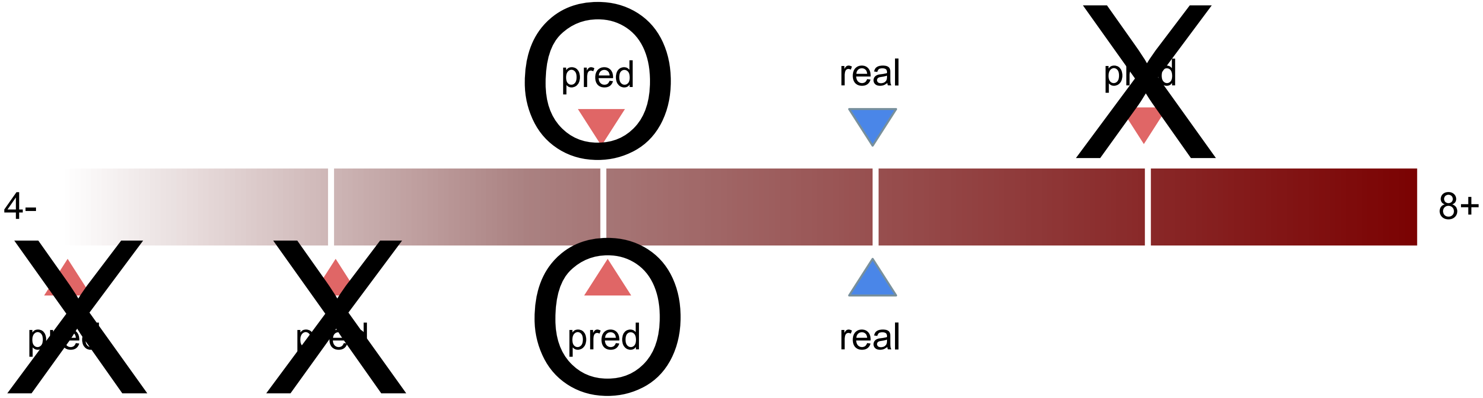
- 와인 산지 평판 하락 가능성
- 소비자 피해 가능성

Quality

PROBLEM α

예측등급 > 실제등급

예측등급이 실제등급보다 낮은 범위



PROBLEM β

예측등급 < 실제등급

1등급 차까지만

Quality

Accurate

+Tolerance

Prediction

Observed

	4-	5	6	7	8+
4-	5	34	15	0	0
5	3	286	108	2	0
6	2	84	462	29	1
7	0	13	103	109	3
8+	0	0	14	12	15

(ExtraTreesClassifier, oversampling)

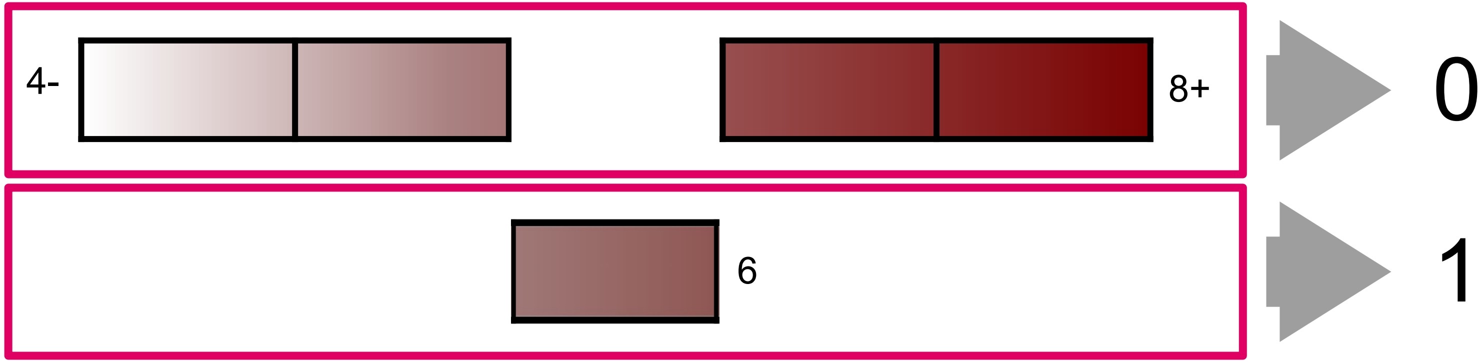
	4-	5	6	7	8+
4-	7	32	8	0	0
5	3	363	71	0	0
6	3	153	381	1	2
7	0	19	121	75	1
8+	0	1	25	3	15

(StackingClassifier, oversampling)

Quality

	Tutorial		StackingClassifier	
	(ExtraTrees, oversampling)		(SVM, original)	(XGB, oversampling)
	Accurate	Tolerance	Accurate	Tolerance
Accuracy	0.6746	0.7232	0.6854	0.8012
Precision	0.6746	0.8747	0.7239	0.9036
Recall	0.6746	0.8300	0.6854	0.8731
F1	0.6590	0.8431	0.6678	0.8822

