Introduction to ML (Part II)

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Plans for today

A. Recap and Supervised Learning
B. Intro. to Supervised Learning algorithms
C. Worries During the Learning
D. Learning Paradigms and Optimization

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$\{(x_i, y_i)\}$

$i = 1, \ldots N$

$y \to$ Class

$y \to$ Res.

$x \in \mathbb{R}^d$

To

Goal: Find fn $f(\ )$

$f(x_i) \to y_i$ $\forall i$ To beyond N

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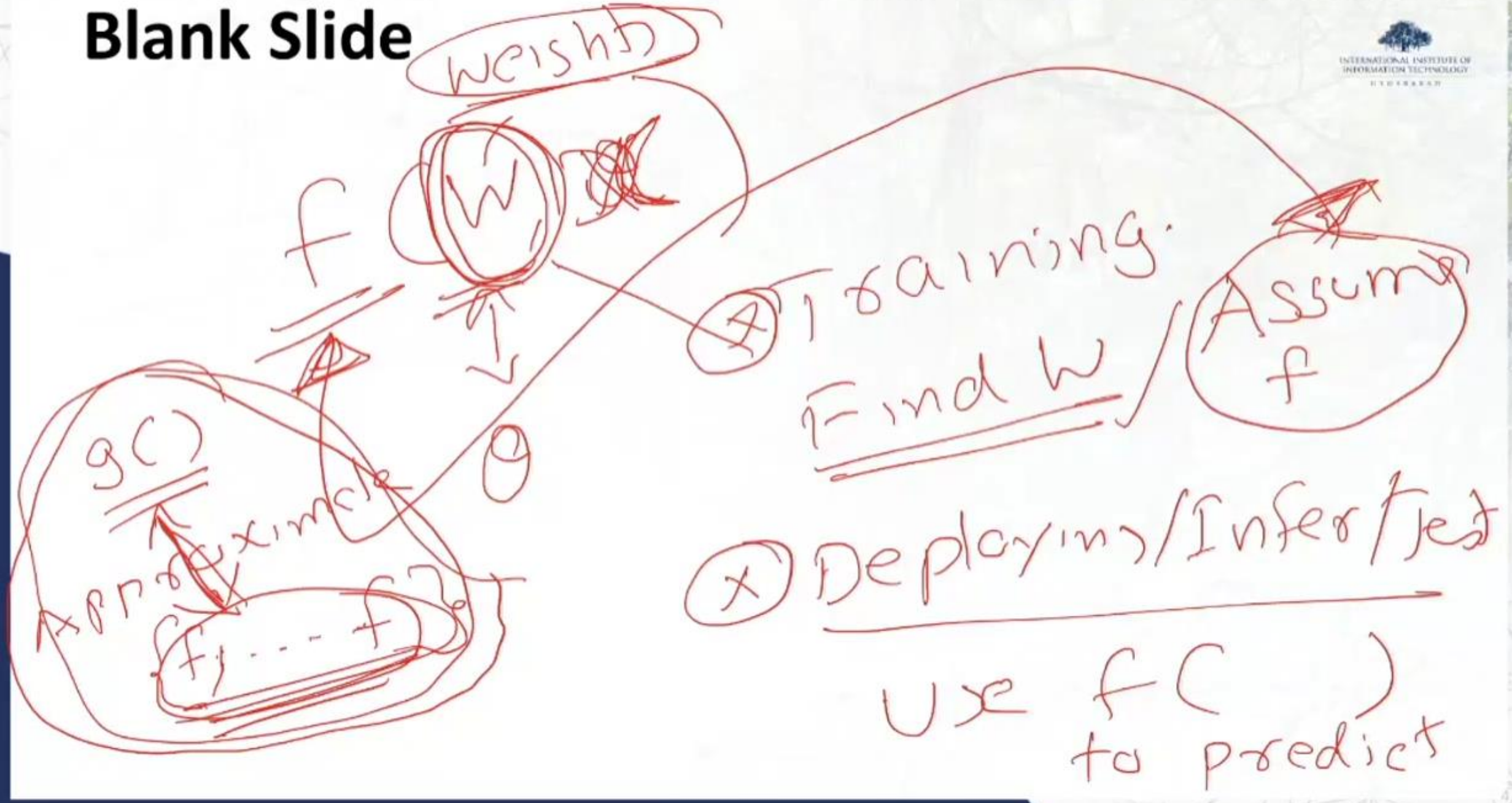
weights
W
f
θ
g()
Approximate
f
(f1 ... fn)
Training.
Find W
Assume
f
Deploying/Infer/Test
Use f( )
to predict

Variations

- Binary Classification

$$\mathbf{X} \longrightarrow l \in L = \{l_1, l_2\}$$

x Class
x Regr

- Multi Class Classification

$$\mathbf{X} \longrightarrow l \in L = \{l_1, l_2, \ldots, l_{\|C\|}\}$$

x -> y
x -> y1, y2 ...

- Multi Label Classification

$$\mathbf{X} \longrightarrow l^X = \{l_1^X, l_2^X, \ldots\} \quad l_i^X \in L = \{l_1, l_2, \ldots, l_{\|C\|}\}$$

- Structured Output Prediction

$$\mathbf{X} \longrightarrow y \in \mathcal{Y} = \{1, \ldots, \mathrm{k}\}^l$$

- $\mathcal{Y}$ are complex (structured outputs)
  - Images, text, audio, folds of protein

Problem Space

- **Feature Extraction:** Find ***X*** corresponding to an entity/item ***I*** (such as an image, web page, ECG etc.)

- **Classification:** Find a parameterized function $f_W(X)$ which can make the right predictions ***Y***.

- **End to End:** Can we learn ***Y*** directly from ***I***.

B. Intro. to Supervised Learning

Machine Learning

Popular Problems

- Classification
- Regression
- Density Estimation

Classification

- K Nearest Neigours
- Naïve Bayes Classifier
- Decision Trees
- Random Forest
- Logistic Regression
- Ensemble Learning
- Neural Networks
- Support Vector Machines

The machine learning framework

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

output

prediction function

feature or representation

- **Training:** given a *training set* of labeled examples $\{(\mathbf{x}_1,y_1), \ldots, (\mathbf{x}_N,y_N)\}$, estimate the prediction function f by minimizing the prediction error.
- **Testing:** apply f to a never before seen *test example* $\mathbf{x}$ and output the predicted value $y = f(\mathbf{x})$

Slide credit: L. Lazebnik

Examples of Loss Function

- Very similar: Loss function, Objective function, Error Function

$$error = \frac{1}{N}\sum_{n=1}^{N}[y_n \neq g(x_n)]$$

- Is error the only measure?
- Many Alternatives:
  - Square error loss.
  - Ranking Loss
  - ??

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Consider the Following Problems

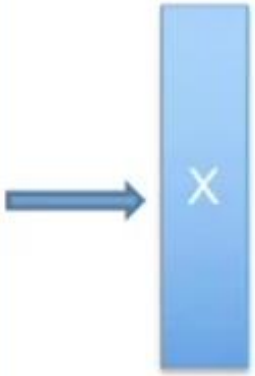
1. Given an email, decide if it is SPAM or not
2. Given the picture of a pet, decide if it is a cat or a dog

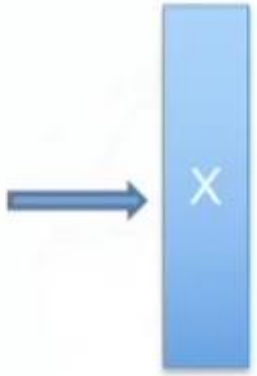
X: Text of email
Y: SPAM / HAM : {1, 0}

X: Image of the pet
Y: Cat / Dog : {1, 0}

- How do we represent the text as a vector?
- What about the image?

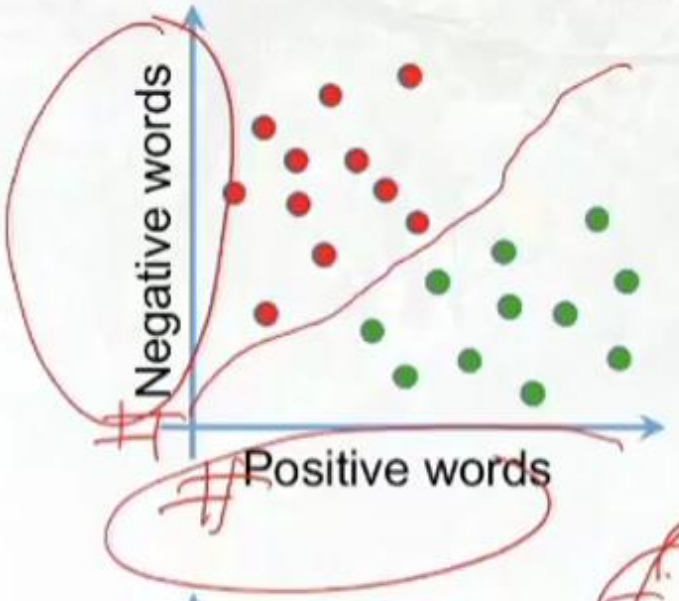
Feature Vector

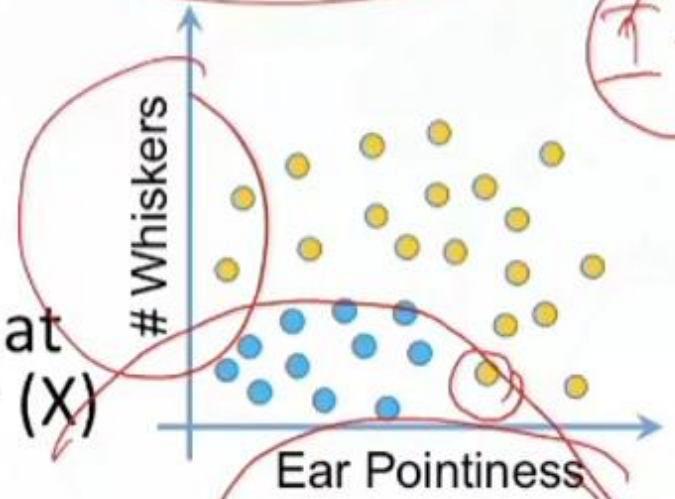




Feature Space

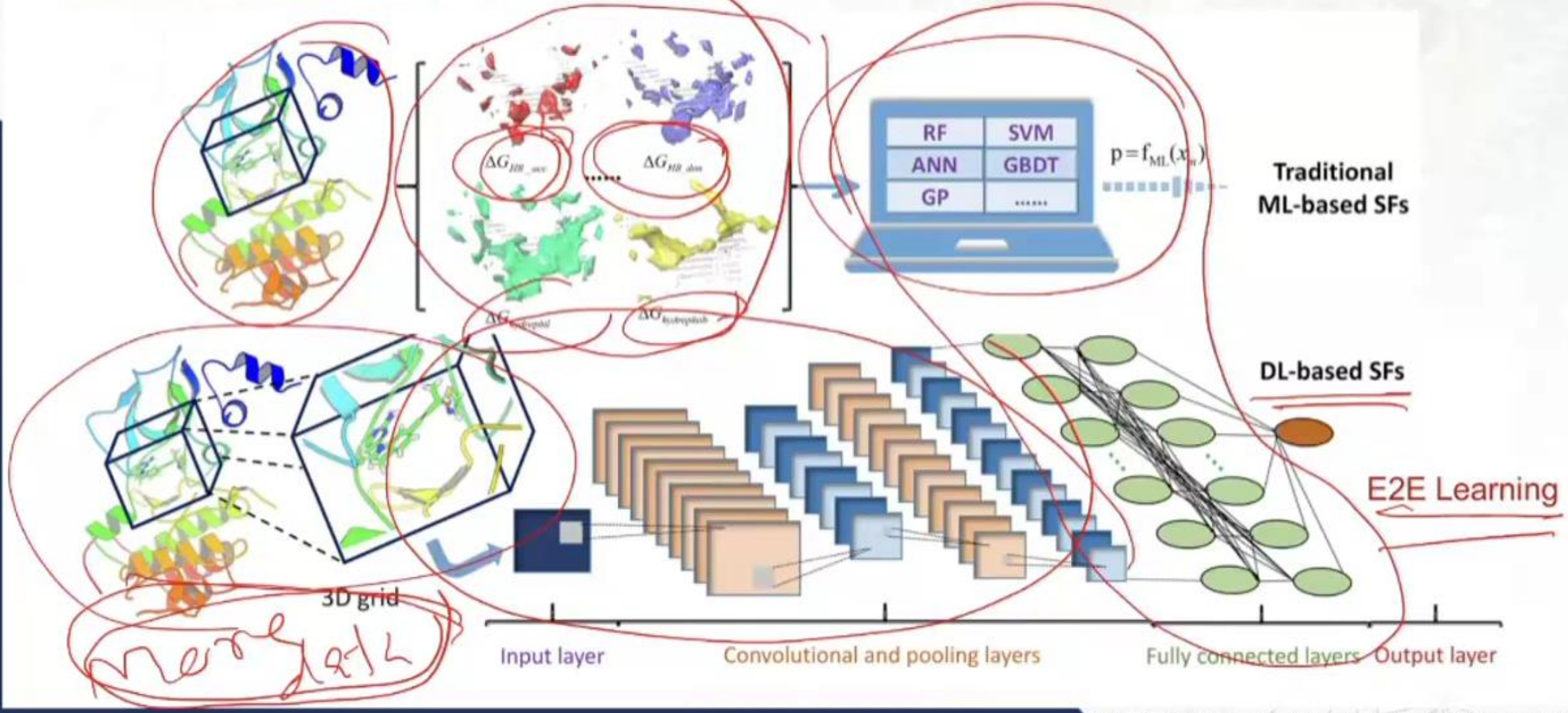
- We need to extract useful information from the input, and avoid 'noise'.
- Email: Count of positive and negative words in the email
- Pet: Pointiness of ears, Number of whiskers
- Now onwards, we assume that a sample is its feature vector (X)





