Classification metrics optimization: AUC and Kappa

In this video

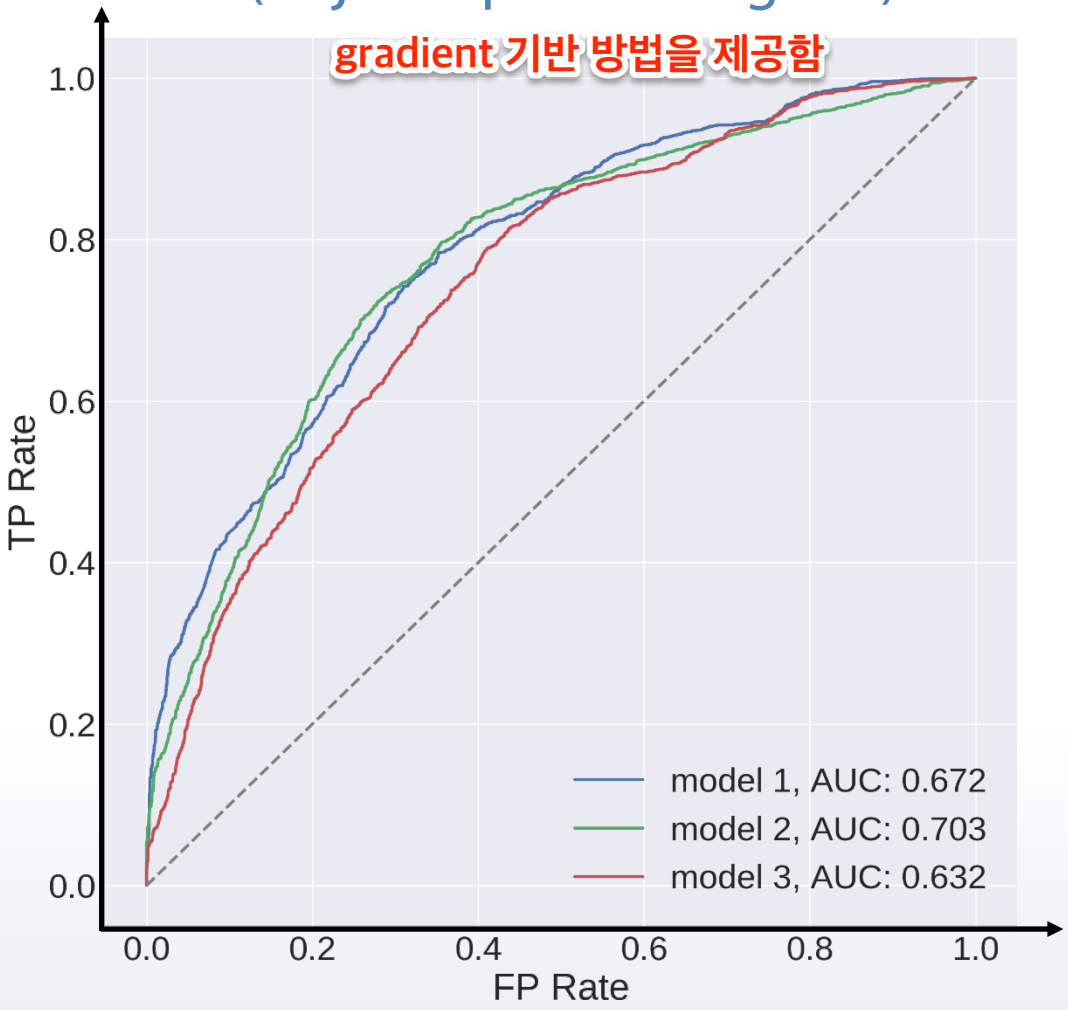
- Logloss
- Accuracy
- AUC
- (Quadratic weighted) Kappa

AUC (ROC)

How do you optimize it?

