



Machine Learning Process #2

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Huawei / IFCE

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Agenda

① Model Validation

- Training and Generalization Error

- Underfitting and Overfitting

- Model capacity

- Bias and Variance

- Model Complexity and Error

② Model Learning Performance Evaluation

- Classification

- Regression

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- The goal of machine learning is that the model obtained after learning should perform well on new samples

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Generalization

- The goal of machine learning is that the model obtained after learning should perform well on new samples
- The capability of applying a model to new samples is called generalization or robustness

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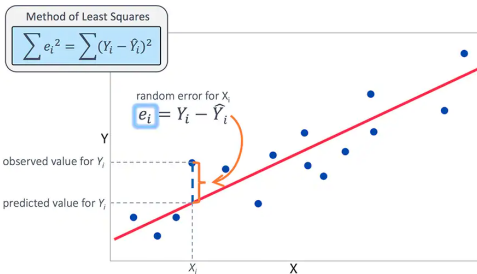
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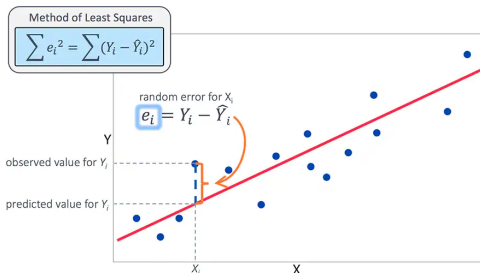
Model Validation

Error



Model Validation

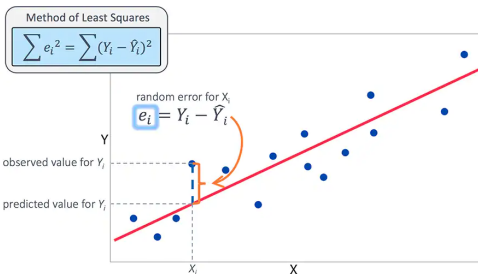
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- Difference between the sample result predicted by the model obtained after learning and the actual sample result.

Model Validation

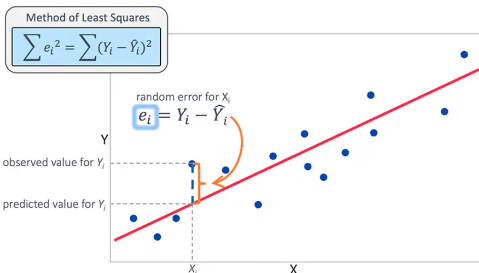
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- Difference between the sample result predicted by the model obtained after learning and the actual sample result.
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Model Validation

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Overfitting

- Occurs when the training error of the model obtained after learning is small but the generalization error is large

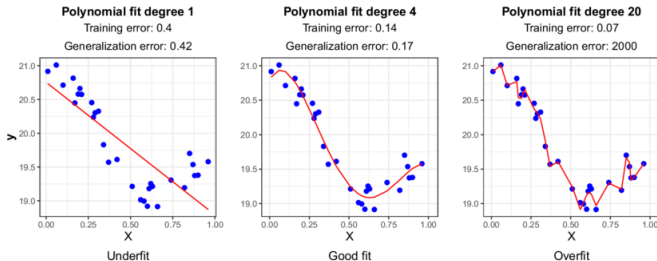
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- When the capacity suits the task complexity and the amount of training data provided, the algorithm effect is usually optimal.
- Models with insufficient capacity cannot solve complex tasks and underfitting may occur.
- A high-capacity model can solve complex tasks, but overfitting may occur if the capacity is higher than that required by a task.

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Bias and Variance

- Let $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$ a data set. We assume there is a relationship between a \mathbf{x}_n and a y_n is

$$y_n = f(\mathbf{x}) + \epsilon \quad (1)$$

Where $\epsilon \sim \mathcal{N}(0, \sigma_e^2)$.

