UVA CS 4774: Machine Learning

Lecture 2: Machine Learning in a Nutshell

Dr. Yanjun Qi

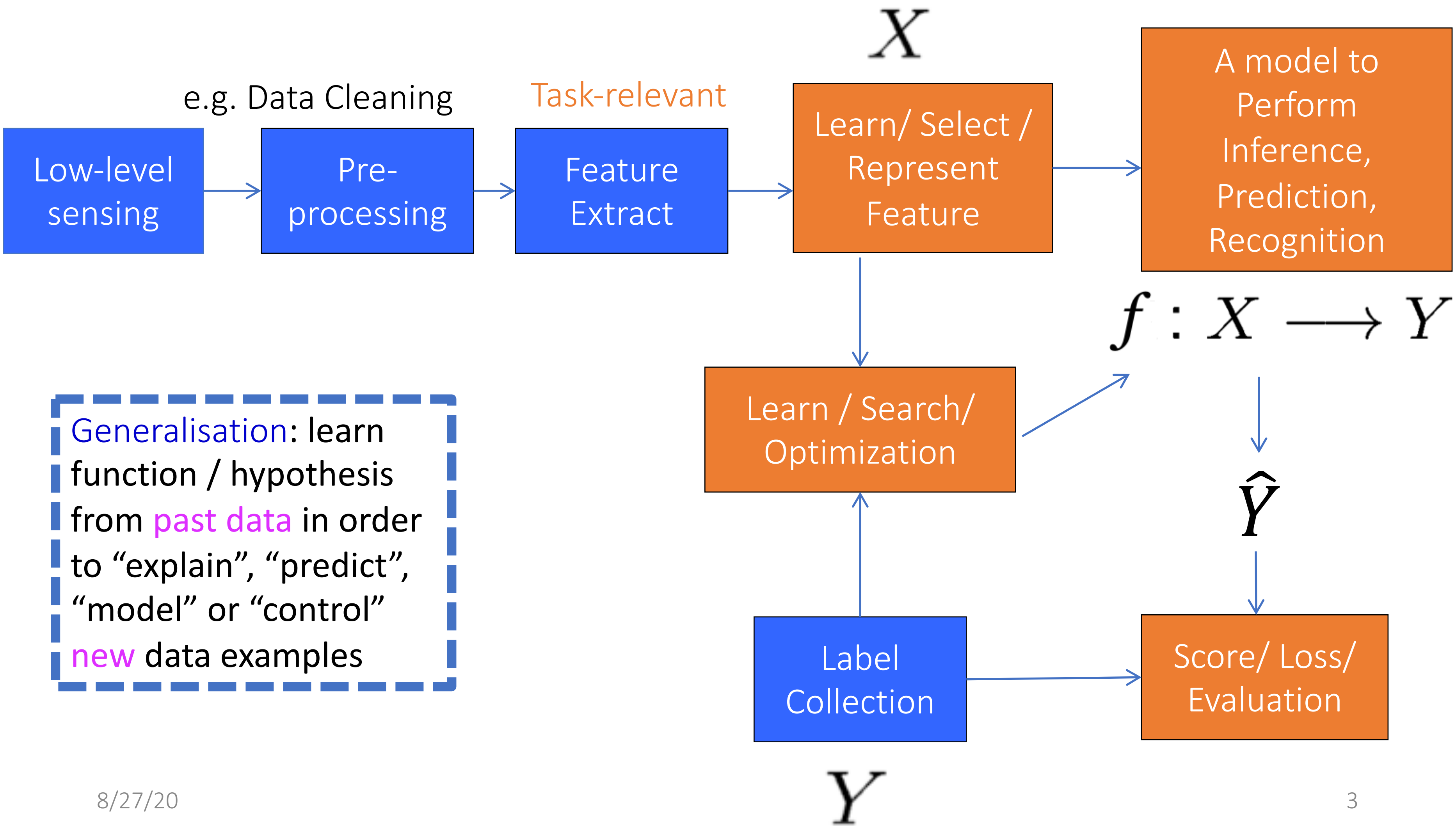
University of Virginia
Department of Computer Science

Roadmap

- Machine Learning in a Nutshell

- Examples of Different Tasks
- Examples of Different Data Types
- Examples of Different Representation Types
- Examples of Different Loss/Cost Types
- Examples of Different Model Properties

A Typical Machine Learning Application’s Pipeline

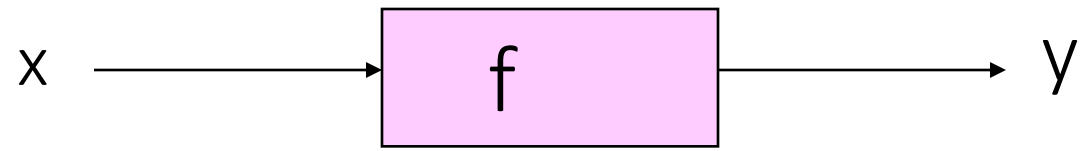


Generalisation: learn function / hypothesis from past data in order to “explain”, “predict”, “model” or “control” new data examples

When to use Machine Learning (Adapt to / learn from data) ?

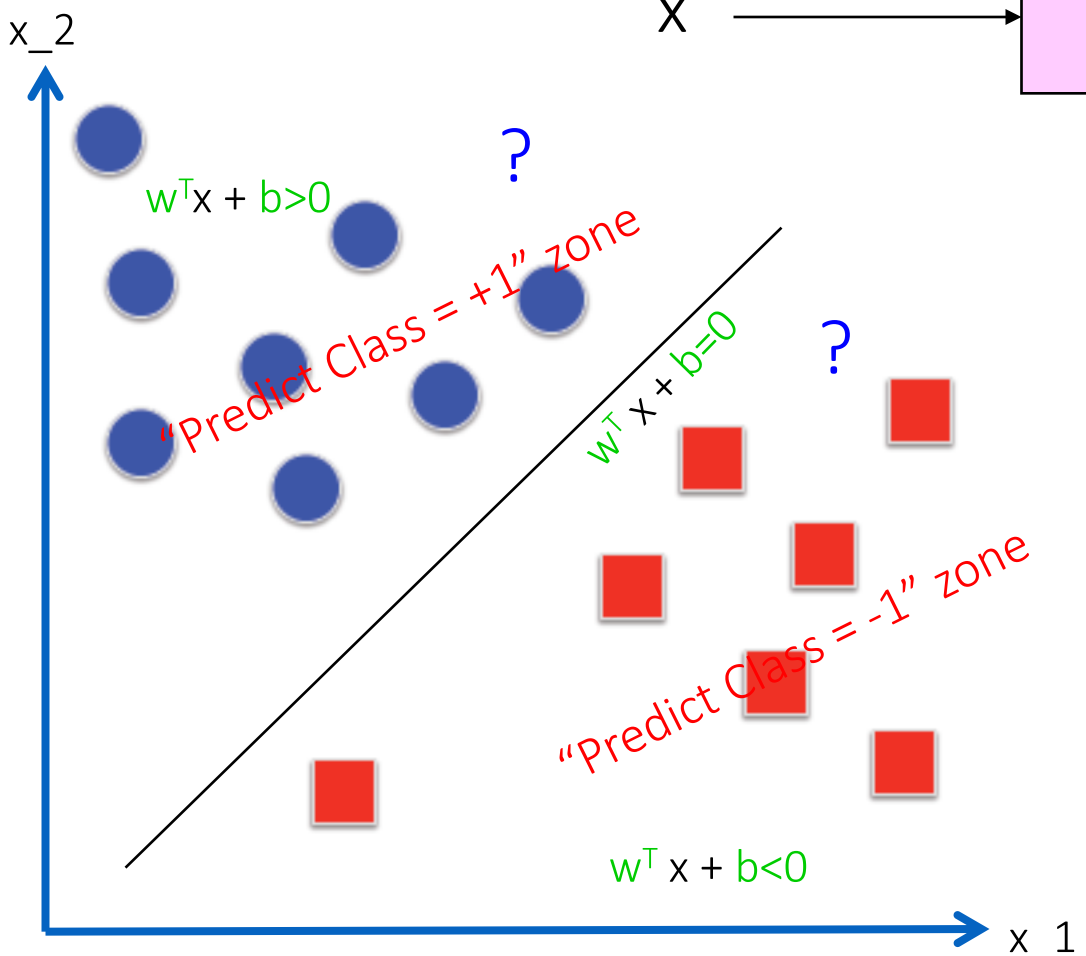
- 1. Extract knowledge from data
  - Relationships and correlations can be hidden within large amounts of data
  - The amount of knowledge available about certain tasks is simply too large for explicit encoding (e.g. rules) by humans
- 2. Learn tasks that are difficult to formalise
  - Hard to be defined well, except by examples, e.g., face recognition
- 3. Create software that improves over time
  - New knowledge is constantly being discovered.
  - Rule or human encoding-based system is difficult to continuously re-design "by hand".

SUPERVISED Linear Binary Classifier
: Binary y / Linear f / X as R^2



$f(x,w,b) = \text{sign}(w^T x + b)$

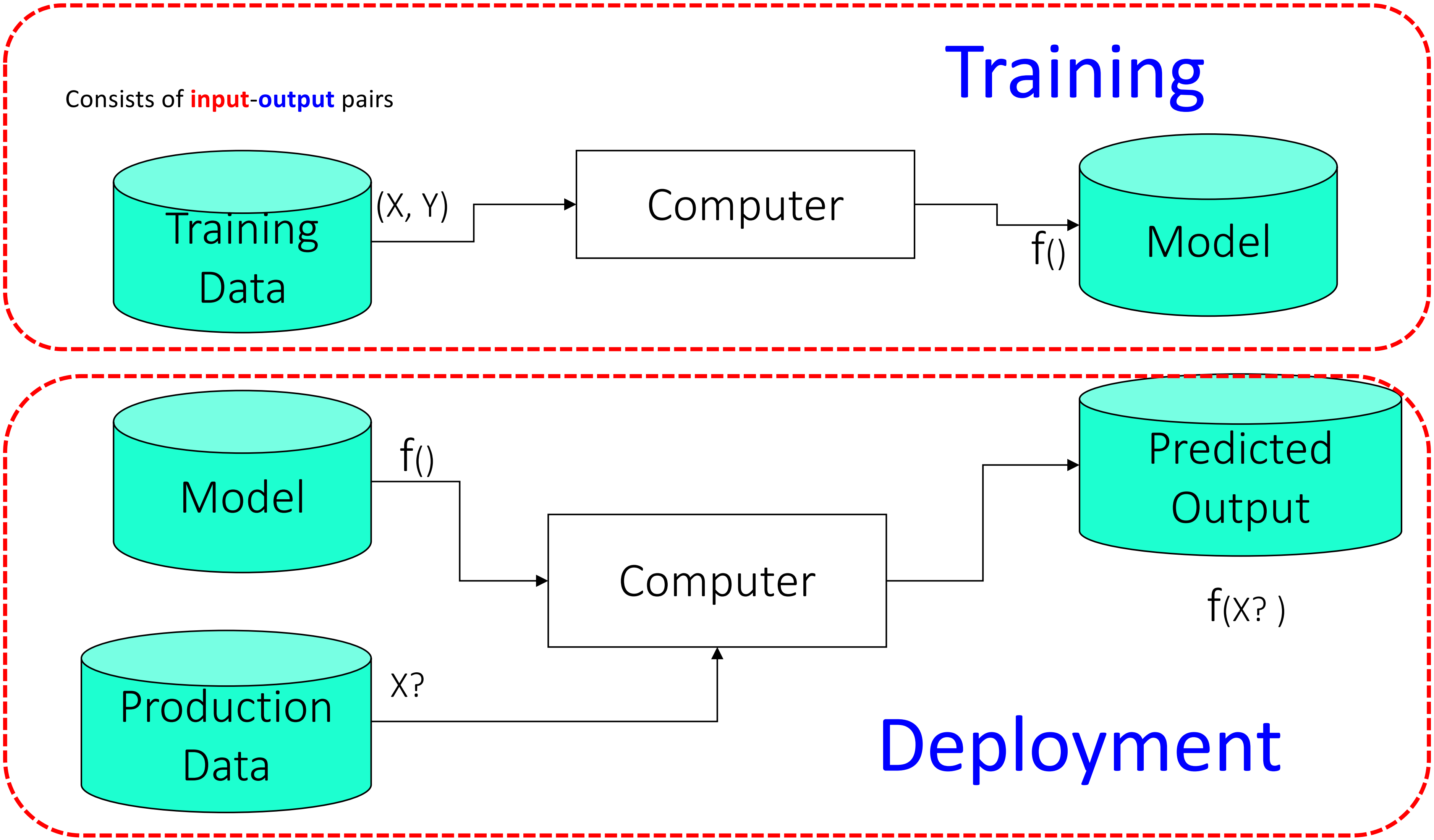
$X = (x\_1, x\_2)$



- denotes +1 point
- denotes -1 point
- ? denotes future points

Courtesy slide from Prof. Andrew Moore's tutorial

Two Modes of Machine Learning



Basic Concepts

- Training (i.e. learning parameters w,b)
  - Training set includes
    - available examples $x_1,\ldots,x_L$
    - available corresponding labels $y_1,\ldots,y_L$

- Find (w,b) by minimizing loss / Cost function L()
  - (i.e. difference between y and f(x) on available examples in training set)

$$(W, b) = \underset{W,\, b}{\operatorname{argmin}} \sum_{i=1}^{L} \ell(f(x_i), y_i)$$

Basic Concepts

- Testing (i.e. evaluating performance on "future" points)
  - Difference between true $y_?$ and the predicted $f(x_?)$ on a set of testing examples (i.e. testing set)
  - Key: example $x_?$ not in the training set

- Generalisation: learn function / hypothesis from past data in order to "explain", "predict", "model" or "control" new data examples