Run the right model

(or just optimize logloss)



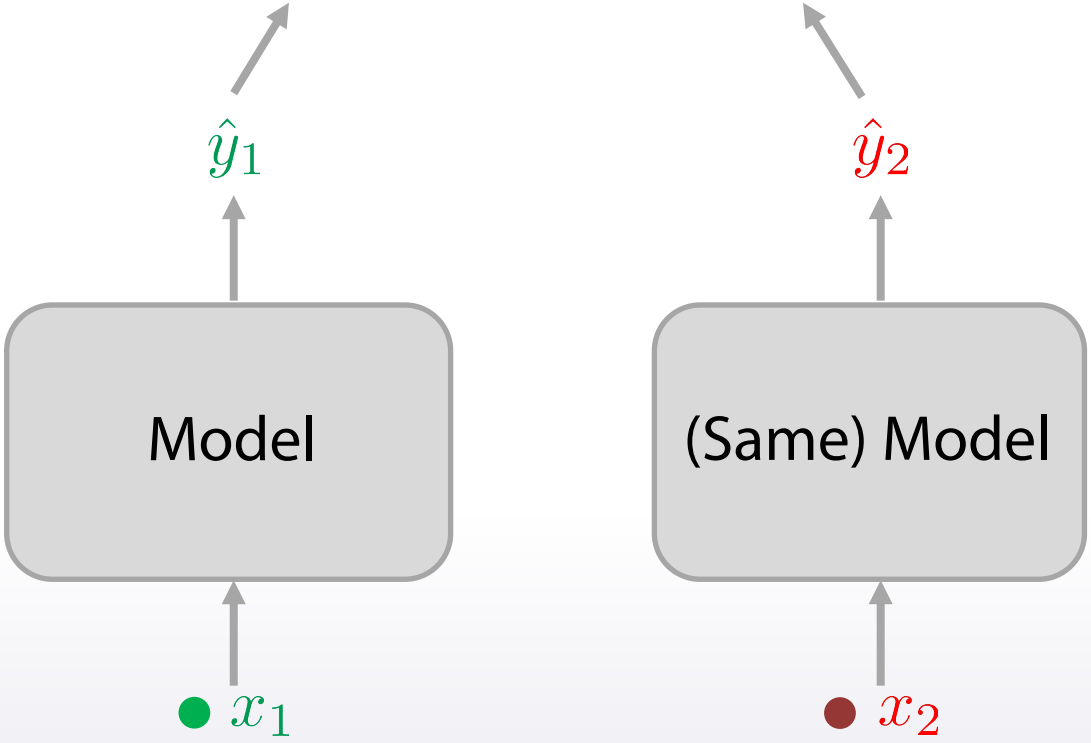
Pointwise loss

object 각각에 대한 loss 계산

$$\min \sum_{i}^{N} l_{point}(\hat{y}_i; y_i)$$

We want:

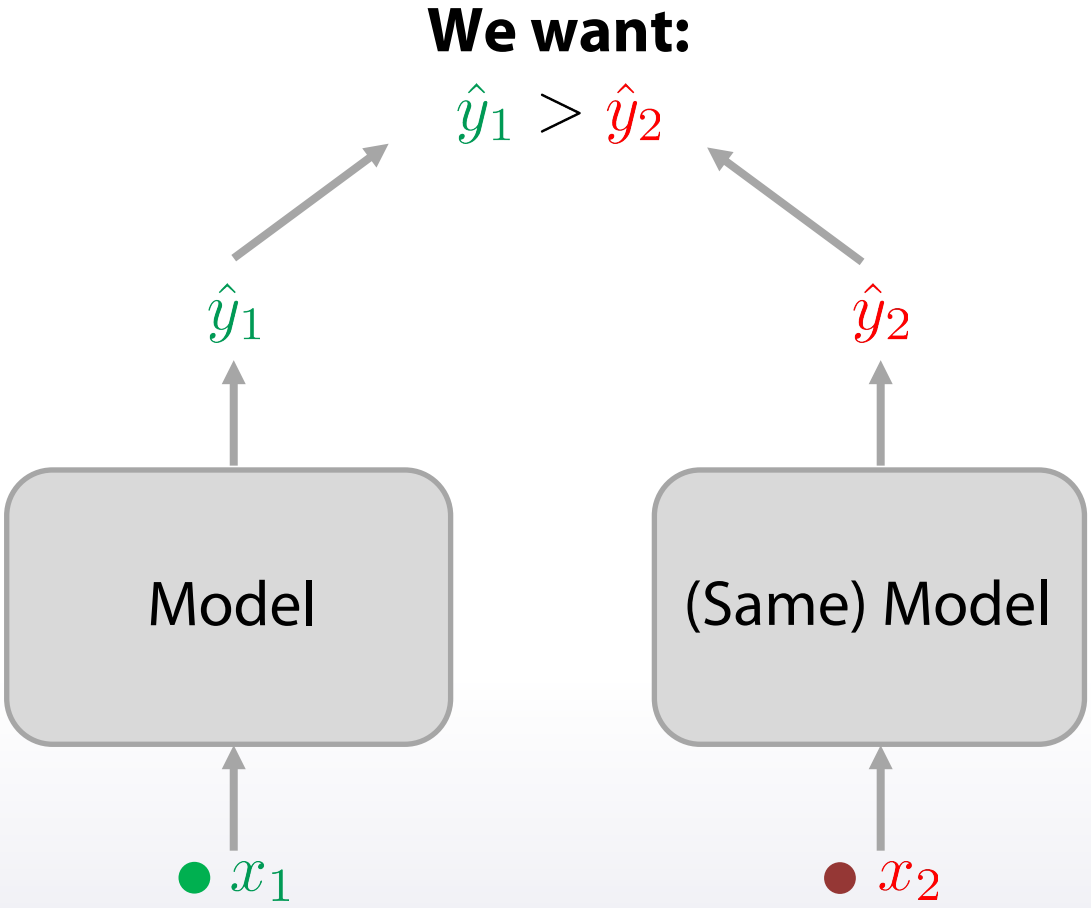
$\hat{y}_1 = 1$ $\hat{y}_2 = 0$



Pairwise loss

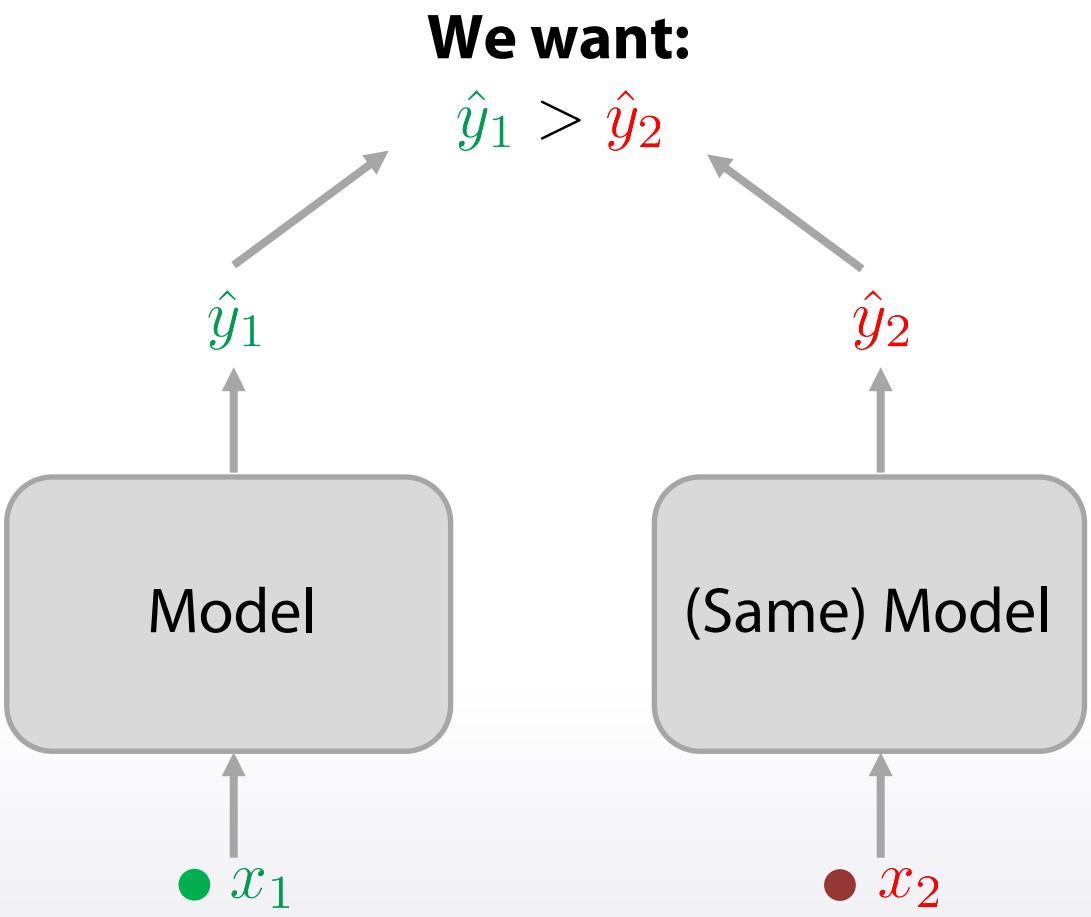
AUC는 순서대로 정렬했을 때 옳은 페어인 확률을 계산한 것
실질적으로 계산하기 어려움

