CS550 - Machine Learning and Business Intelligence

Using Overfitting to Evaluate Models

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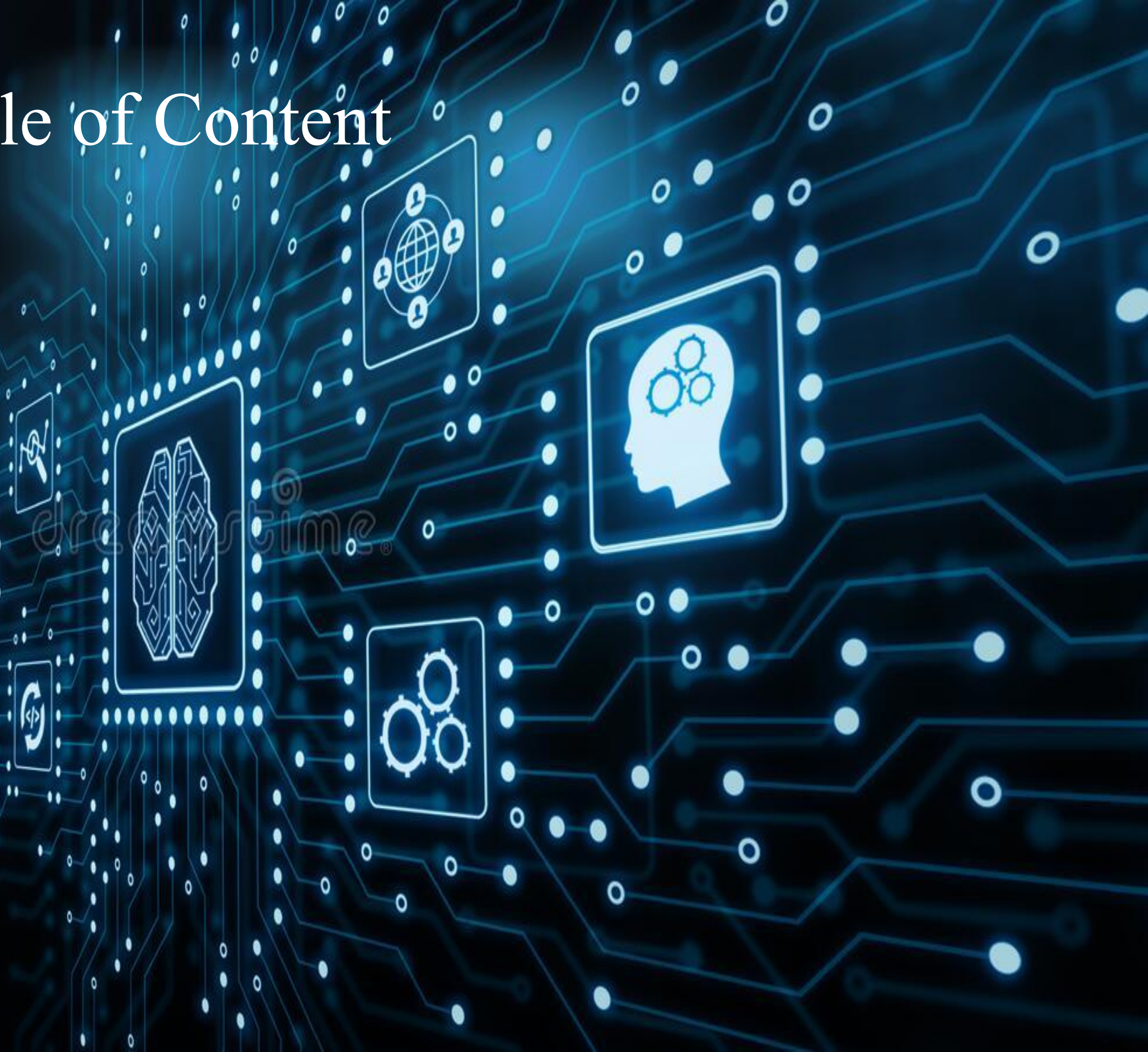
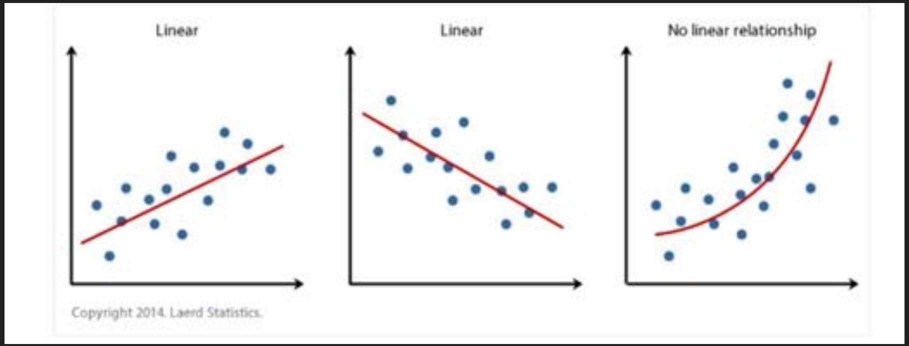