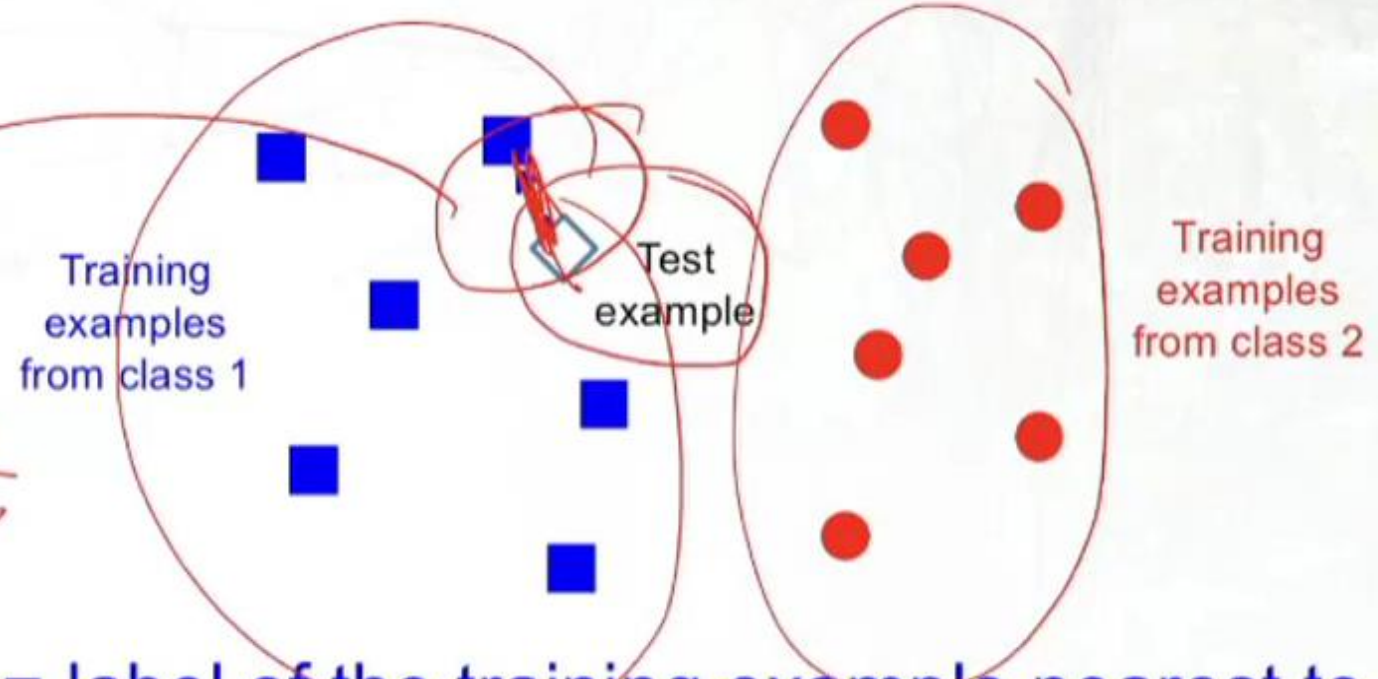
Protein-Ligand Binding Affinity Prediction

Regression: Predict Scoring Function/Scores



WIREs Comp. Mol. Sci. 2019, e1429

Classifiers: Nearest neighbor



Distance

f(x)

lazy learr

f(**x**) = label of the training example nearest to **x**

- All we need is a distance function for our inputs
- No training required!

Slide credit: L. Lazebnik

Classifiers: Linear

$w_1 = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ $w_1 x_1 + w_2 x_2 + b$

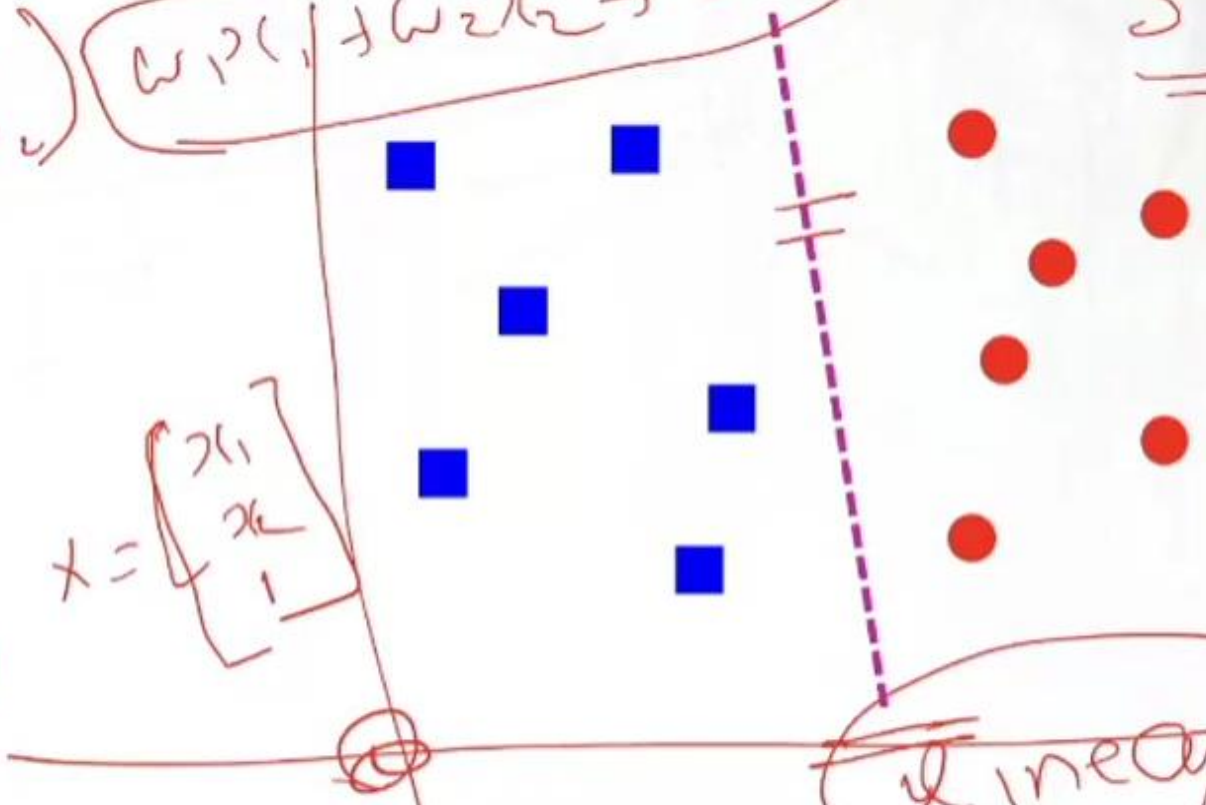
$\text{sign}(w^T x)$

$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$x = \begin{bmatrix} x_1 \\ x_2 \\ 1 \end{bmatrix}$

$w = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix}$

$x^T \begin{bmatrix} x \\ 1 \end{bmatrix}^T \begin{bmatrix} w \\ b \end{bmatrix}$



linear

bias

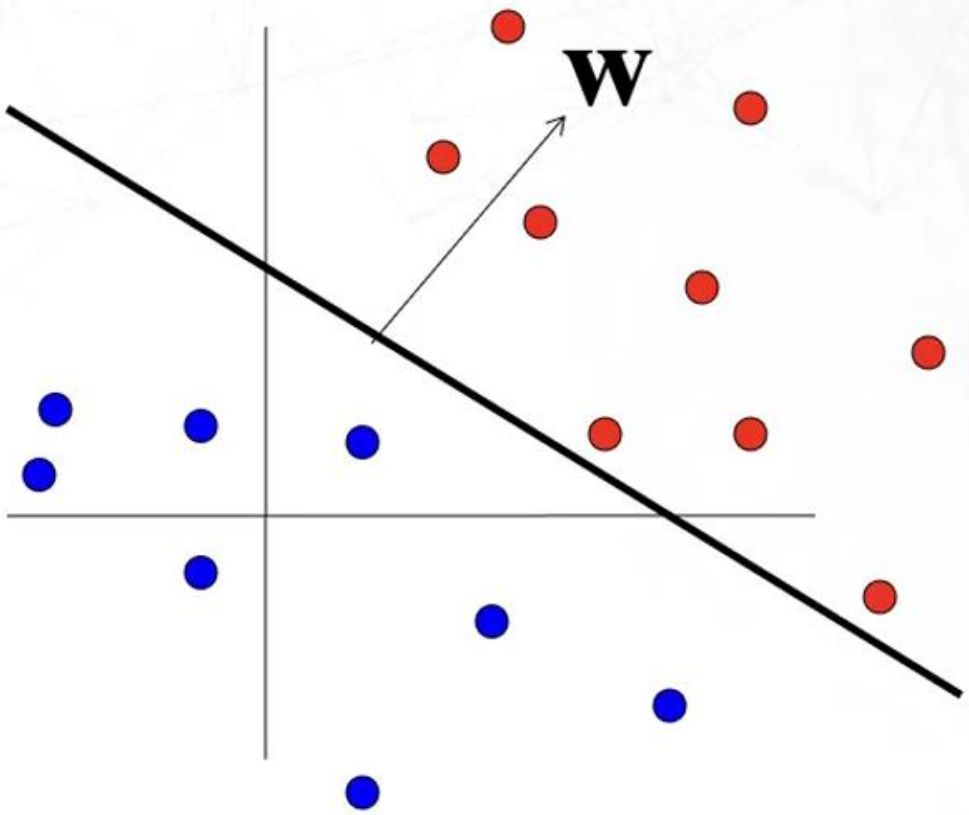
- Find a linear function to separate the classes:

$w^T x$

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w}^T \cdot \mathbf{x} + b)$$

Slide credit: L. Lazebnik

Linear Classifiers

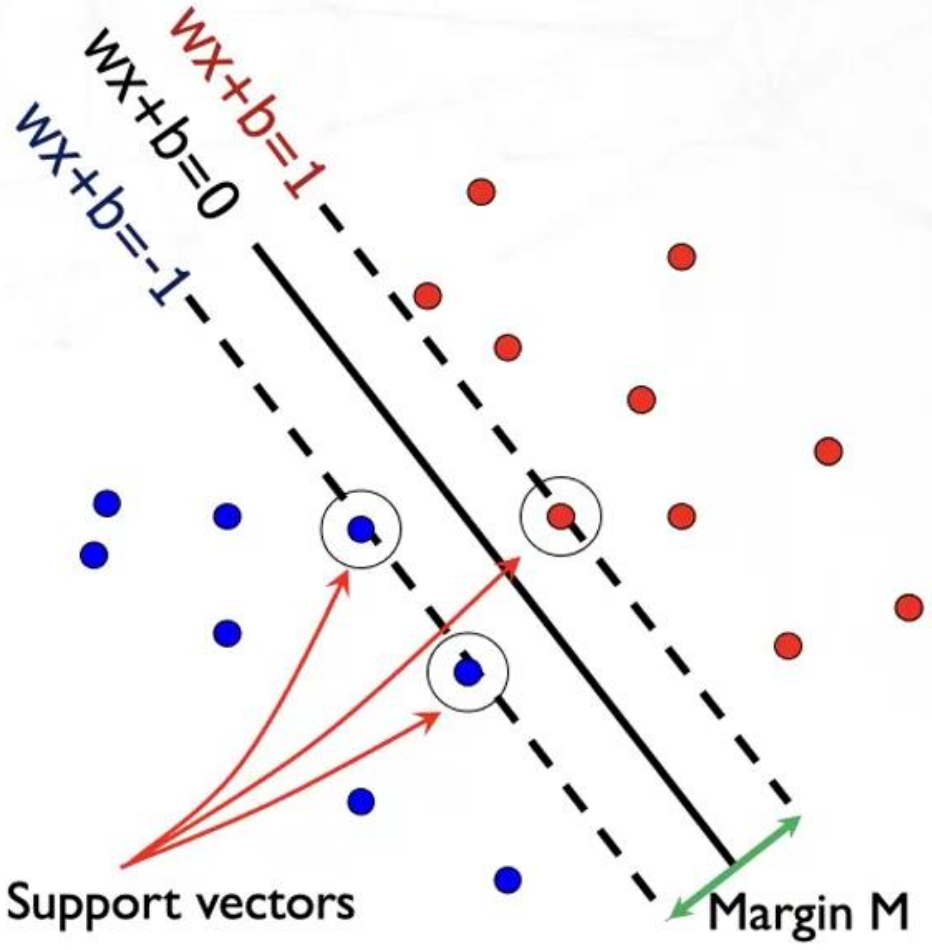


$$ax + by + cz + d = 0$$

$$\mathbf{w} \cdot \mathbf{x} + d = 0$$

$$D = \frac{|ax_0 + by_0 + cz_0 + d|}{\sqrt{a^2 + b^2 + c^2}} = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{x} + d}{\|\mathbf{w}\|}$$ distance from point to plane

Support Vector Machines



$\mathbf{x}_i$ positive $(y_i = 1)$: $\quad \mathbf{x}_i \cdot \mathbf{w} + b \geq 1$

$\mathbf{x}_i$ negative $(y_i = -1)$: $\quad \mathbf{x}_i \cdot \mathbf{w} + b \leq -1$

$$\mathbf{x}_i \cdot \mathbf{w} + b = \pm 1$$

For support, vectors,

Distance between point and line: $\dfrac{|\mathbf{x}_i \cdot \mathbf{w} + b|}{\|\mathbf{w}\|}$

For support vectors:

$$\frac{\mathbf{w}^T\mathbf{x} + b}{\|\mathbf{w}\|} = \frac{\pm 1}{\|\mathbf{w}\|} \qquad M = \left| \frac{1}{\|\mathbf{w}\|} - \frac{-1}{\|\mathbf{w}\|} \right| = \frac{2}{\|\mathbf{w}\|}$$

Finding the Maximum Margin Plane

$$\mathbf{x}_i \text{ positive } (y_i = 1): \quad \mathbf{x}_i \cdot \mathbf{w} + b \geq 1$$

$$\mathbf{x}_i \text{ negative } (y_i = -1): \mathbf{x}_i \cdot \mathbf{w} + b \leq -1$$

$$\text{Min } \frac{1}{2} \| w \|^2 + C \sum_{i=1}^{M} \xi_i$$

$$\text{subject to: } y_i(w^T x_i) \geq \mathbf{1} - \xi_i, \xi_i \geq \mathbf{0}$$

One constraint for each training point.

Note sign trick.

