Machine Learning: The Basics

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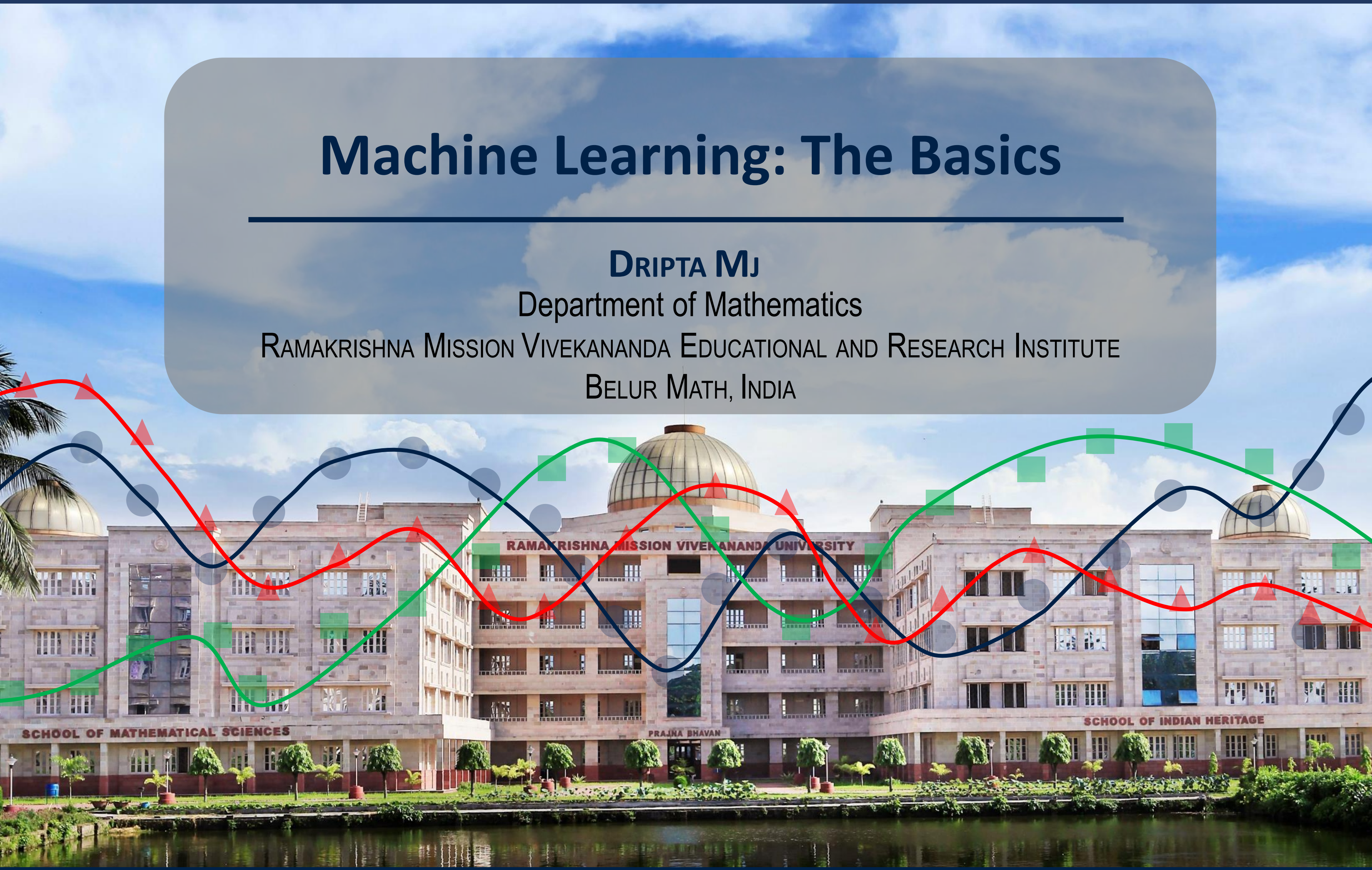


Machine Learning is everywhere . . . .

Astronomy

Social Networks

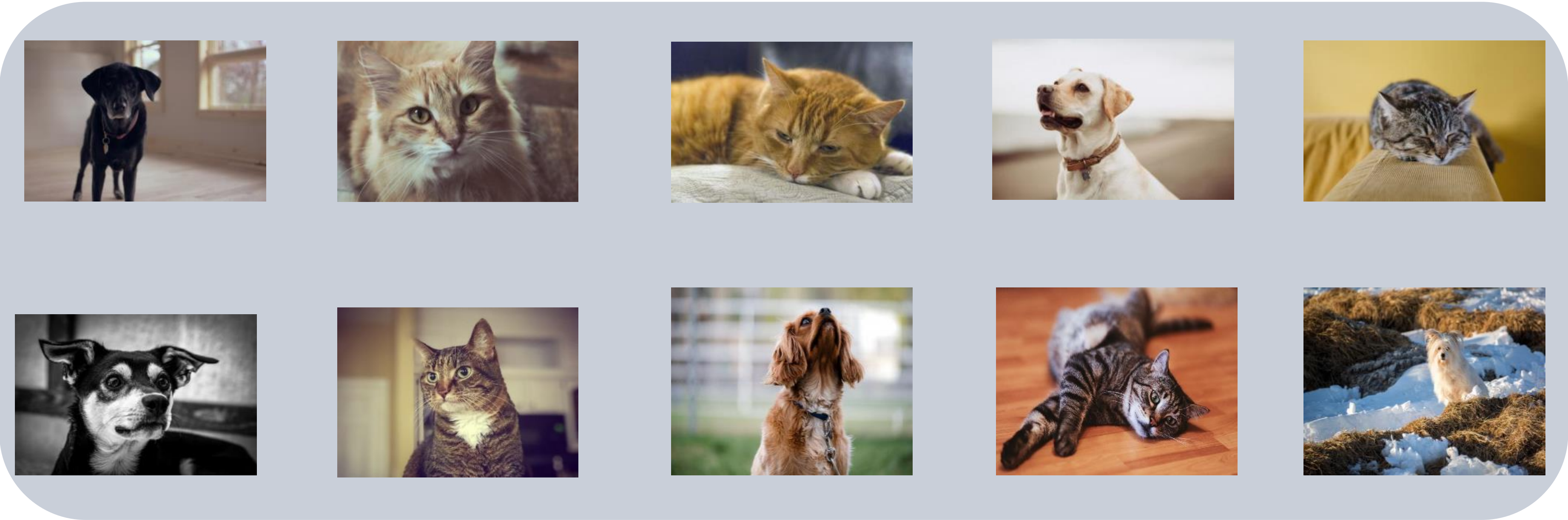
Healthcare

Banking

Genomics

Weather predictions

Dogs and Cats …..