Machine Learning in a Nutshell

Data

↓

Task

↓

Representation

↓

Score Function

↓

Search/Optimization

↓

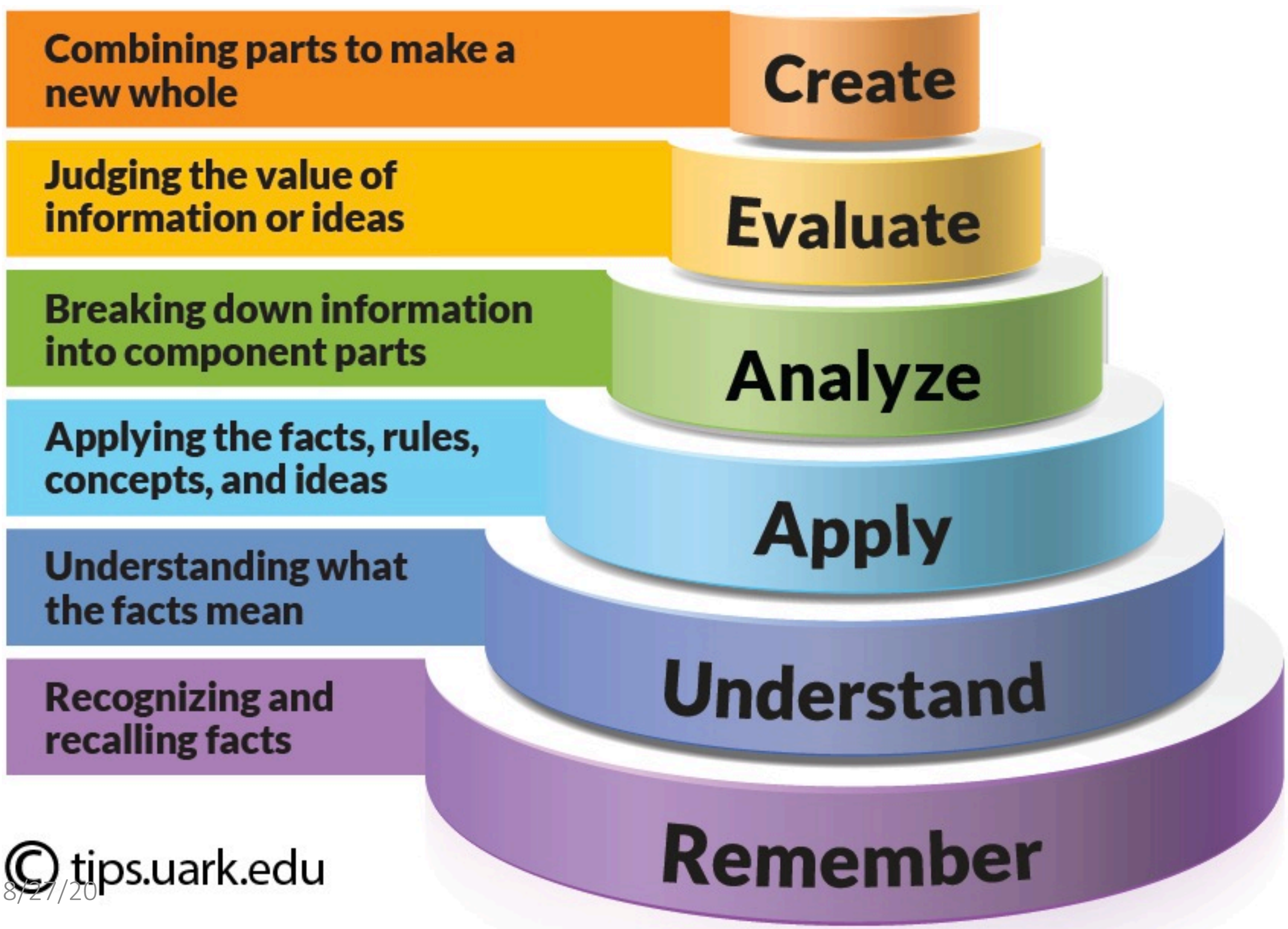
Models, Parameters

ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

My Teaching Guide: Bloom's Taxonomy on Cognitive Learning



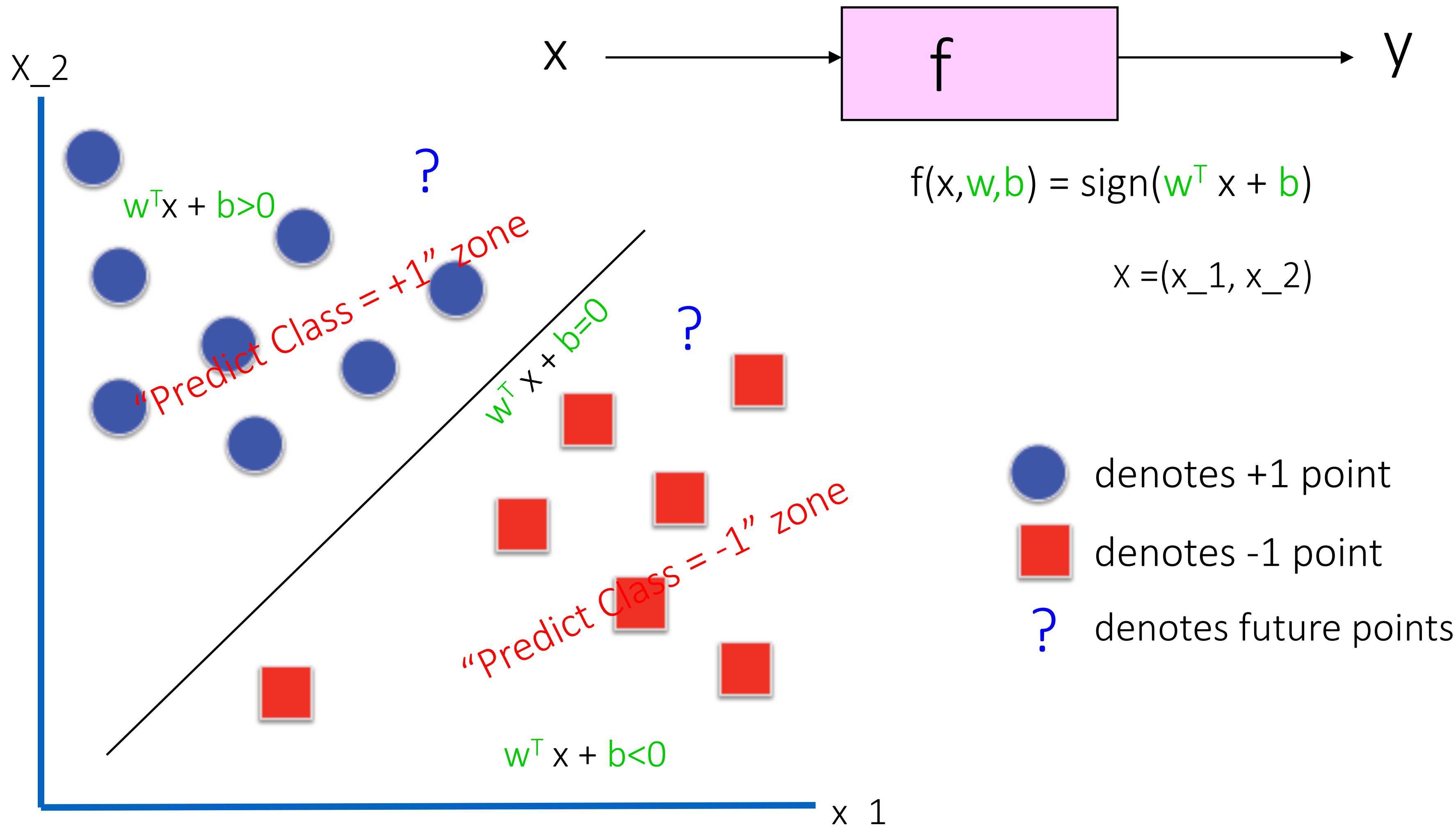
What we have covered

Data	
Task	
Representation	
Score Function	
Search/Optimization	
Models, Parameters	

What we will cover

Data	Tabular, 1-D sequential, 2-D Grid like Imaging, 3-D VR, Graph, Set
Task	Regression, classification, clustering, dimen-reduction
Representation	Linear func, nonlinear function (e.g. polynomial expansion), local linear, logistic function (e.g. p(c|x)), tree, **multi-layer, prob-density family (e.g. Bernoulli, multinomial, Gaussian, mixture of Gaussians), local func smoothness, kernel matrix, local smoothness, partition of feature space,**
Score Function	MSE, Margin, log-likelihood, EPE (e.g. L2 loss for KNN, 0-1 loss for Bayes classifier), cross-entropy, cluster points distance to centers, variance, conditional log-likelihood, complete data-likelihood, regularized loss **func (e.g. L1, L2) , goodness of inter-cluster similar**
Search/ Optimization	Normal equation, gradient descent, stochastic GD, Newton, Linear programming, Quadratic programming (quadratic objective with linear constraints), greedy, EM, asyn-SGD, **eigenDecomp, backprop**
Models, Parameters	Linear weight vector, basis weight vector, local weight vector, dual weights, training samples, tree-**dendrogram, multi-layer weights, principle components, member (soft/hard) assignment, cluster centroid, cluster covariance (shape), …**

SUPERVISED Linear Binary Classifier



$f(x,w,b) = sign(w^T x + b)$

$X = (x\_1, x\_2)$

Courtesy slide from Prof. Andrew Moore's tutorial

Nutshell for the simple Linear Supervised Classifier

Data

↓

Task

↓

Representation

↓

Score Function

↓

Search/Optimization

↓

Models,
Parameters,
Metrics

Tabular (R^2)

↓

Classification: Output Y is binary

↓

Linear Decision Boundary

$f(x, w, b) = \text{sign}(w^T x + b)$

↓

$$(W, b) = \underset{W,\, b}{\text{argmin}} \sum_{i=1}^{L} \ell(f(x_i), y_i)$$

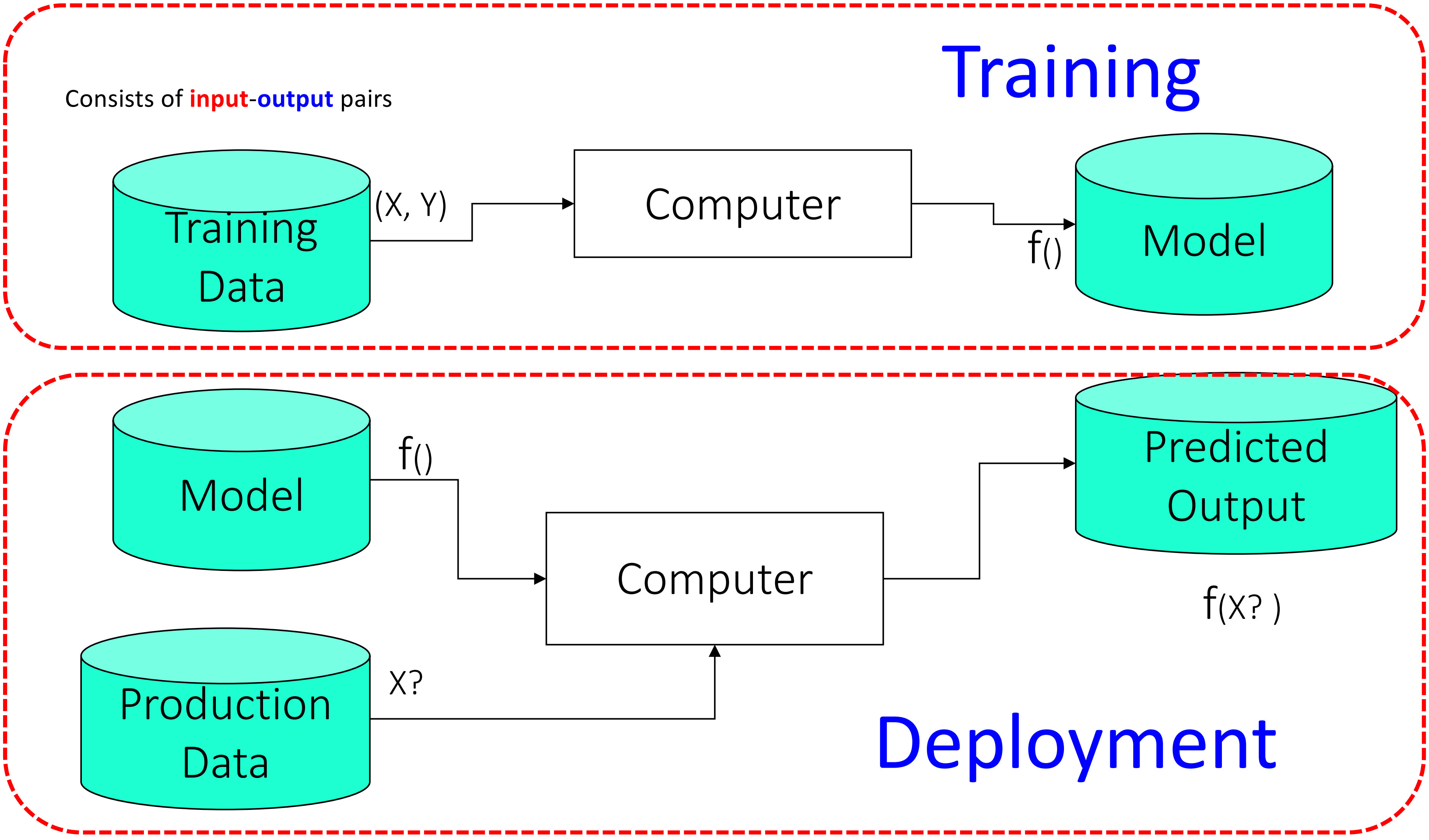
↓

?

↓

e.g., Classification Error on
future points (Testing Data)

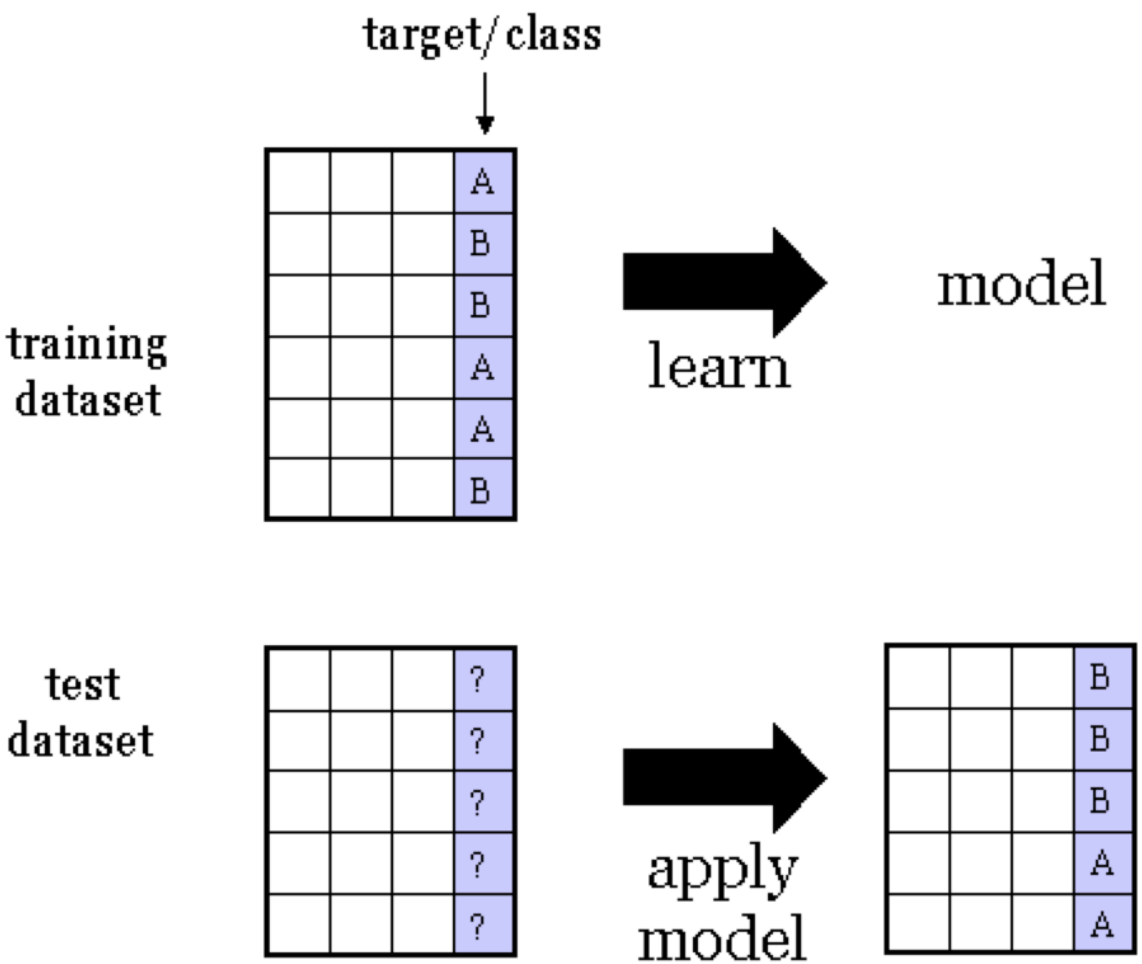
Two Modes of Machine Learning



https://scikit-learn.org/stable/tutorial/basic/tutorial.html

https://colab.research.google.com/drive/1oEGNhQ55iBNElYqfZpueSE2l_g3tQxSD?usp=sharing

I will code-run through: Recognizing hand-written digits with L2.ipynb
Adapted from: ScikitLearn Tutorial plot_digits_classification.ipynb



Training dataset consists of input-output pairs


Thank You

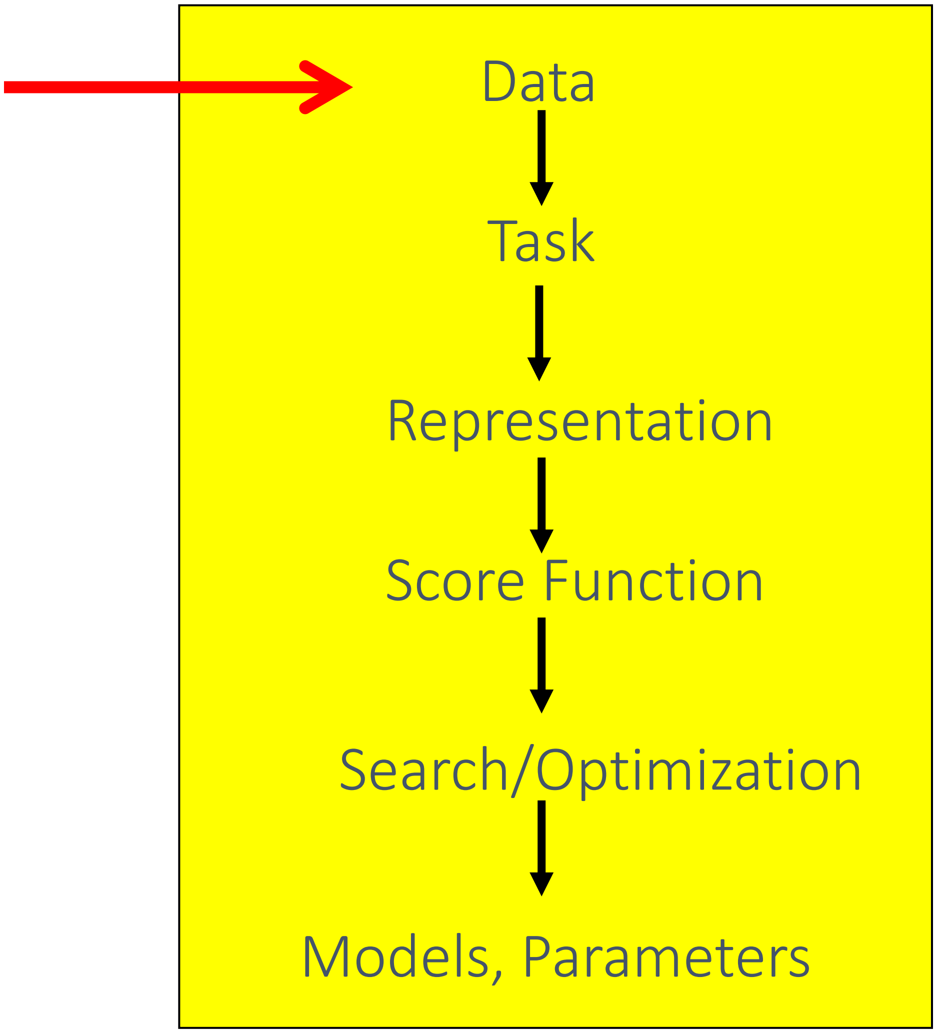
Roadmap

- Machine Learning in a Nutshell

- Examples of Different Data Types
- Examples of Different Tasks

- Examples of Different Representation Types
- Examples of Different Loss/Cost Types
- Examples of Different Model Properties