$$\min \sum_{i}^{N} \sum_{j}^{N} l_{pair}(\hat{y}_i, \hat{y}_j; y_i, y_j)$$



Pairwise loss ordering 대신 logloss를 사용

$$\text{Loss} = -\frac{1}{N_0 N_2} \sum_{j:y_j=1}^{N_1} \sum_{i:y_i=0}^{N_0} \log(\text{prob}(\hat{y}_j - \hat{y}_i))$$



AUC

- **Tree-based**
  - `XGBoost, LightGBM`
  - ~~`sklearn.RandomForestClassifier`~~
- **Linear models**
  - ~~`sklearn. LogisticRegression`~~
  - ~~`sklearn.SGDRegressor`~~
  - ~~`Vowpal Wabbit`~~
- **Neural nets**
  - `PyTorch, Keras, TF` – not out of the box

Read the docs!

Quadratic weighted Kappa

How do you optimize it?

- **Optimize *MSE* and find right *thresholds***
  - *Simple*
- **Custom smooth loss for GBDT or neural nets**
  - Harder

MSE + tresholds

1. **Optimize MSE**

$$\text{Kappa}(y, \hat{y}) \approx 1 - \frac{\frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}{\text{hard to deal with part}} =$$

$$= 1 - \frac{\text{MSE}(y, \hat{y})}{\text{hard to deal with part}}$$

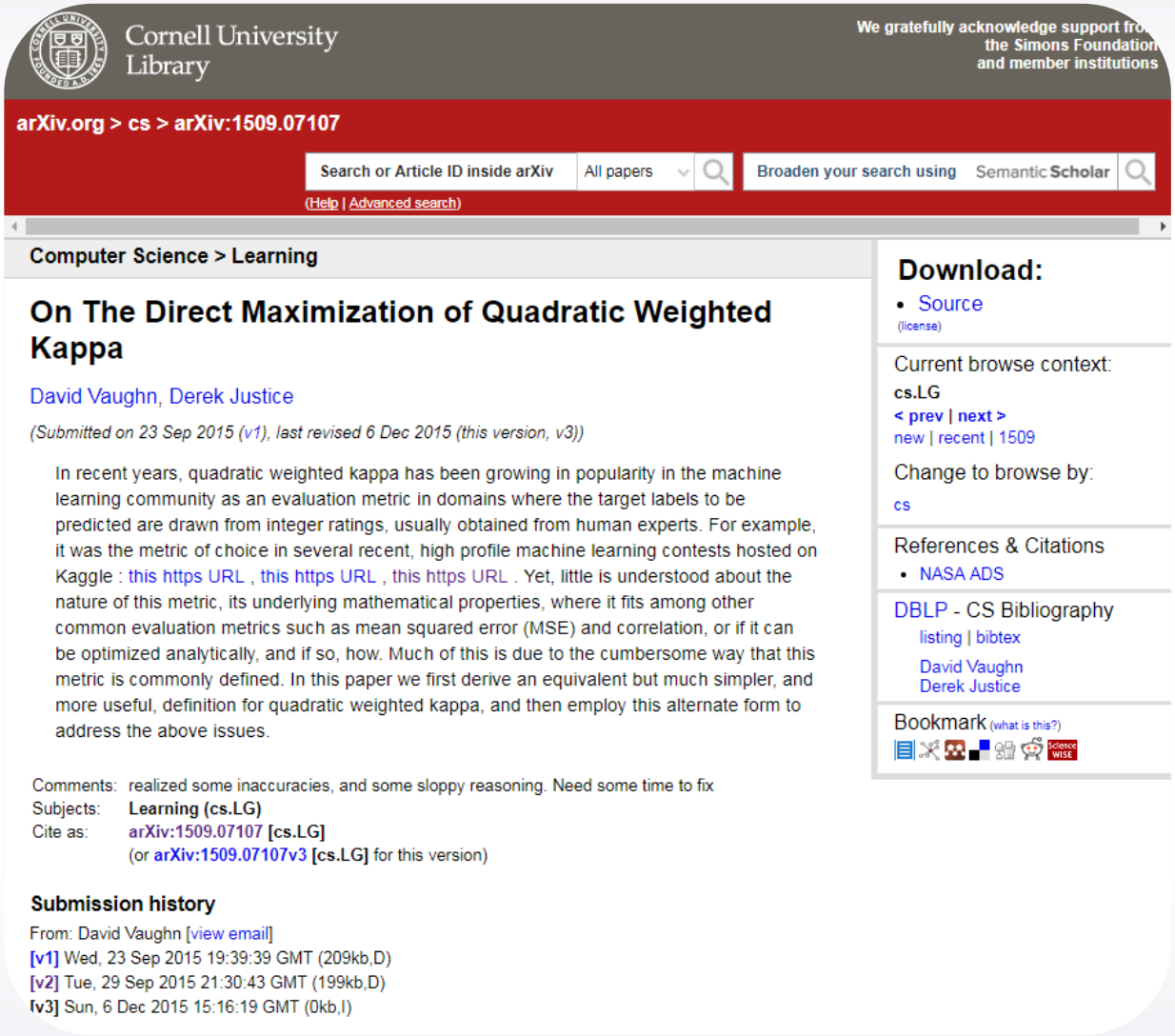
MSE와 비슷하지만 다른 값, 분모는 중요하지 않음

2. **Find right *thresholds***

분류 문제이므로 레이블로 사후 변환해야함

- Bad: `np.round(predictions)` 3.5 < x < 4.5 ---> 4
- Better: optimize thresholds grid search

Smooth loss 분모에 관한 설명



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On The Direct Maximization of Quadratic Weighted Kappa

David Vaughn, Derek Justice

(Submitted on 23 Sep 2015 (v1), last revised 6 Dec 2015 (this version, v3))

