The Three Pillars of Machine Learning

- **1. Learning Theory**
- The key to neural network and machine learning: Learning theory
- The role of learning theory has grown a great deal in:
 - Mathematics
 - Statistics

- Finance
- Computational Biology
- Neurosciences, e.g., theory of plasticity, workings of visual cortex



University of Washington Computer science, e.g., vision theory, graphics, speech synthesis



T. Poggio/MIT

Face identification:



MIT

People classification or detection:



Poggio/MIT

What is the theory behind such learning algorithms?

2. The problem: Learning theory

Given an unknown function $f(\mathbf{x})$ whose graph is unknown, learn the function from examples.

Example 1: $\mathbf{x} = (x_1, x_2, \dots, x_k)$ is retinal activation pattern (i.e., x_1 = activation level of retinal neuron 1, etc.), and $y = f(\mathbf{x}) > 0$ if the retinal pattern is a chair; $y = f(\mathbf{x}) < 0$ otherwise.

[Thus: $f(\mathbf{x})$ encodes concept of a chair]

Given: examples of chairs (and non-chairs): $\mathbf{x}_1, \mathbf{x}_2$ etc., together with proper outputs y_1, y_2 , etc. This is the *training information*.



Goal: Give best possible estimate of the unknown function f, i.e., try to learn the concept f from the above examples.

But: given a few pieces of information about the graph of *f* not sufficient: which is the "right" $f(\mathbf{x})$ given the data points (\mathbf{x}, y) below?

Example 2: (Here **x** is just 1 dimensional)



(a)





[How to decide?]

Note: there is no unique solution for $f(\mathbf{x})$ - finding f is an *ill-posed problem*.

Hint: a good machine will choose the simplest f(x) - this is Occam's razor.

MACHINE LEARNING: BASICS

1. Motivation: machine learning for high dimensional problems

Computational biology

Example in Computational Biology: RNA-Seq Machine



Computational biology

Process: for each subject tissue sample s, obtain feature vector

$$\Phi(s) = \mathbf{X} = (x_1, \dots, x_{20,000})$$

= vector of gene expression levels

E.G., $x_1 = expression$ level of gene 1, etc.

Can we classify tissues this way?

If this is an ovarian cancer tissue sample:

Questions:

- (a) What type of cancer is it?
- (b) What is prognosis if untreated?
- (c) What will be the reaction to standard chemotherapies?

Goals:

- 1. Differentiate two different but similar cancers.
- 2. Differentiate different cancer prognoses or potential therapies
- 3. Understand genetic origins and pathways of the cancer

Basic difficulties: few samples to train with (e.g., 30-200); high dimension (e.g., 5,000 - 100,000).

Curse of dimensionality - too few samples and too many parameters (dimensions) to fit them.

Tool: Support vector machine (SVM)

Procedure: look at feature space F in which $\Phi(s)$ lives, and separate examples of one and the other cancer with a hyperplane:

Computational biology



e.g. Red vs. Green points represent tissues that were responsive (green) vs.

Computational biology

unresponsive (red) to a particular therapy T.

Train machine: take n = 50 subjects with different responses to therapy T, and locate their feature vectors in the space F, labeling them red (unresponsive) or green (responsive).

Find separating hyperplane, and use this plane to separate feature vectors of future subjects into 'responsive' and 'unresponsive'.

There are a number of other *machine learning methods* (often with non-linear separating boundaries) that can discriminate (classify) tissue feature vectors $\Phi(s)$ this way, with respect to prognosis, response to therapies, metastatic/nonmetastatic cancer etc.

Such cancer data has often been very reliable and obtained from TCGA (the Cancer Genome Atlas) and its iterates.

2. The principle: more is more

Past beliefs: too many variables spoil the statistics; < 50 variables was typical requirement

Present: more is better

Machine learning allows massive integration of information about any object (e.g. a tissue sample): On a gene level: for any gene in a tissue sample we get a series of numbers describing it, from basic measurements and databases of:

- protein-protein interactions
- co-expression (when genes activate together)
- gene ontology relationships (keywords referring to given genes in the literature)
- pathway correlations (when genes appear in the same biological pathways)

Computational biology

 epigenetic information (methylation, phosphorylation levels of genes in DNA)

Machine Learning and Suport Vector Machines (SVM)

1. Machine learning: SVM

Support vector machine (SVM) is one of the most well-known machine learning tools.