Machine Learning in a Nutshell

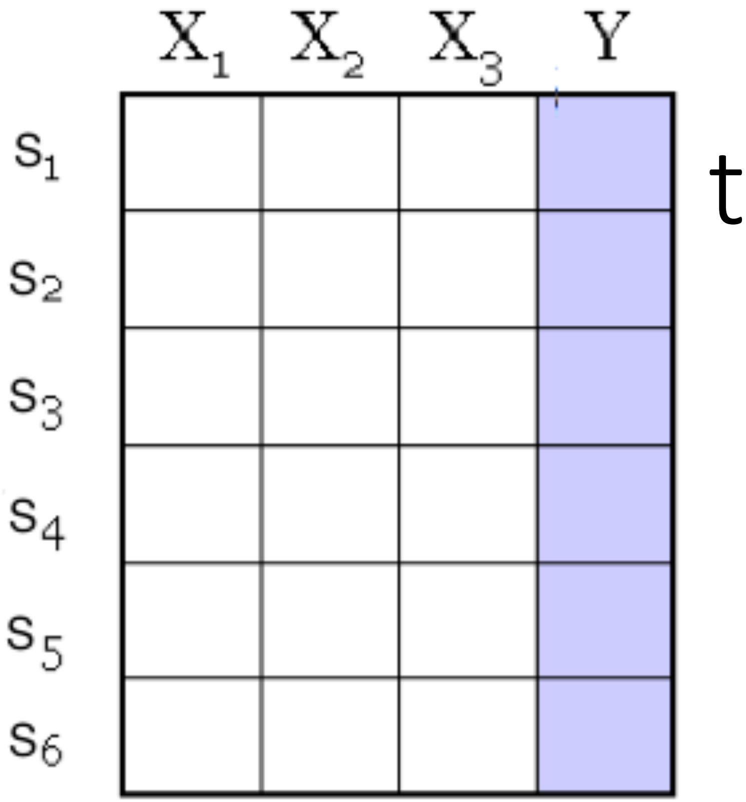


ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

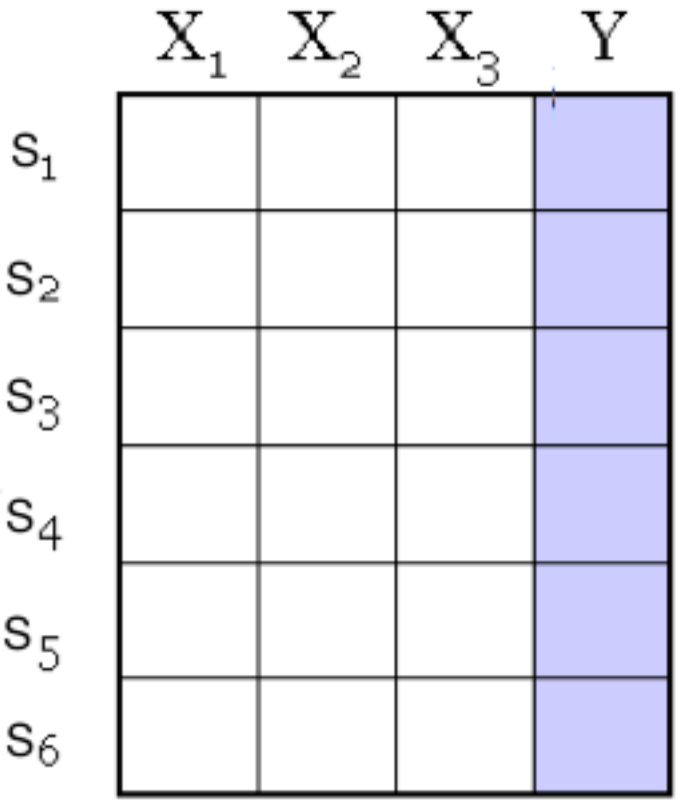
Tabular Data Type



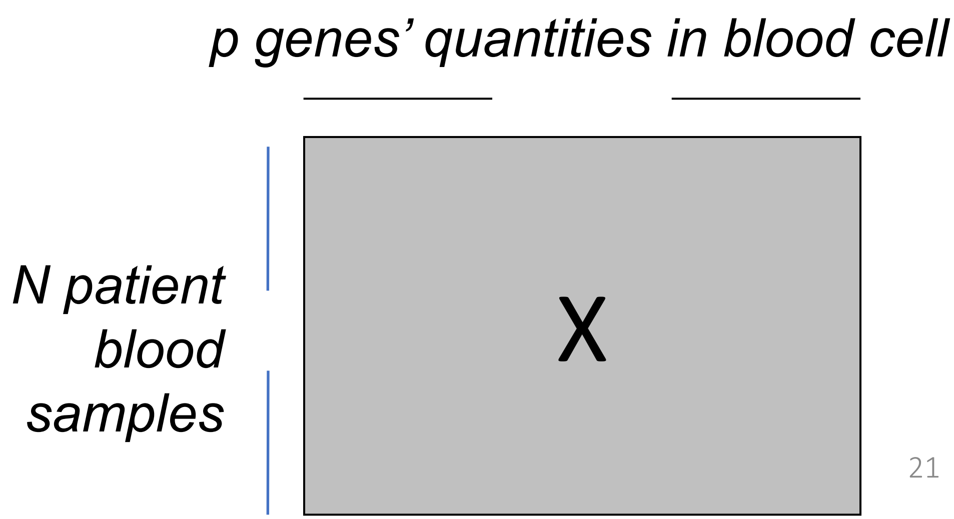
$$f : \boxed{X} \longrightarrow \boxed{Y}$$

- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target**/*outcome/response/label/dependent variable*: special column to be predicted [last column]

Main Types of Columns



- *Continuous*: a real number, for example, weight
- *Discrete*: a symbol, like “Good” or “Bad”



$$\mathbf{X}_{train} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y}_{train} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

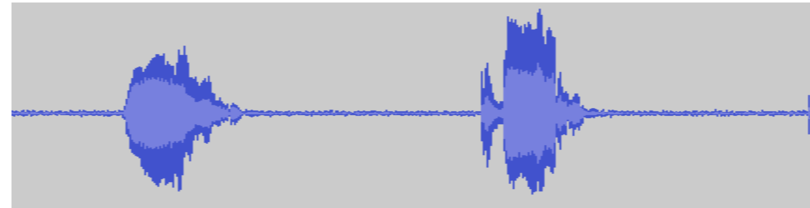
training dataset

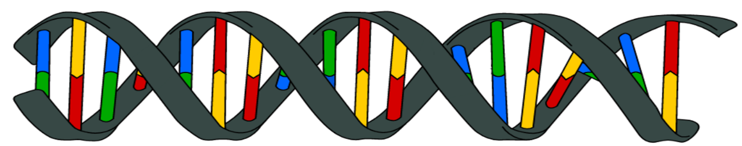
test dataset

$$\mathbf{X}_{test} = \begin{bmatrix} -- & \mathbf{x}_{n+1}^T & -- \\ -- & \mathbf{x}_{n+2}^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_{n+m}^T & -- \end{bmatrix} \qquad \vec{y}_{test} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \\ y_{n+m} \end{bmatrix}$$

Sequence Data Type (eg. Language, Genome, Audio)

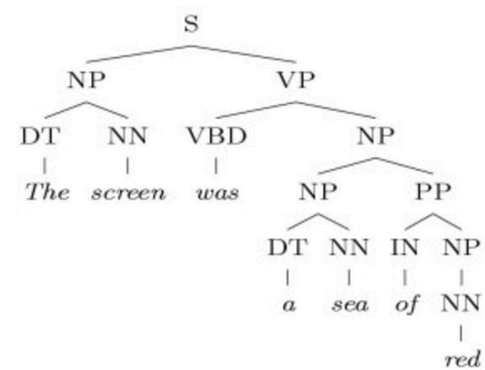
x I believe that this book is not at all helpful since it does not explain thoroughly the material . it just provides the reader with tables and calculations that sometimes are not easily understood …



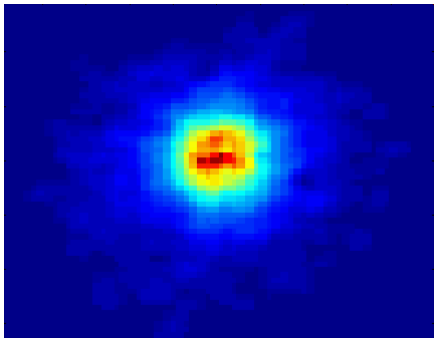


The screen was a sea of red

Language Parsing →



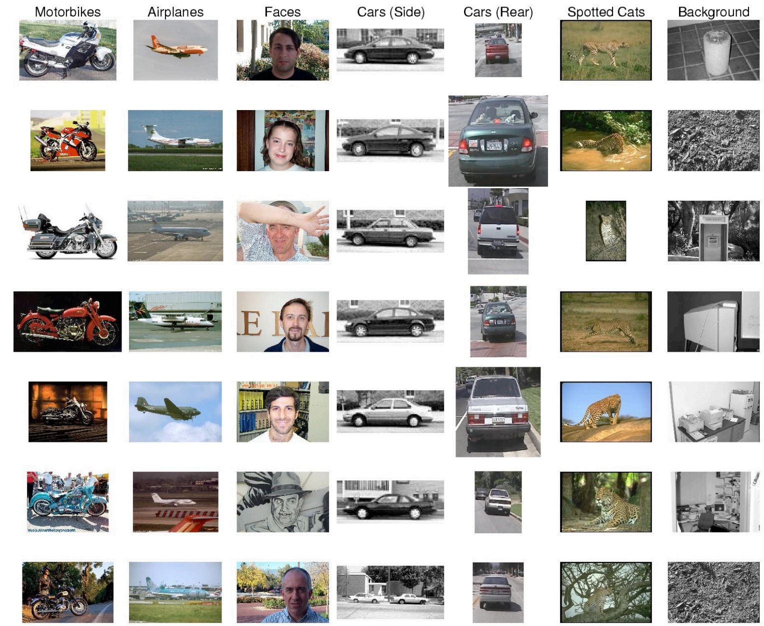
2D Grid Data Type (eg. Images)



e.g.,
- 72 million stars, 20 million galaxies
- Object Catalog: 9 GB
- Image Database: 150 GB

Figure S6 Illustrative Examples of Chest X-Rays in Patients with Pneumonia,

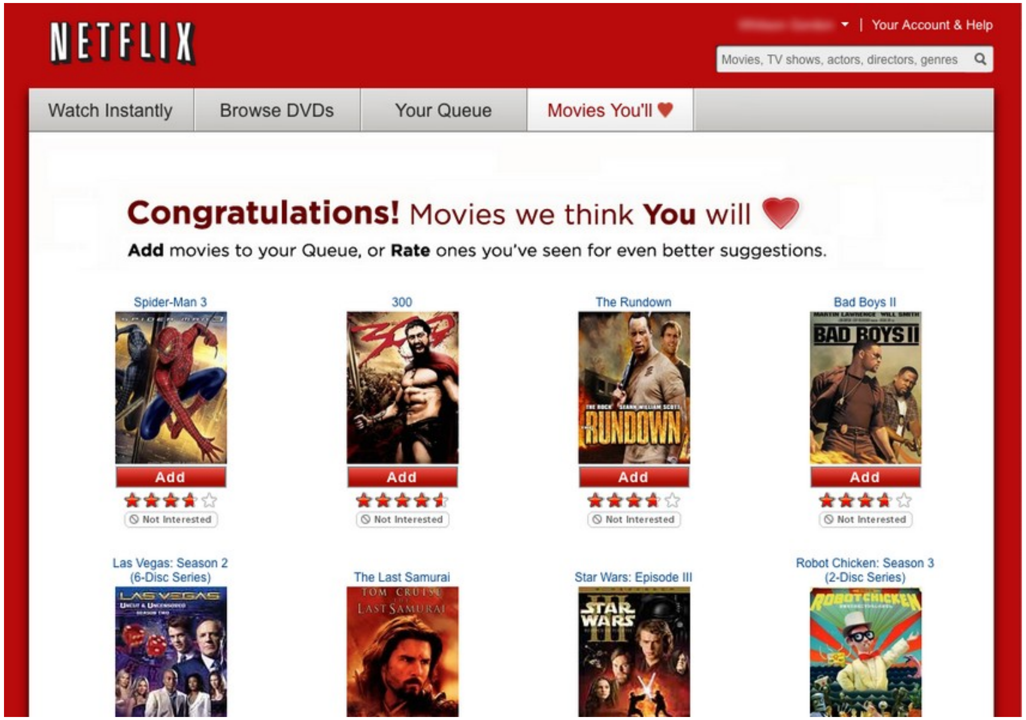
5,232 chest X-ray images from children, including 3,883 characterized as depicting pneumonia (2,538 bacterial and 1,345 viral) and 1,349 normal, from a total of 5,856 patients

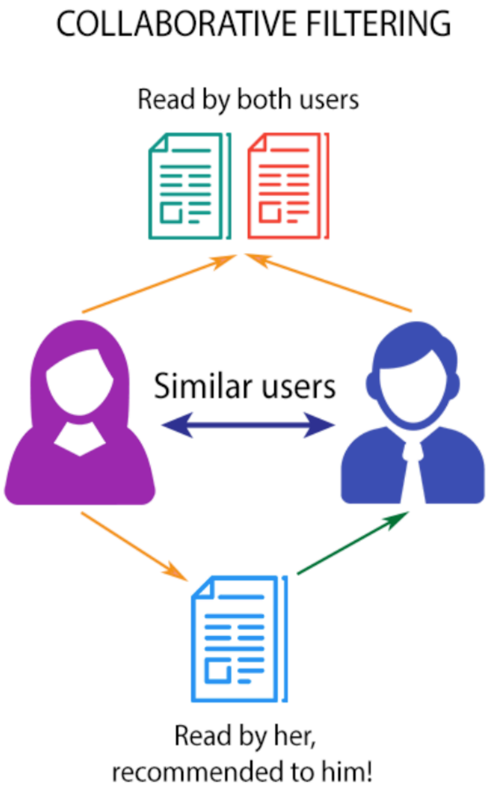


ImageNet Competition:

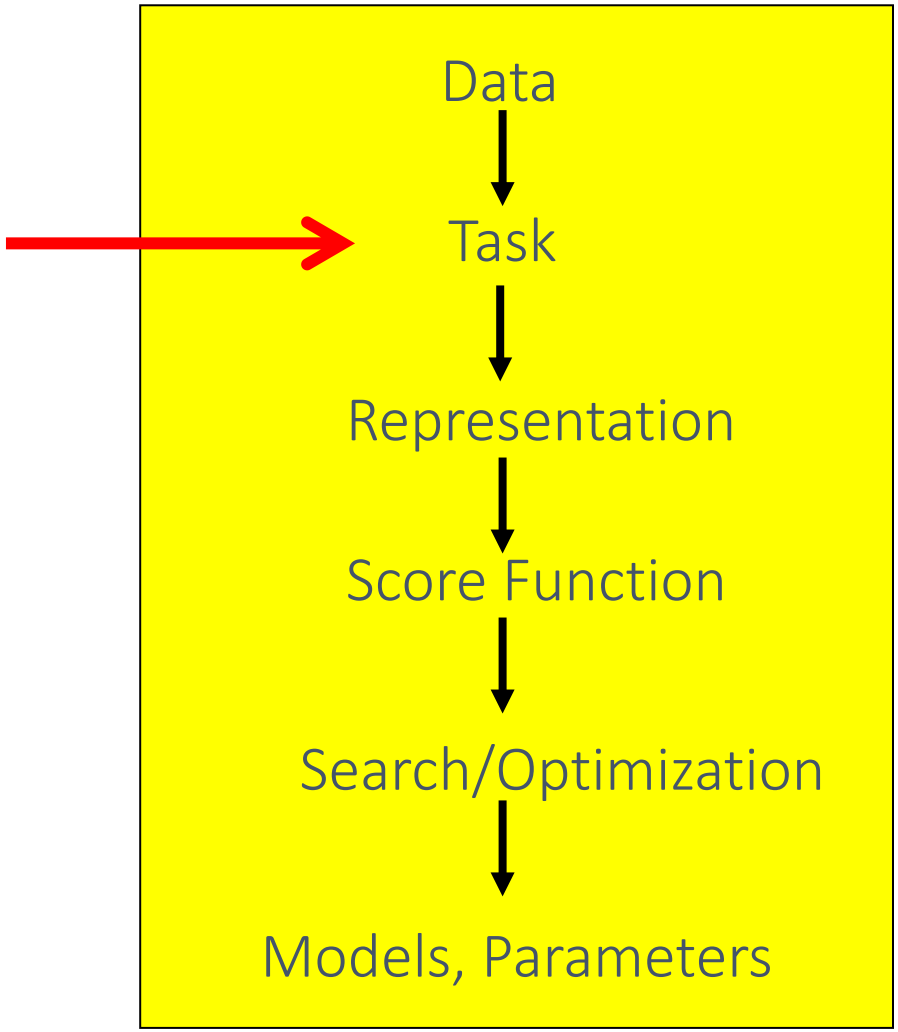
[Training on 1.2 million images [X] vs. 1000 different word labels [Y]]