1. Introduction

In this presentation, we will discuss about using overfitting to evaluate Linear Regression Model and Non-Linear Regression Model for Machine Learning.

2. Linear Regression & Non-Linear Regression

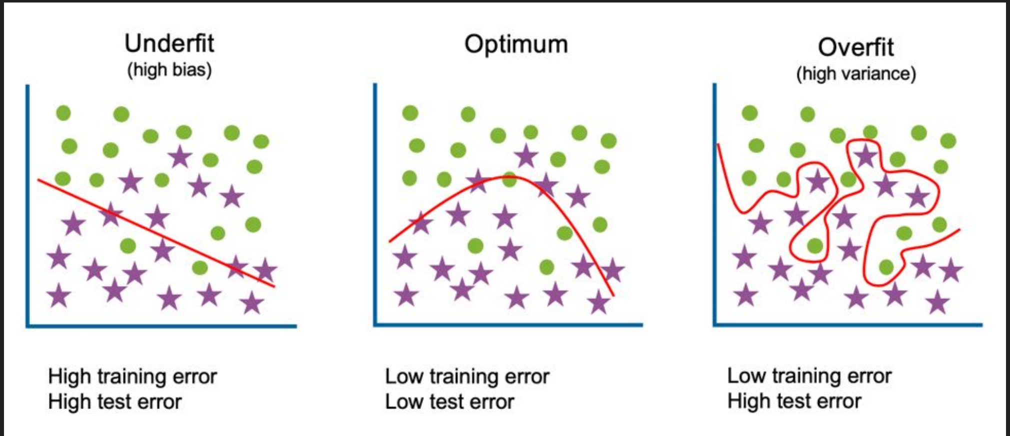
Linear Regression is the supervised Machine Learning model in which the model finds the best fit linear line between the independent and dependent variable i.e it finds the linear relationship between the dependent and independent variable.

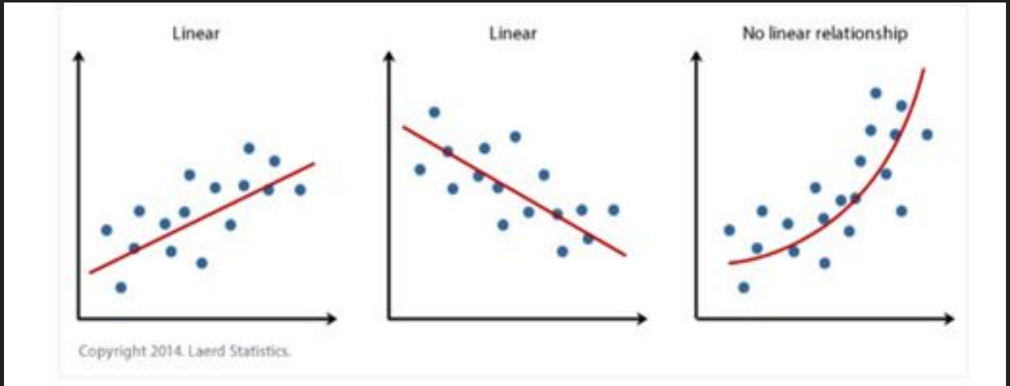


Non-Linear Regression is a form of regression analysis in which observational data are modeled by a function which is a nonlinear combination of the model parameters and depends on one or more independent variables. The data are fitted by a method of successive approximations.