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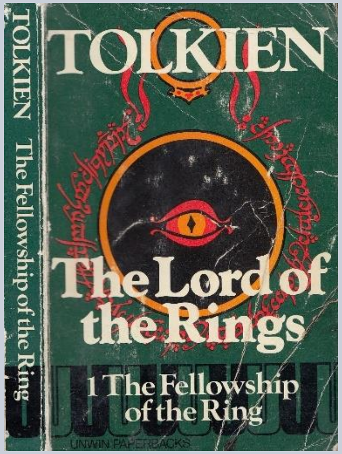
Product recommendation



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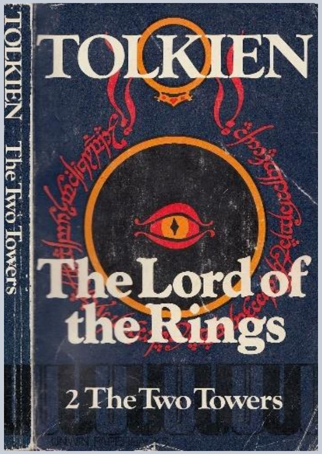

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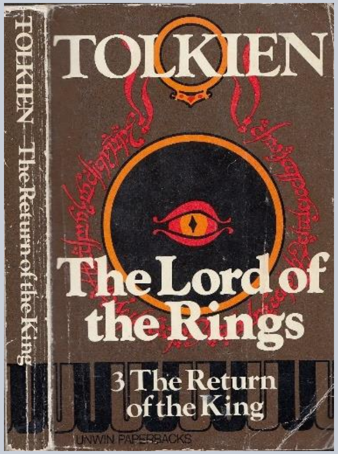
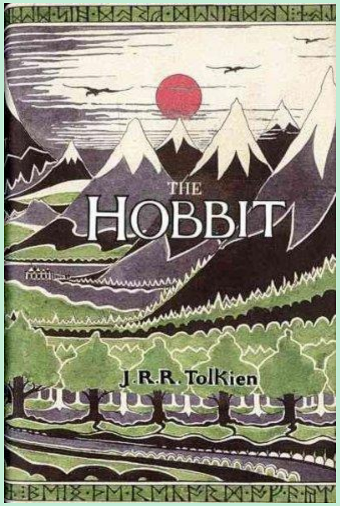
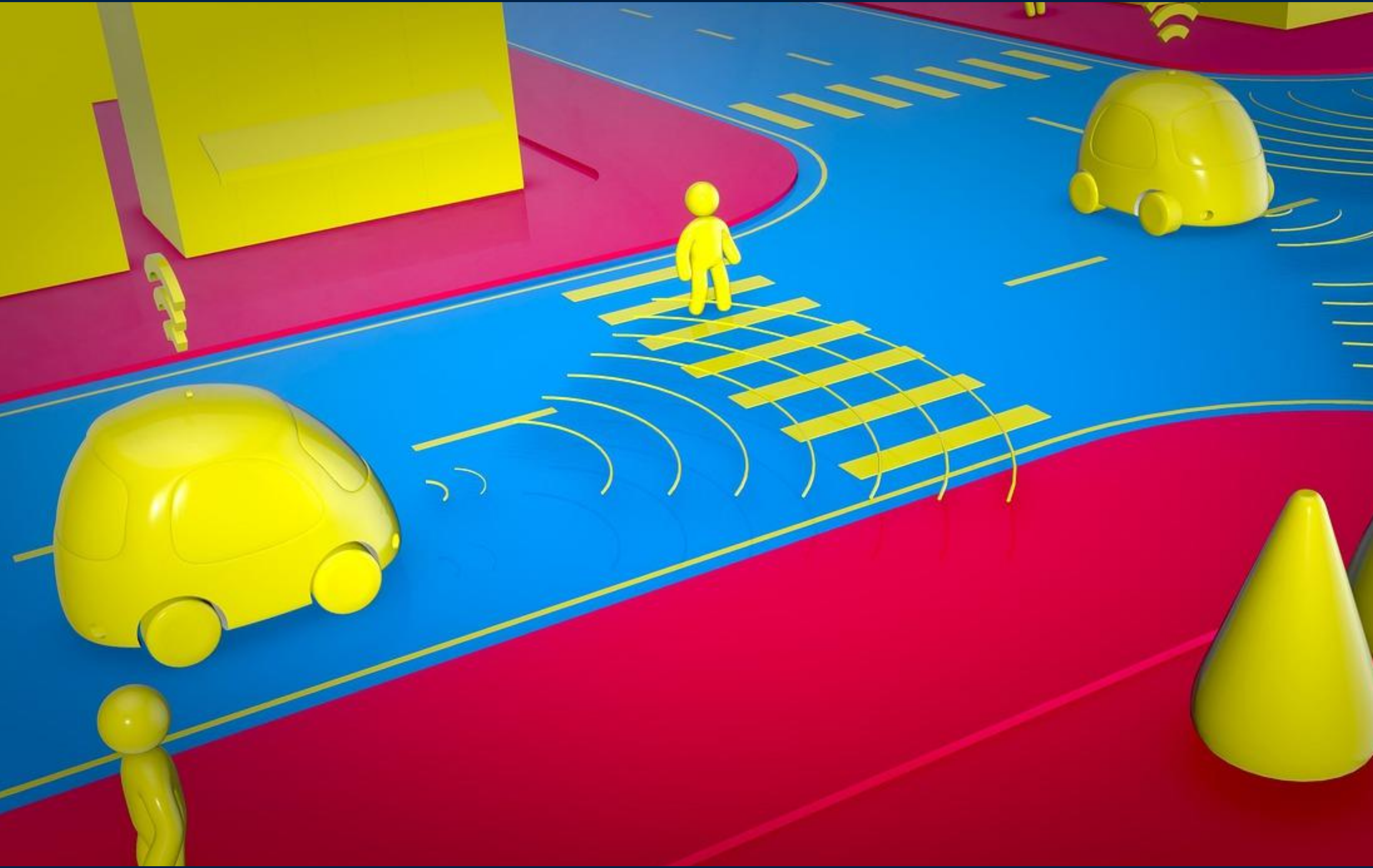