Graph Data Type (eg. Social Network)





Machine Learning in a Nutshell

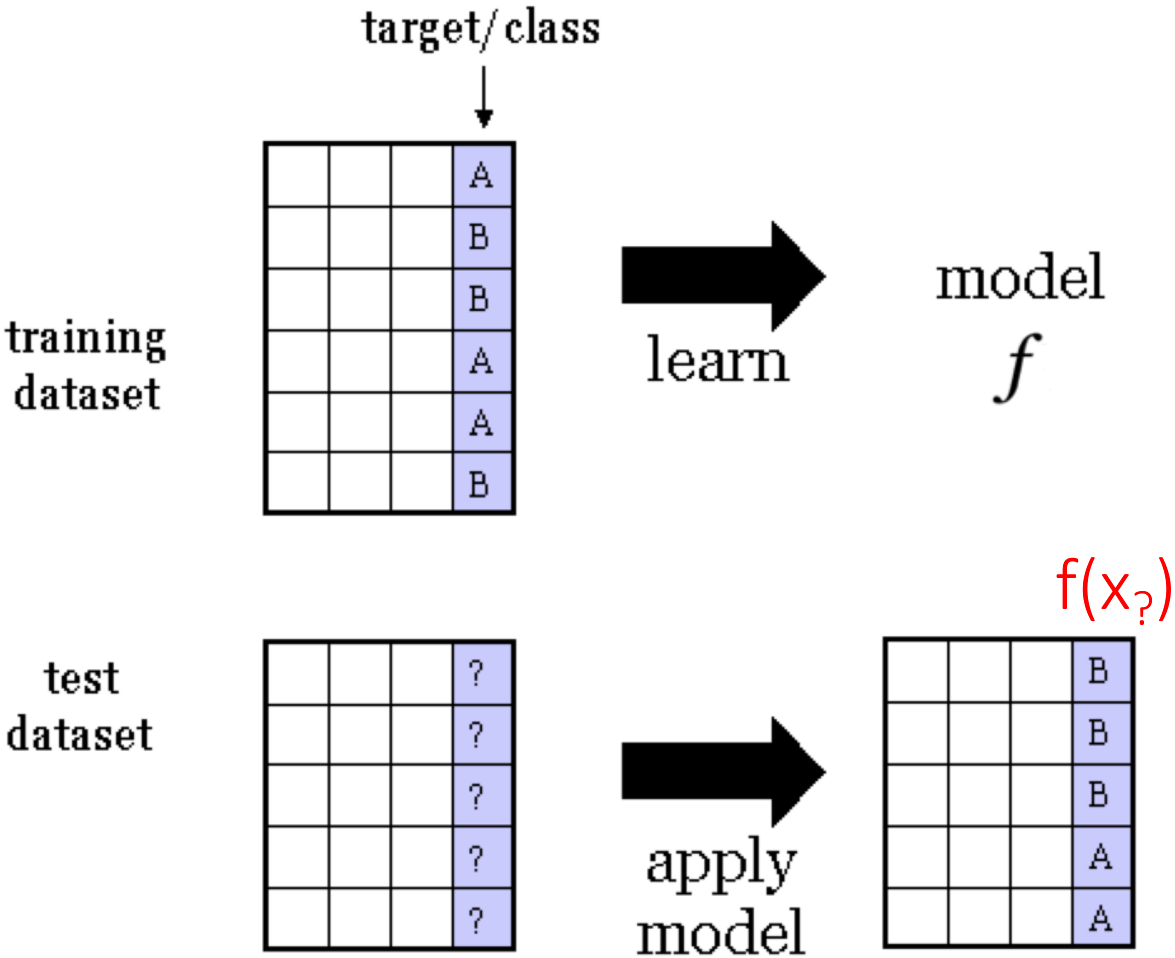


ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

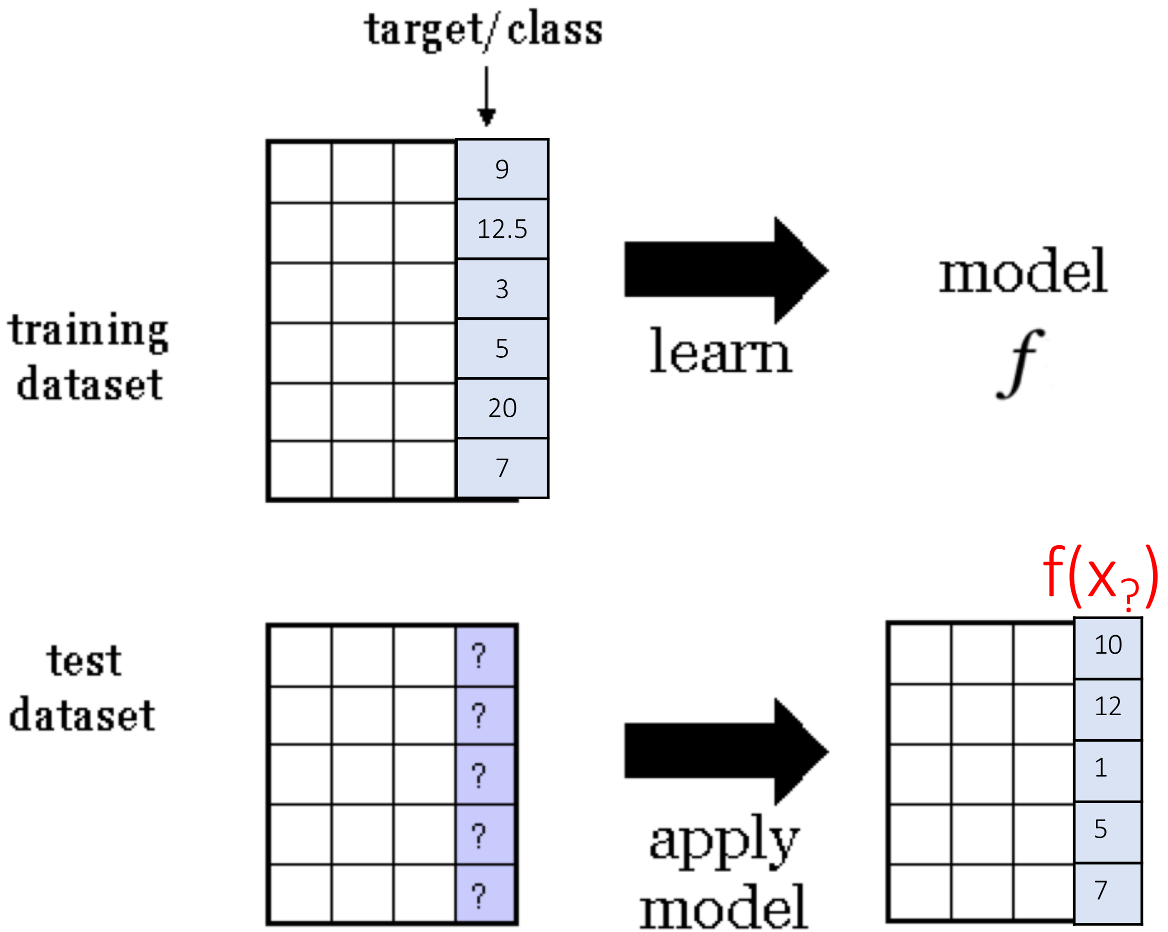
e.g. SUPERVISED Classification



Training dataset consists of input-output pairs

- e.g. target Y can be a discrete target variable

e.g. SUPERVISED Regression

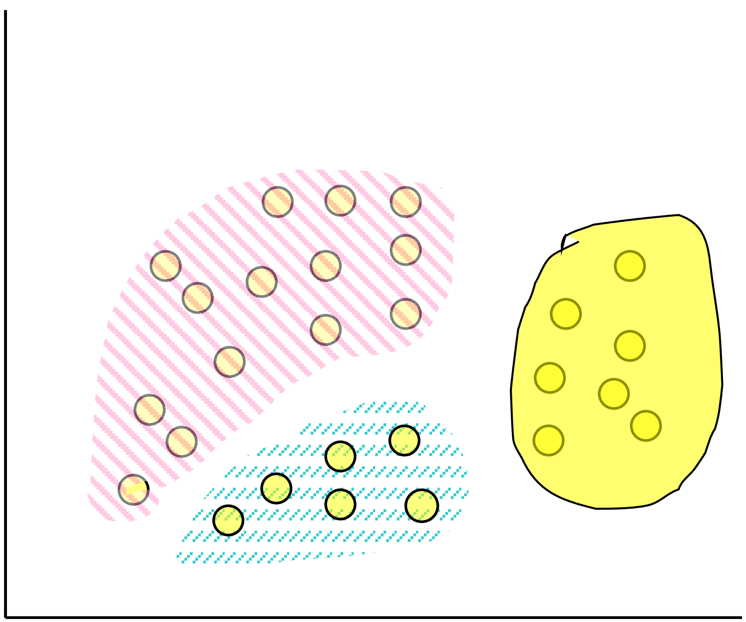


Training dataset consists of input-output pairs

- e.g. target Y can be a continuous target variable

Unsupervised LEARNING : [No Given Y]

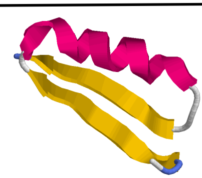
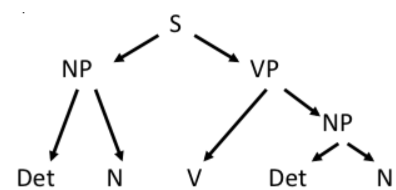
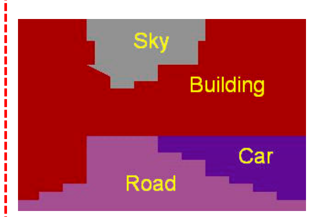
- No labels are provided (e.g. No Y provided)
- Find patterns from unlabeled data, e.g. clustering



e.g. clustering => to find "natural" grouping of instances given un-labeled data

Structured Output LEARNING : [Complex Y]

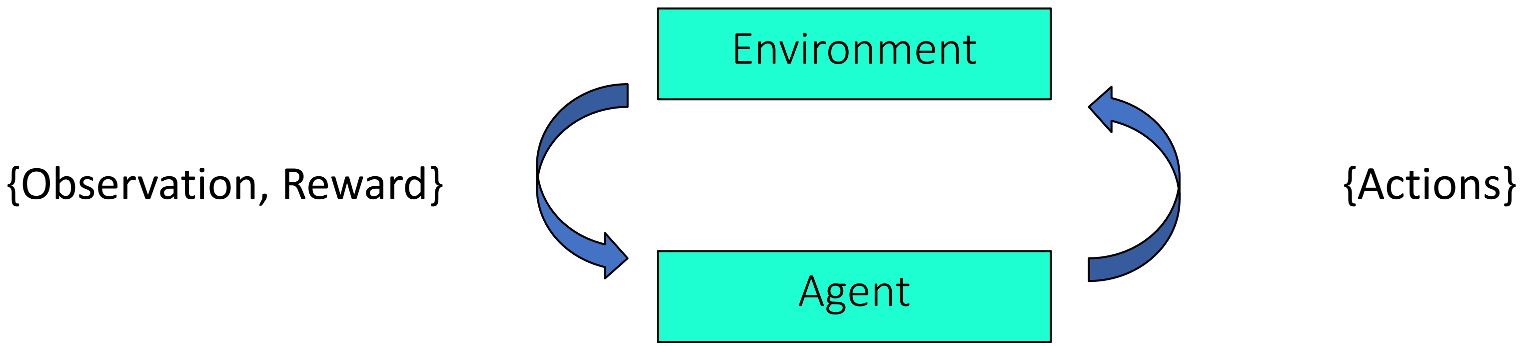
- Many prediction tasks involve output labels having structured correlations or constraints among instances

Structured Dependency between Examples' Y	Sequence	Tree	Grid
Input X	APAFSVSPASGACGPECA…	The dog chased the cat	
Output Y	 CCEEEEECCCCCHHHCCC…		

Many more possible structures between y_i , e.g. spatial , temporal, relational …

Reinforcement Learning (RL) [Not IID, Sequential]

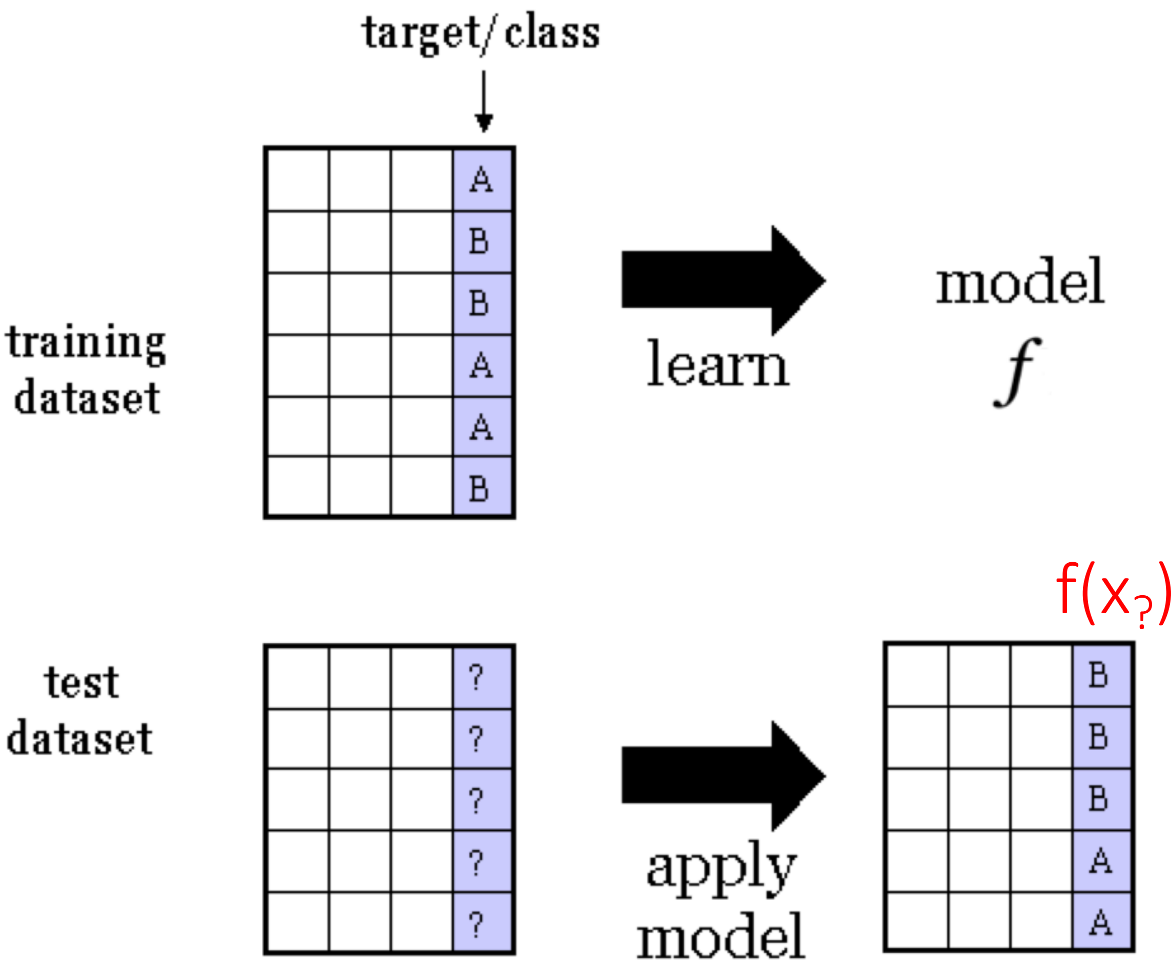
- What’s Reinforcement Learning?