In recent years, quadratic weighted kappa has been growing in popularity in the machine learning community as an evaluation metric in domains where the target labels to be predicted are drawn from integer ratings, usually obtained from human experts. For example, it was the metric of choice in several recent, high profile machine learning contests hosted on Kaggle : this https URL , this https URL , this https URL . Yet, little is understood about the nature of this metric, its underlying mathematical properties, where it fits among other common evaluation metrics such as mean squared error (MSE) and correlation, or if it can be optimized analytically, and if so, how. Much of this is due to the cumbersome way that this metric is commonly defined. In this paper we first derive an equivalent but much simpler, and more useful, definition for quadratic weighted kappa, and then employ this alternate form to address the above issues.

Comments: realized some inaccuracies, and some sloppy reasoning. Need some time to fix
Subjects: **Learning (cs.LG)**
Cite as: **arXiv:1509.07107 [cs.LG]**
(or **arXiv:1509.07107v3 [cs.LG]** for this version)

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Lesson conclusion

- **Target metric is how competitors are scored**
- **Target metric VS optimization loss**
- **Regression metrics**
  - MSE, RMSE, R-squared
  - MAE
  - MSPE, MAPE
  - RMSLE
- **Classification metrics**
  - Accuracy
  - Logloss
  - AUC
  - (Quadratic weighted) Kappa