Images from *amazon.com*

Autonomous vehicles



Creativity

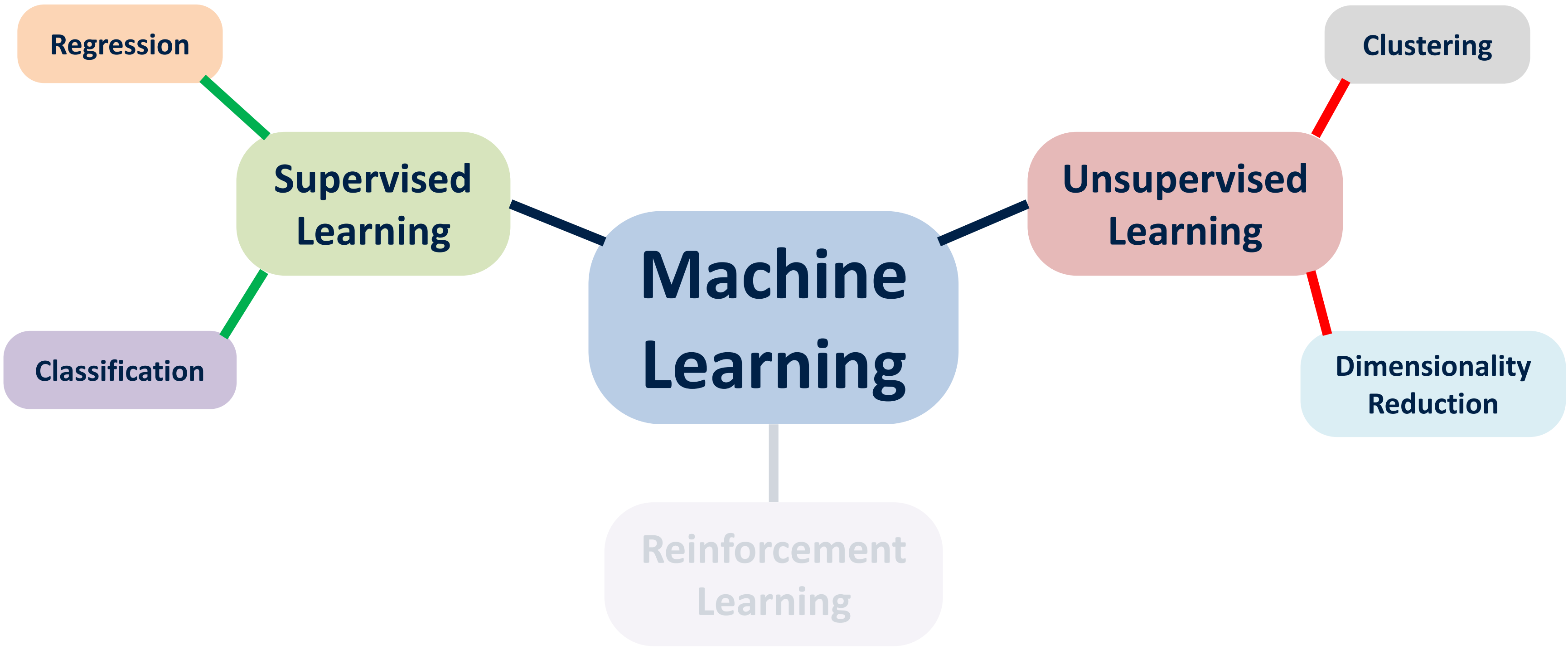
Figure source: Gatys, Ecker and Bethge, Image style transfer using convolutional neural networks, CVPR 2016.

ML depends on

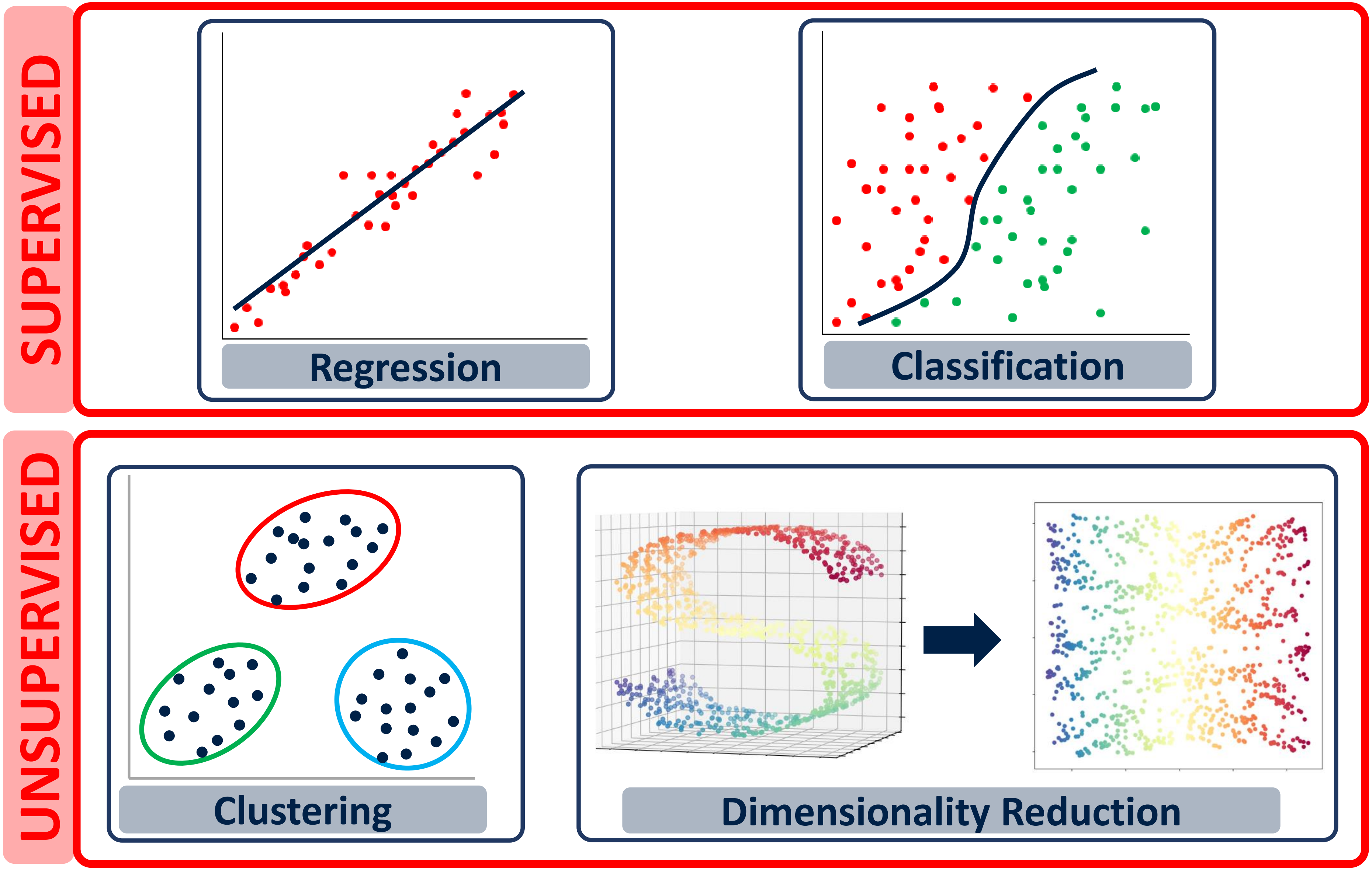
- Statistics: Probability theory, Sampling .....
- Mathematics: Linear Algebra, Multivariate Calculus,....
- Computer Science: Data structures, Programming .....
- Some domain knowledge.