Some applications of SVM in computational biology:



• Protein binding prediction

Will protein *A* bind to protein *B*?



http://3dsig.weizmann.ac.il/usersfiles/3dsig/abstracts/2004/13.html

SVM

• Text and topic mining Does this paper discuss transcription factor binding to DNA?





http://3dsig.weizmann.ac.il/3dsig/2004/abstracts/allabs.html http://www.informatik.hu-

berlin.de/forschung/gebiete/wbi/research/projects/textmining/k meddbx.jpg

2. SVM illustration in cancer classification

Example 1: Myeloid vs. Lymphoblastic leukemias [Golub]

ALL: acute lymphoblastic leukemia AML: acute myeloblastic leukemia

SVM training: leave one out cross-validation

SVM

Dataset	Algorithm	Total Samples	Total error s	Class 1 errors	Class 0 errors	Number Genes
Leukemia Monphology (trest) AML vs ALL	SVM	35	0/35	0/21	0/14	40
	¥	35	2/35	1/21	1/14	50
	k-NN	35	3/35	1/21	2/14	10
Leukemia Lineage (ALL) B vsT	SVM	23	0/23	0/15	0/8	10
	w	23	0/23	0/15	0/8	9
	k-NN	23	0/23	0/15	0/8	10
Lymphoma FS vs DLCL	SVM	77	4/77	2/32	2/35	200
	w	77	6/77	1/32	5/35	30
	k-NN	77	3/77	1/32	2/35	250
Brain MD vs Glioma	SVM	41	1/41	1/27	0/14	100
	w	41	1/41	1/27	0/14	3
	k-NN	41	0/41	0/27	0/14	5

S. Mukherjee

fig. 1: Myeloid and Lymphoblastic Leukemia classification by SVM, along with other discrimination tasks; k-NN is *k*-nearest neighbors; WV is weighted voting





S. Mukherjee

fig 2: AML vs. ALL error rates with increasing sample size; Above curves are error rates within test sets after training of machine with a training set.
3. Result: SVM on cancer (Alon, et al., PNAS)

Recall: 40 samples colon cancer tissue 22 samples of normal colon tissue (62 total).

For each sample computed

 $\mathbf{x} = (x_1, \dots, x_p) =$ gene expression array



Let

$$D = \{(\mathbf{x}_i, y_i)\}_{i=1}^{62}$$

be collection of samples and correct classifications:

$$y_i = \begin{cases} 1 & \text{if } \mathbf{x}_i \text{ cancerous} \\ -1 & \text{if } \mathbf{x}_i \text{ non-cancerous} \end{cases}$$

Feature space *F* is 6,500 dimensional (6,500 genes)

SVM

Result: using leave one out cross validation (leave one sample out and train a machine on the others) obtained:

Misclassification of 6/62 tissues.



4. Example application: handwritten digit recognition - USPS (Scholkopf, Burges, Vapnik)

Handwritten digits:



0	0	0	0	0
/	/	/	1	/
2	Z	2	2	2
F	3	3	3	3
4	4	4	4	4
2	5	5	5	5
6	6	6	6	6
1	7	7	7	7
8	8	8	8	8
9	9	9	9	9



Training set (sample size): 7300; Test set: 2000

10 class classifier; each class has a separating SVM function: Results:

SVM

polynomial : $K(\mathbf{x}, \mathbf{y}) = ((\mathbf{x} \cdot \mathbf{y})/256)^{\text{degree}}$									
degree	1	2	3	4	5	6			
raw error/ $\%$	8.9	4.7	4.0	4.2	4.5	4.5			
av. $\#$ of SVs	282	237	274	321	374	422			

degree ~

RBF : $K(\mathbf{x}, \mathbf{y}) = \exp\left(- \mathbf{x} - \mathbf{y} ^2/(256 \ \sigma^2)\right)$									
σ^2		1.0	0.8	0.5	0.2	0.1			
raw error/%		4.7	4.3	4.4	4.4	4.5			
av. $\#$ of SVs		234	235	251	366	722			

sigmoid: $K(\mathbf{x}, \mathbf{y}) = 1.04 \tanh(2(\mathbf{x} \cdot \mathbf{y})/256 - \Theta)$