3. Overfitting Issue

Non-linear regression has more serious overfitting issue. Linear regression is less prone to overfitting than non-linear regression because it has a simpler model structure.





We are going to figure out which model is the best to choose for test phase.

<table>
<tr><th colspan="4">Training Phase</th><th colspan="4">Validation Phase</th><th colspan="2">Test Phase</th></tr>
<tr><td colspan="2">Real Data Set 1 50% of the collcted data</td><td>Model 1: Linear Regression</td><td>Model 2: Non-Linear Regression</td><td colspan="2">Real Data Set 2 25% of the collcted data</td><td>Model 1: Linear Regression</td><td>Model 2: Non-Linear Regression</td><td>Real Data Set 3 25% of the collcted data</td><td>The better model (Model 1 or Model 2) selected from the Validation Phase based on the analysis of overfitting will be used to calculate $\hat{y}$</td></tr>
<tr><td colspan="10">

- After calculating a1, b1, a2, b2 in Training Phase, the values are not changed with the new Real Data Sets in Validation Phase and Test Phase.
- Only $\hat{y}$ values are changed with the new Real Data Sets.

</td></tr>
<tr><td>x</td><td>y</td><td>$\hat{y}=a1 + b1 * x$</td><td>$\hat{y}=a2 + b2 * x^2$</td><td>x</td><td>y</td><td>$\hat{y}=a1 + b1 * x$</td><td>$\hat{y}=a2 + b2 * x^2$</td><td>x</td><td>$\hat{y}=a1 + b1 * x$
or
$\hat{y}=a2 + b2 * x^2$</td></tr>
<tr><td>1</td><td>1.8</td><td></td><td></td><td>1.5</td><td>1.7</td><td></td><td></td><td>1.4</td><td></td></tr>
<tr><td>2</td><td>2.4</td><td></td><td></td><td>2.9</td><td>2.7</td><td></td><td></td><td>2.5</td><td></td></tr>
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<tr><td>5.3</td><td>5.3</td><td></td><td></td><td>5.1</td><td>5.5</td><td></td><td></td><td>5.4</td><td></td></tr>
<tr><td>1.4</td><td>1.5</td><td></td><td></td><td>X</td><td>X</td><td>X</td><td>X</td><td>X</td><td>X</td></tr>
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4. Training Phase

First and foremost, the values for X^2, Y^2, X*Y, X*X*Y, P*P and summation of each are calculated to be used in the equations.

Then we will calculate Slope(b) and Intercept(a) values for both **Model 1 (Linear Regression)** and **Model 2 (Non-Linear Regression)**.

X and Y values are from Real **Data Set 1**, 50% of the collected data.

Training Phase

	X	Y	X^2	Y^2	XY	XXY	P*P
	1	1.8	1	3.24	1.8	1.8	1
	2	2.4	4	5.76	4.8	9.6	16
	3.3	2.3	10.89	5.29	7.59	25.047	118.5921
	4.3	3.8	18.49	14.44	16.34	70.262	341.8801
	5.3	5.3	28.09	28.09	28.09	148.877	789.0481
	1.4	1.5	1.96	2.25	2.1	2.94	3.8416
	2.5	2.2	6.25	4.84	5.5	13.75	39.0625
	2.8	3.8	7.84	14.44	10.64	29.792	61.4656
	4.1	4	16.81	16	16.4	67.24	282.5761
	5.1	5.4	26.01	29.16	27.54	140.454	676.5201
Sum	31.8	32.5	121.34	123.51	120.8	509.762	2329.9862