Machine Learning

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E" Tom Mitchell



Machine Learning



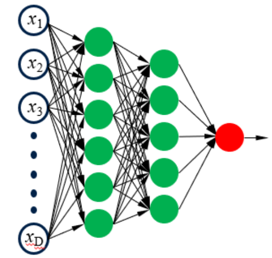
Some key components

Data pre-processing

x_1	x_2	x_3	y
2.2	0.8	2.7	1
4.9	3.1	1.6	-1

- Data cleaning
- Training-test data splitting
- Feature engineering ……

ML Model



Linear Regression

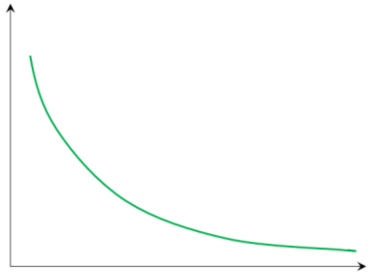
*k*NN | SVM | Decision Tree

Neural Network | ……..

Training

- Loss function
- Optimization algorithm
- Regularization ……

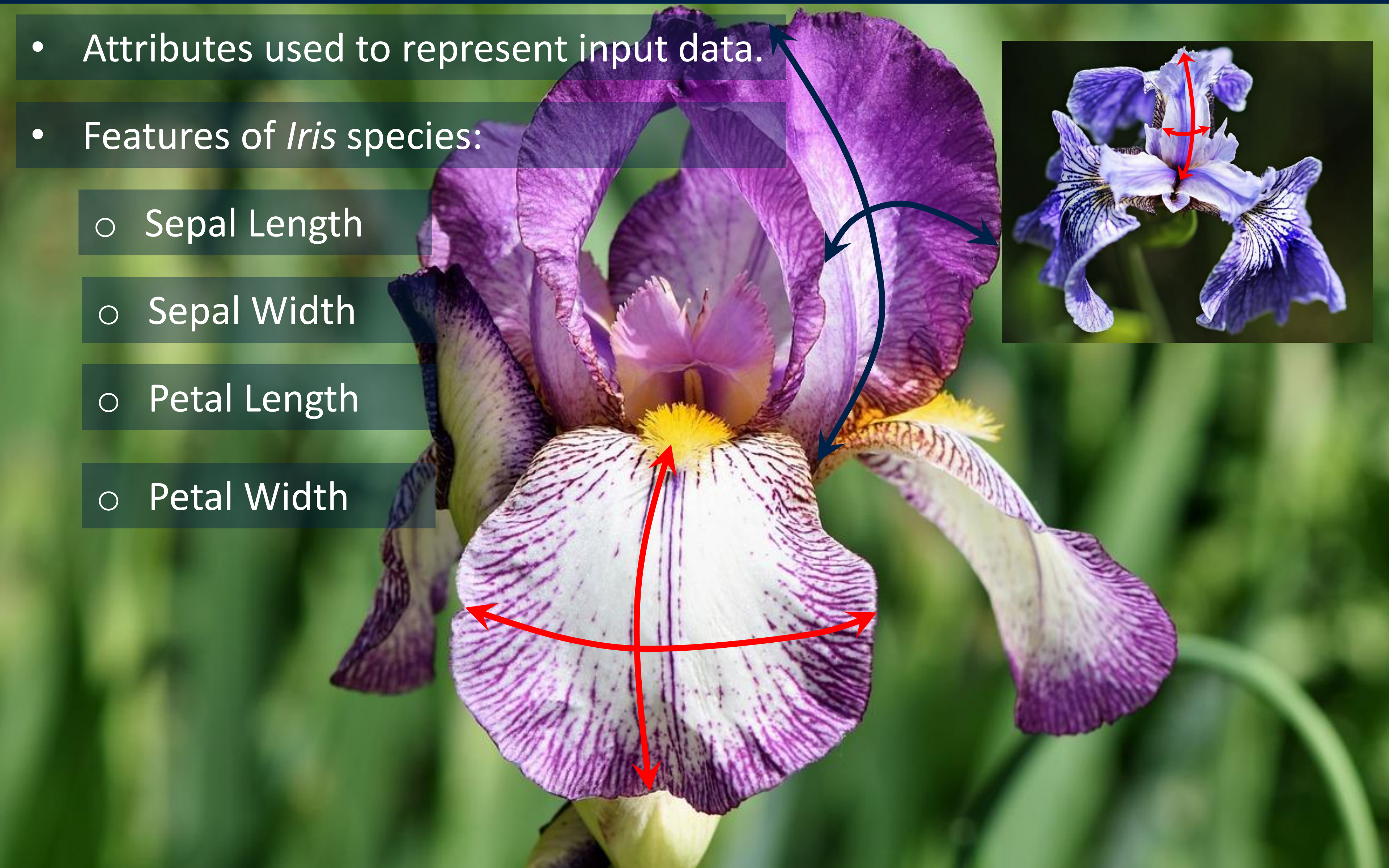
Evaluation



- Generalization error
- Cross-validation
- Metric ……….