Θ		0.9	1.0	1.2	1.3	1.4
raw error/%	4	4.8	4.1	4.3	4.4	4.8
av. $\#$ of SVs	2	242	254	278	289	296

5. Example: machine learning and finance

A note on machines and neural networks:

The notion of machine learning includes neural network architectures.

The vector of inputs to such a network is $\mathbf{x} = (x_1, \dots, x_p)$ and the output (prediction) is q.

Thus we are implementing the function $f(\mathbf{x}) = q$.

Neural net:



Input: feature vector $\mathbf{x} = (x_1, \dots, x_p)$ Output: number q.

Training: show the network examples of known 'correct' outputs q_i based on input (training) vectors \mathbf{x}_i :

$$\{(\mathbf{X}_1, q_1), \dots, (\mathbf{X}_N, q_N)\}.$$

Example 2: \mathbf{x}_1 is a time series of consecutive daily prices of a given stock, while q_1 is a predicted return on the stock

over the day immediately following this time series.

This machine is a neural network trained with weights (parameters) that transform input vector $\mathbf{x} = (x_1, \dots, x_p)$ entering on the left layer into a single ouptut number $q = f(\mathbf{x}) =$ predicted stock price formed on the right.

Other Machine Learning methods are really generalized versions of the above inputoutput network.

Input: feature vector

$$\mathbf{X} = (x_1, \dots, x_p)$$

desired ouptut: q = predicted stock price.

6. The simplest machine: linear regression

Example: Let's build a regression machine to predict stock price from time series.

Training data:

$$\{(\mathbf{X}_1, q_1), \ldots, (\mathbf{X}_N, q_N)\}.$$

Machine will find a rule that takes prior prices x_i to today's predicted price q:

$$\mathbf{X} = (x_1, \dots, x_p) \to q.$$

Regression machine:



$$q = \beta_1 x_1 + \ldots + \beta_p x_p + \beta_0 = q = \boldsymbol{\beta} \cdot \mathbf{X} + \beta_0$$

$$\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_p) \longrightarrow q = \boldsymbol{\beta} \cdot \mathbf{x} + \boldsymbol{\beta}_0 \longrightarrow q$$

How do we train the machine? Find coefficients β_0, \ldots, β_p from ordinary regression based on the training data set

$$\{(\mathbf{X}_1,q_1),\ldots,(\mathbf{X}_N,q_N)\}$$
 .



http://www.aboutdm.com

ML Pillars

The Three Pillars of Machine Learning:

 The world can be injected into any computer using feature vectors - any object can be summarized as a string of numbers. Example -

ML Pillars



This object (a face) can be converted to a feature vector (numbers) in different ways:

 (a) for example a face is just 10⁶ numbers (photograph pixel intensities).



(b) or a face is a list of distances between the primary facial features (e.g. eye, ears, lip corners), or (better) distance ratios.

Main point: feature vectors are the language of learning machines - objects are now strings of numbers.

ML Pillars

- (2) Geometrization of data: a *n*dimensional feature vector is a string of numbers that become coordinates in an *n* more dimensional space (feature space).
- Thus objects to be classified become geometric points in a space.
- Identifying an object becomes identifying its location in feature space:

ML Pillars



Kernel Trick

(3) Kernel trick: Sometimes feature vectors are large (e.g. 10⁶ numbers = 10⁶ dimensional space). Keeping track of 10⁶ numbers for each example - too much!

Computers will protest ... curse of dimensionality!

Trick: fix the data matrix:

Kernel Trick

Example 3: *N* independent company daily price histories x_1, \ldots, x_p followed by a predicted price *q* after x_p .