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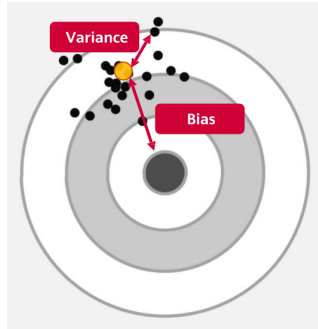
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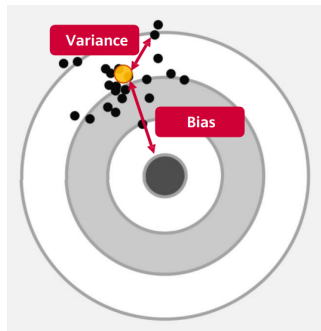
$$\begin{aligned} \text{Error}(\mathbf{x}) &= \mathbb{E} \left[(y - \hat{f}(\mathbf{x}))^2 \right] \quad (2) \\ &= \underbrace{\left(\mathbb{E} [f(\mathbf{x})] - \hat{f}(\mathbf{x}) \right)^2}_{\text{bias}^2} + \underbrace{\mathbb{E} \left[\left(\hat{f}(\mathbf{x}) - \mathbb{E} [\hat{f}(\mathbf{x})] \right)^2 \right]}_{\text{variance}} \\ &\quad + \underbrace{\sigma_e^2}_{\text{irreducible error}} \end{aligned}$$

Bias and Variance

Bias and Variance



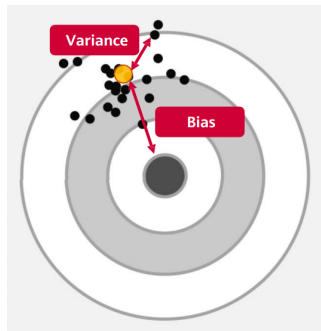
Bias and Variance



Variance

- Offset of the prediction result from the average value

Bias and Variance



Variance

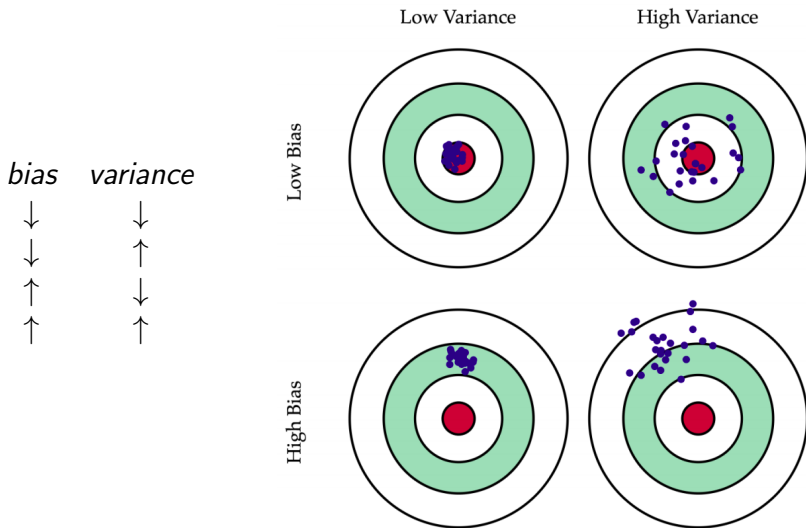
- Offset of the prediction result from the average value

Bias

- Difference between the expected prediction value and the correct

Bias and Variance

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Model Complexity and Error

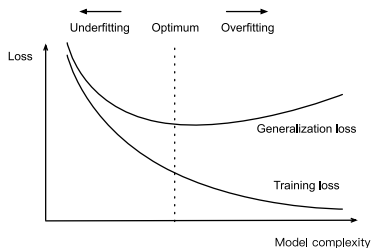
As the model complexity increases

- The training error decreases
- The test error decreases to a certain point and then increases in the reverse direction, forming a convex curve.

Model Complexity and Error

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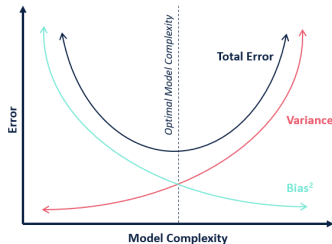
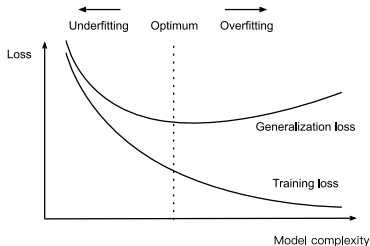
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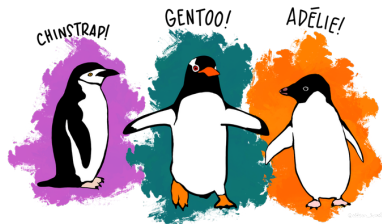
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- Classification is the process of predicting the class of given data points.