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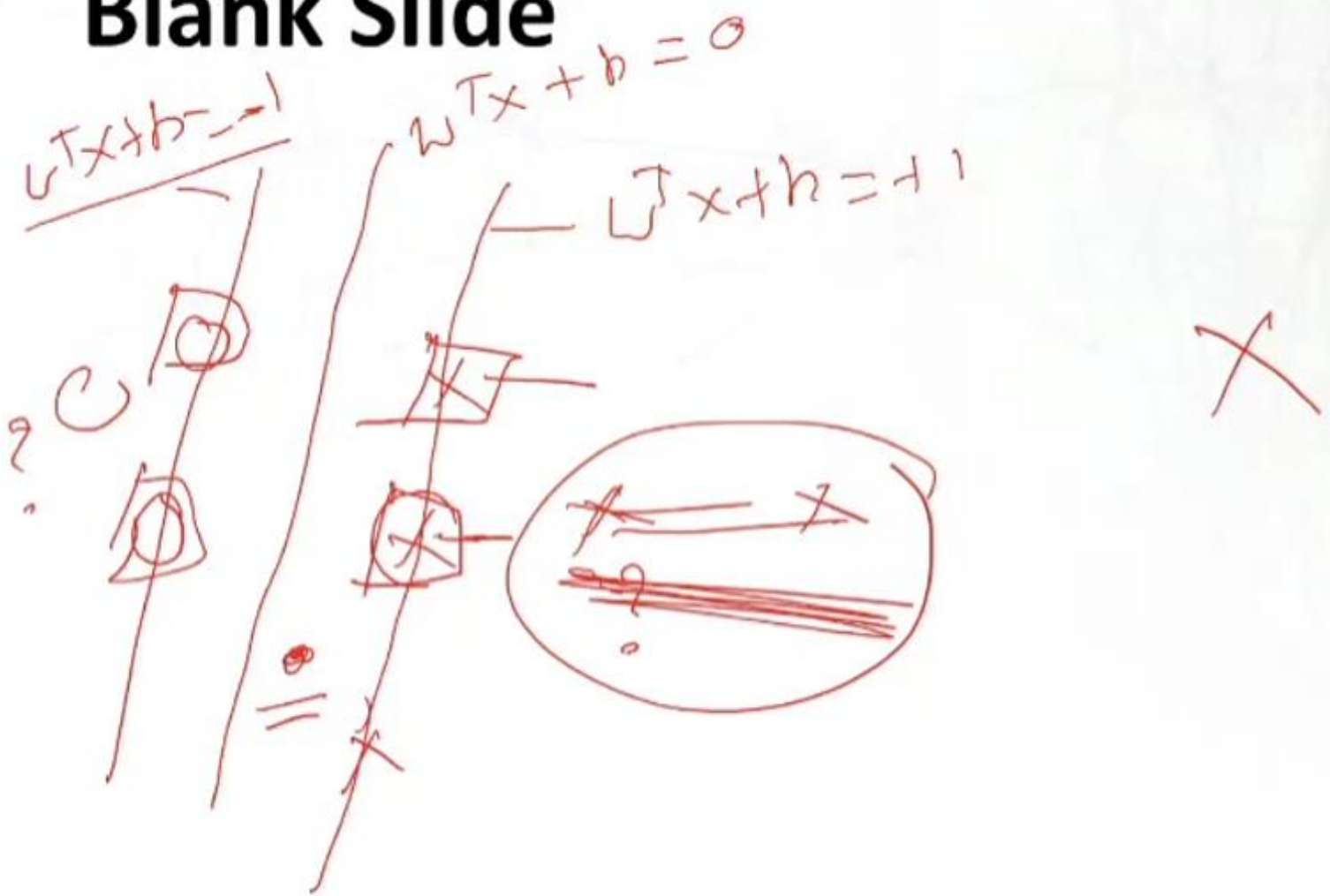

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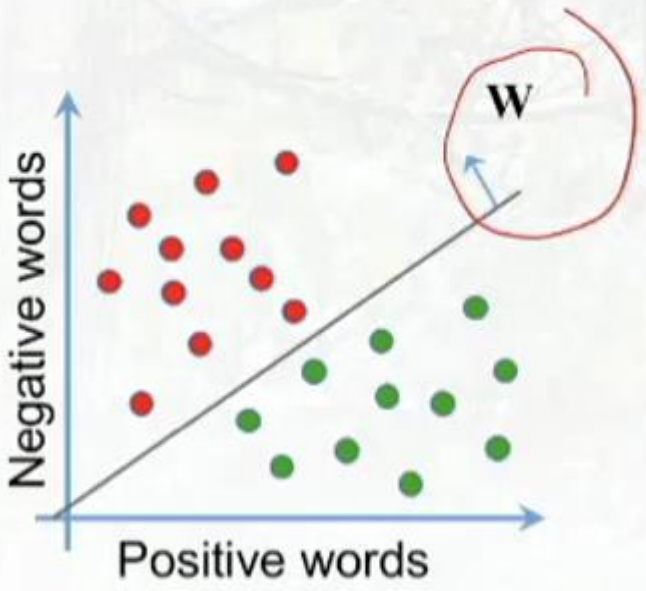
Creating a SPAM Filter

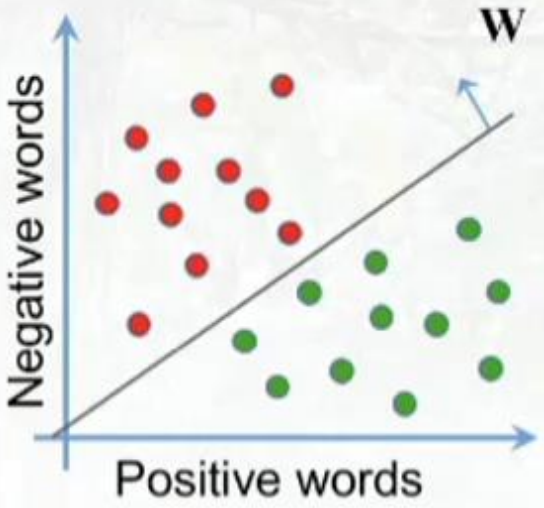
- Can we separate SPAM from Non-SPAM ?

1. Collect a set of example emails (training data)
2. Convert the emails to vector representation
3. Label the examples as SPAM or not
4. Learn a separator in the feature space

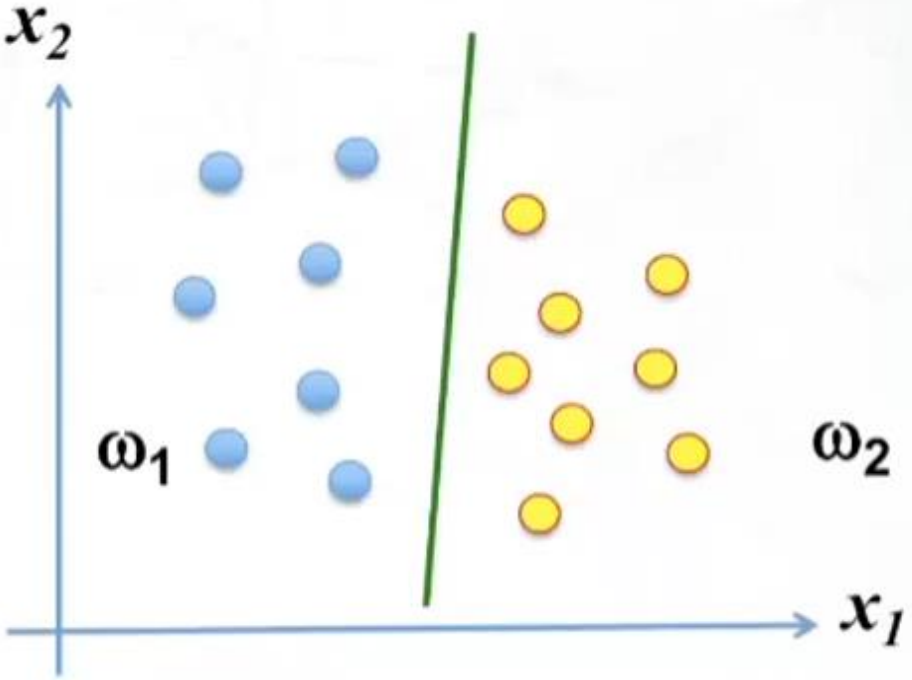


Training vs Testing

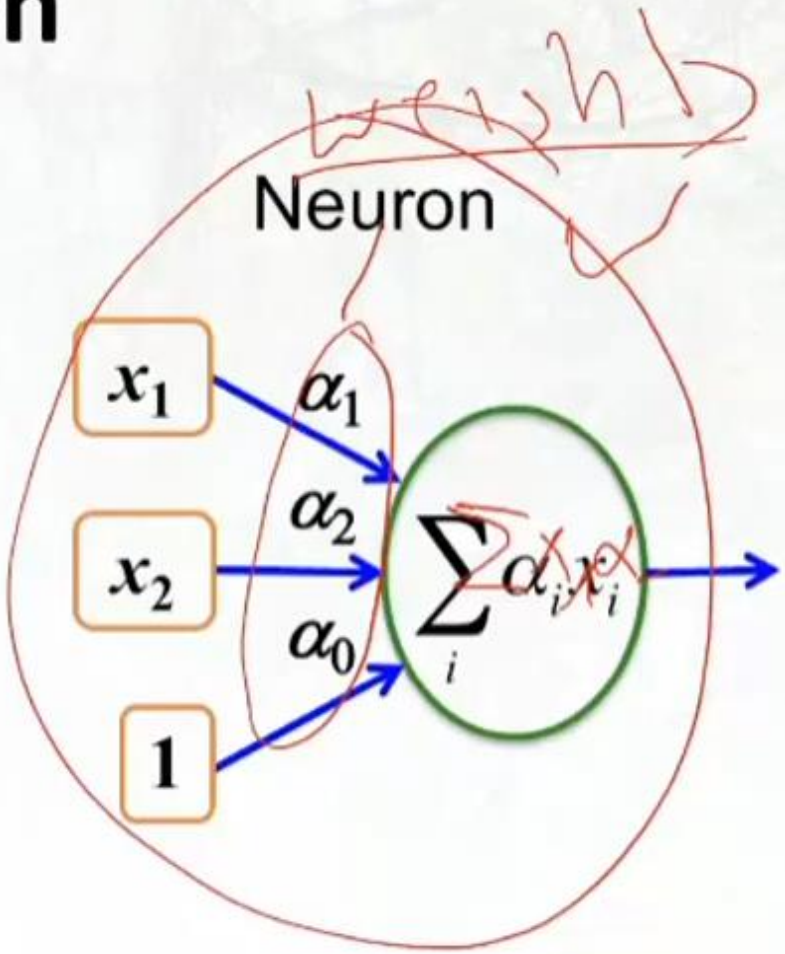
- Training
  - Using examples to 'learn' a classifier model
  - $y = f(\mathbf{W}, \mathbf{X})$: We learn the parameters $\mathbf{W}$ during training
- Testing
  - Predict the y values for new samples
  - Why **new** samples?
    - Using training samples to test may give a false sense of capability



Linear Classifier: A Neuron



$$\alpha_1 x_1 + \alpha_2 x_2 + \alpha_0 = 0$$



- A linear boundary separates two classes.
- Learning the classifier means learning the weights, α_i.

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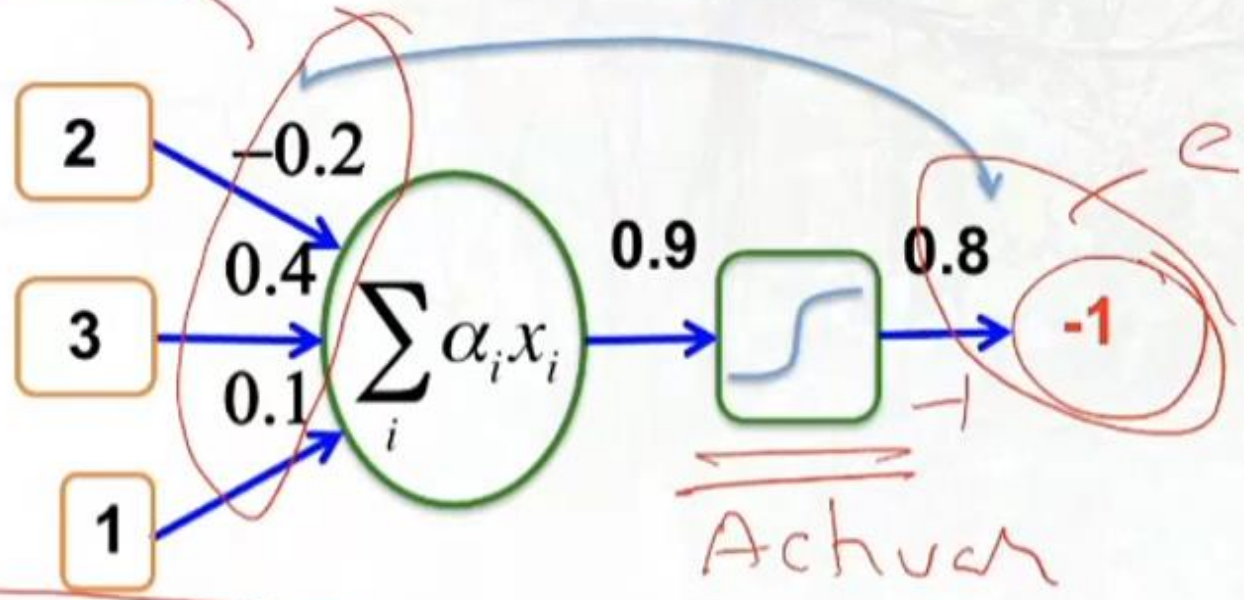
Learning



weight update

error

Actual

error is small

Repeat until weights stabilize

1. Take a training sample and pass it through the neuron
2. Find the difference between the output and expected values (loss function)
3. Update the weights to reduce this loss

