AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

LESSON 8: Model-capacity, Under- and Overfitting, Generalization

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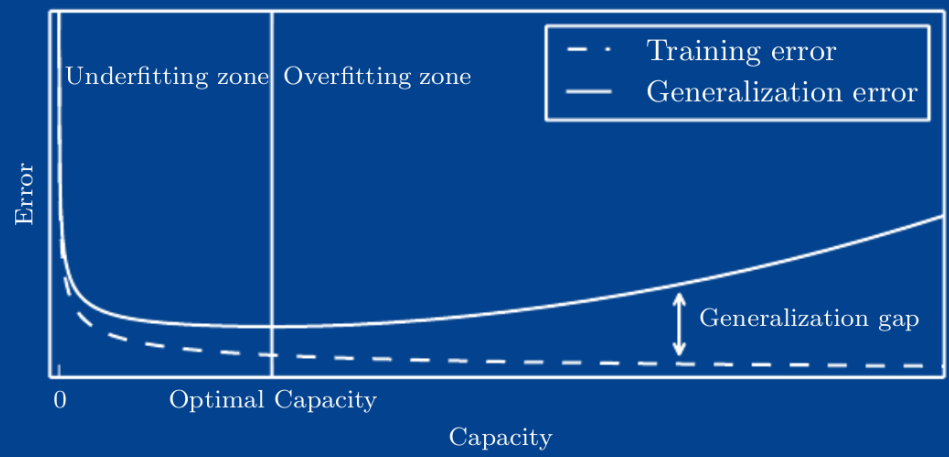


The Map

ML algo+ model selection

model hyperparms

gridsearch/random search, minimize J ; θ^*

minimize J ; θ^*

model; θ

L_2 , L_1, cross-entropy

$J(\mathbf{X}, \mathbf{y}, \theta)^{(train)}$

$\mathbf{X}^{(train)}$

$\mathbf{y}^{(train)}_{true}$

train $h(\mathbf{X}^{(train)}, \theta)$

$\mathbf{y}^{(train)}_{pred}$

loss; L_α $\mathbf{y}^{(train)}_{pred}$; $\mathbf{y}^{(train)}_{true}$

training done

$J(\mathbf{X}, \mathbf{y}, \theta)^{(test)}$

$\mathbf{X}^{(test)}$

$\mathbf{y}^{(test)}_{true}$

test $h(\mathbf{X}^{(test)}, \theta)$

$\mathbf{y}^{(test)}_{pred}$

loss; L_α $\mathbf{y}^{(test)}_{pred}$; $\mathbf{y}^{(test)}_{true}$

train-test split

preprocessing

trained model; θ

generalization

performance metrics/scores

inference/run $h(\mathbf{X}^{(new)}, \theta)$

$\mathbf{y}^{(new)}_{pred}$

$\mathbf{X}$

$\mathbf{y}_{true}$

K-fold cross val.
stratification
shuffling

new data

$\mathbf{X}^{(new)}$

precision, p
recall, r
accuracy, a
F-score, F_1
confusion matrix, $\mathbf{M}$

R^2,
Pearson's r

Pipelines

Brief intro to Scikit-learn pipelines..

Python code from `capacity_under_overfitting.ipynb`

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score

..

polynomial_features = PolynomialFeatures(degree=degrees[i], ..
linear_regression = LinearRegression()

pipeline = Pipeline([
        ("polynomial_features", polynomial_features),
        ("linear_regression", linear_regression)
    ])
pipeline.fit(X[:, np.newaxis], y)