Result - Binary

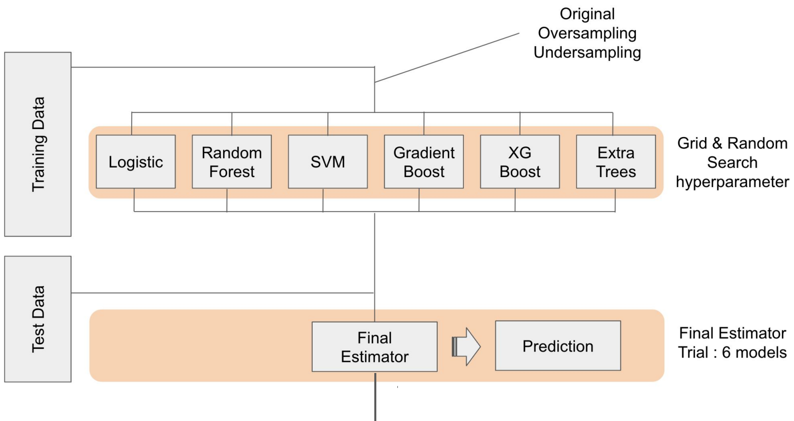


Loss

Expected Gain

이진화하면 순서정보 상실 > 이진화하면 모델별로 잘 예측하는 변수의 결과만 취합 가능 + 클래스별 over/undersampling 적용 가능

Result - Ordinal



Final Estimator : SVM			
Accuracy	**Precision**	**Recall**	**F1-score**
0.6854	0.7239	0.6854	0.6678

- **트리기반 모델의 성능이 전반적으로 우수한 이유**
    - 트리모델은 분기 기준에 따라 이산적인 결정을 내리므로 각 클래스의 상대적인 순서 파악 가능
    - 특히 Extratrees의 경우 데이터 불균형 문제를 가중치를 부여하는 방식으로 해결하여 클래스간 imbalance의 문제를 효과적으로 해결
    - 트리모델은 샘플별로 차이가 없었음

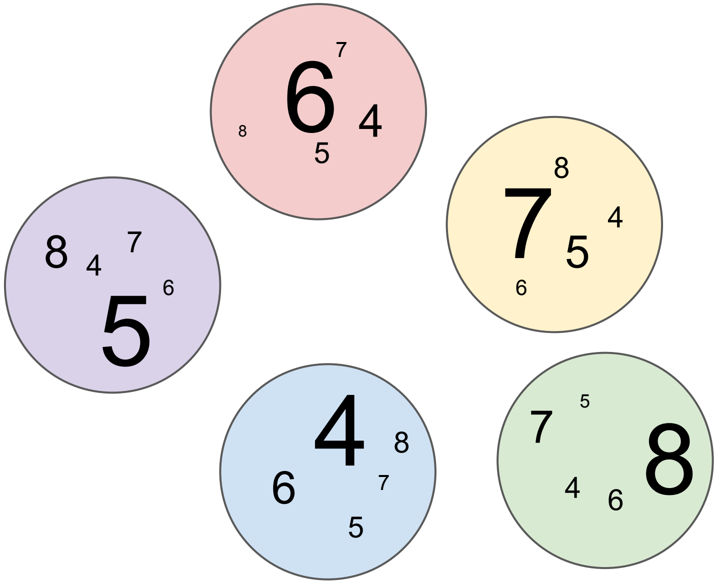
- **SVM**
    - svm은 가장 수가 많은 중간 등급에 대해서 예측을 진행하므로써 성능을 높이려고 시도한 것으로 보임
    - 즉, 가장 수가 적은, 그리고 극단의 등급(ordered class이므로) 에 대해서 decision boundary를 좁게 설정하여 자연스럽게 중간 등급으로 예측하는 오류가 있었을 것으로 보임

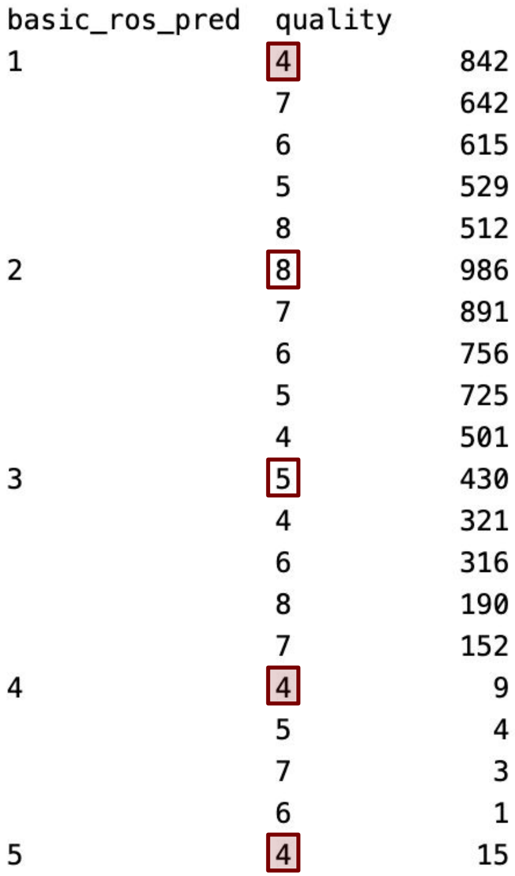
- **StackingClassifier에서 Final Estimator에 트리기반 외 SVM등 다른 모델들이 우수한 성능을 보였던 이유**
    - 멀티클래스의 분류가 아닌 기초모델들의 결과를 취합하는 역할의 수행이라는 점에서 멀티클래스 분류의 역할보다는 더 좋은 결과
    - Final estimator가 다루는 샘플은 사실상 6개이므로, 트리와 부스팅 모델은 샘플이 적은 상황에서는 svm보다 불리한 것으로 판단, svm이 최종 평가자인 모형이 좀 더 나은 결과를 도출한 것으로 보임

Unsupervised

K-Means Clustering

1. 5 clusters vs 15 clusters and re-clustering(by fcluster())
2. No Dimension Reduction vs PCA vs Kernel PCA
3. Origin / Oversampling / Undersampling Data





```
basic_ros_pred  quality
1               4          842
                7          642
                6          615
                5          529
                8          512
2               8          986
                7          891
                6          756
                5          725
                4          501
3               5          430
                4          321
                6          316
                8          190
                7          152
4               4            9
                5            4
                7            3
                6            1
5               4           15
```

감사합니다.