Training Phase				Validation Phase				Test Phase	
Real Data Set 1 50% of the collcted data		Model 1: Linear Regression	Model 2: Non-Linear Regression	Real Data Set 2 25% of the collcted data		Model 1: Linear Regression	Model 2: Non-Linear Regression	Real Data Set 3 25% of the collcted data	The better model (Model 1 or Model 2) selected from the Validation Phase based on the analysis of overfitting will be used to calculate ŷ
x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	ŷ=a1 + b1 * x or ŷ=a2 + b2 * x^2
1	1.8			1.5	1.7			1.4	
2	2.4			2.9	2.7			2.5	
3.3	2.3			3.7	2.5			3.6	
4.3	3.8			4.7	2.8			4.5	
5.3	5.3			5.1	5.5			5.4	
1.4	1.5			X	X	X	X	X	X
2.5	2.2			X	X	X	X	X	X
2.8	3.8			X	X	X	X	X	X
4.1	4.0			X	X	X	X	X	X
5.1	5.4			X	X	X	X	X	X

- After calculating a1, b1, a2, b2 in Training Phase, the values are not changed with the new Real Data Sets in Validation Phase and Test Phase.
- Only ŷ values are changed with the new Real Data Sets.

Equations for Linear Regression

Slope(b1) = $(N\Sigma XY - (\Sigma X)(\Sigma Y)) / (N\Sigma X2 - (\Sigma X)2)$

Intercept(a1) = $(\Sigma Y - b(\Sigma X)) / N$

Equations for Non-Linear Equation

Slope(b2) = $(N\Sigma PY - (\Sigma P)(\Sigma Y)) / (N\Sigma P2 - (\Sigma P)2)$

Intercept(a2) = $(\Sigma Y - b(\Sigma P)) / N$

Where $P = X * X$

Slope(b1)	0.8631777
Intercept(a1)	0.505095

Slope(b) = $(N\Sigma XY - (\Sigma X)(\Sigma Y)) / (N\Sigma X^2 - (\Sigma X)^2)$

Intercept(a) = $(\Sigma Y - b(\Sigma X)) / N$

Slope(b2)	0.1345624
Intercept(a2)	1.617249

Slope(b) = $(N\Sigma \underline{P}Y - (\Sigma \underline{P})(\Sigma Y)) / (N\Sigma \underline{P}^2 - (\Sigma \underline{P})^2)$

Intercept(a) = $(\Sigma Y - b(\Sigma \underline{P})) / N$

Where $\underline{P} = X * X$

By using the values calculated above, we can calculate $\hat{y}$ values for both **Model 1** and **Model 2**.

* The value of N is 10 for Training Phase.

$\hat{y}=a1 + b1 * x$	$\hat{y}=a2 + b2 * x^2$
1.36826	1.751809
2.23143	2.155489
3.353551	3.0826074
4.216721	4.1052634
5.079891	5.3970394
1.713528	1.8809866
2.663015	2.458249
2.921966	2.6721994
4.044087	3.8792026
4.907257	5.1171546

5. Validation Phase

Values for X^2, Y^2, X*Y, X*X*Y, P*P and summation of each are calculated to be used in the equations.

Then we will calculate Slope(b) and Intercept(a) values for both **Model 1 (Linear Regression)** and **Model 2 (Non-Linear Regression)**.

X and Y values are from **Real Data Set 2**, 25% of the collected data.