scores = cross_val_score(pipeline, X[:, np.newaxis], y, scoring=
    "neg_mean_squared_error", cv=10)
..
score_mean = -scores.mean()
```

RESUMÉ: L02/performance_metrics.ipynb

Classification metrics

See the Classification metrics section of the user guide for further details.

`metrics.accuracy_score` (y_true, y_pred[, ...])	Accuracy classification score.
`metrics.auc` (x, y[, reorder])	Compute Area Under the Curve (AUC) using the trapezoidal rule
`metrics.average_precision_score` (y_true, y_score)	Compute average precision (AP) from prediction scores
`metrics.cohen_kappa_score` (y1, y2[, labels, ...])	Cohen's kappa: a statistic that measures inter-annotator agreement.
`metrics.confusion_matrix` (y_true, y_pred[, ...])	Compute confusion matrix to evaluate the accuracy of a classification
`metrics.f1_score` (y_true, y_pred[, labels, ...])	Compute the F1 score, also known as balanced F-score or F-measure
`metrics.log_loss` (y_true, y_pred[, eps, ...])	Log loss, aka logistic loss or cross-entropy loss.
`metrics.precision_score` (y_true, y_pred[, ...])	Compute the precision
`metrics.recall_score` (y_true, y_pred[, ...])	Compute the recall
`metrics.roc_auc_score` (y_true, y_score[, ...])	Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.
`metrics.roc_curve` (y_true, y_score[, ...])	Compute Receiver operating characteristic (ROC)
`metrics.zero_one_loss` (y_true, y_pred[, ...])	Zero-one classification loss.

Regression metrics

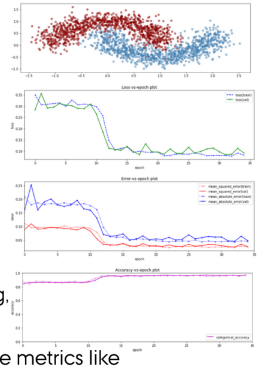
See the Regression metrics section of the user guide for further details.

`metrics.explained_variance_score` (y_true, y_pred)	Explained variance regression score function
`metrics.max_error` (y_true, y_pred)	max_error metric calculates the maximum residual error.
`metrics.mean_absolute_error` (y_true, y_pred)	Mean absolute error regression loss
`metrics.mean_squared_error` (y_true, y_pred[, ...])	Mean squared error regression loss
`metrics.mean_squared_log_error` (y_true, y_pred)	Mean squared logarithmic error regression loss
`metrics.median_absolute_error` (y_true, y_pred)	Median absolute error regression loss