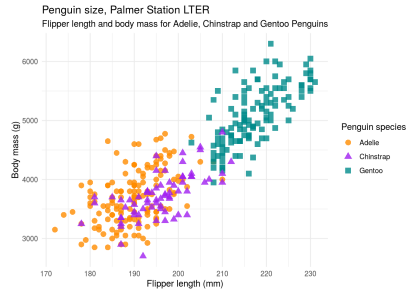
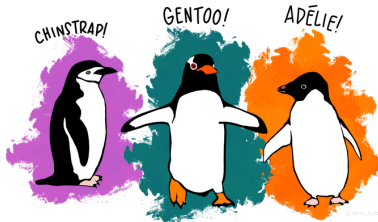
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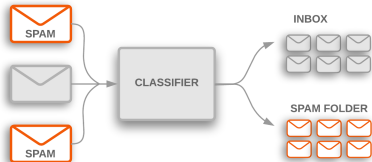
Classification

Classification

- Binary classification

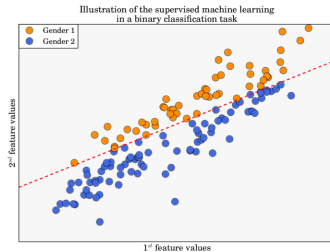
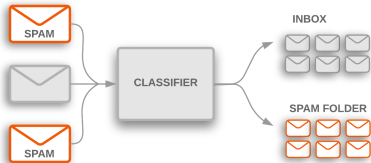
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Classification

Terms and definitions

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Confusion matrix

- A table used to describe the performance of a classifier on a set of test data for which the true values are known.

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Confusion matrix

- A table used to describe the performance of a classifier on a set of test data for which the true values are known.

		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) Type II Error	Sensitivity $\frac{TP}{(TP + FN)}$
	Negative	False Positive (FP) Type I Error	True Negative (TN)	Specificity $\frac{TN}{(TN + FP)}$
		Precision $\frac{TP}{(TP + FP)}$	Negative Predictive Value $\frac{TN}{(TN + FN)}$	Accuracy $\frac{TP + TN}{(TP + TN + FP + FN)}$

Classification

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Confusion matrix example and accuracy rate

		Predicted Class	
		Spam	Non-Spam
Actual Class	Spam	TP=45	FN=20
	Non-Spam	FP=5	TN=30

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Confusion matrix example and accuracy rate

		Predicted Class	
		Spam	Non-Spam
Actual Class	Spam	TP=45	FN=20
	Non-Spam	FP=5	TN=30

$$\text{ACC} \left(\hat{f}(\mathcal{D}_{\text{test}}; \mathcal{D}_{\text{train}}, \boldsymbol{\theta}) \right) = \frac{TP + TN}{TP + FP + TN + FN} \quad (3)$$

Classification

¹where β is a non-negative real number

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Other metrics

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Error rate and misclassification rate

$$\frac{FN+FP}{TP+FP+TN+FN}$$

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$$\frac{TP}{TP+FP}$$

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Other metrics

Error rate and misclassification rate	$\frac{FN+FP}{TP+FP+TN+FN}$
Precision	$\frac{TP}{TP+FP}$
Sensitivity or recall	$\frac{TP}{TP+FN}$

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Error rate and misclassification rate	$\frac{FN+FP}{TP+FP+TN+FN}$
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Specificity and true negative rate	$\frac{TN}{TN+FP}$
F_1 -score	$2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$

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F_1 -score	$2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$
F_β -score ¹	$(1 - \beta^2) \times \frac{\text{precision} \times \text{recall}}{\beta^2 \times \text{precision} + \text{recall}}$

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Receiving Operating Characteristic (ROC) curves

- Shows the sensitivity/specificity trade-off of a classifier for all possible classification thresholds