Validation Phase							
	X	**Y**	**X^2**	**Y^2**	**XY**	**XXY**	**P*P**
	1.5	1.7	2.25	2.89	2.55	3.825	5.0625
	2.9	2.7	8.41	7.29	7.83	22.707	70.7281
	3.7	2.5	13.69	6.25	9.25	34.225	187.416
	4.7	2.8	22.09	7.84	13.16	61.852	487.968
	5.1	5.5	26.01	30.25	28.05	143.055	676.52
			0	0	0	0	0
			0	0	0	0	0
			0	0	0	0	0
			0	0	0	0	0
			0	0	0	0	0
Sum	17.9	15.2	72.45	54.52	60.84	265.664	1427.69

Training Phase				Validation Phase				Test Phase	
Real Data Set 1 50% of the collcted data		Model 1: Linear Regression	Model 2: Non-Linear Regression	Real Data Set 2 25% of the collcted data		Model 1: Linear Regression	Model 2: Non-Linear Regression	Real Data Set 3 25% of the collcted data	The better model (Model 1 or Model 2) selected from the Validation Phase based on the analysis of overfitting will be used to calculate ŷ
▪ After calculating a1, b1, a2, b2 in Training Phase, the values are not changed with the new Real Data Sets in Validation Phase and Test Phase. ▪ Only ŷ values are changed with the new Real Data Sets.									
x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	ŷ=a1 + b1 * x or ŷ=a2 + b2 * x^2
1	1.8			1.5	1.7			1.4	
2	2.4			2.9	2.7			2.5	
3.3	2.3			3.7	2.5			3.6	
4.3	3.8			4.7	2.8			4.5	
5.3	5.3			5.1	5.5			5.4	
1.4	1.5			X	X	X	X	X	X
2.5	2.2			X	X	X	X	X	X
2.8	3.8			X	X	X	X	X	X
4.1	4.0			X	X	X	X	X	X
5.1	5.4			X	X	X	X	X	X

Equations for Linear Regression

$Slope(b1) = (N\Sigma XY - (\Sigma X)(\Sigma Y)) / (N\Sigma X2 - (\Sigma X)2)$

$Intercept(a1) = (\Sigma Y - b(\Sigma X)) / N$

Equations for Non-Linear Equation

$Slope(b2) = (N\Sigma PY - (\Sigma P)(\Sigma Y)) / (N\Sigma P2 - (\Sigma P)2)$

$Intercept(a2) = (\Sigma Y - b(\Sigma P)) / N$

Where $P = X * X$

Slope(b1)	0.83229
Intercept(a1)	0.0302

$Slope(b) = (N\Sigma XY - (\Sigma X)(\Sigma Y)) / (N\Sigma X^2 - (\Sigma X)^2)$

$Intercept(a) = (\Sigma Y - b(\Sigma X)) / N$

Slope(b2)	0.17229
Intercept(a2)	0.54511

$Slope(b) = (N\Sigma PY - (\Sigma P)(\Sigma Y)) / (N\Sigma P^2 - (\Sigma P)^2)$

$Intercept(a) = (\Sigma Y - b(\Sigma P)) / N$

Where $P = X * X$

* The value of N is 5 for Validation Phase.

By using the values calculated above, we can calculate $\hat{y}$ values for both **Model 1** and **Model 2**.

$\hat{y}=a1 + b1 * x$	$\hat{y}=a2 + b2 * x^2$
1.799845	1.920009
3.008283	2.7488986
3.698819	3.4593754
4.561989	4.5896794
4.907257	5.1171546

5. Test Phase

X values are from Real **Data Set 3**, 25% of the collected data.

Before initiating the test phase, we need to calculate mean squared error (MSE) for both **Model 1** and **Model 2** by using the following equation.

$$MSE = \frac{\sum(y_i - \hat{y}_i)^2}{n}$$

Then we will decide which Model to choose by using the following equation.

max(Training_Set_MSE, Validation_Set_MSE) / min(Training_Set_MSE, Validation_Set_MSE)

Training Set

y - ŷ Model 1	y - ŷ Model 2
0.186399428	0.002322372
0.028415845	0.059785629
1.10996971	0.612474343
0.173656392	0.093185743
0.048447972	0.009416645
0.045594207	0.145150789
0.21438289	0.066692546
0.770943705	1.271934193
0.001943664	0.014592012
0.242795664	0.08000152
2.822549476	2.355555794
0.282254948	0.235555579

Validation Set

y - ŷ Model 1	y - ŷ Model 2
0.009969024	0.04840396
0.095038408	0.002391073
1.437166995	0.920401158
3.104605236	3.202952355
0.351344264	0.1465706
4.998123927	4.320719146
0.999624785	0.864143829

max(Training_Set_MSE, Validation_Set_MSE) / min(Training_Set_MSE, Validation_Set_MSE)

5. Test Phase

According to the calculation, **Model 1** is the better model. So, we will use the values of b and a from **Model 1**.