`metrics.r2_score` (y_true, y_pred[, ...])	R^2 (coefficient of determination) regression

Notes on Keras MLPs

Typical Keras MLP Supervised Classifier setup..

- loss function
  `loss='categorical_crossentropy'`
- metrics collected via history
  `metrics=['categorical_accuracy', 'mean_squared_error', 'mean_absolute_error']`
- input lay.: categorical encoding,
- output lay.: softmax function,

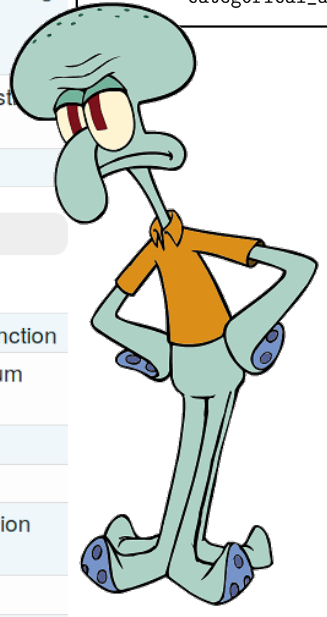


And notice that Keras do *not* provide metrics like

`precision, recall, F1`

but instead

`categorical_accuracy, binary_accuracy`



Model capacity

Exercise: `capacity_under_overfitting.ipynb`

Dummy and Paradox classifier:

capacity fixed ~ 0, cannot generalize at all!

Linear regression for a polynomial model:

capacity $\sim$ degree of the polynomial, x^n

Neural Network model:

capacity $\propto$ number of neurons/layers

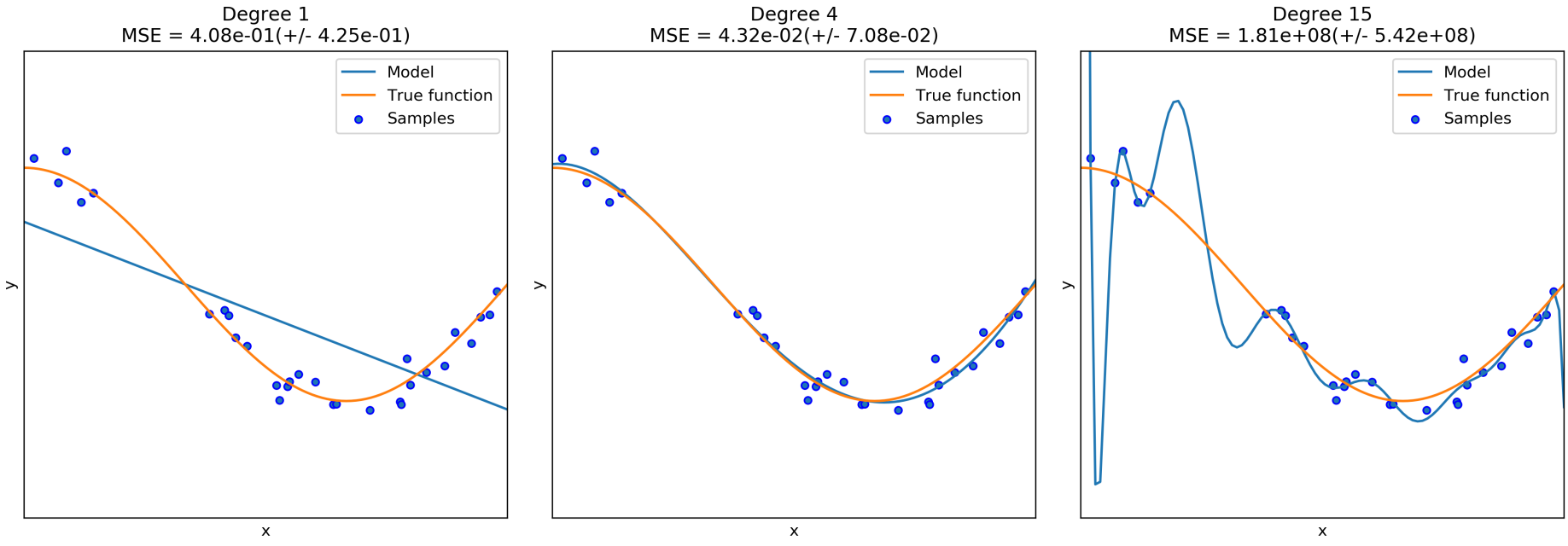
$\Rightarrow$ **Capacity** can be hard to express as a quantity for some models, but you need to choose..

$\Longrightarrow$ how to choose the **optimal** *capacity*?

Under- and overfitting

Exercise: `capacity_under_overfitting.ipynb`

Polynomial linear reg. fit for underlying model: `cos(x)`



- underfitting: capacity of model too low,
- overfitting: capacity to high.

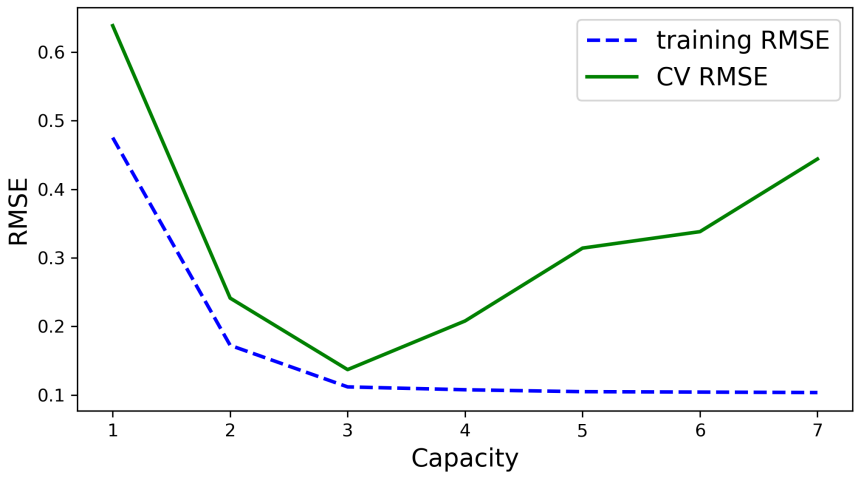
$\Longrightarrow$ how to choose the **optimal** capacity?

Generalization Error

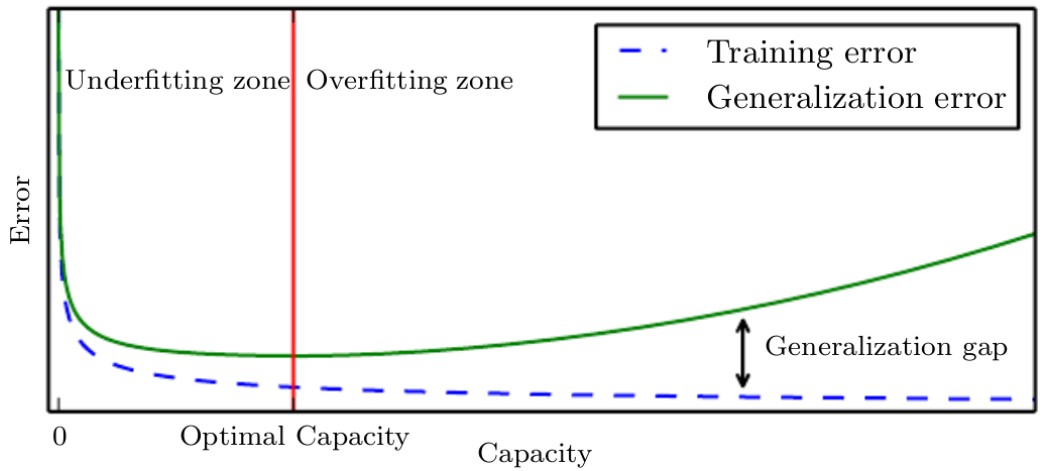
Exercise: `generalization_error.ipynb`

RMSE-capacity plot for lin. reg. with polynomial features

(capacity $\sim$ degree of poly)



(Figure 5.3 from [DL])



Inspecting the plots from the exercise (`.ipynb`) and [DL], extracting the concepts:

- training/generalization error,
- generalization gab,
- underfit/overfit zone,
- optimal capacity (best-model, early stop),
- (and the two axes: x/capacity, y/error.)

Generalization Error

Exercise: `generalization_error.ipynb`

NOTE: three methods/plots:

i) via **learning curves** as in [HOML],
ii) via an **error-capacity** plot as in [GITHOML] and[DL],
ii) via an **error-epoch** plot as in [GITHOML].