- Agent interacts with an environment and learns by maximizing a scalar reward signal
  - Basic version: No labels or any other supervision signal.
  - Variation like imitation learning: supervised

Adapt from Professor Qiang Yang of HK UST

(Most popular:) SUPERVISED Classification



Training dataset consists of input-output pairs

- e.g. target Y can be a discrete target variable

Many Variants of SUPERVISED Classification

- Binary Classification
- Multi-class Classification
- Hierarchical Classification
- Multi-label Classification
- Structured Predictions
- ……

Binary: Text Review-based Sentiment Classification

x

I believe that this book is not at all helpful since it does not explain thoroughly the material . it just provides the reader with tables and calculations that sometimes are not easily understood …

Input X : e.g. a piece of English text

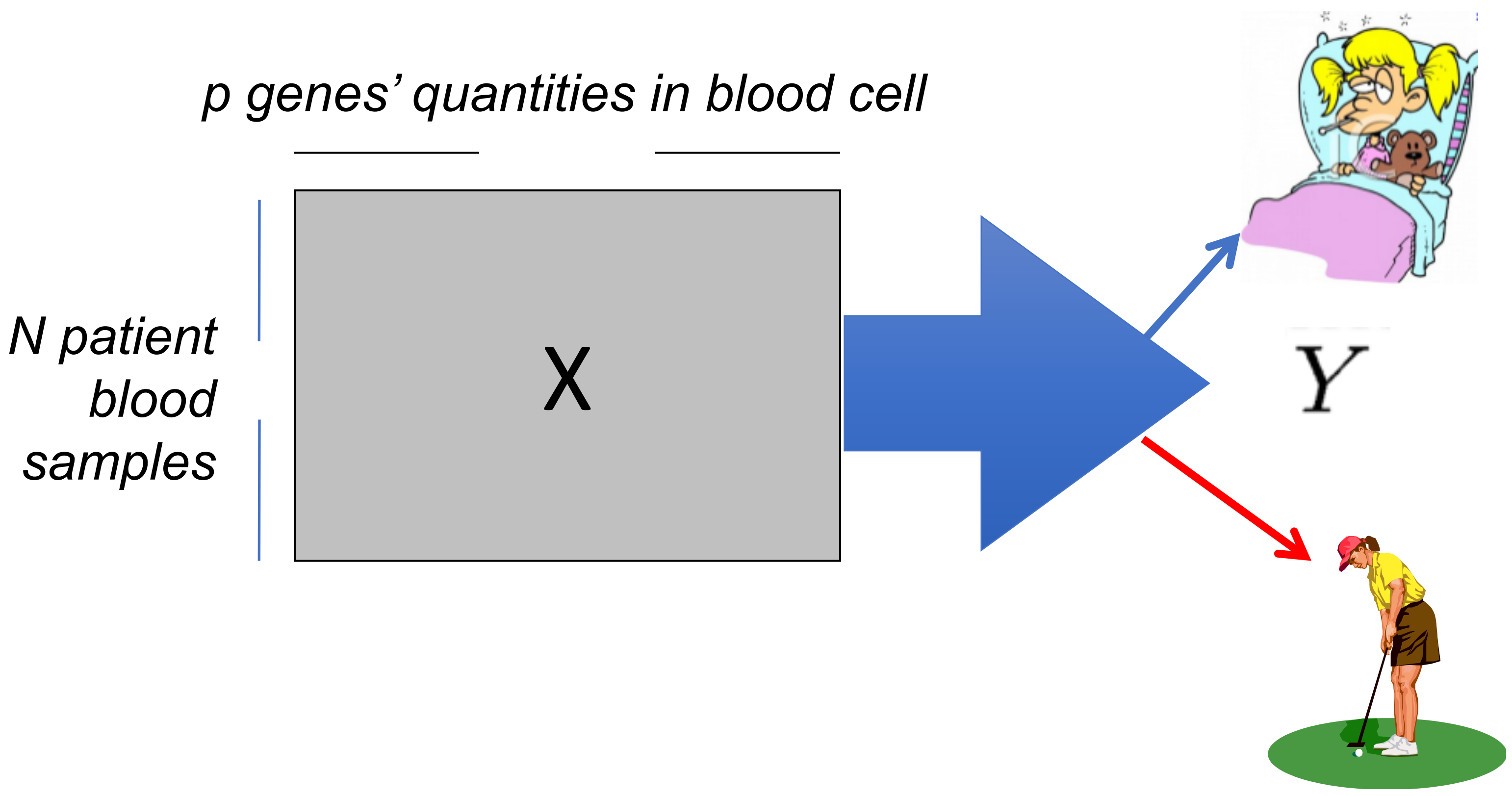
$\longrightarrow$

y -1

Output Y: {1 / Yes , -1 / No }

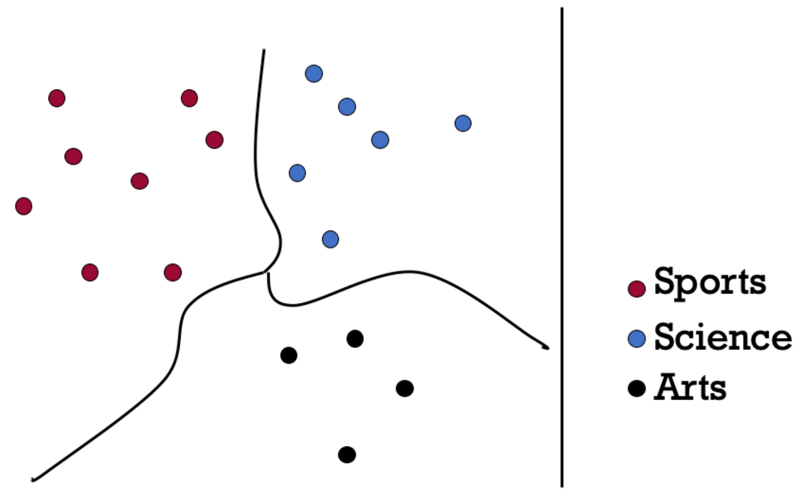
e.g. Is this a positive product review ?

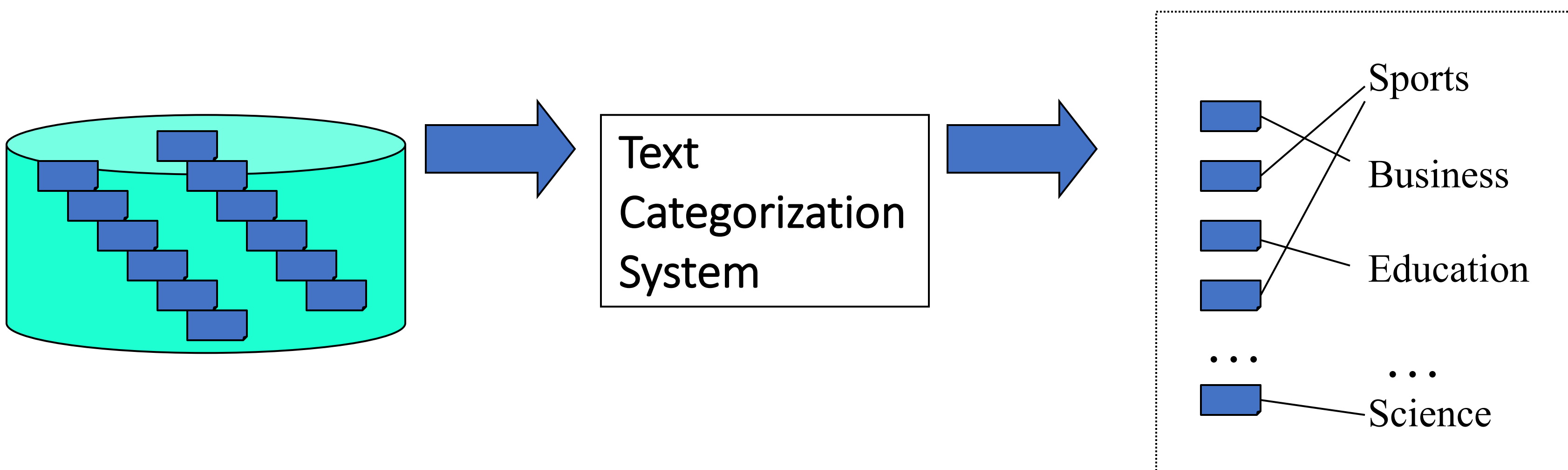
Binary: : Disease Classification using gene expression



Multi-Class: Text Categorization

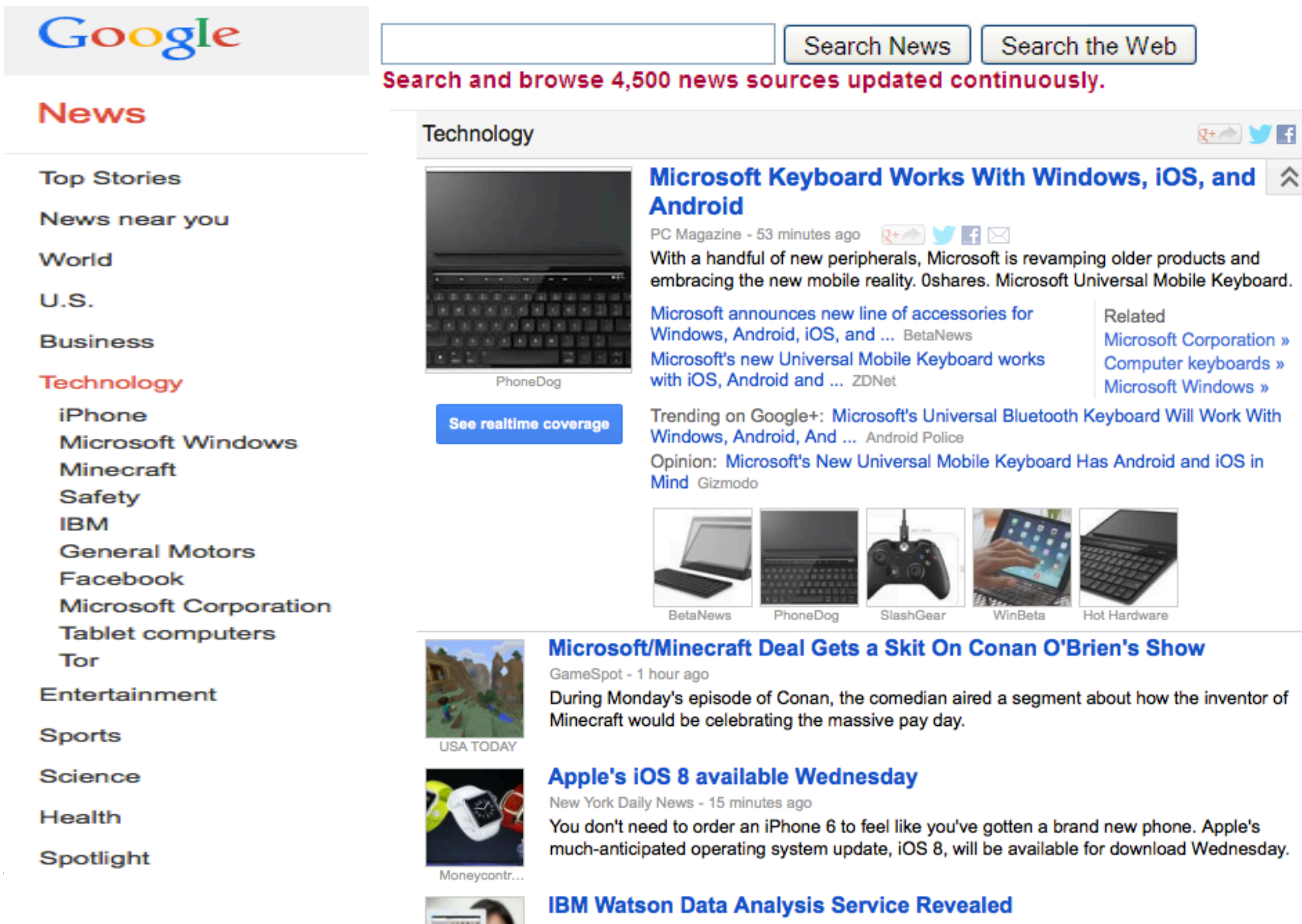
- Almost the most basic/ standard supervised classification problem





$$\hat{y} = f(x)$$

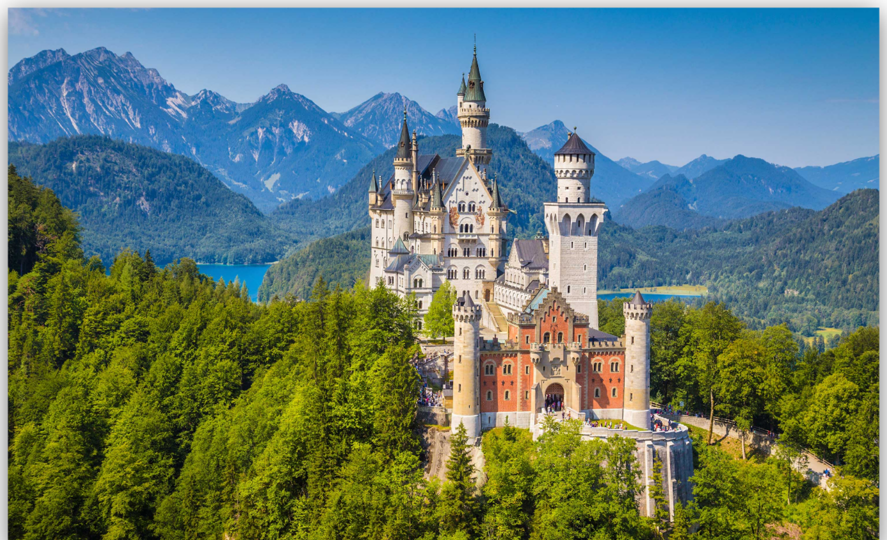
Hierarchical: Text Categorization, e.g. Google News



Multi Label Classification (MLC)

- MLC is the task of assigning a set of target labels for a given sample
- Given input ***x***, predict the set of labels $\{ y_1, y_2, \ldots, y_L \}$, $y_i \in \{0,1\}$

x



y_1 **Castle** ✓

y_2 **City** ✗

y_3 **Mountains** ✓

y_4 **Car** ✗

y_5 **Road** ✓

Edges2Image

[Isola et al. CVPR 2017]

Text2Image

this small bird has a pink breast and crown, and black primaries and secondaries.

this magnificent fellow is almost all black with a red crest, and white cheek patch.

the flower has petals that are bright pinkish purple with white stigma

this white and yellow flower have thin white petals and a round yellow stamen

[Reed et al. ICML 2016]

Thank You

Roadmap

- Machine Learning in a Nutshell

- Examples of Different Tasks
- Examples of Different Data Types

- Examples of Different Representation Types
- Examples of Different Loss/Cost Types
- Examples of Different Model Properties

Machine Learning in a Nutshell

Data

↓

Task

↓

→ Representation

↓

Score Function

↓

Search/Optimization

↓

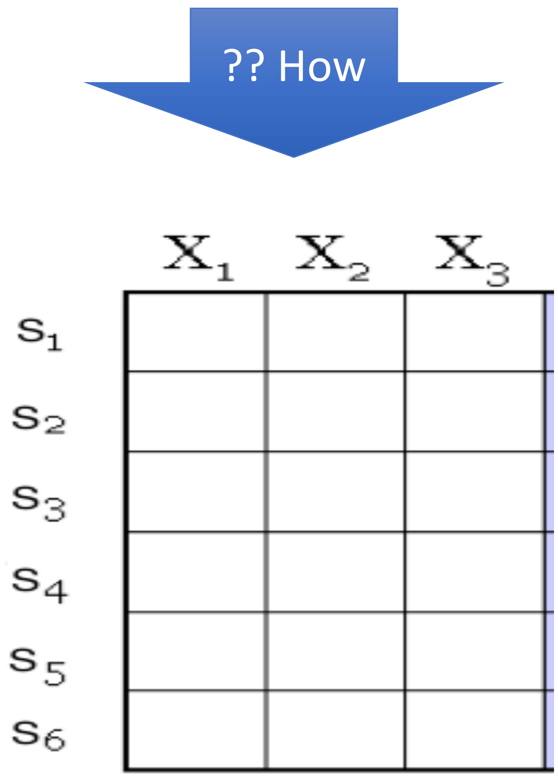
Models, Parameters

ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

- Text / String / Symbolic
- Sequences / Sets / Graph
  - Variable length
  - Discrete
  - Combinatorial
  - Spatial ordering among units

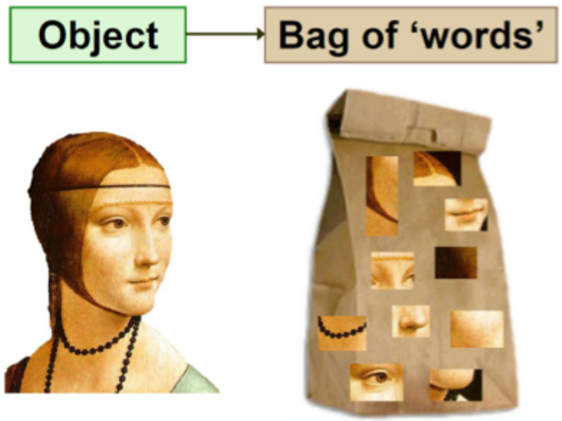


Vector Space Representation: Bag of Words Trick

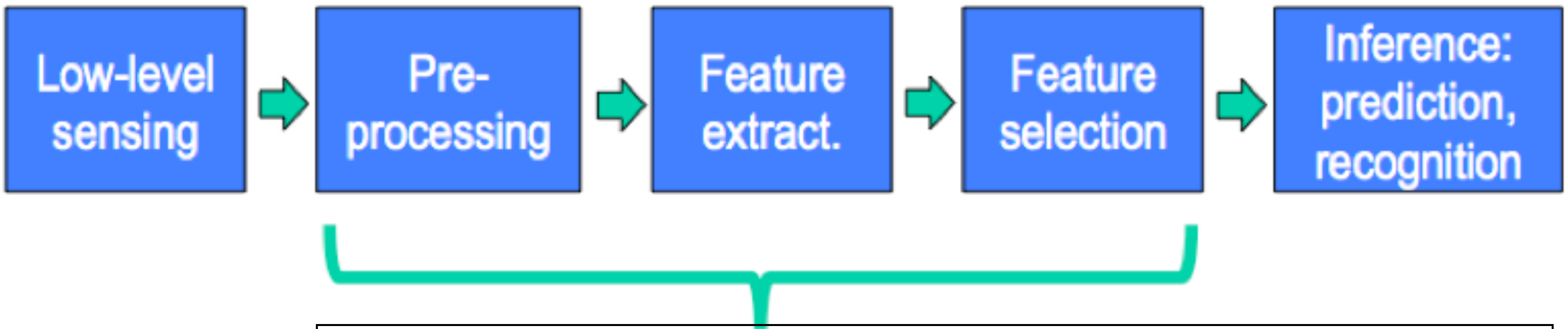
- Each document is a vector, one component for each term (= word).