	Fea	ature	Outcome			
Company 1	x_1	x_2	x_3	• • •	x_p	q
Company 2	x_1	x_2	x_3	•••	x_p	q
• •	• •					• •
Company N	x_1	x_2	x_3	•••	x_p	q

features = p = dimensions# samples = N

Often p >> N (i.e., very high frequency price samples can have more time slices k than sample companies N)

 \Rightarrow (Curse of dimensionality)

Kernel Trick

Data matrix:

$\mathbf{X} = k$ rows

	$\begin{array}{c} x_1 \\ x_1 \end{array}$	x_2 x_2	$\frac{x_3}{x_2}$	•••	x_p x_n	$\begin{array}{c} q \\ a \end{array}$	
ł	$\begin{array}{c} x_1 \\ x_1 \end{array}$	x_2	x_3		x_p	$\begin{array}{c} q \\ q \end{array}$	
	:	•			•••		
	$\lfloor x_1$	x_2	x_3	•••	x_p	q	

N columns

Kernel Trick



Then: usually use the final matrix to be the covariance matrix

$\mathbf{X}^T \cdot \mathbf{X}$

[note this is $p \times p = huge matrix!$]

Now use the *kernel matrix*

$\mathbf{X} \cdot \mathbf{X}^T$

[now this is an $N \times N$ matrix - can be much smaller!]

But both the large and the small matrix encode exactly the same information!



Thus high dimensional problem $(k \times k)$ becomes low dimensional problem $(N \times N)$

 \rightarrow Kernel trick!

Equities

7. Example (continued): Machine Learning and Stock Trading:



https://blogs.msdn.microsoft.com/meechao/2017/01/19/buildingan-experimental-stock-trading-system-using-machine-learningand-python/

Equities

HIGH FREQUENCY TRADING USING ML:

For a specific company (say IBM), train a machine to predict return y (percentage change in stock value) in the next *millisecond* based on the pattern of stock values over the last p milliseconds, (x_1, \ldots, x_p) .

That is, find a machine M to implement the best approximate map



$$y = f_M(x_1, \ldots, x_p).$$

High frequency methods are well developed (sometimes not publicized).



FUNAMENTALS (LOW FREQUENCY) TRADING USING ML:

Also important:

Try a feature vector

$$\mathbf{X} = (x_1, \ldots, x_p).$$

where x_1, x_2, \ldots are:

 company fundamental numbers (say month to month or quarterly)



- US Economic indicators (leading economic indicators, interest rates, etc.)
- Sentiment indicators (possibly only low frequency updates)


Main point:

Fundamentals dominate low frequency trading;

Psychology/game theory dominate high frequency trading.

Machine learning can be used in both!

More about low frequency trading

• Focus on low frequency trading by identifying by predicting price from slowly changing fundamental performance indicators (x_1, \ldots, x_p)

- Lots (hundreds) of performance indicators x_i (e.g. taxes, operating income etc.) are available for thousands of companies.
- ML techniques can explore and combine large numbers of indicators x_i to identify extreme performers (likely to have very high earnings or large losses).

- Each stock at any time is now a point in a high-dimensional space (one dimension per performance indicator). Can have hundreds or thousands of indicators x_i.
- Goal is always the same: use indicators (x_1, \ldots, x_p) to predict return y in the next time period
- One can use an ensemble of ML methods not just Support Vector Machines.

Low Frequency Trading







Note: If only two classes *A* and *B* are to be predicted, there are many ways to choose the separator between class *A* (good companies, blue) and class *B* (not good companies, red) when they are placed in the feature space *F*.

 If over-fitting occurs, performance on the test set will be poor; i.e. there is little predictive value.

Low Frequency Trading



- Solution: numerous highly technical approaches can be implemented to prevent overfitting
- Most important rule of thumb: keep your separator simple!

Performance

Sample portfolios: Thirty years



1994-2013

Extensions

Sentiment Analysis is a New Application

Machine learning tools for predicting a company stock may be extended to include news items (textual analysis of newspapers), analyst rankings of companies, and company sentiments from social networks (twitter, stocktwit, facebook, G+)

8. The latest machines

• Self-driving Ubers:

How a Car Drives Itself



By Guilbert Gates | Source: Google | Note: Car is a Lexus model modified by Google.