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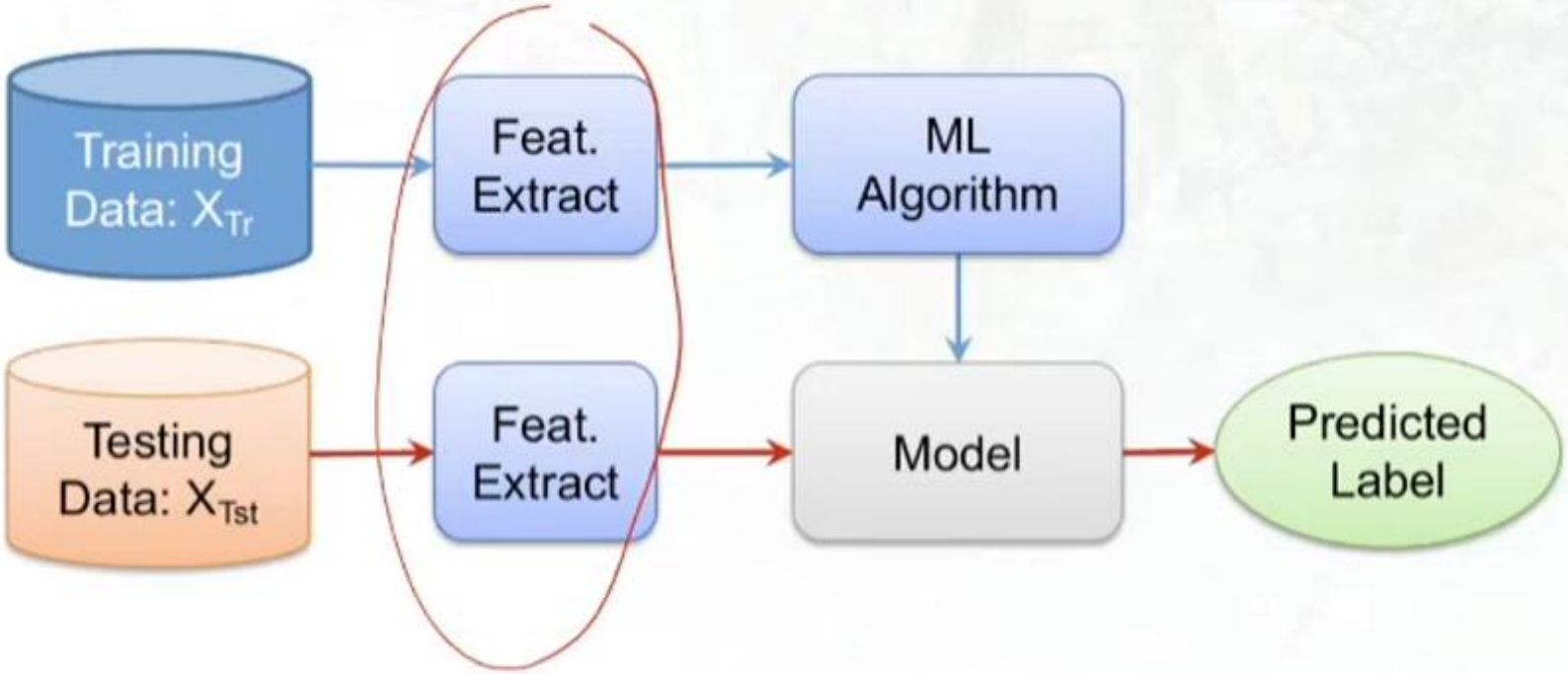
Summary: The ML Pipeline



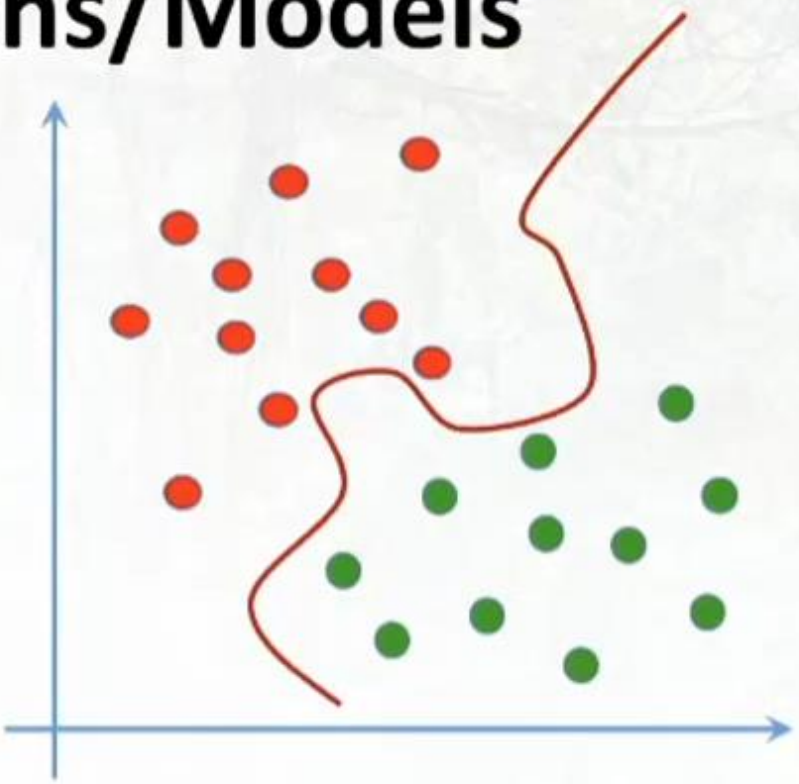
In traditional AI models,
the features used to be engineered and learning was limited to the classifier

C. Worries During Learning

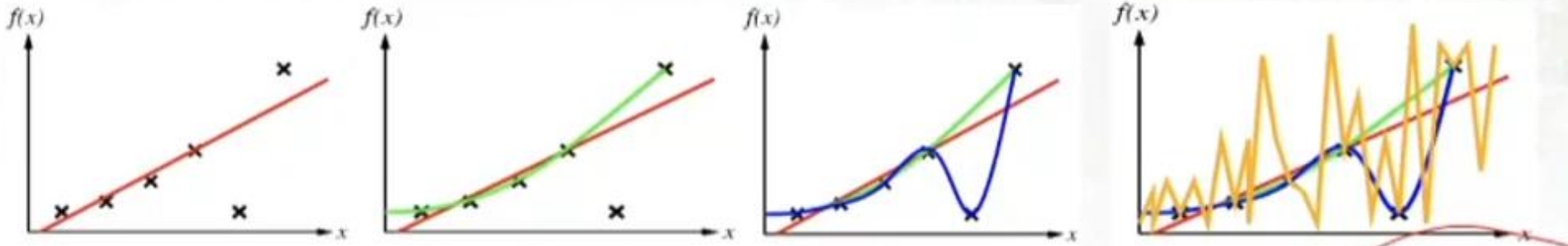
Wide Ranges of Functions/Models

Models for Learning

- If-Else: Axis-Parallel (Decision Trees)
- Linear Classifier
- Distance based (Nearest Neighbor)
- Non-linear (Neural Network)



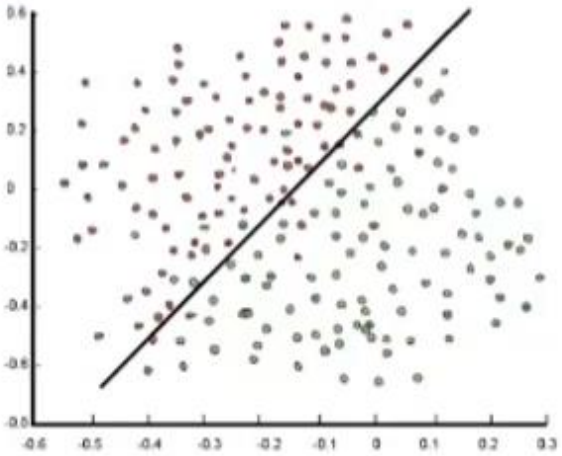
Remember: Generalization and Overfitting

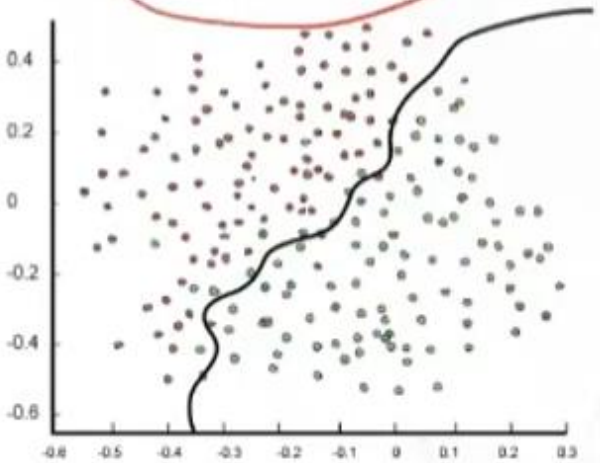


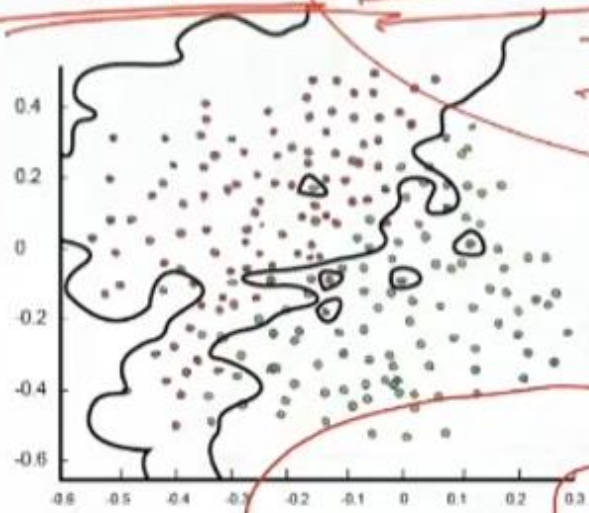
Comp ↓ Tr ↑

?

Comp ↑ Tr err = 0







X

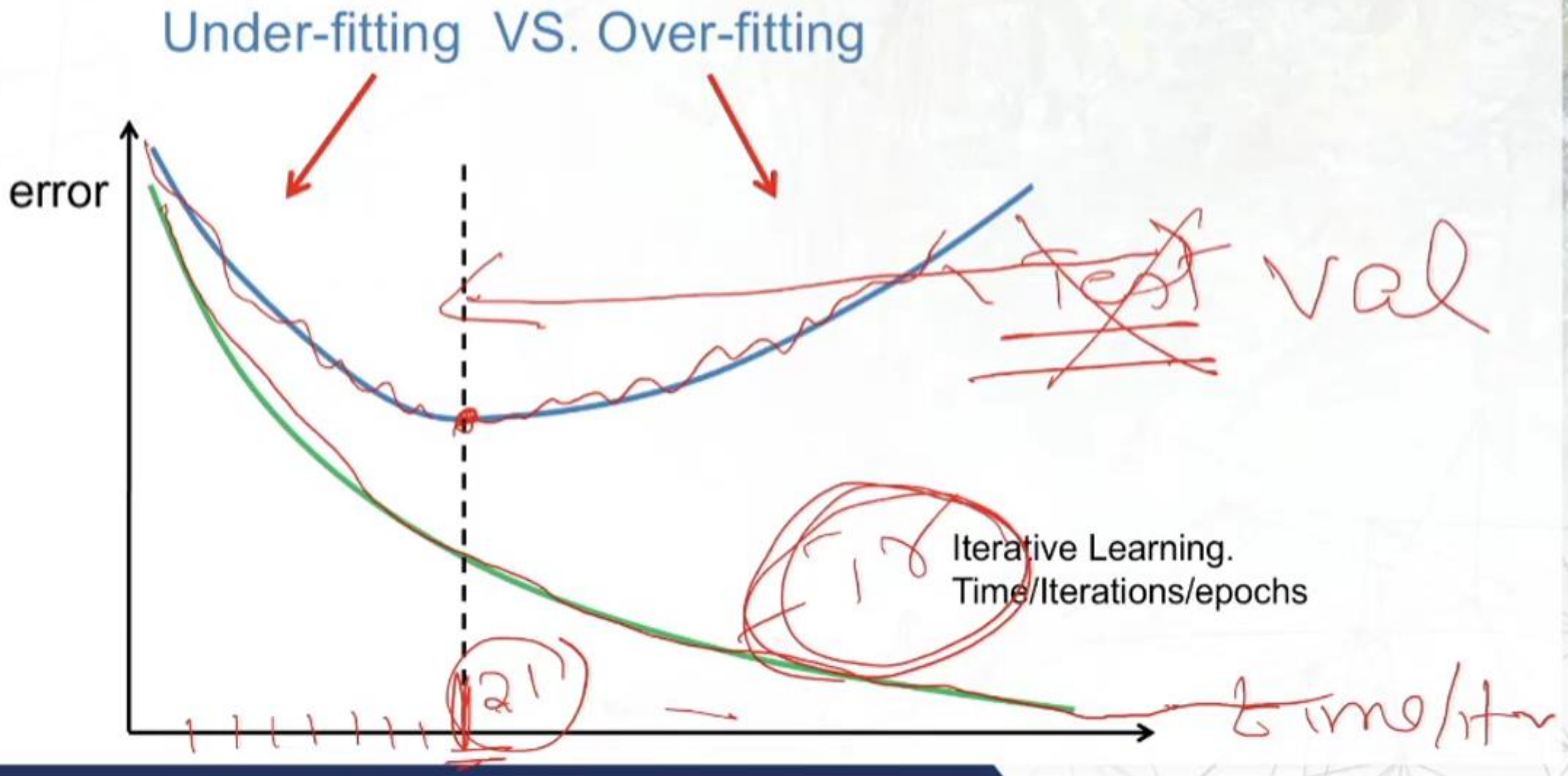
overfitting

Overfitting

- Performance on the training data is too good
- Performance on the test data is bad.

- Why?
  - Algorithm has remembered the data/solutions.

What are we seeking?