	Doc 1	Doc 2	Doc 3	...
Word 1	3	0	0	...
Word 2	0	8	1	...
Word 3	12	1	10	...
...	0	1	3	...
...	0	0	0	...

- Normalize to unit length.
- High-dimensional vector space:
  - Terms are axes, 10,000+ dimensions, or even 100,000+
  - Docs are vectors in this space



DEEP LEARNING / FEATURE LEARNING :



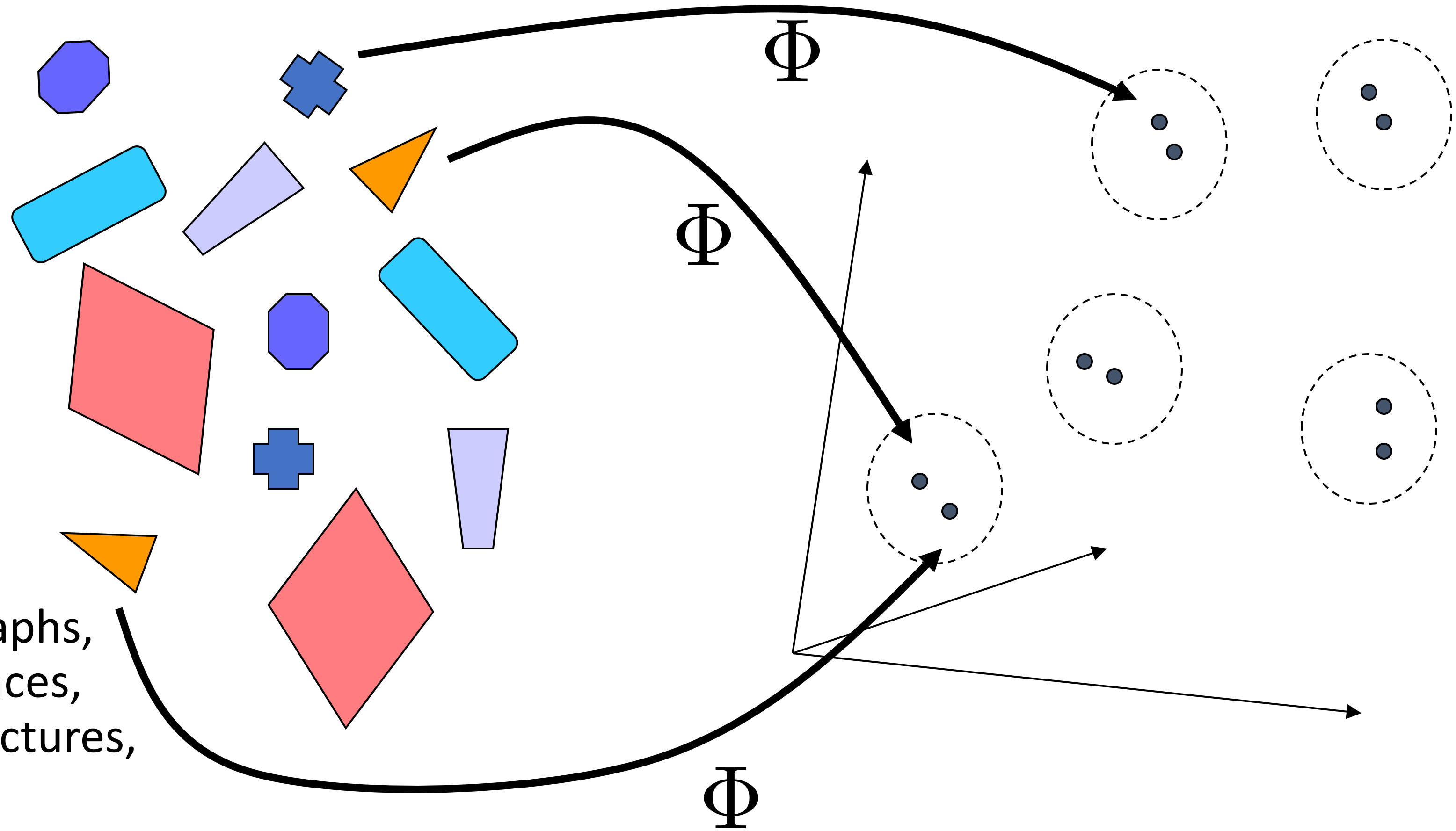
Feature Engineering (before 2012)

- ✓ Most critical for accuracy
- ✓ Account for most of the computation for testing
- ✓ Most time-consuming in development cycle
- ✓ Often hand-craft and task dependent in practice

Feature Learning

- ✓ Easily adaptable to new similar tasks
- ✓ Layerwise representation
- ✓ Layer-by-layer unsupervised training
- ✓ Layer-by-layer supervised training

STRUCTURAL INPUT : Kernel Methods [Complex X]



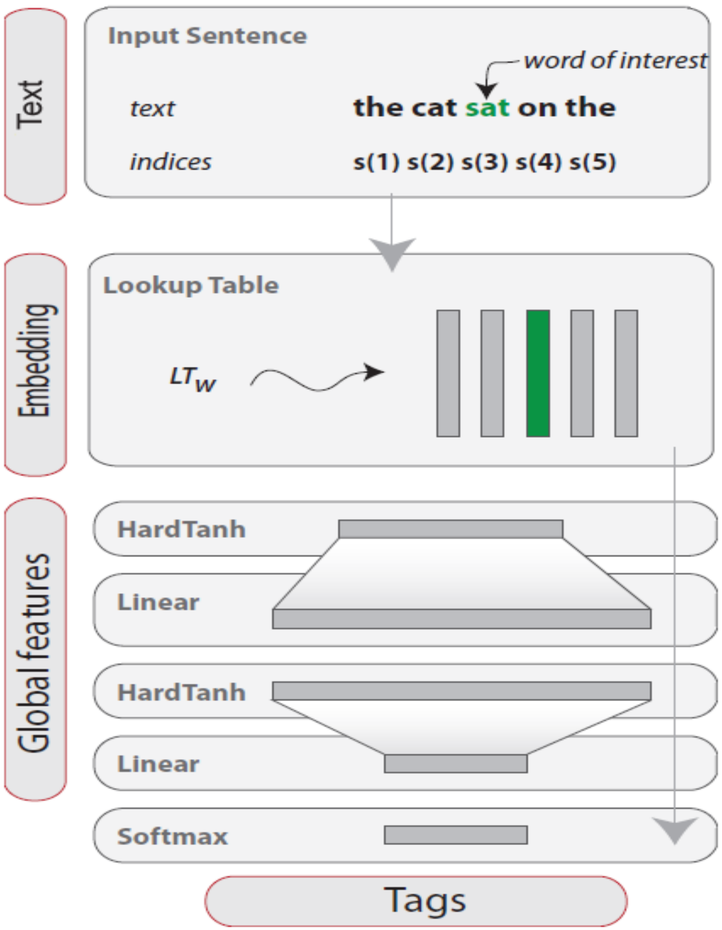
e.g. Graphs,
Sequences,
3D structures,

Original Space

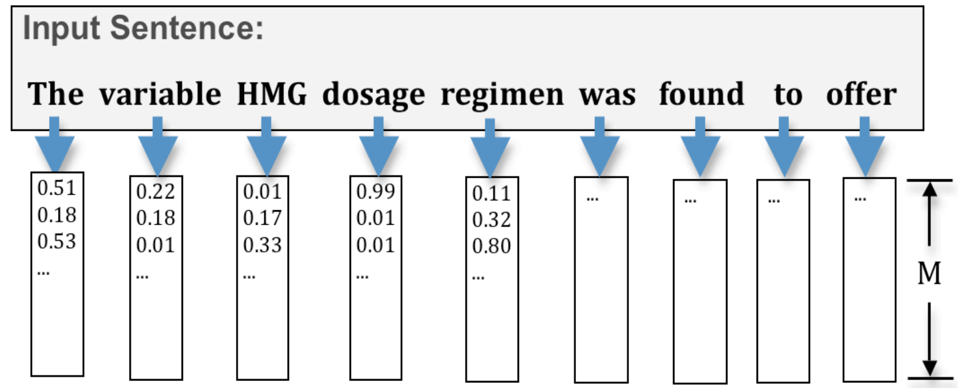
Feature Space

MORE RECENT: Deep Learning Based

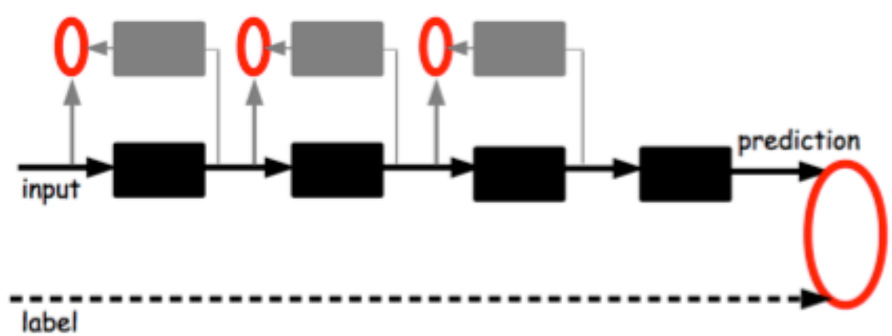
Deep Multi-Layer Learning



Supervised Embedding



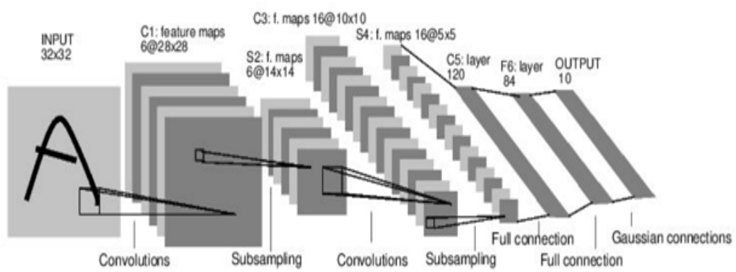
Layer-wise Pretraining



History of ConvNets

1998

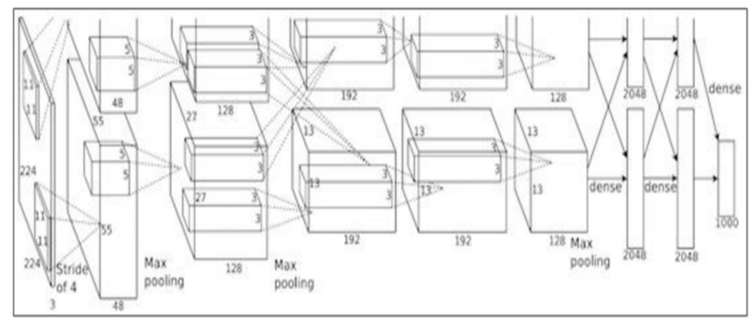
Gradient-based learning applied to document recognition [LeCun, Bottou, Bengio, Haffner]



LeNet-5

2012

ImageNet Classification with Deep Convolutional Neural Networks [Krizhevsky, Sutskever, Hinton, 2012]



"AlexNet"

Machine Learning in a Nutshell

Data

↓

Task

↓

Representation

↓

Score Function

↓

Search/Optimization

↓

Models, Parameters

ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

Basic Concepts

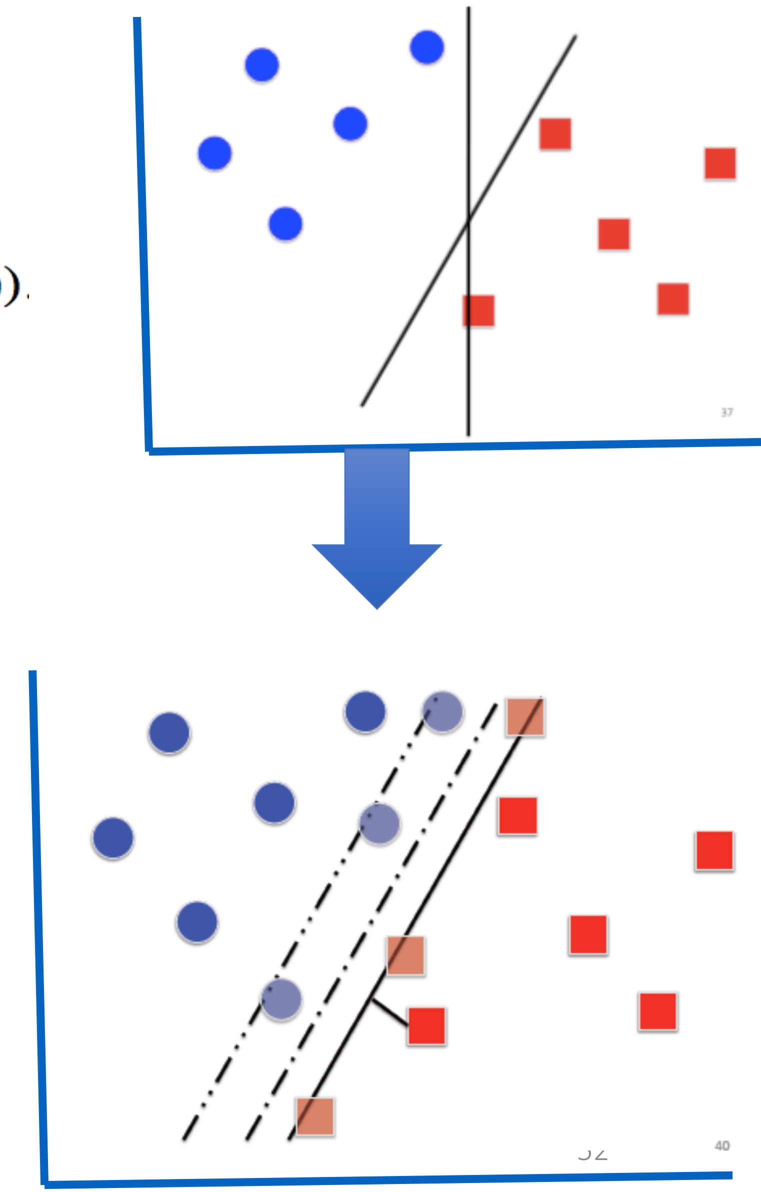
- Training (i.e. learning parameters w,b)
  - Training set includes
    - available examples $x_1,\ldots,x_L$
    - available corresponding labels $y_1,\ldots,y_L$
  - Find (w,b) by minimizing loss
    - (i.e. difference between y and f(x) on available examples in training set)

$$(W, b) = \underset{W,\, b}{\text{argmin}} \sum_{i=1}^{L} \ell(f(x_i), y_i)$$

Basic Concepts

- Loss function
  - e.g. hinge loss for binary classification task

$$\sum_{i=1}^{L} \ell(f(x_i), y_i) = \sum_{i=1}^{L} \max(0, 1 - y_i f(x_i)).$$

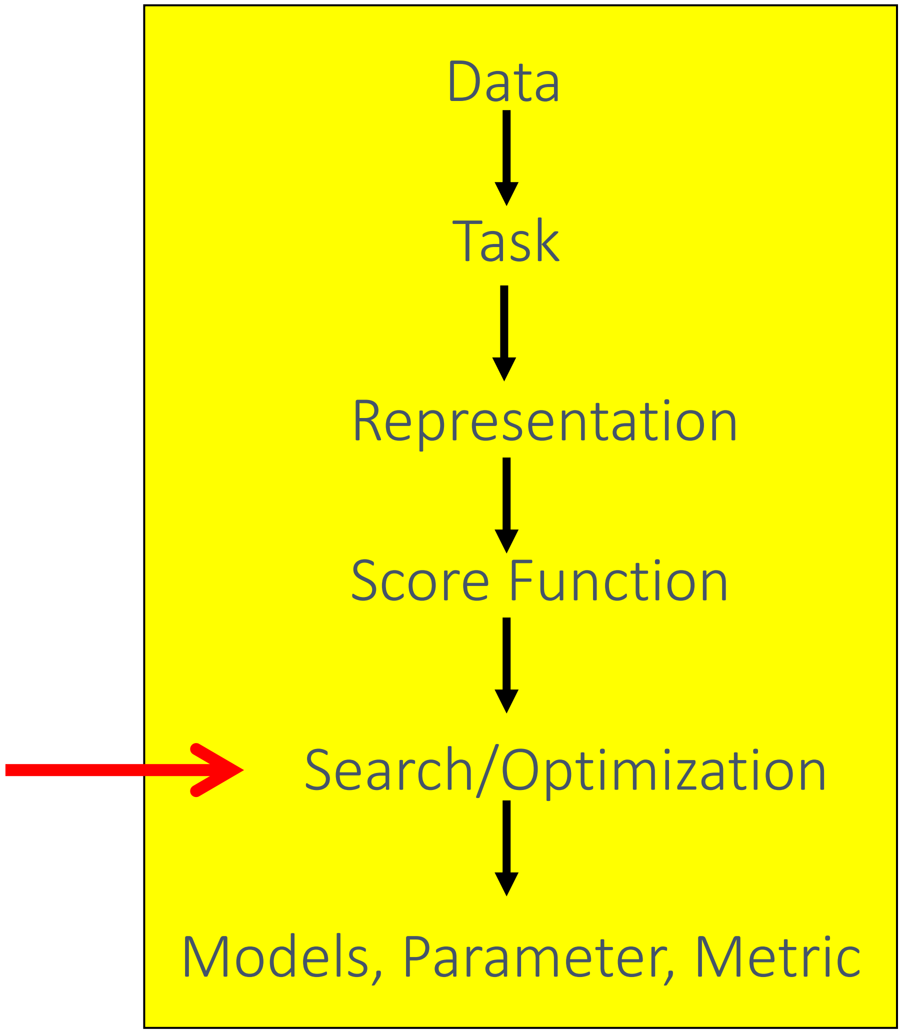


- Regularization
  - E.g. additional information added

on loss function to control f

$$C \sum_{i=1}^{L} \ell(f(x_i), y_i) + \frac{1}{2}\|w\|^2;$$

Machine Learning in a Nutshell



ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

Large-Scale Machine Learning: SIZE MATTERS

- One thousand data instances
- One million data instances
- One billion data instances
- One trillion data instances

Those are not different numbers, those are different mindsets !!!