Features

- Attributes used to represent input data.
- Features of *Iris* species:
  - Sepal Length
  - Sepal Width
  - Petal Length
  - Petal Width



Iris dataset

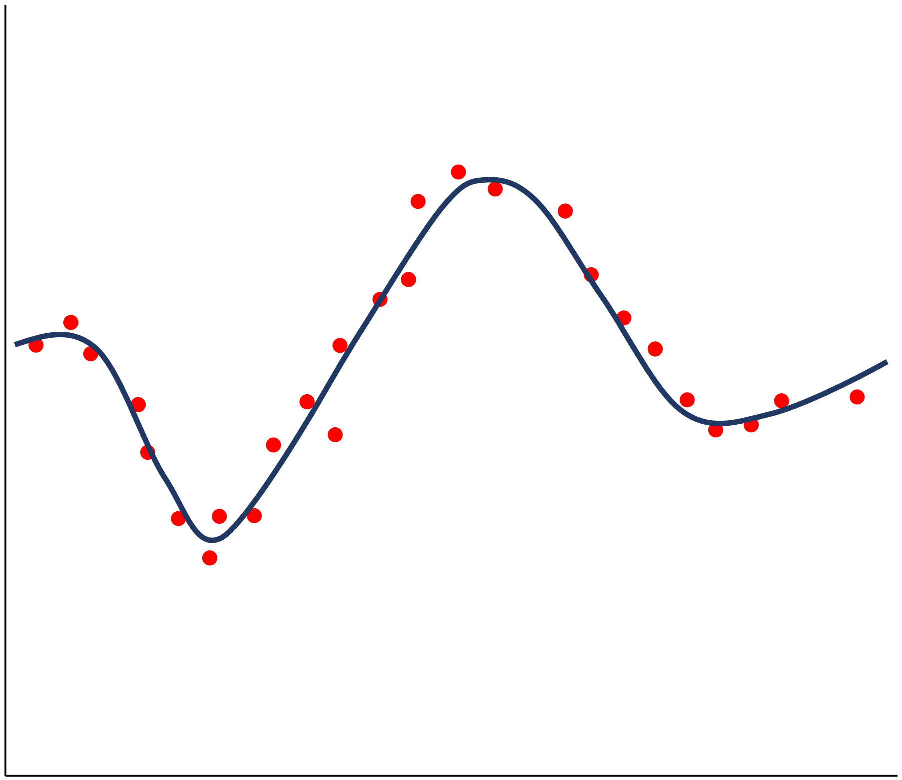
Inputs

Sepal Length (cm)	Sepal Width (cm)	Petal Length (cm)	Petal Width (cm)
5.1	3.5	1.4	0.2
4.9	3	1.4	0.2
4.7	3.2	1.3	0.2
4.6	3.1	1.5	0.2
5	3.6	1.4	0.2
5.4	3.9	1.7	0.4
4.6	3.4	1.4	0.3
5	3.4	1.5	0.2
4.4	2.9	1.4	0.2
.	.	.	.
.	.	.	.

Outputs

Species	
Iris Setosa	0
Iris Virginica	1
Iris Versicolor	2

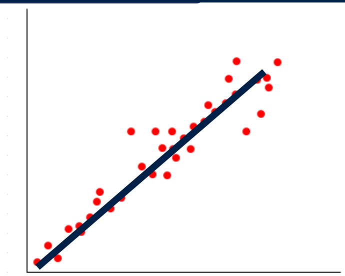
Training and Test data



- Training data: Used for training the ML algorithm.
- Test data: Used for assessing the performance of the ML algorithm.

Loss function

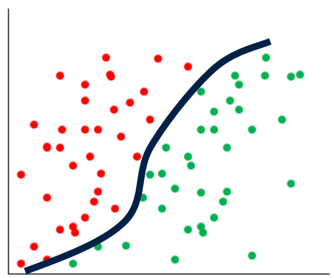
REGRESSION



Squared loss:

$$\mathcal{L}(\mathbf{y}^{(n)}, \mathbf{y}^{*(n)}) = \frac{1}{2}\sum_{j=1}^{J}\left(y_j^{(n)} - y_j^{*(n)}\right)^2$$

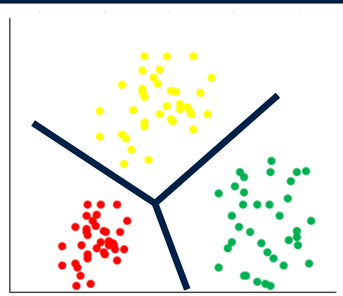
BINARY CLASSIFICATION



Binary cross-entropy loss:

$$\mathcal{L}(y^{(n)}, y^{*(n)}) = -y^{(n)}\log(y^{*(n)}) - (1 - y^{(n)})\log(1 - y^{*(n)})$$

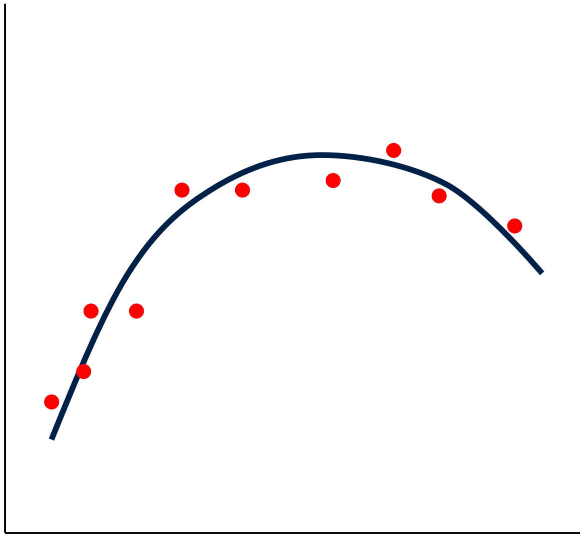
MULTI-CLASS CLASSIFICATION



Cross-entropy loss:

$$\mathcal{L}(\mathbf{y}^{(n)}, \mathbf{y}^{*(n)}) = -\sum_{j=1}^{J} y_j^{(n)} \log y_j^{*(n)}$$