Idealization of input-output:

feature vector $\mathbf{x} = (x_1, \dots, x_p)$

For example:

 $x_1 = \text{distance to nearest obstacle in the front}$ of car (0 degrees from front direction)

 $x_2 = \text{distance to nearest obstacle 10 degrees}$ from front direction.

 $x_3 =$ distance to nearest obstacle 20 degrees from front direction. Etc.

Another possible feature vector

$$\mathbf{y} = (y_1, \dots, y_p)$$

 $y_1 =$ direction of motion of object at x_1 $y_2 =$ direction of motion of object at x_2 $y_3 =$ direction of motion of object at x_3

Etc.

$$\mathbf{z} = (z_1, \dots, z_p)$$

 $z_1 =$ speed of motion of object at x_1 $z_2 =$ speed of motion of object at x_2

Etc.

How to combine information in feature vectors?

Super-feature vector

$$\mathbf{V} = (x_1, \dots, x_p; y_1, \dots, y_p; z_1, \dots, z_p, \dots)$$

[a very large vector containing all numbers the machine might be interested in] OR: Use the kernel trick: use a *kernel* function $K_1(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})$ where $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ are independent copies of **x** (vector of object distances).

Now form another kernel function $K_2(\mathbf{y}^{(1)}, \mathbf{y}^{(2)})$ where $\mathbf{y}^{(1)}, \mathbf{y}^{(2)}$ are independent copies of variable \mathbf{y} (vector of object directions).

Etc.

Training (the car machine)

Example of training: Now take lots of example measured values of high dimensional super-vectors **v** in many different situations:

$$\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \dots, \mathbf{v}^{(N)}$$

Desired machine output for input v:

 $f(\mathbf{v}) \left\{ \begin{array}{ll} > 0 & \text{if brakes should be applied} \\ \leq 0 & \text{if brakes should not be applied} \end{array} \right.$

For SVM machine, if **v** is the current measured super-vector, then there is an appropriate kernel function $K(\mathbf{v}^{(1)}, \mathbf{v}^{(2)})$ defined on independent copies $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}$ of the super-vector **v**, such that

$$f(\mathbf{v}) = \sum_{i=1}^{N} a_i K(\mathbf{v}, \mathbf{v}^{(N)}) + a_0.$$

Note this gives a *curved* (non-plane) separation between the two regions, $f(\mathbf{v}) > 0$ and $f(\mathbf{v}) \le 0$,

i.e., the separation is $f(\mathbf{v}) = 0$.

The coefficients a_i can be obtained using a linear algebra algorithm from the $k \times k$ kernel matrix **K** with entries

$$\mathbf{K}_{ij} = K(\mathbf{v}^{(i)}, \mathbf{v}^{(j)})$$

 $(i, j = 1, \dots, N).$

The good news: if we have already derived a good kernel matrix **K**_x for the **x** variables, **K**_y for the **y** variables, **K**_z for the **z** variables, etc., then the *correct* full kernel matrix incorporating all of this information is the sum matrix

$$\mathbf{K} = \mathbf{K}_{x} + \mathbf{K}_{y} + \mathbf{K}_{z} + \dots$$

integrating all of the variables **x**, **y**, **z** *automatically.* Again the utility of the kernel trick!

More about the kernel trick: Can we use just any function $K(\mathbf{v}, \mathbf{w})$ above?

Almost - the function $K(\mathbf{v}, \mathbf{w})$ must be positive definite, i.e., if take any fixed set of measured super-vectors $\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(k)}$, the kernel matrix

$$\mathbf{K}_{ij} = K(\mathbf{v}^{(i)}, \mathbf{v}^{(j)})$$

is positive definite, i.e. has only nonnegative eigenvalues.