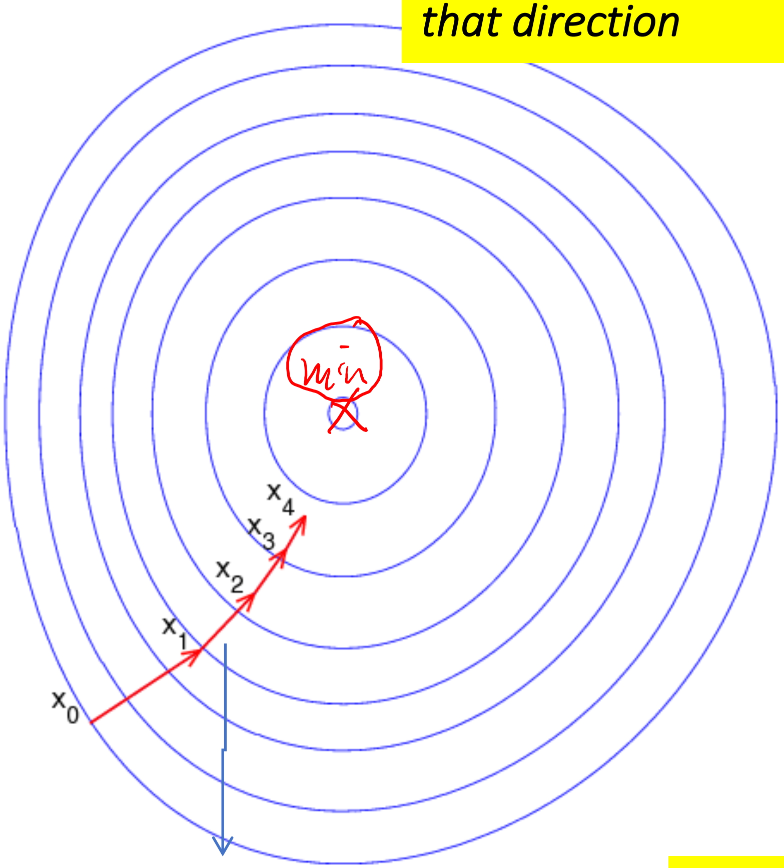
Not the focus, being covered in my advanced-level course

Gradient Descent (Steepest Descent) – contour map view

The gradient (in the variable space) points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the surface graph in that direction

A first-order optimization algorithm.

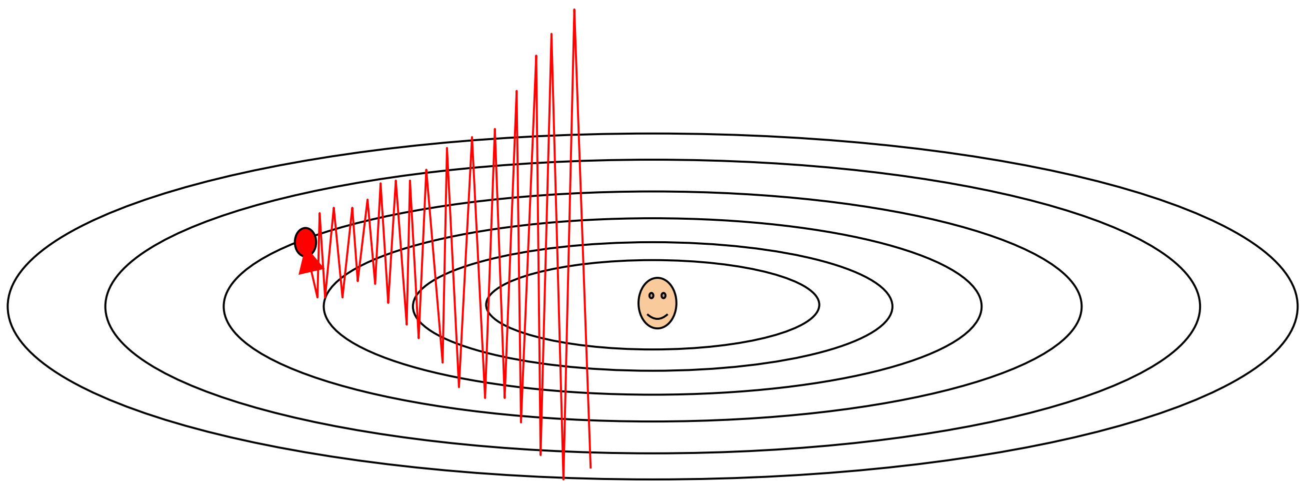
To find a local minimum of a function using gradient descent, one takes steps proportional to the *negative* of the gradient of the function at the current point.



$$-\nabla_x F(x_{k-1})$$

Contour map view

Gradient Magnitudes:

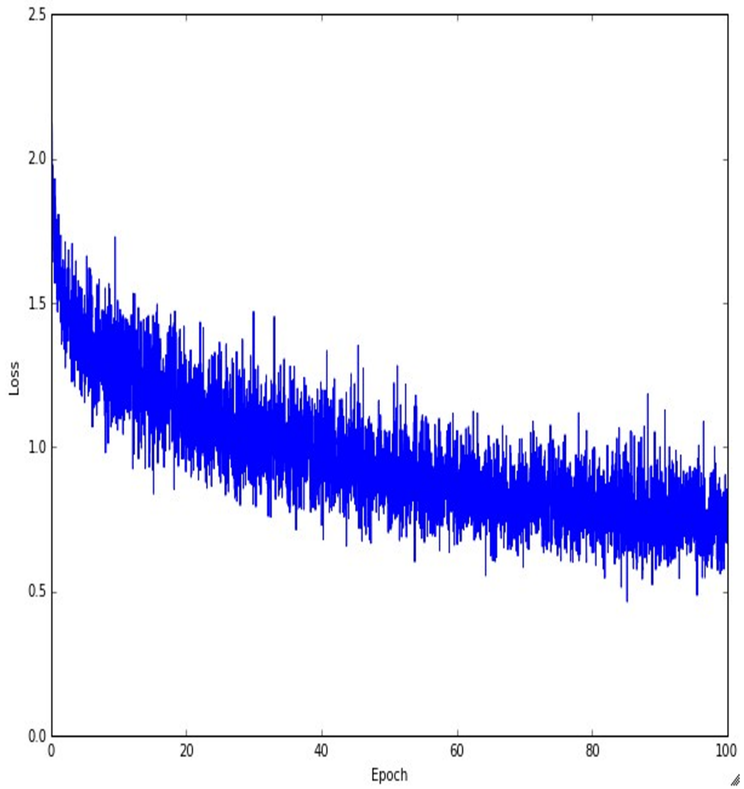


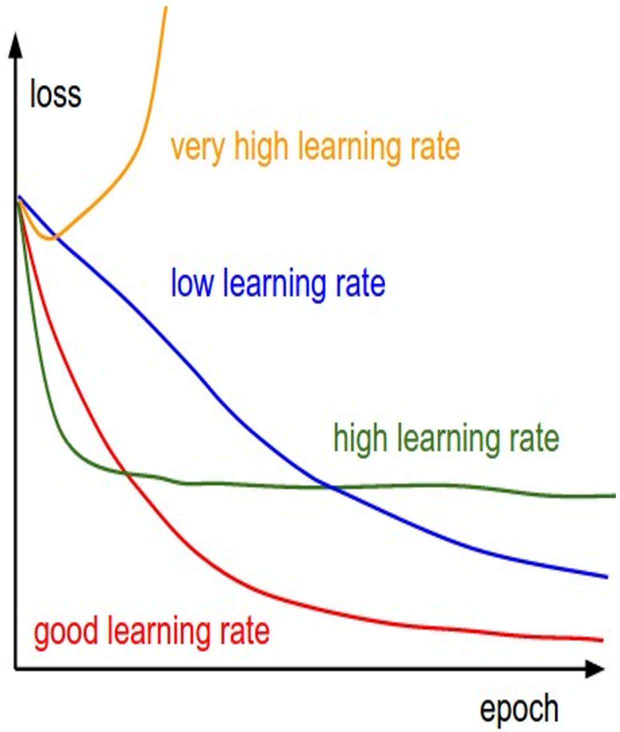
Gradients too big → divergence
Gradients too small → slow convergence

Divergence is much worse!

Many great tools, e.g., Adam
https://arxiv.org/abs/1609.04747

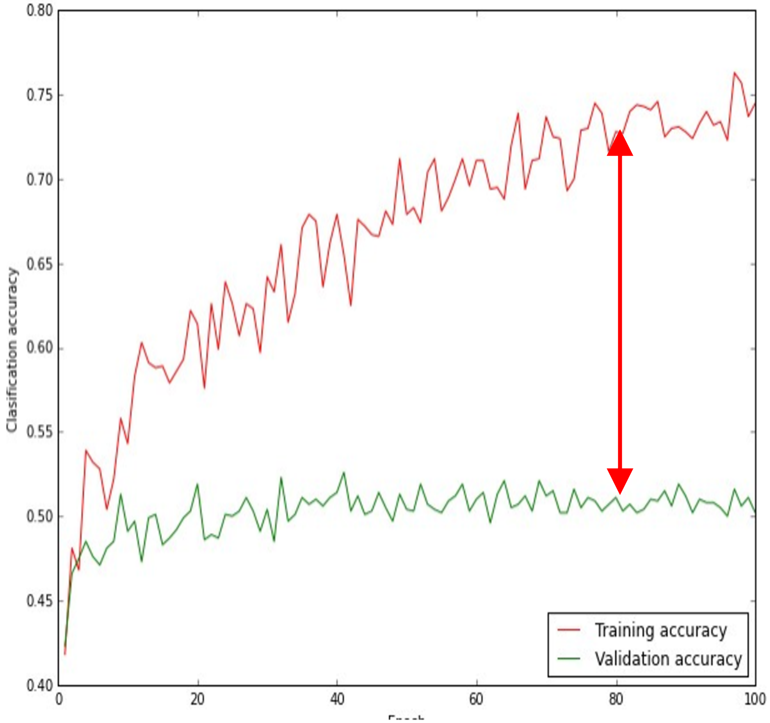
Monitor and visualize the loss curve





From Feifei Li Stanford Cousre

Monitor and visualize the train / validation loss / accuracy: Bias Variance Tradeoff



big gap = overfitting

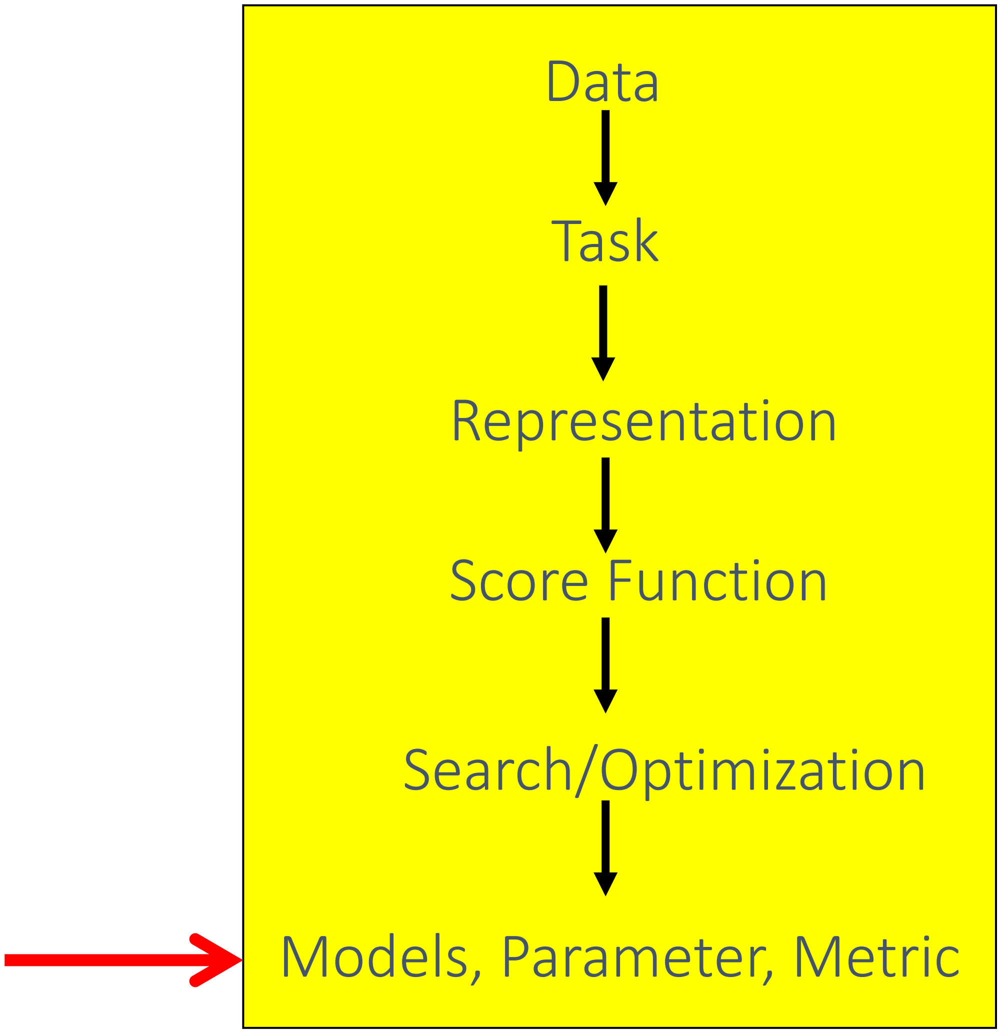
=> increase regularization strength?

no gap, e.g. underfitting / both bad

=> increase model capacity?