Generalization

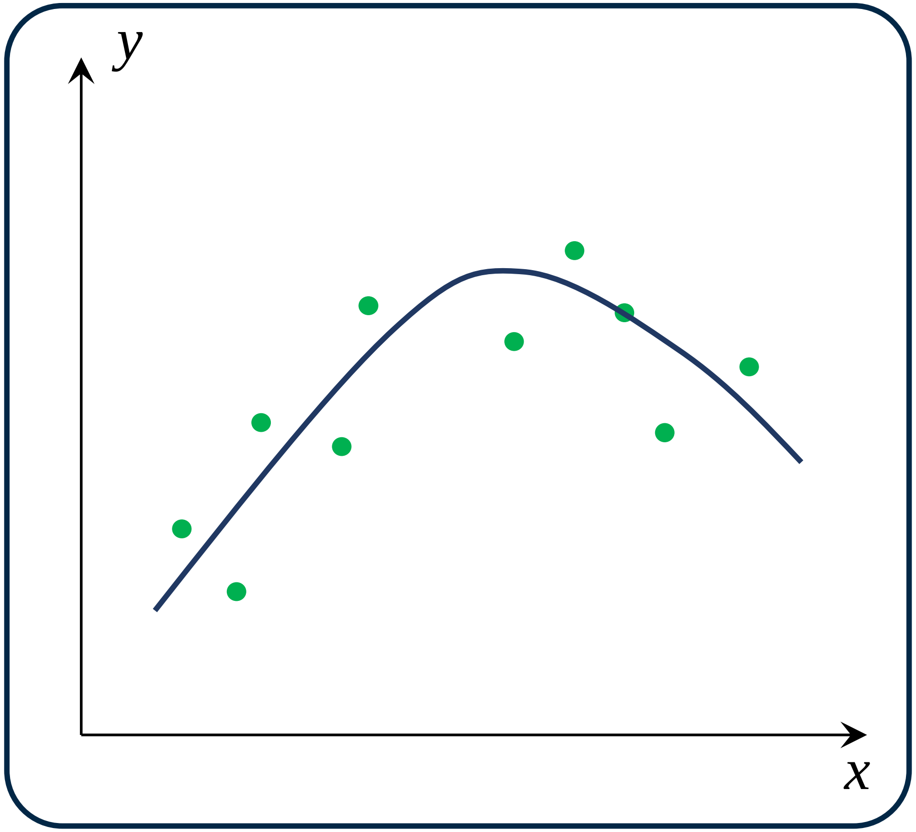


- Larger class of functions $\rightarrow$ more complexity of the hypothesis class $\mathcal{C}(\mathbb{H})$.

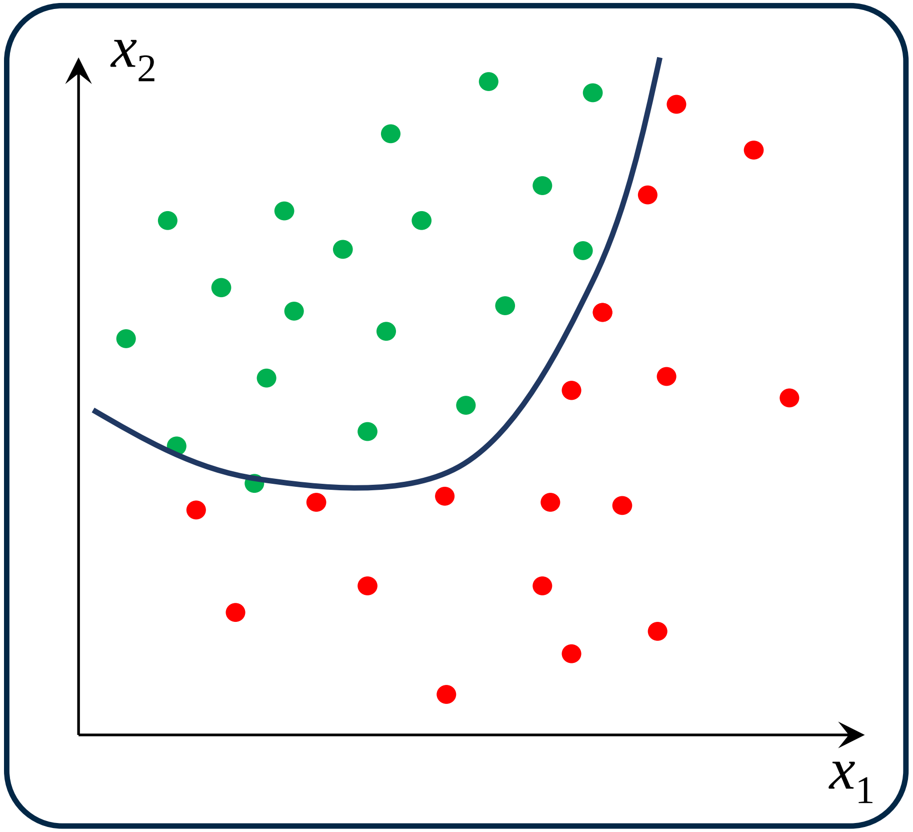
- Objective: Good prediction at unobserved locations $\rightarrow$ good **generalization**.