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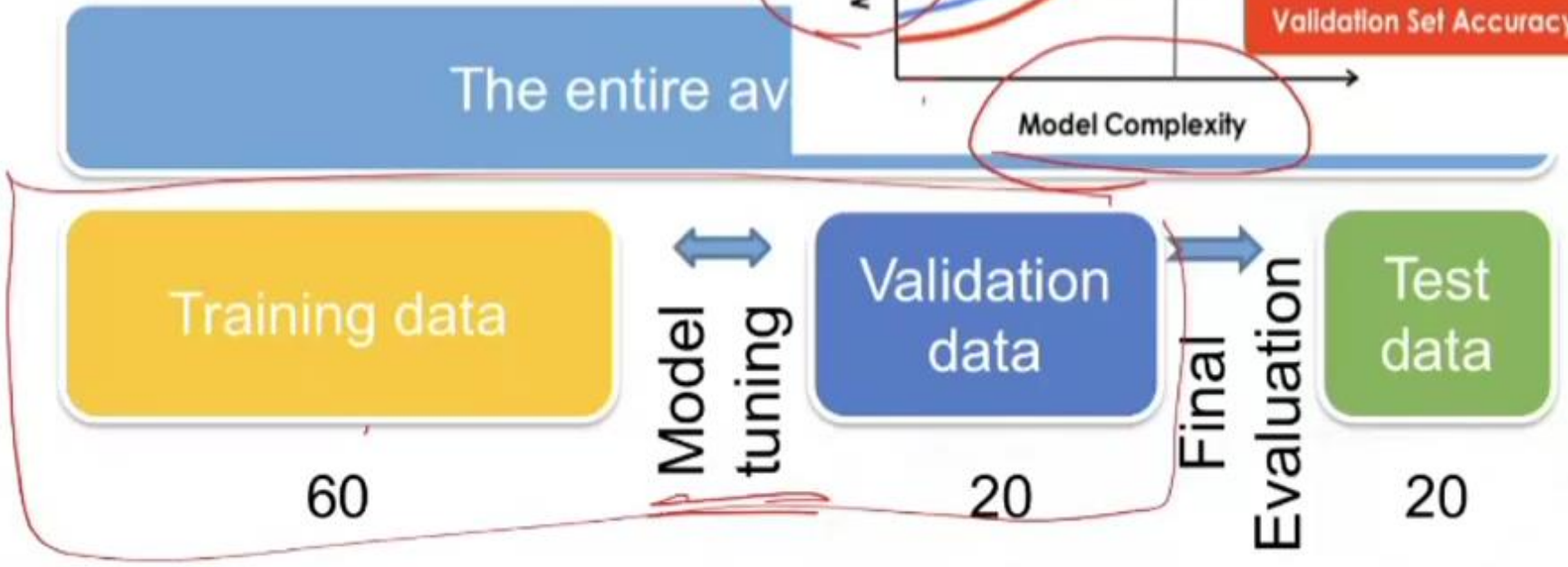
Detecting Overfitting

- When do we overfit?
  - Model is powerful/complex
  - Limited training samples
  - Large number of features
- Empirical Detection

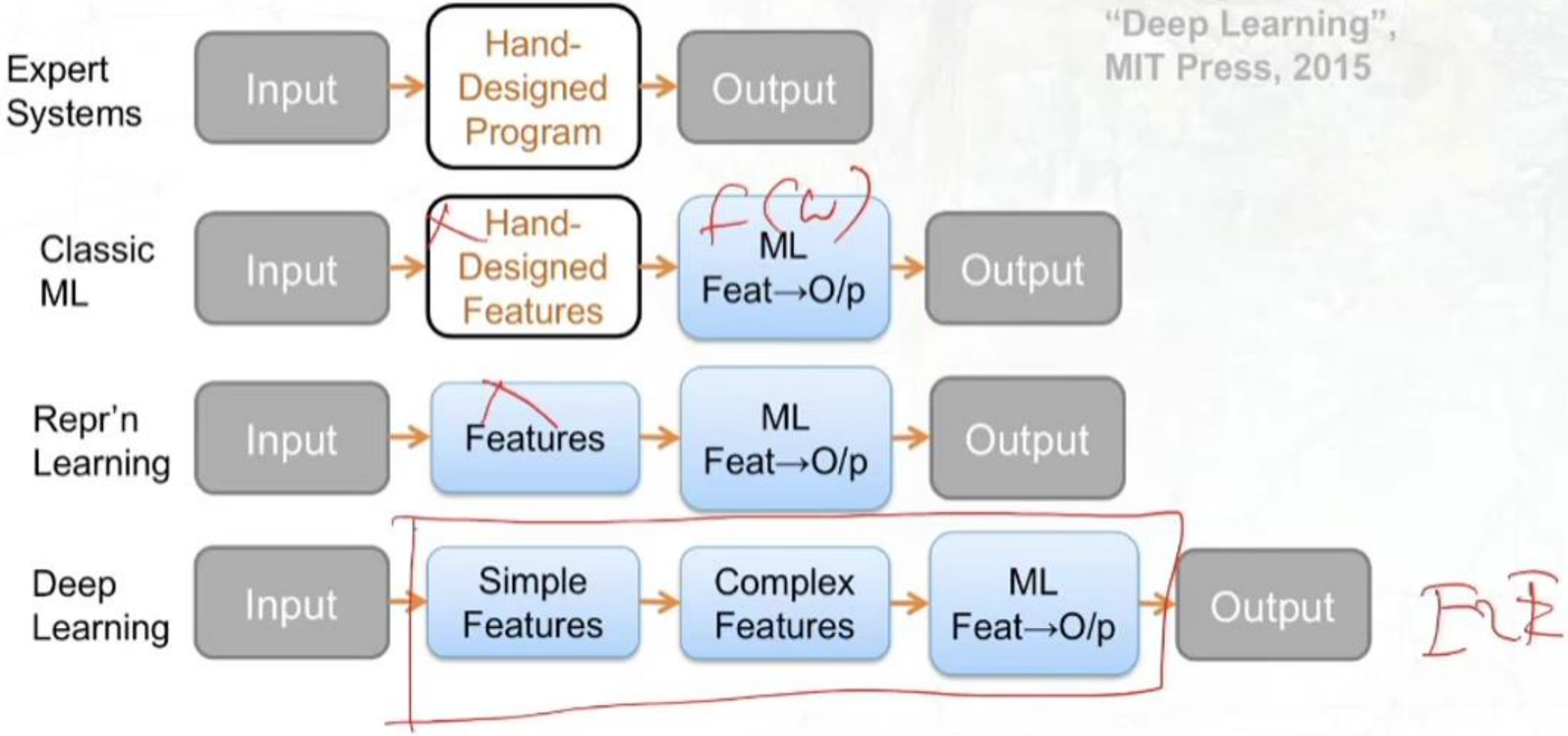


Overfitting: Solutions

- Reduce the model complexity
  - Regularization
  - Ensemble Techniques
- Increase the number of training samples
  - Data Augmentation
- Reduce the number of features
  - Dimensionality Reduction
- Model-specific methods
  - Early Stopping
  - Pruning
  - Large-margin methods

Evolution of Learning

Y. Bengio et al,
"Deep Learning",
MIT Press, 2015

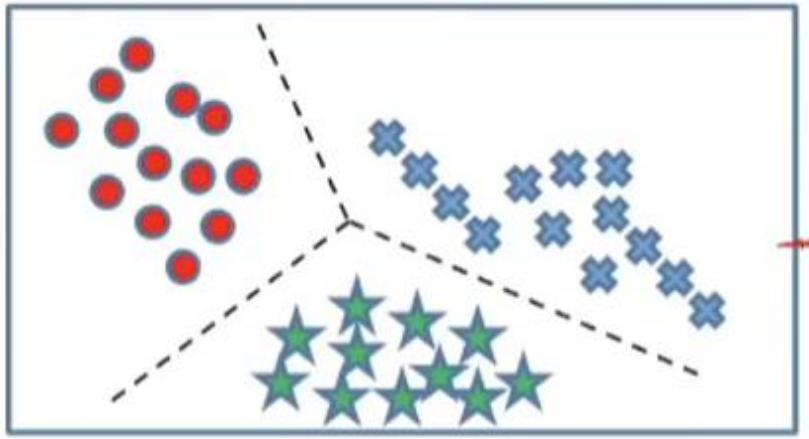


Summary

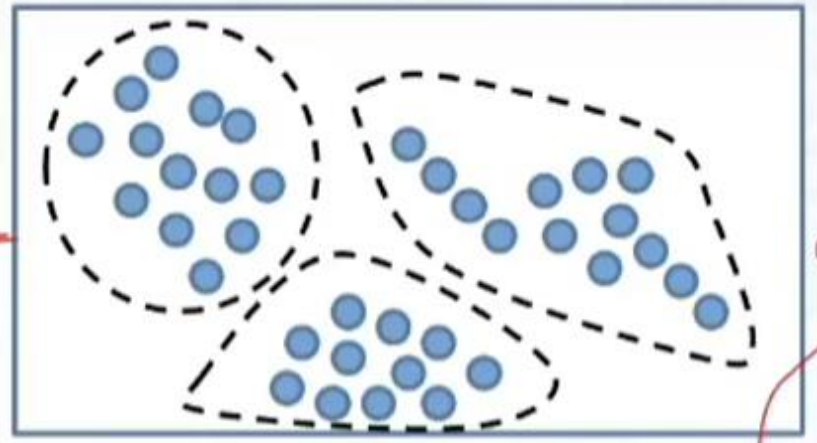
- Data driven problem solving
  - Modelling vs Learning/Generalization
  - Classification, Regression, Structured Prediction
  - Many other formulations/problems
- Function Class
  - Simple Models: DT, Nearest Neighbour, Linear
  - Powerful, Popular Neural Networks
- Problem of Learning
  - Optimization: Convex and non-convex
  - Learning as "finding the W"
  - Deep Architectures (more next lecture)

D. Learning Paradigms and Optimization

Class of ML Algorithms

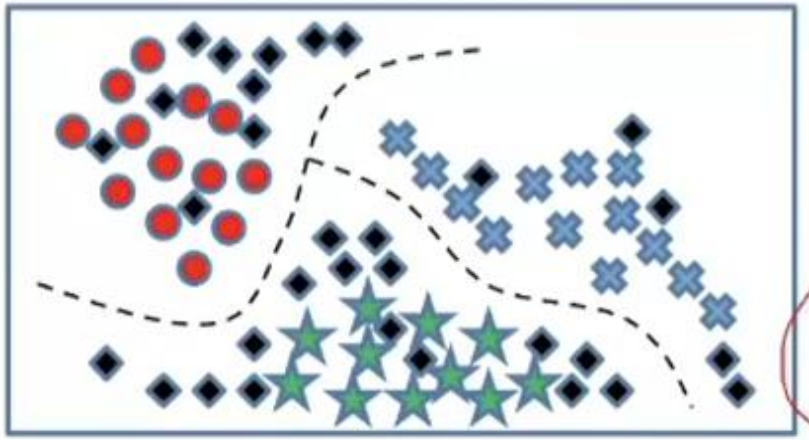


Supervised learning



cluster

Unsupervised learning



W. Sup
Self sup.

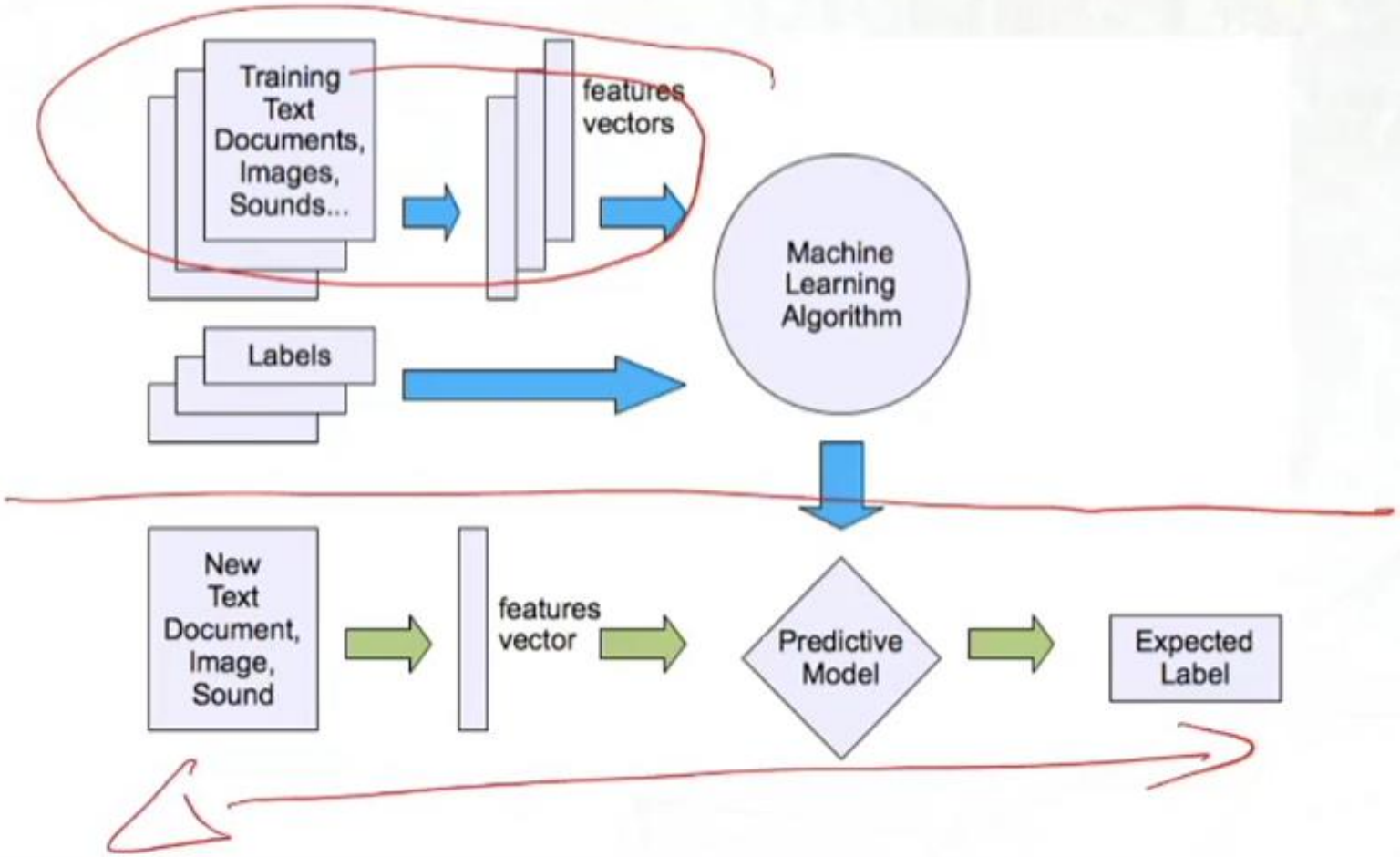
Semi-supervised learning

Algorithms

- **Supervised learning** ($\{x_n \in R^d, y_n \in R\}_{n=1}^N$)
  - Prediction
  - Classification (discrete labels), Regression (real values)
- **Unsupervised learning** ($\{x_n \in R^d\}_{n=1}^N$)
  - Clustering
  - Probability distribution estimation
  - Finding association (in features)
  - Dimension reduction
- **Semi-supervised learning**
- **Reinforcement learning**
  - Decision making (robot, chess machine)