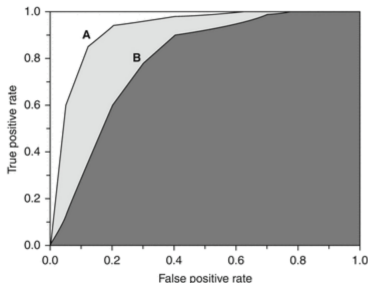
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Receiving Operating Characteristic (ROC) curves

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Area under a ROC curve

- Abbreviated as AUC, is a single scalar value that measures the overall performance of a binary classifier



Classification

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Performance evaluation example

- We have trained a machine learning model to identify whether the object in an image is a cat. Now we use 200 pictures to verify the model performance. Among the 200 images, objects in 170 images are cats, while others are not. The identification result of the model is that objects in 160 images are cats, while others are not.

	yes	no
yes	140	30
no	20	10

Classification

Performance evaluation example

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- Accuracy rate?

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- Accuracy rate? $\frac{150}{200} = 0.75$

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	yes	no
yes	140	30
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- Accuracy rate? $\frac{150}{200} = 0.75$
- Precision? $\frac{140}{140+20} = 0.875$

Classification

Performance evaluation example

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	yes	no
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- Precision? $\frac{140}{140+20} = 0.875$
- Recall?

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	yes	no
yes	140	30
no	20	10

- Accuracy rate? $\frac{150}{200} = 0.75$
- Precision? $\frac{140}{140+20} = 0.875$
- Recall? $\frac{140}{140+30} = 0.824$

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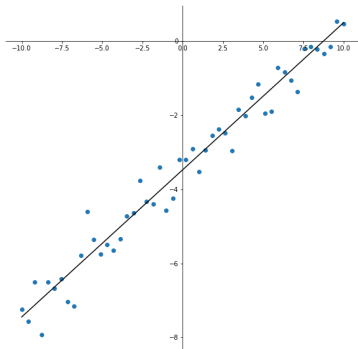
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Regression

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- The most common type of regression is linear regression.

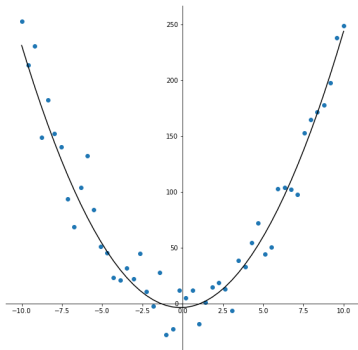
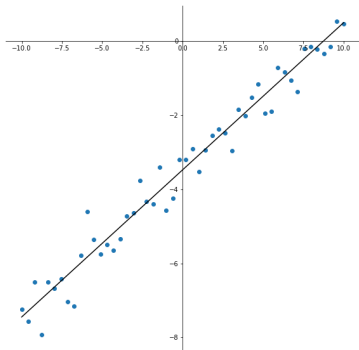
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Regression

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Mean Squared Error (MSE)

$$\text{MSE} = \frac{1}{N} \sum_{n=1}^N (y_n - \hat{y}_n)^2$$

Regression metrics

Mean Squared Error (MSE)	$\text{MSE} = \frac{1}{N} \sum_{n=1}^N (y_n - \hat{y}_n)^2$
--------------------------	-------------------------------------------------------------

Mean Absolute Error (MAE)	$\text{MAE} = \frac{1}{N} \sum_{n=1}^N y_n - \hat{y}_n $
---------------------------	-----------------------------------------------------------

Regression metrics

Mean Squared Error (MSE)	$\text{MSE} = \frac{1}{N} \sum_{n=1}^N (y_n - \hat{y}_n)^2$
--------------------------	-------------------------------------------------------------

Mean Absolute Error (MAE)	$\text{MAE} = \frac{1}{N} \sum_{n=1}^N y_n - \hat{y}_n $
---------------------------	-----------------------------------------------------------

R-squared (R^2)	$R^2 = 1 - \frac{\sum_{n=1}^N (y_n - \hat{y}_n)^2}{\sum_{n=1}^N (y_n - \bar{y}_n)^2}$
---------------------	---------------------------------------------------------------------------------------