Generalization

REGRESSION



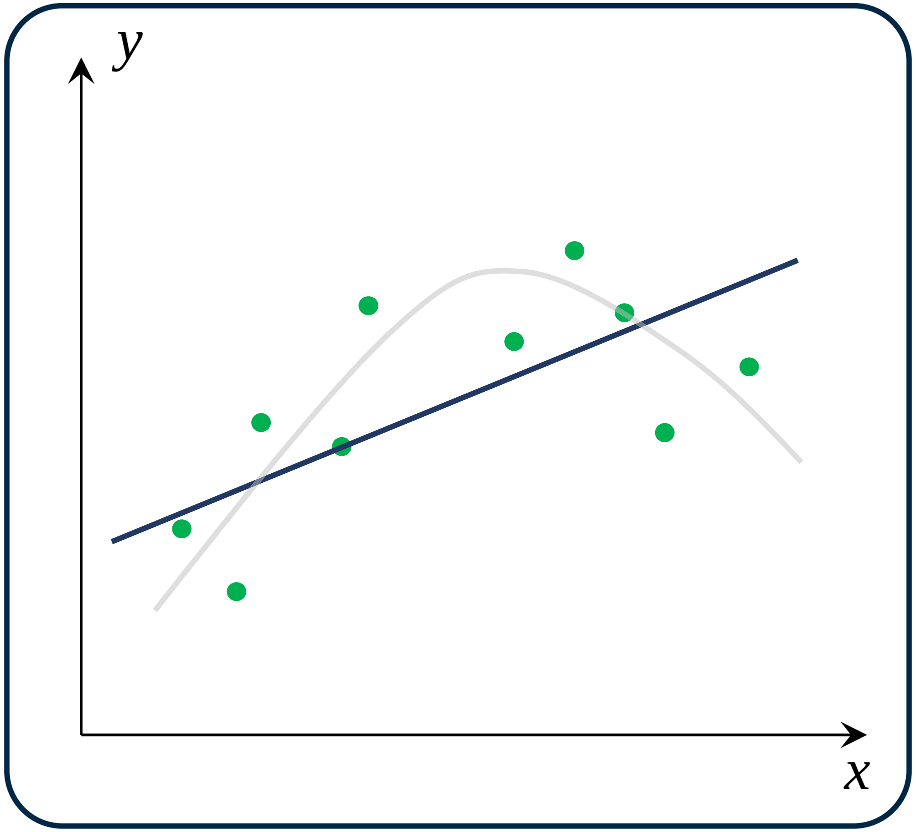
CLASSIFICATION



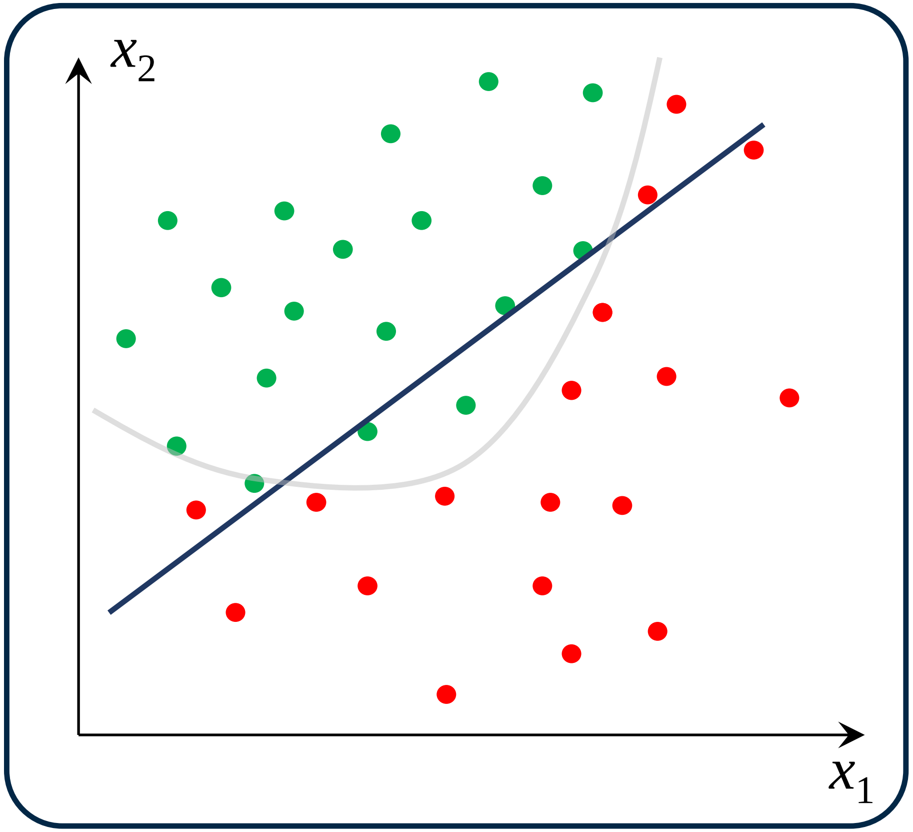
Figures for illustration only.

Simple models

REGRESSION



CLASSIFICATION



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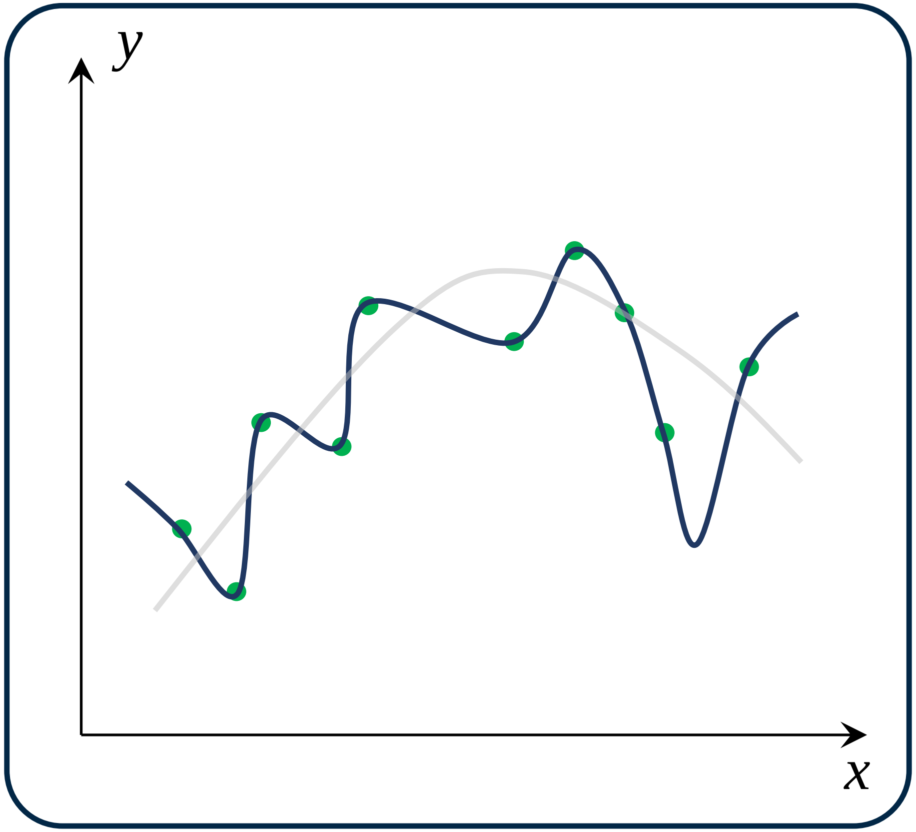
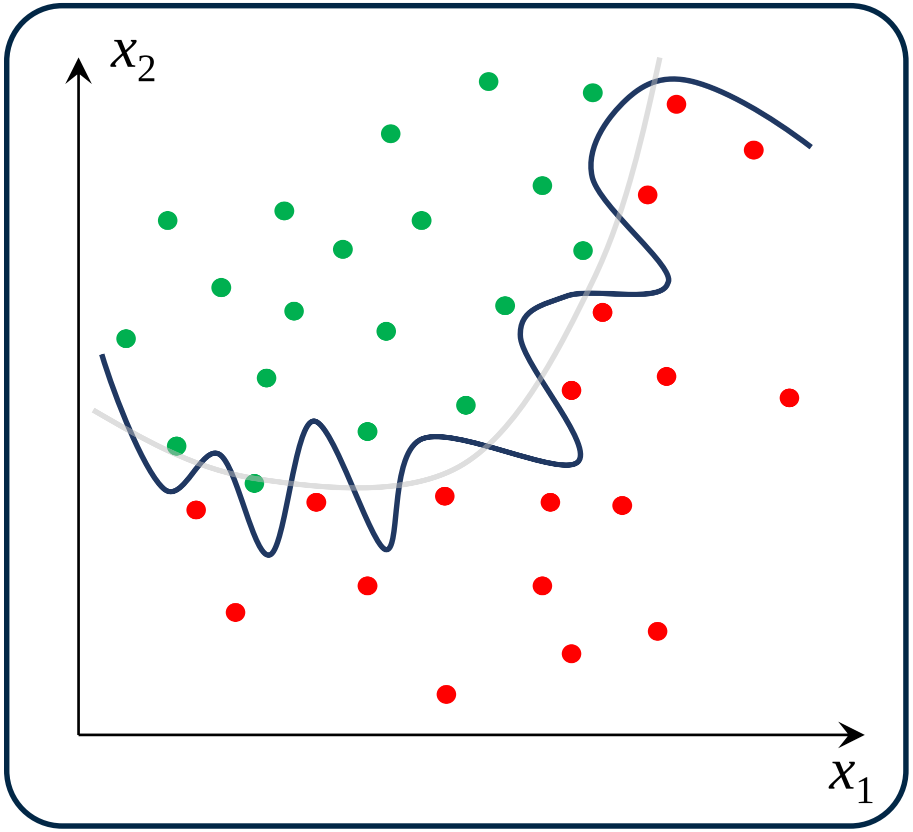
Complex models