Machine learning structure

- **Supervised learning**



Optimization: Find the *best* W

$$\text{Min } \frac{1}{2} \| w \|^2 + C \sum_{i=1}^{M} \xi_i$$

$$\text{subject to: } y_i(w^T x_i) \geq \mathbf{1} - \xi_i, \xi_i \geq \mathbf{0}$$

Eg. SVM

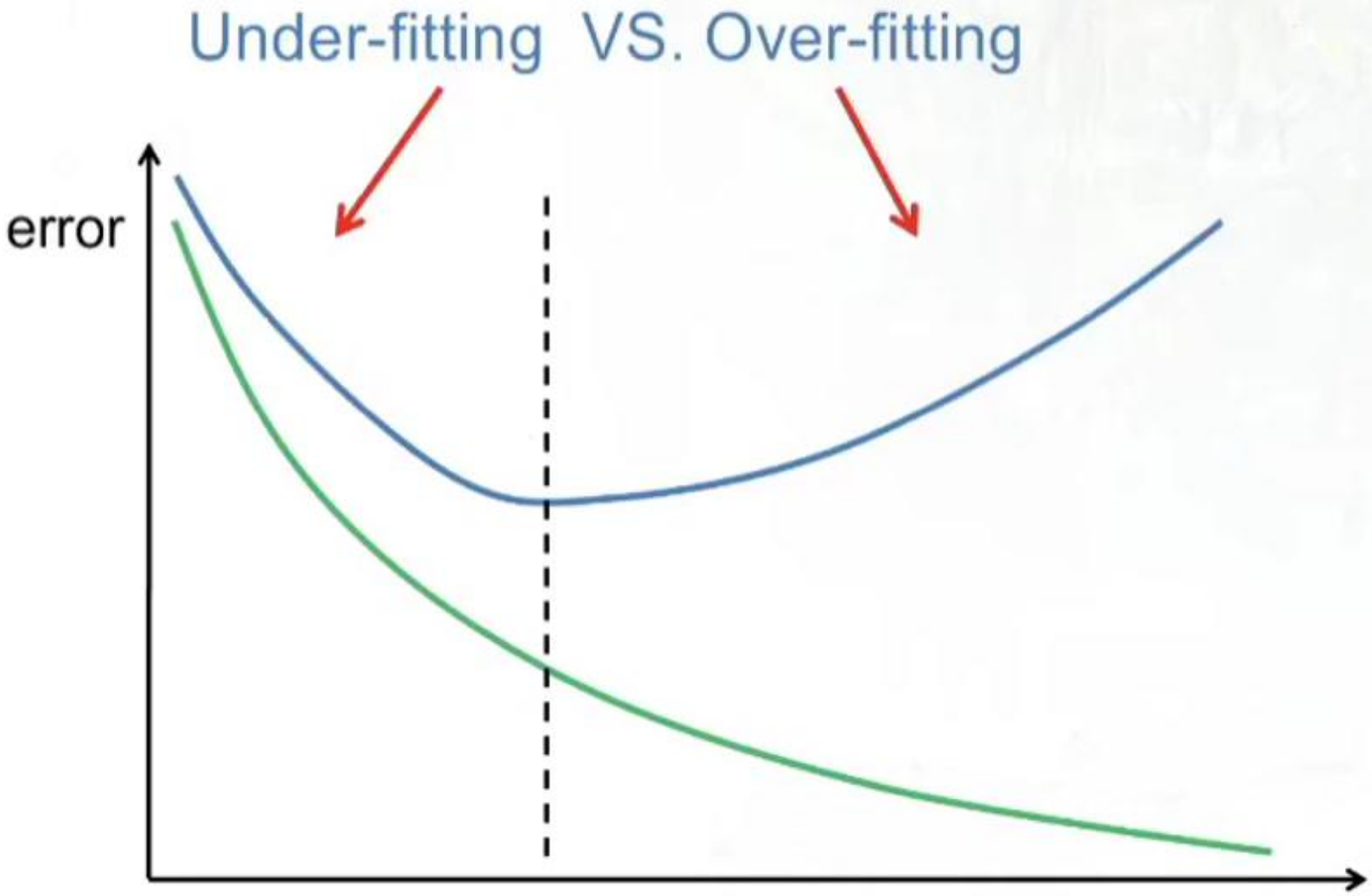
Often problem is formulated as an optimization problem on the set of known examples

Some More Key Words

- Training: Find f and W
- Testing: Evaluate f on a specific example
- Training, Testing and Validation splits of the data
- Generalization: Goal is to do well on "unseen data"
- Error, Loss, Objective Functions
- Complexity of the solution (eg. Number of free parameters)
- Generative classifiers try to model the data. Discriminative classifiers try to predict the label.

V.C. Dimension

What are we seeking?



Example: Linear Classification

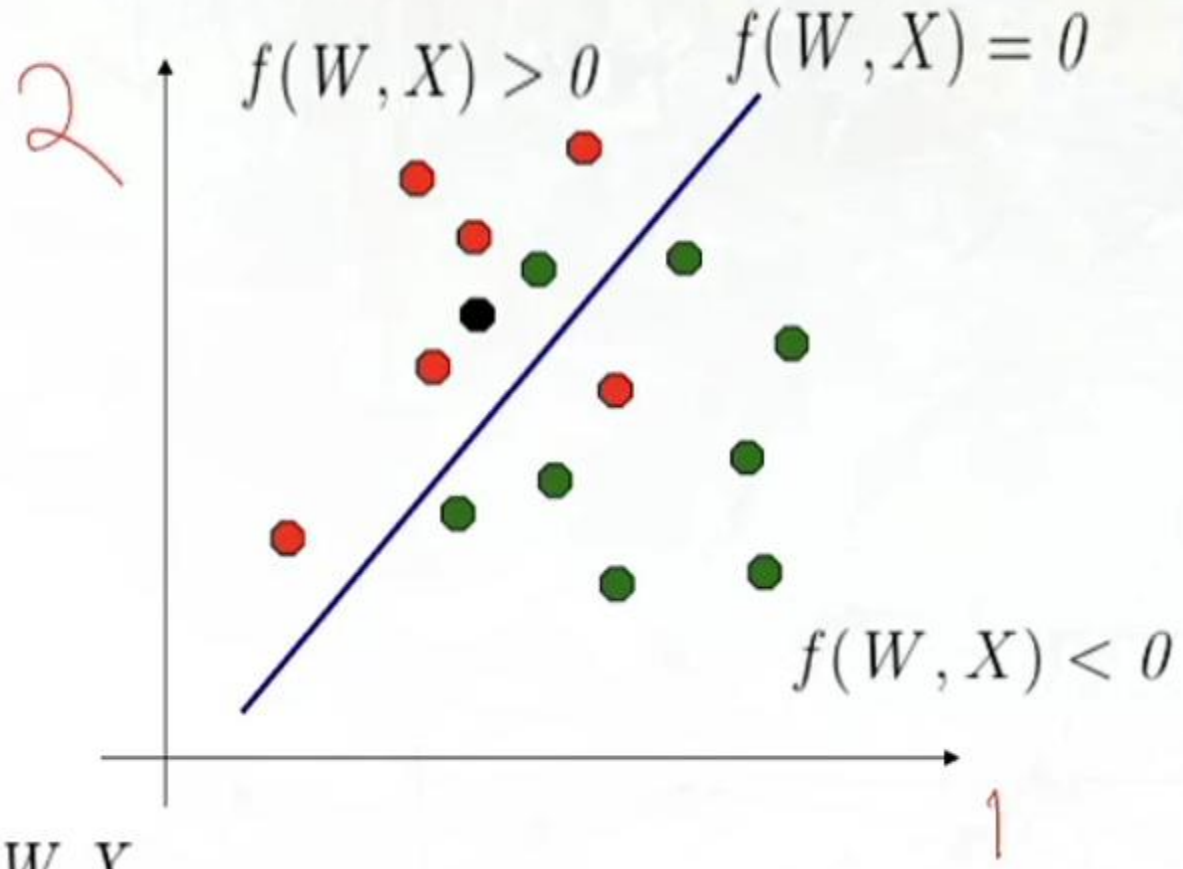
$$f(W, X) = w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

=1

d - dimensi.

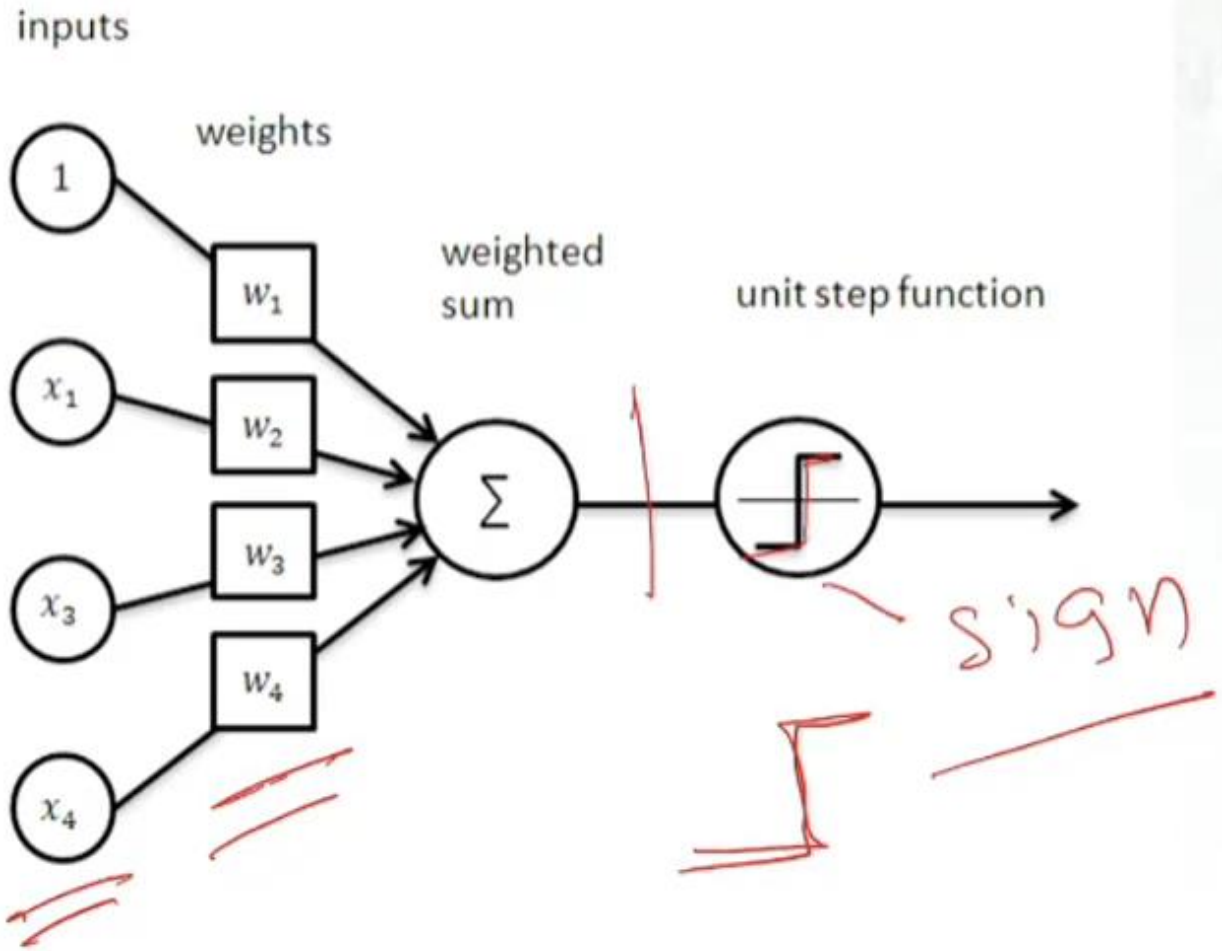
Feature Vector $X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$

Parameters to be learned $W = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}$



Compactly: $f(W, X) = W^T X$ or $W.X$

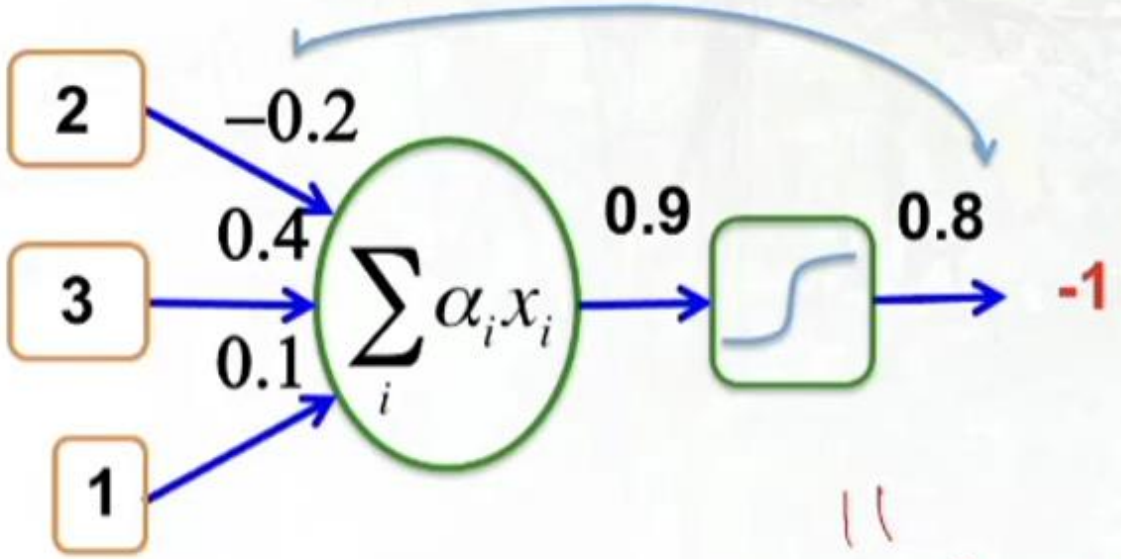
Example: A "Neural Network" Perspective



Predicted Label:

Sign ($\mathbf{w}^T\mathbf{x}$)

Basics: Learning



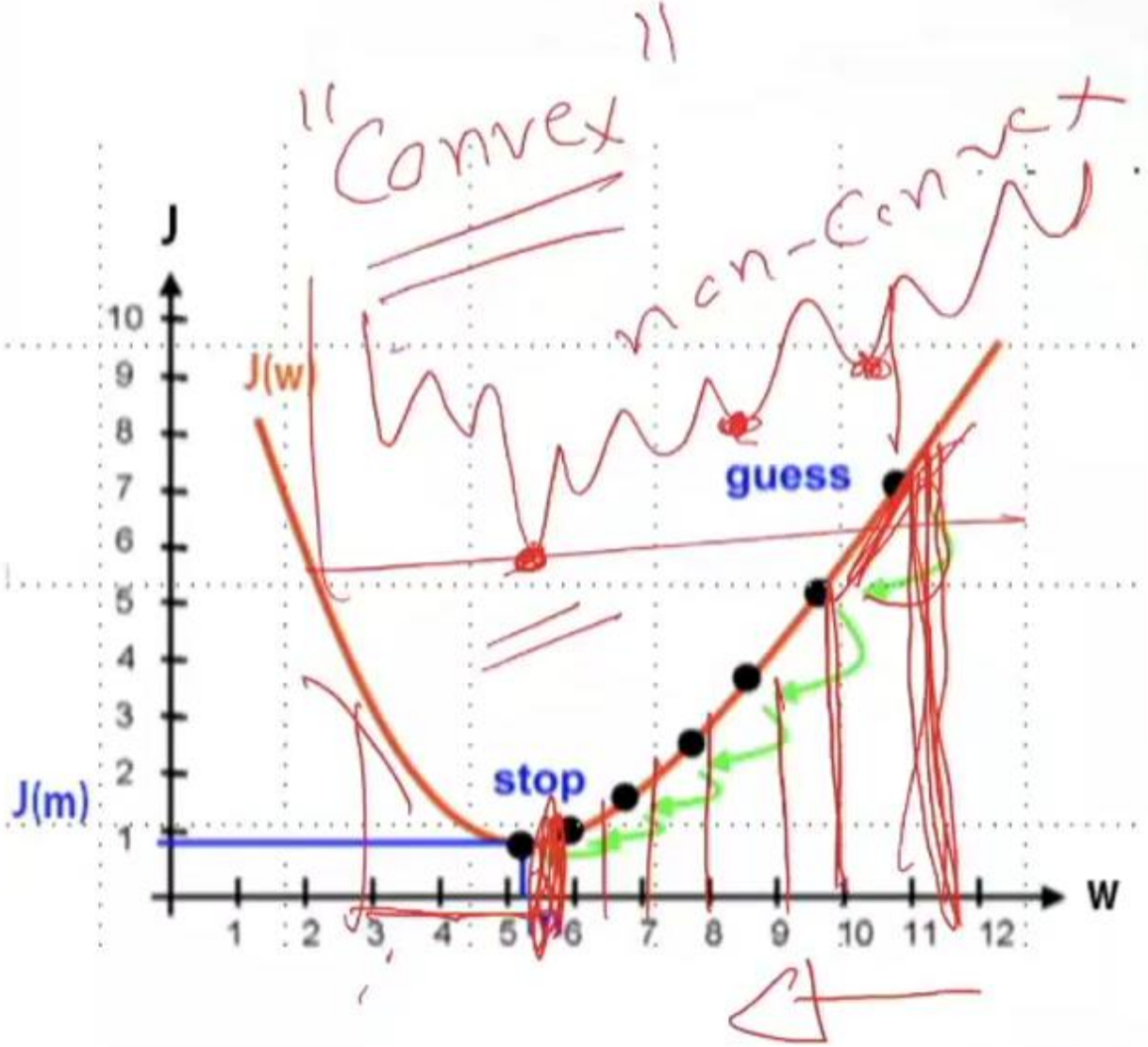
weight update

"Gradient Desc"

Repeat until weights stabilize

1. Take a training sample and pass it through the neuron
2. Find the difference between the output and expected values (loss function)
3. Update the weights to reduce this loss

Basics: Gradient Descent: Intuition



Problem: Minimize J(w).

1. Start with an initial guess.
2. Update your guess by moving along the negative slope (gradient).

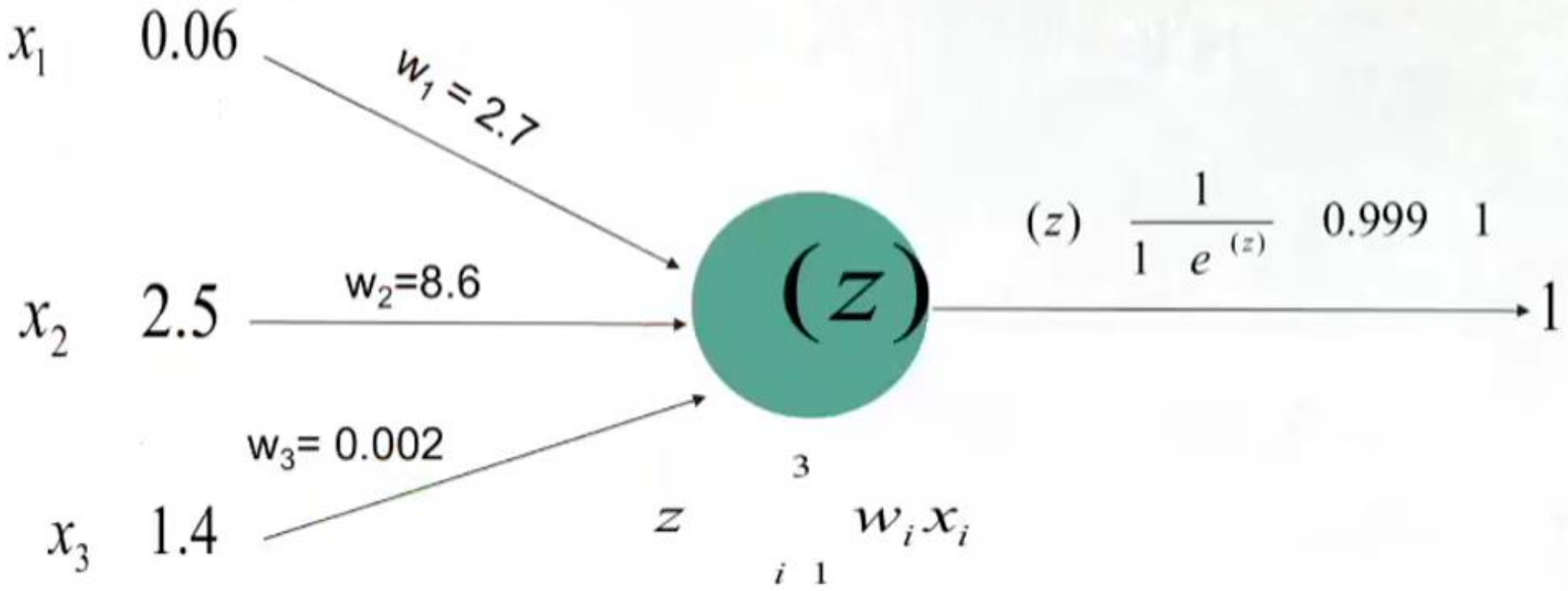
$$\mathbf{w_{n+1}} = \mathbf{w_n} + \eta \Delta \mathbf{w}$$

Notes:

1. We do not have an analytic form of J(w) to differentiate and find the optima/best/minima.
2. We can differentiate "locally" at the samples and update the weights/parameters.