Slope(b1) = 0.8631777

Intercept(a1) = 0.505095

Model 1

Training_Set_MSE = 0.28225

Validation_Set_MSE = 0.99962

0.99962/0.28225 = **3.54**

Model 2

Training_Set_MSE = 0.23555

Validation_Set_MSE = 0.86414

0.86414/0.23555 = 3.668

Test Phase

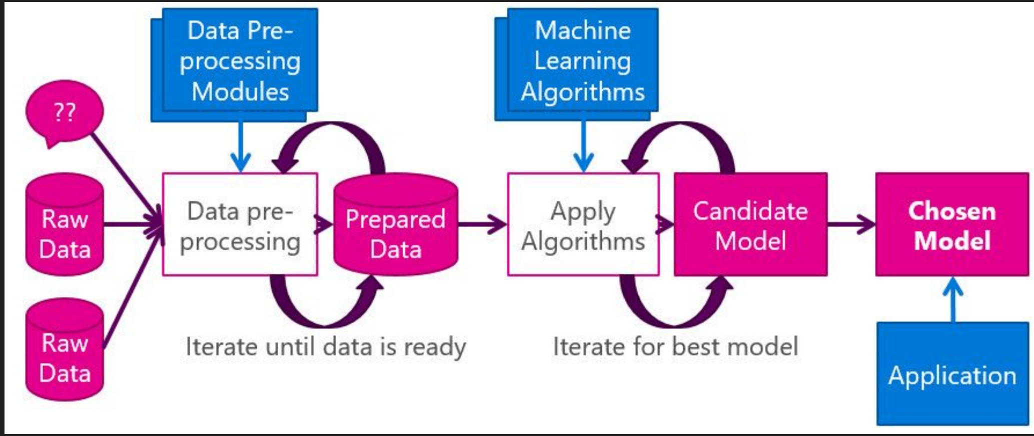
	Model 1
X	ŷ=a1 + b1 * x
1.4	1.71354378
2.5	2.66303925
3.6	3.61253472
4.5	4.38939465
5.4	5.16625458

Final Result

x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	y	ŷ=a1 + b1 * x	ŷ=a2 + b2 * x^2	x	ŷ=a1 + b1 * x
1	1.8	1.36826	1.751809	1.5	1.7	1.799845	1.920009	1.4	1.71354378
2	2.4	2.23143	2.155489	2.9	2.7	3.008283	2.7488986	2.5	2.66303925
3.3	2.3	3.353551	3.0826074	3.7	2.5	3.698819	3.4593754	3.6	3.61253472
4.3	3.8	4.216721	4.1052634	4.7	2.8	4.561989	4.5896794	4.5	4.38939465
5.3	5.3	5.079891	5.3970394	5.1	5.5	4.907257	5.1171546	5.4	5.16625458
1.4	1.5	1.713528	1.8809866	X	X	X	X	X	X
2.5	2.2	2.663015	2.458249	X	X	X	X	X	X
2.8	3.8	2.921966	2.6721994	X	X	X	X	X	X
4.1	4	4.044087	3.8792026	X	X	X	X	X	X
5.1	5.4	4.907257	5.1171546	X	X	X	X	X	X