REGRESSION



CLASSIFICATION

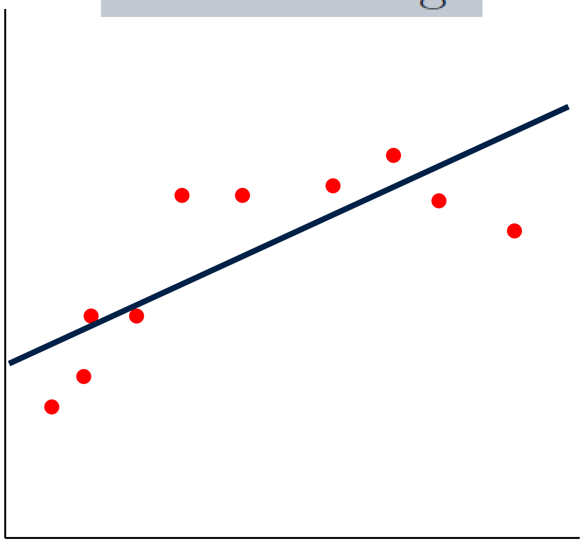


Figures for illustration only.

Model selection

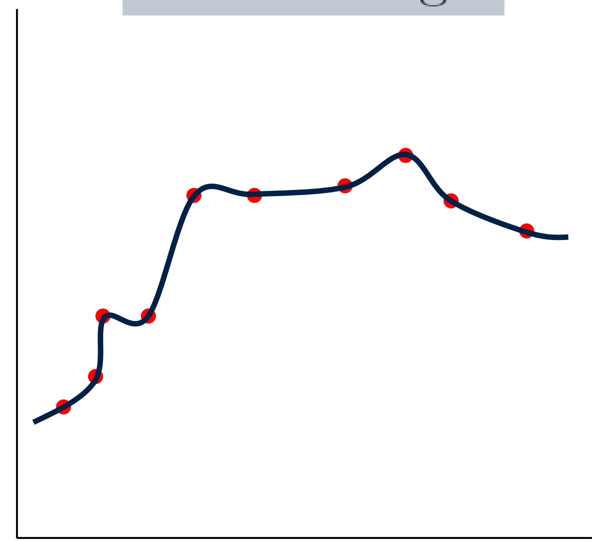
- Inductive bias of the ML algorithm.
- Hypothesis class (of functions) $\mathbb{H}$.

Underfitting



Complexity of $\mathbb{H}$ is low.

Overfitting

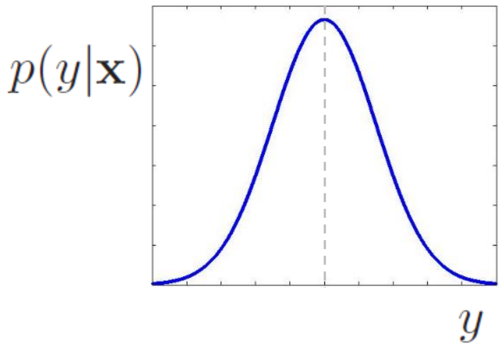


Complexity of $\mathbb{H}$ is high.

- Very complex hypothesis could lead to overfitting.
- Model selection $\rightarrow$ choosing the right $\mathbb{H}$.

Probabilistic modelling

- Many cases of supervised learning need estimation of the distribution $p(y|\mathbf{x})$ over possible outputs y for input $\mathbf{x}$.



- Expected value of the output is the mean of the distribution.
- Gives an estimate of the uncertainty of predictions.
- Two major types of probabilistic modelling approaches:
  - Discriminative modelling: The conditional distribution $p(y|\mathbf{x})$ is estimated directly. The distribution $p(\mathbf{x})$ is not modelled. For example, using $p(y|\mathbf{x},\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}^{\mathrm{T}}\mathbf{x}, \sigma^2)$ to model regression problem.
  - Generative modelling: The conditional distribution $p(y|\mathbf{x})$ is estimated using the joint distribution $p(y,\mathbf{x})$ and the distribution $p(\mathbf{x})$ as $p(y|\mathbf{x},\boldsymbol{\theta}) = p(y,\mathbf{x}|\boldsymbol{\theta})/p(\mathbf{x}|\boldsymbol{\theta})$. These type of approaches model both y and $\mathbf{x}$.

Training and Test datasets

- Dataset is split into two groups:
  - Training dataset is used to train the ML algorithm.
  - Test dataset is used to estimate the error rate of the trained model.

- Shortcomings:
  - If the size of the dataset is small, then keeping aside a separate test dataset can lead to loss of some vital information in the model training stage.
  - "Unfortunate" data split can result in misleading error estimates.
- Solution:
  - K-fold cross-validation
  - Leave-one-out cross-validation