Lots of functions work though. For example

$$\begin{split} K(\mathbf{v},\mathbf{w}) &= \mathbf{v} \cdot \mathbf{w} \text{ (linear kernel)} \\ K(\mathbf{v},\mathbf{w}) &= e^{-|\mathbf{v}-\mathbf{w}|^2/\sigma^2} \text{ (Gaussian kernel) with} \\ & \text{width } \sigma \\ K(\mathbf{v},\mathbf{w}) &= (1+\mathbf{v}\cdot\mathbf{w})^d \text{ (polynomial kernel)} \end{split}$$

See:

(1)

More generally: can let

 $K(\mathbf{V},\mathbf{W}) = \Phi(\mathbf{V})\Phi(\mathbf{W})$

for any continuous function $\Phi: \mathbb{R}^m \to \mathbb{R}^n$ ($m = \text{dimension of } \mathbf{v}$)

Can show: using this kernel K in (1) is equivalent to mapping *all* feature vectors **v** that we encounter into $\Phi(\mathbf{v})$ in *all* ML operations.

After this mapping just use the simple linear kernel function $K(\mathbf{v}, \mathbf{w}) = \mathbf{v} \cdot \mathbf{w}$ (the one that gives a linear boundary between the two categories), *but always replacing* $\mathbf{v} \rightarrow \Phi(\mathbf{v})$ *and* $\mathbf{w} \rightarrow \Phi(\mathbf{w})$ before starting the calculation. Φ is called a *feature map*.

When is a feature map useful? When a linear separation does not work between the blue and red dots:

See:

https://www.youtube.com/watch?v=3liCbRZP rZA • Deep neural networks:

Replace single middle (hidden) layer of neurons by 3 or more hidden layers.



Input layer has neural activations that form a vector **x** :

$$\mathbf{X} = (x_1, \dots, x_p)$$

Hidden layer 1 activations:

$$\mathbf{y} = (y_1, \ldots, y_n)$$

Hidden layer 2 activations:

$$\mathbf{Z}=(z_1,\ldots,z_n)$$

Final (output) layer activations:

$$\mathbf{q} = (q_1, \ldots, q_n).$$

Feedforward function from **x** to **y** is *almost* a linear map:

$$\mathbf{y} = \mathbf{W} \cdot \mathbf{x},$$

where matrix entries

 $w_{ij} = \mathbf{W}_{ij} = \text{connection strength from neuron}$ x_i to neuron y_j

Almost: now apply a sigmoid function $\phi(y) = \frac{1}{1+e^{-x}}$ that for each component y of **y** looks like



Note ϕ is bounded to prevent your neurons y_i from burning out. Thus we actually have:

$$\mathbf{y} = \phi(\mathbf{W} \cdot \mathbf{x}).$$

Now repeat same map from **y** to **z** :

$$\mathsf{z} = \phi(\mathbf{V} \cdot \mathbf{y})$$
,

where **V** is now matrix of weights from **y** layer to **z** layer, etc.

Each layer encodes more abstract information about the input information **x** (image with pixel intensites x_i).

Finally, the output layer (with enough layers) tells you whether the painting you showed to the first layer **x** is a Da Vinci or not.
Deep Networks



The trick: you need lots of layers.

x (first) layer encodes visual pixels of painting

y (second) layer encodes directionalities of edges at nearby pixels

z (third) layer encodes presence of shapes (circles, triangles) at nearby pixels.

Each successive layer encodes higher levels of abstract information.

q (last) layer encodes identity of the painter

(after sufficient training of your network machine!).

Who knew that iterated maps (applying matrix multiplications and the sigmoid function φ repeatedly to get from input **x** to output **q**) had such power!

Final remark

Just as standard computers can emulate our ability to perform precise calculational tasks (and even linguistic tasks)

Machine learning (e.g. in a neural network or SVM or elsewhere) emulates our *intuition*.

Yin and Yang

Intuition is what takes an input situation consisting of feature vectors **x**, **y**, **z** representing our Uber car's current environment and then tells it what to do next.

Intuition will also be emulated by computers, using machine learning -- already our precise calculational abilities have been emulated (very well!) by standard computers.

Yin and Yang



The combination of precise calculation and intuitive thinking are the *yin* and *yang* of our thinking, and will also be the *yin* and *yang* of the thinking of future Artificial Intelligences.

Yin and Yang



https://medium.com/fluxx-studio-notes/ai-virtual-assistants-and-chat-bots-beforenow-and-in-the-future-df979529ad5f