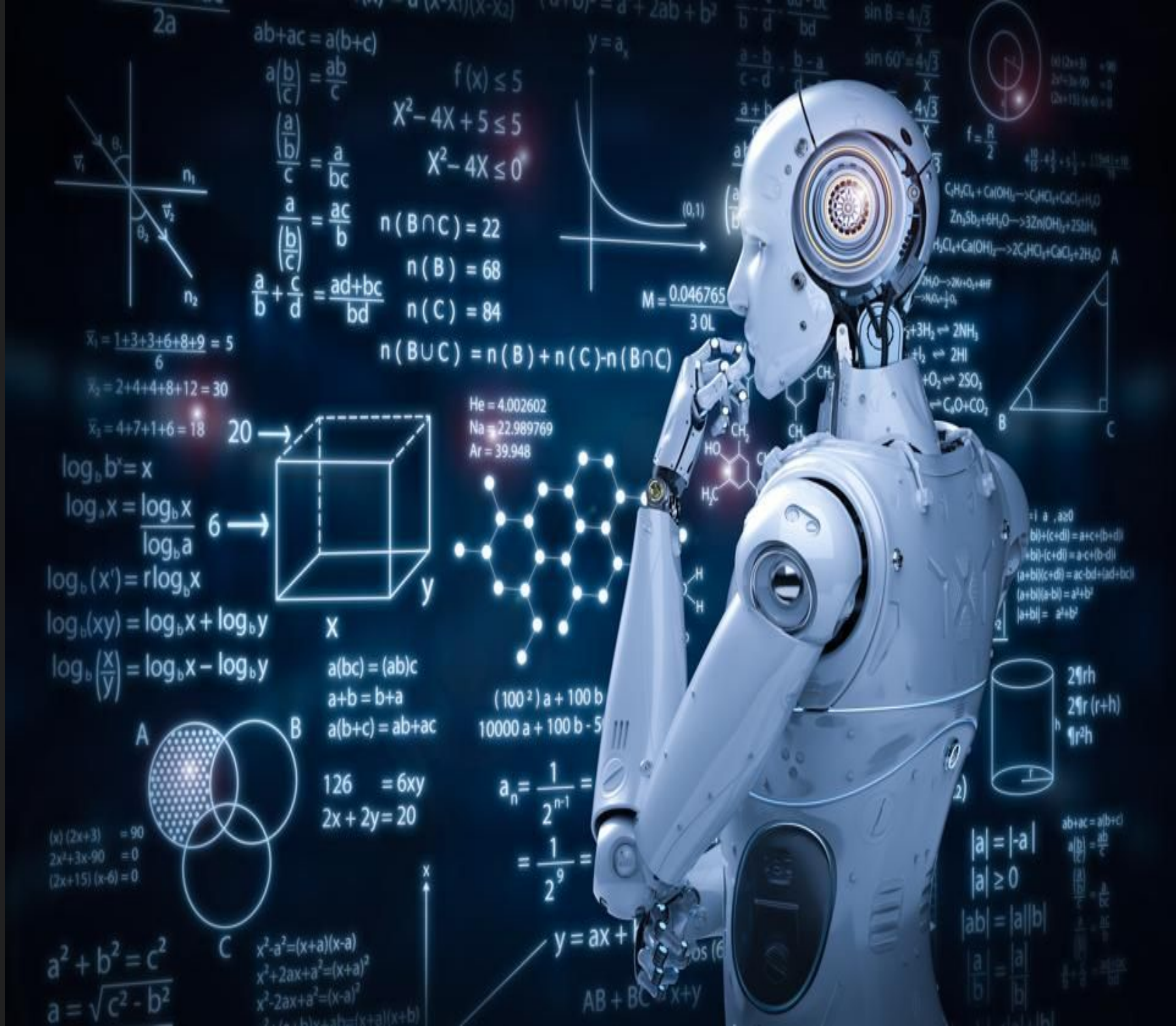
6. Machine Learning Model Selection

Model selection is the process of selecting one final machine learning model from among a collection of candidate machine learning models for a training dataset. Model selection is a process that can be applied both across different types of models (e.g. logistic regression, SVM, KNN, etc.)



7. Conclusion

Conclusion Machine learning is a powerful tool for making predictions from data. However, it is important to remember that machine learning is only as good as the data that is used to train the algorithms.



8. References

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