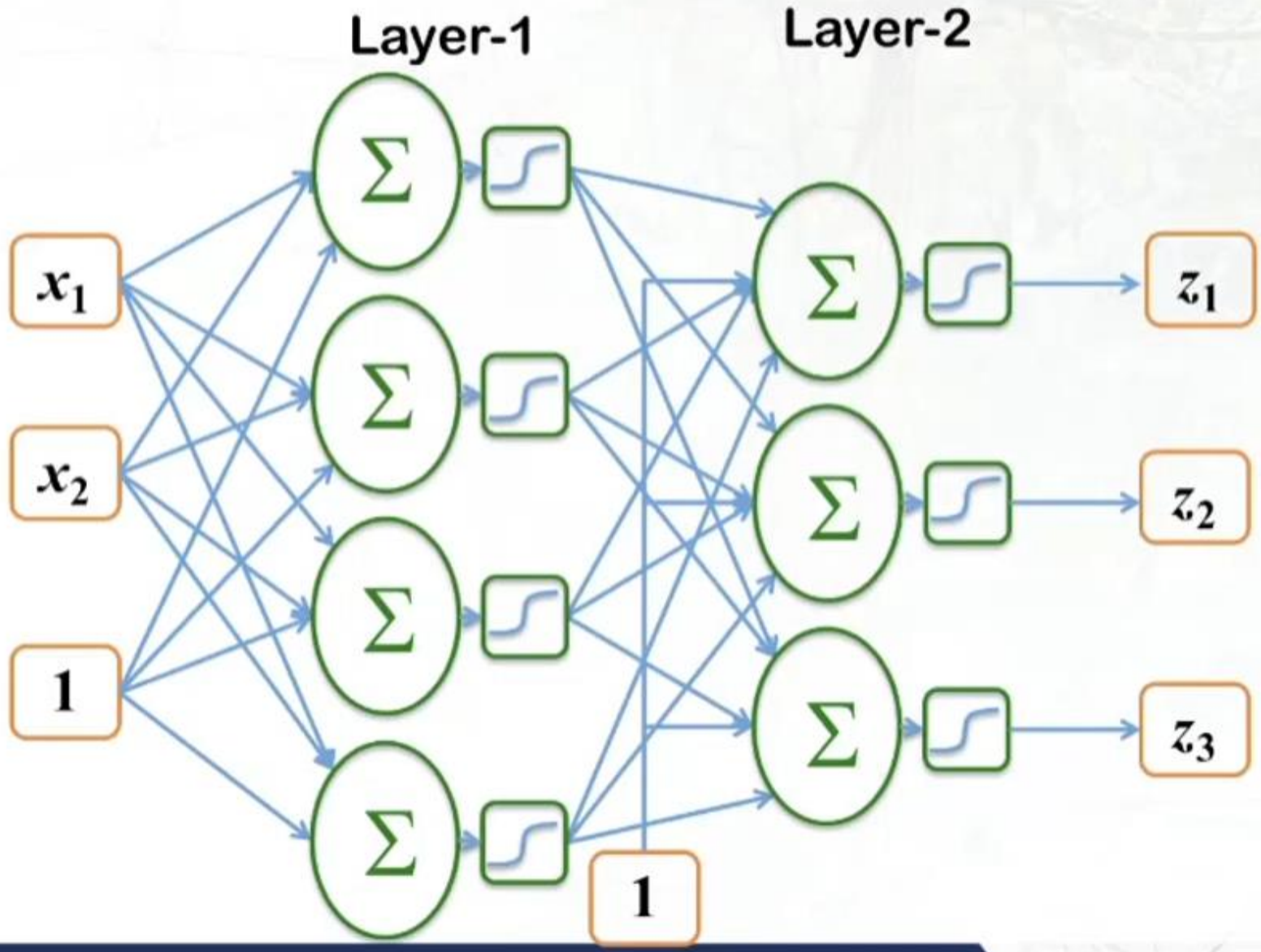
Learning in Neural Networks

Learning = Finding the best or optimal weights

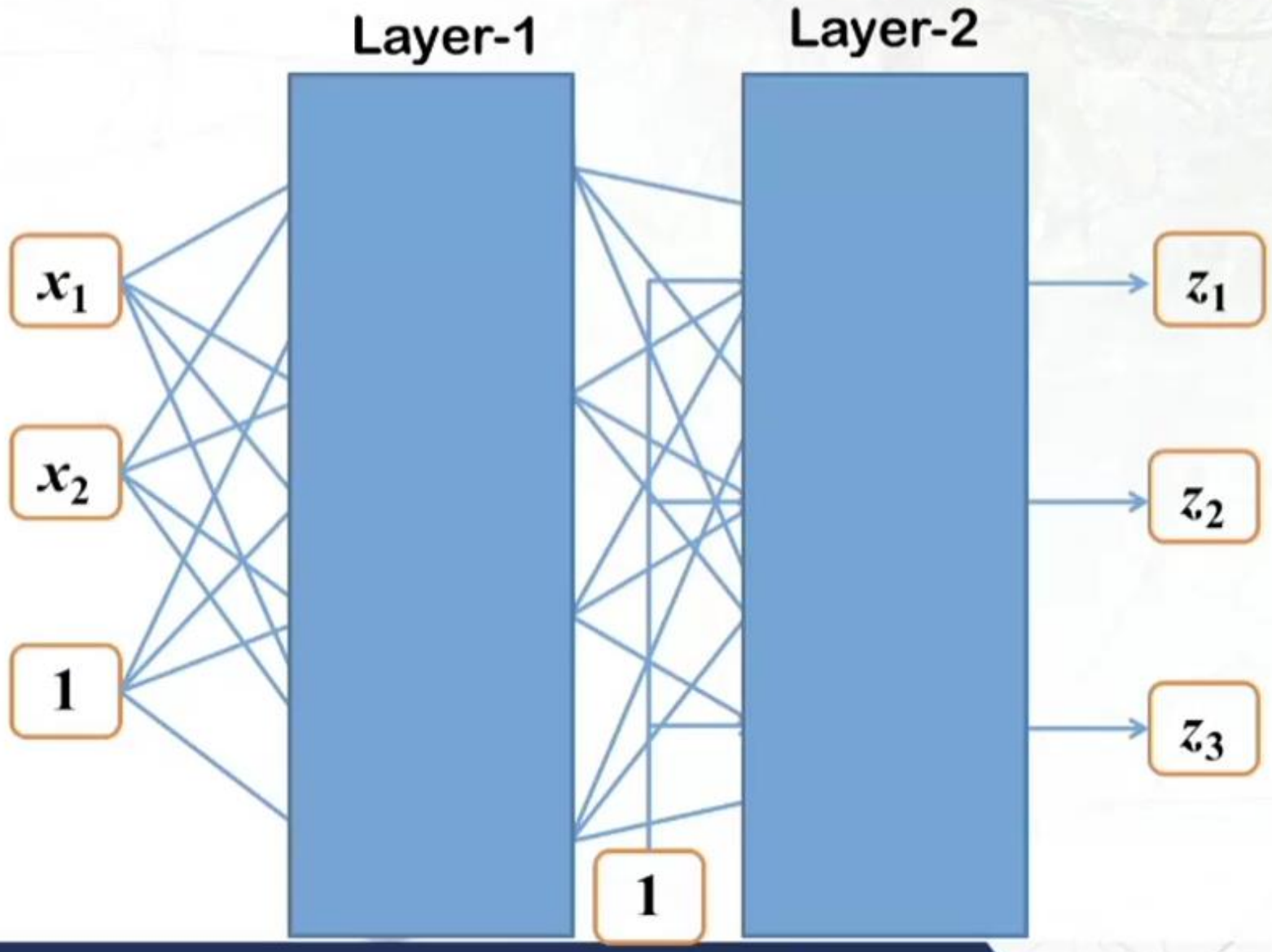


z -0.06 2.7 2.5 8.6 1.4 0.002 21.34

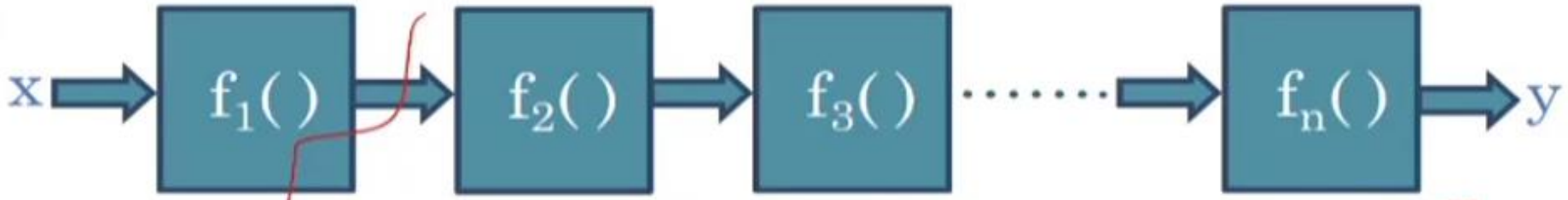
Neural Network

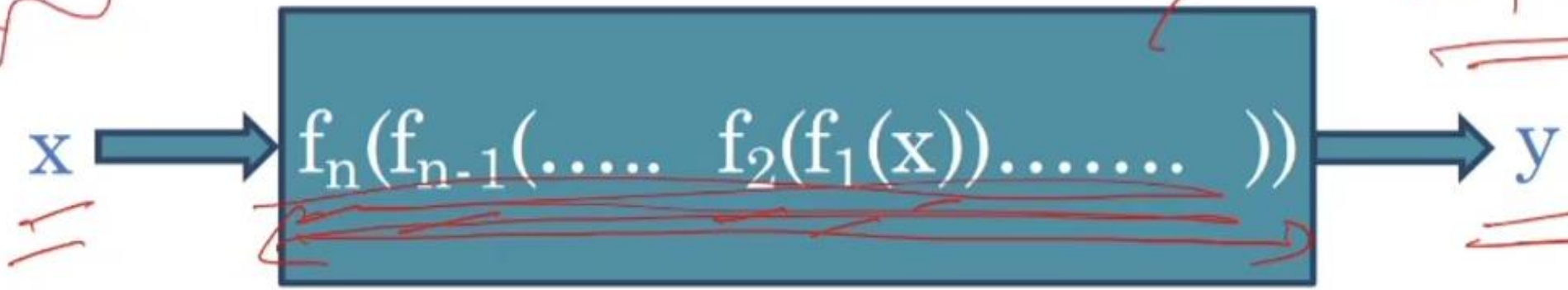


Neural Network

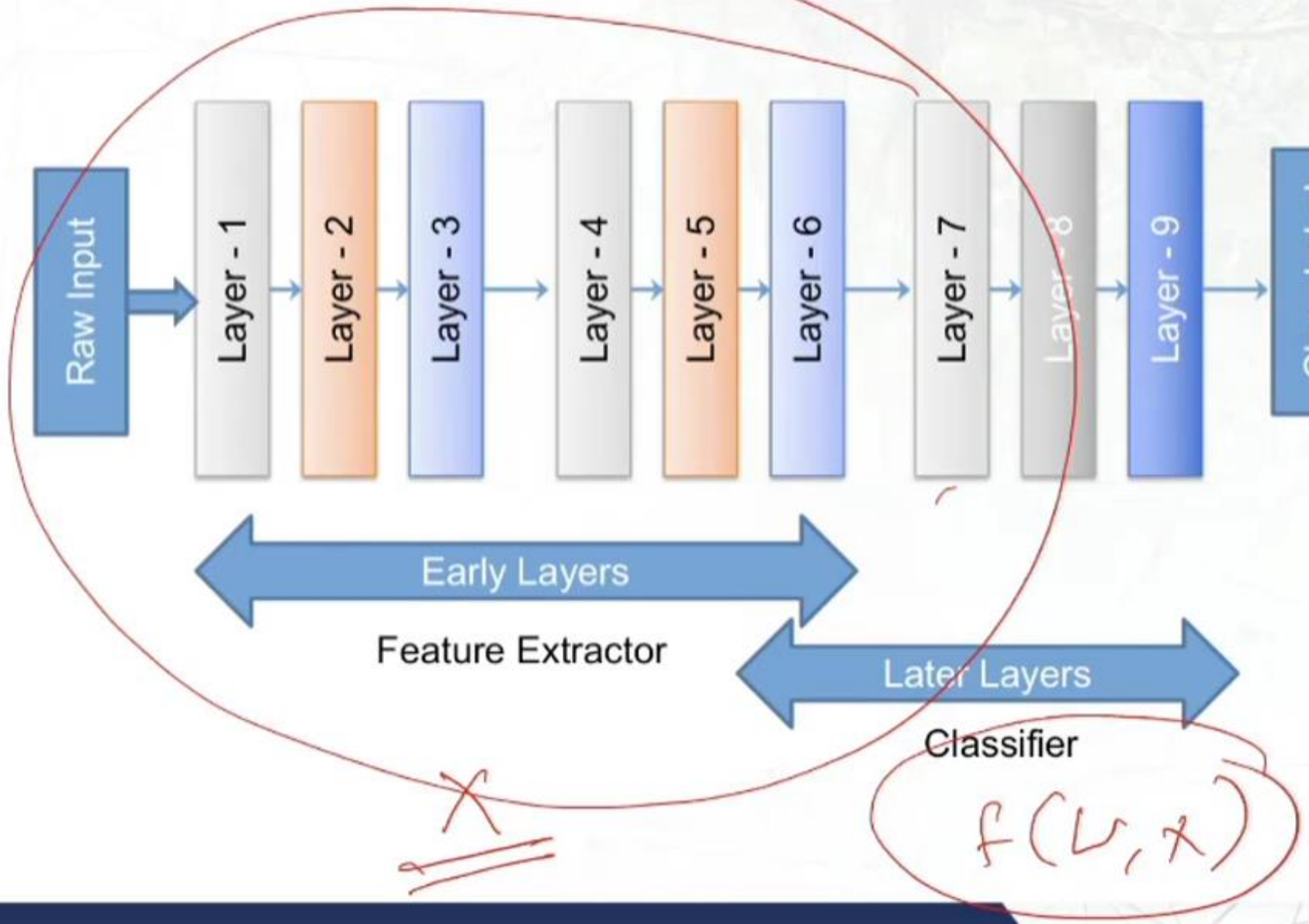


Complex Functions and Richer Features

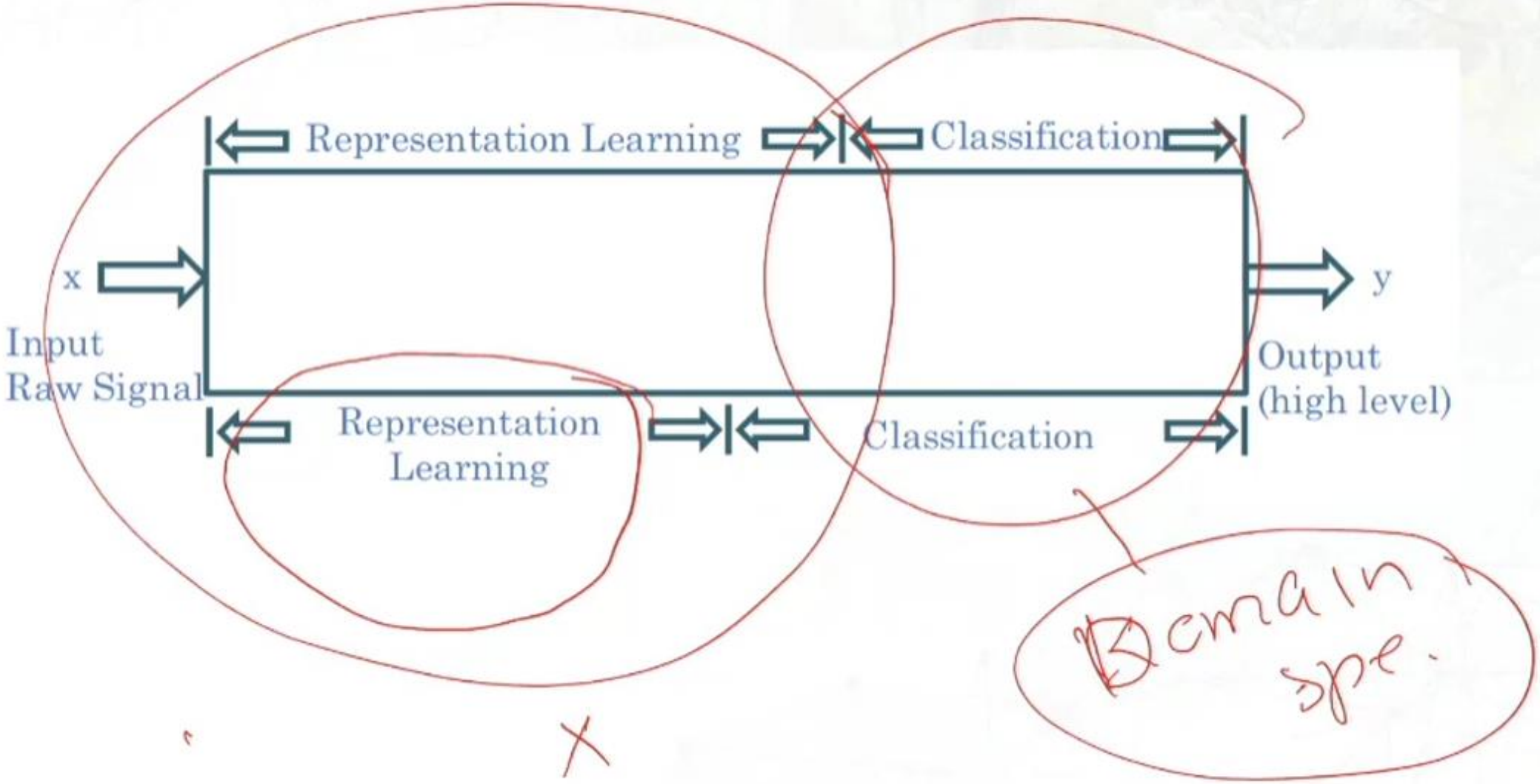




Deep Neural Networks



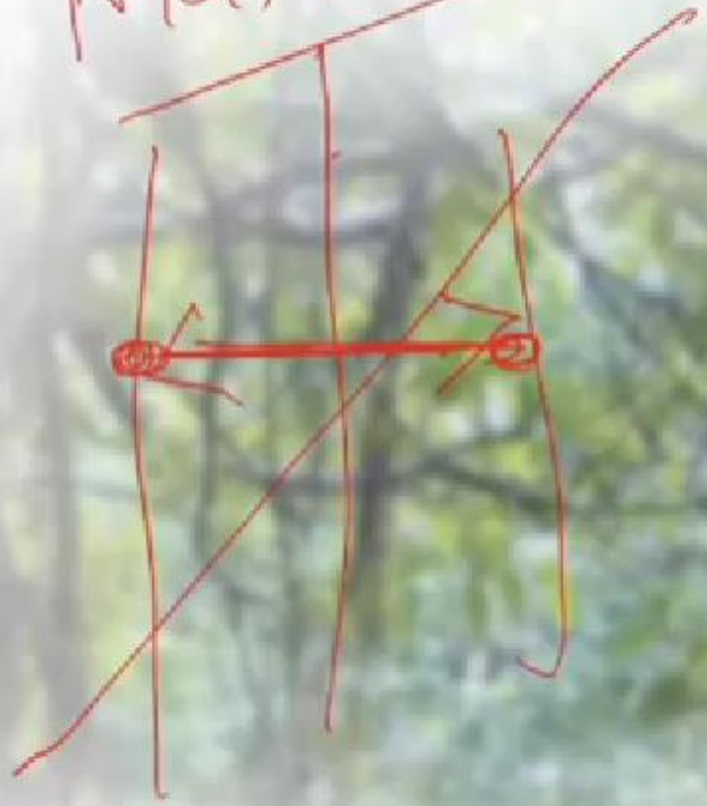
View Point


Representation Learning
Classification
x
Input
Raw Signal
y
Output
(high level)
Representation
Learning
Classification
Domain
spe.

Summary

- **Popular methods of today are**
  - Supervised
  - Discriminative
- **SVMs were/are popular.** Nice optimization problem to solve
- **Deep neural networks are becoming the standard for many problems**
  - Feature extraction
  - End to end training
  - Trained models for evaluation
  - Porting/Transforming network to network.

max-margin



$\min_{w} L + \|w\|$ # norm

Thanks!!

L-fn

Questions/Comments?

Regularize

S SS P