From Feifei Li Stanford Cousre

Machine Learning in a Nutshell

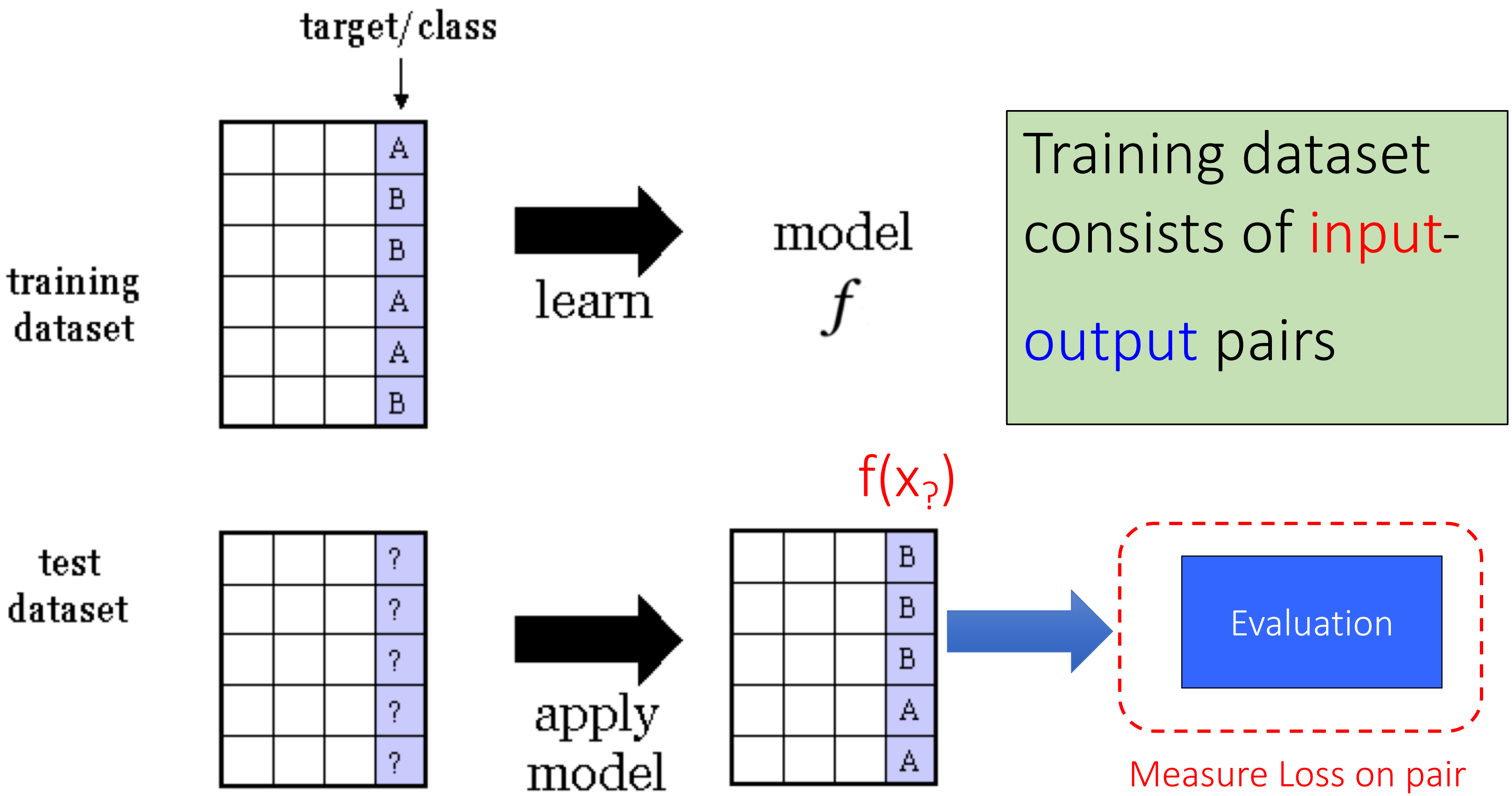


ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

How to know the program works well: Measure Prediction Accuracy on Test Data



Measure Loss on pair

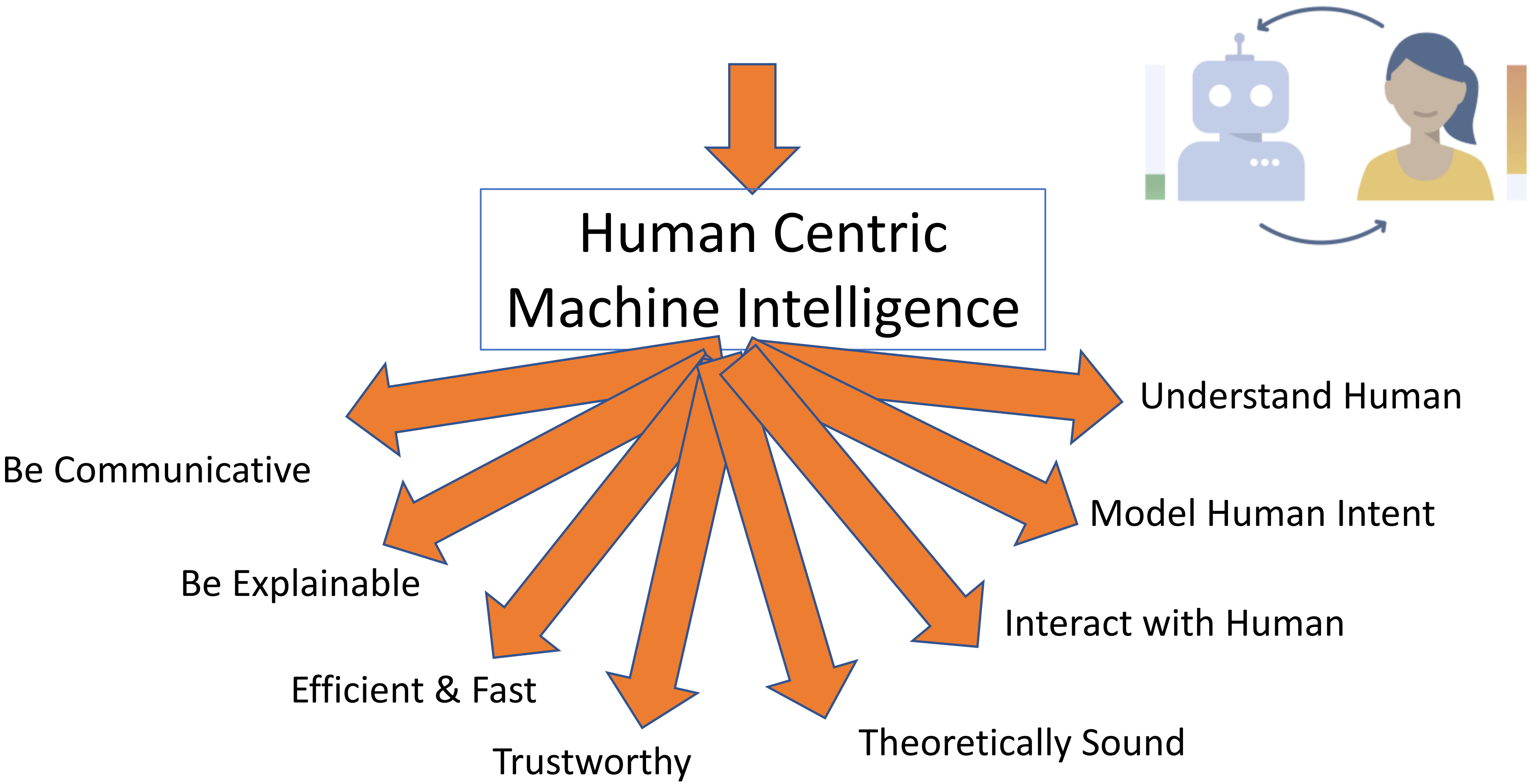
→ Error ($f(x_?)$, $y_?$)

Many Metric for Supervised Classification

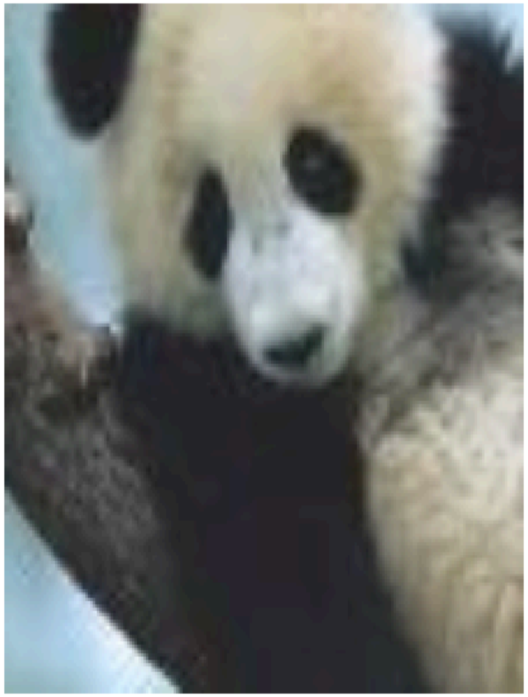
Metric	Formula	Interpretation
Accuracy	$\frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}$	Overall performance of model
Precision	$\frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FP}}$	How accurate the positive predictions are
Recall Sensitivity	$\frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}$	Coverage of actual positive sample
Specificity	$\frac{\mathrm{TN}}{\mathrm{TN}+\mathrm{FP}}$	Coverage of actual negative sample
F1 score	$\frac{2\mathrm{TP}}{2\mathrm{TP}+\mathrm{FP}+\mathrm{FN}}$	Hybrid metric useful for unbalanced classes

Credit: Stanford Machine Learning course

Go Beyond Prediction Accuracy: e.g., ML and AI Research @ UVA CS



Evade DNN, e.g. Adversarial Examples (AE)

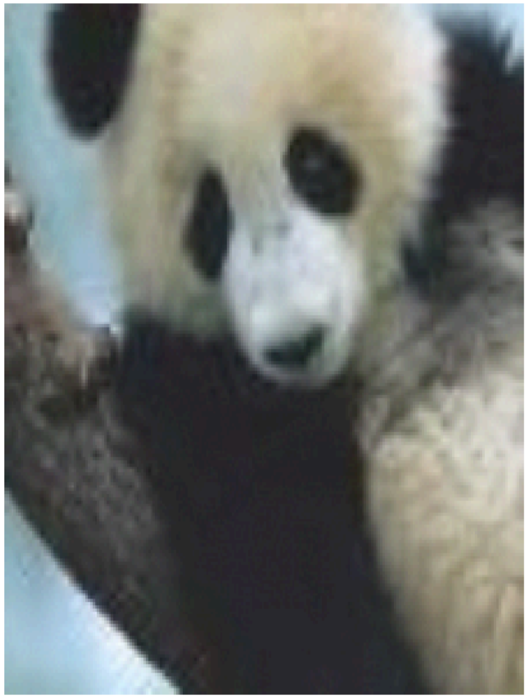


“panda”

+

$0.007 \times [noise]$

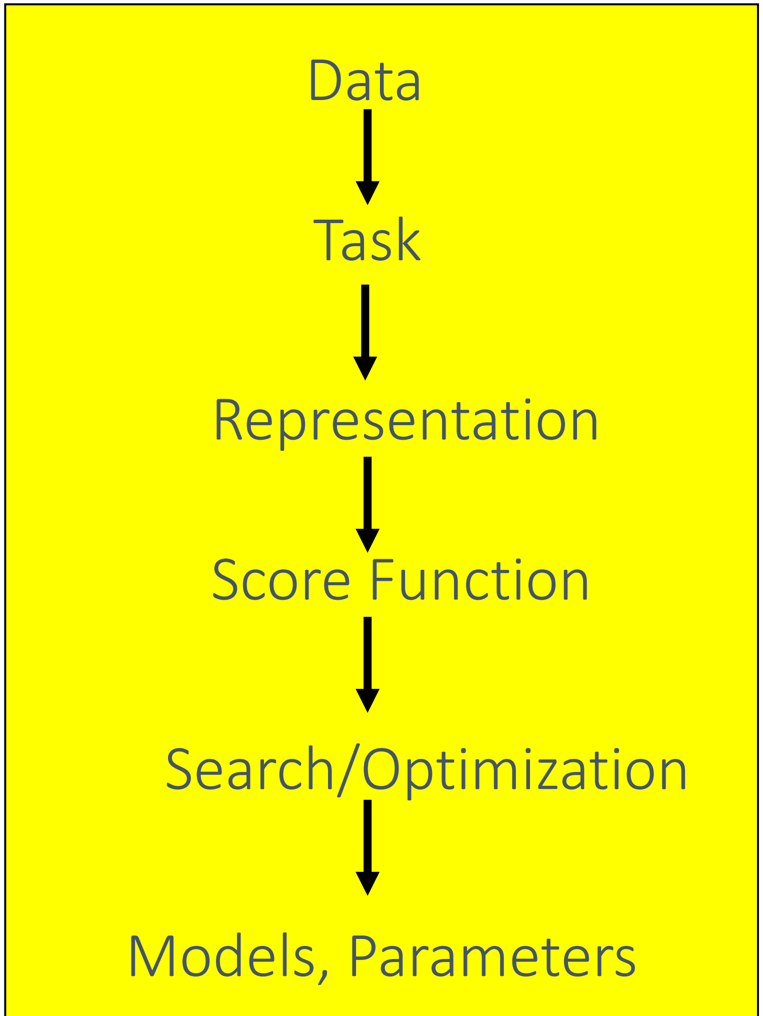
=



“gibbon”

Example from: Ian J. Goodfellow, Jonathon Shlens, Christian Szegedy. *Explaining and Harnessing Adversarial Examples*. ICLR 2015.

Machine Learning in a Nutshell



ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

Rough Sectioning of this Course

- 1. Basic Supervised Regression + Tabular Data
- 2. Basic Deep Learning + 2D Imaging Data
- 3. Advanced Supervised learning + Tabular Data
- 4. Generative and Deep + 1D Sequence Text Data
- 5. Not Supervised

Section 1 - Basics & On Tabular Input Type

Extra	Extra		Algebra Review	Slides: S1-AlgbReview		Notes: S1-linalg-extra.pdf	video	Useful Math
Platform	Platform		Basics scikit-learn	Slides: S1-scikit-learn	**library**			TA survey scikit-learn
0827	W1		Linear Regression	Slides: S1-LinearReg	**tabular**		video	LR more + ELS Ch3.2
0901	W2	Q1	Optimization for LR	Slides: S1-LR optimization	**tabular**		video	Useful SGD
0903	W2		Nonlinear Regression	Slides: S1-lrExtend SelectModel	**tabular**	Notes: S1-nonparametricR	video	NonLinear + API + ELS Ch5
0908	W3	Q2	Linear Prediction with Regularization	Slides: S1-lr Regularized	**tabular**		video	More Ridge
Extra	Extra		Lasso and Elastic Net	Slides: S1-lr Sparse	**tabular**	Notes: S1-Extra-lrReguOpm	video	Elastic paper
0910	W3		supervised classification	Slides: S1-Classify			video	Error Metrics
0915	W4	Q3	KNN and Theory	Slides: S1-kNearestN	**tabular**	Notes: S1-KNN-extra	video	Useful BiasVar
0917	W4		Bias Variance Tradeoff	Slides: S1-biasVariance		Notes: S1-Tibshirani-modelbasics	video	ESL Ch7
Platform	Platform		machine leanring in the cloud	Slides: S1-CloudML	**library**		video	Invited Speaker

Section 2 - Deep and 2D Grid Type (e.g. Imaging)								
0922	W5	Q4	ProbReview + MLE	Slides: S2-ProbReview		Notes: S2-MLE	video	MLE / MLE code
0924	W5		Logistic and NN	Slides: S2-LogisticReg	**structured**	Notes: L14extra-Logistic	video	code + compare classifiers
0929	W6	Q5	NN and Deep Learning	Slides: S2-basicDeepNN	**structured**	Notes: L15-lecun-98b	MLP video	
1001	W6		CNN	Slides: S2-CovNN	**2d(vision)**	Notes: L16-PCA	video	CNN
Extra	Extra		Quick survey of recent deep learning	Slides: S2-deepSurvey	**structured**	Notes: L16-PCA	video	DNN Cheatsheets
1006	W7	Q6	PCA, TSNE, UMAP	Slides: S2-PCA-VAE	**tabular**	Notes: L07-feaSelc		DNN Cheatsheets
Extra	Extra		semi-supervised	Slides: S2-semi-self-learning				
Extra	Extra		auto differentiation	Slides: S2-auto-grad	**library**			
Platform	Platform		S2 L09 Ta Pytorch	Slides: S2-pytorch	**library**			TA survey pytorch
Section 3 - More Advanced Supervsied on Tabular Type								
1008	W7		SVM	Slides: S3-SVM-basic	**tabular**	Notes: L11-LibSVMGuide	video	More SVM
1015	W8	Q7	SVM, Kernel	Slides: S3-SVM-kernel		Notes: L11-LibSVMGuide	video	VC Theory
Extra	Extra		SVM, Dual	Slides: S3-SVM-optimDual		Notes: L11Extra-SVMoptimDual	video	SMO + Paper SMO
1020	W9		DecisionTree and Bagging	Slides: S3-DecisionTree	**tabular**	Notes: L22-review	video	xgboost

Section 4 - on 1D Sequence Type (e.g. Language Text)								
1027	W10		Generative Classification	Slides: S4-BayesClassify		Notes: L16-PCA	video	
1029	W10	Q9	Gaussian BC	Slides: S4-GenerDiscr		Notes: L17c-NBCtext	video	Paper Discr vs. Genera
1103	W11		NaiveBC on Text	Slides: S5-NBCtext	**1D(Text)**	Notes: L20-review	video	Multinomial MLE
1105	W11	Q10	Recent deep learning on Text	Slides: S4-deepText	**1D(Text)**	Notes: L16-PCA	video	DNN Cheatsheets
1110	W12		Learning to Recommend on Text	Slides: S4-deepRecommend	**1D(Text)**		video	
Extra	Extra		probabilistic programming	Slides: S2-prob-program				
Extra	Extra		Feature Selection and Model Selection	Slides: S4-feaSelc		Notes: L07-FeatureSelect-jmlrPaper	video	API + ELS Ch3.4 and Ch3.3
Section 5 - Not Supervised								
1112	W12	Q11	Clustering Hier	Slides: S5-clustering-Hier	**tabular**	Notes: L19c-clustering3-GMM	video	compare Hier clusterings
1117	W13		Clustering Partition	Slides: S5-clustering-kMeans	**tabular**	Notes: L19d-EMextra-EM	video	compare clusterings
Extra	Extra		Clustering GMM	Slides: S5-clustering-GMM	**1DSignal(Audio)**	Notes: L19d-EMextra-EM	video	EM primer
1119	W13	Q12	RL	Slides: S5-reinforcement-learning	**None-IID**	Notes: L18c-More-Boosting	video	xgboost

Thank You

References

- Prof. Andrew Moore’s tutorials
- Prof. Raymond J. Mooney’s slides
- Prof. Alexander Gray’s slides
- Prof. Eric Xing’s slides
- http://scikit-learn.org/
- Hastie, Trevor, et al. The elements of statistical learning. Vol. 2. No. 1. New York: Springer, 2009.
- Prof. M.A. Papalaskar’s slides