

Regression metrics optimization

Metrics optimization: our plan

1) Regression

- MSE, (R)MSE, R-squared
- MAE
- (R)MSPE, MAPE
- (R)MSLE

2) Classification:

- Accuracy
- Logloss
- AUC
- Cohen's Kappa

RMSE, MSE, R-squared

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$$

How do you optimize them?

Just fit the right model!

$$\text{RMSE} = \sqrt{\text{MSE}} \qquad R^2 = 1 - \frac{\text{MSE}}{\frac{1}{N} \sum_{i=1}^N (y_i - \bar{y})^2}$$

RMSE, MSE, R-squared

- **Tree-based**

- XGBoost, LightGBM

- `sklearn.RandomForestRegressor`

- **Linear models**

- `sklearn.<>Regression`

- `sklearn.SGDRegressor`

- Vowpal Wabbit (*quantile loss*)

- **Neural nets**

- PyTorch, Keras, TF, etc.

Synonyms: L2 loss

Read the docs!

MAE

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i|$$

How do you optimize it?

Again, just run the right model!

MAE

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- ~~XGBoost~~, LightGBM

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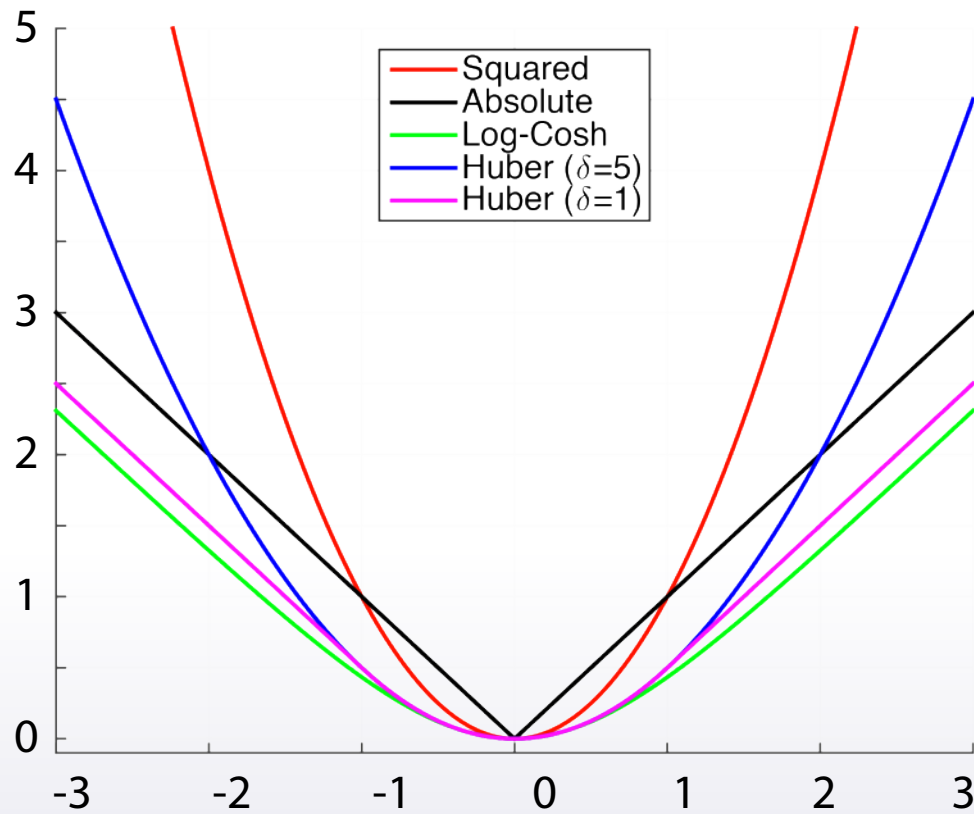
- PyTorch, Keras, TF, etc.

Synonyms: L1, Median regression

Read the docs!

MAE: optimal constant

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i|$$



MSPE and MAPE

$$\text{MSPE} = \frac{100\%}{N} \sum_{i=1}^N \left(\frac{y_i - \hat{y}_i}{y_i} \right)^2 \quad \text{MAPE} = \frac{100\%}{N} \sum_{i=1}^N \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

How do you optimize them?

~~Just run the right model!~~

MSPE (MAPE) as weighted MSE (MAE)

Sample weights

$$\text{MSPE} = \frac{100\%}{N} \sum_{i=1}^N \left(\frac{y_i - \hat{y}_i}{y_i} \right)^2 \quad w_i = \frac{1/y_i^2}{\sum_{i=1}^N 1/y_i^2}$$

$$\text{MAPE} = \frac{100\%}{N} \sum_{i=1}^N \left| \frac{y_i - \hat{y}_i}{y_i} \right| \quad w_i = \frac{1/y_i}{\sum_{i=1}^N 1/y_i}$$

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- **Use weights for samples (`sample_weights`)**
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 - `df.sample(weights=sample_weights)`
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 - And use *any* model that optimizes MSE (MAE)
 - Usually need to resample many times and average

RMSLE

$$\begin{aligned}\text{RMSLE} &= \sqrt{\frac{1}{N} \sum_{i=1}^N (\log(y_i + 1) - \log(\hat{y}_i + 1))^2} = \\ &= \sqrt{\text{MSE}(\log(y_i + 1), \log(\hat{y}_i + 1))}\end{aligned}$$

Train:

1. Transform target:

$$z_i = \log(y_i + 1)$$

2. Fit a model with MSE loss

Test:

- Transform predictions back:

$$\hat{y}_i = \exp(\hat{z}_i) - 1$$

Conclusion

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