ML with numerical optimization
brief introduction

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What is this ?

example 1:

sépal		pétal		
long.	larg.	long.	larg.	type
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
.	.	.	.	.
7.0	3.2	4.7	1.4	versic.
6.4	3.2	4.5	1.5	versic.
.	.	.	.	.
6.3	3.3	6.0	2.5	virgin.
5.8	2.7	5.1	1.9	virgin.
.	.	.	.	.

Aim: find a simple numerical function f such that:

- computing $f(x)$ provides the class of x
- x is a vector of numerical values (i.e. a row in the table) 4 ici
- the class is just 0 or 1 (or 1 and -1)
- for instance:

$$f(x) = \alpha sepal.long + \beta speal.larg + \dots$$

- Classifier: if f(x)< 5.1 then class = setosa
  .....

Another example: letters and pixels

Example 2:

40	39	39	39	38	37	37	36	36	35	34	34	34	33	33	33
32	31	31	30	30	29	28	28	27	26	27	26	26	25	25	25
24	23	23	22	21	19	18	16	15	17	20	21	22	23	18	14
25	28	25	23	23	22	21	19	18	16	13	13	13	12	17	19
18	19	14	18	21	22	23	24	25	25	25	25	26	26	26	27
28	28	28	28	29	30	30	30	32	32	32	32	32	31	33	33
34	35	36	36	36	37	37	37	38	39	39	39	39	39	41	40
40	41	41	41	40	42	41	41	41	41	42	41	42	42	41	41
40	40	39	38	38	37	37	36	36	35	35	35	33	34	32	32
31	31	30	29	29	29	29	28	28	27	27	27	26	25	25	25
24	24	23	22	22	20	19	17	16	18	22	22	24	24	19	13
25	28	26	24	24	23	22	21	20	18	16	15	14	13	18	19

- a matrix of pixel, each pixel is a grey level (black and white image)
- each image is a letter
- find c such that $f(x_1, \ldots, x_n) \in \{1, -1\}$ tells us if the image is letter a: too hard
- find h such that $h(x_1, \ldots, x_n) \in \mathbb{R}$ and $\forall z = (x, y) \in TS, h(x) \times y > 0$

The signe of h give the class since h(x) and y have the same sign.

How to compute f ?

What do we have?

- as usual, a finite set of examples $TS = \{z_1, \ldots, z_m\}$ with their class
  Training Set
- $class : \mathbb{R}^n \rightarrow \{+1, -1\}$
- if no noise, $z = (x, class(x))$, if noise we can have $z = (x, y)$ with $y \neq class(x)$
  le bruit entraine les erreurs

How to compute f ?

What do we have?

- as usual, a finite set of examples $TS = \{z_1, \ldots, z_m\}$ with their class
- $class : \mathbb{R}^n \rightarrow \{1, -1\}$
- if no noise, $z = (x, class(x))$, if noise we can have $z = (x, y)$ with $y \neq class(x)$

Separable versus linearly separable

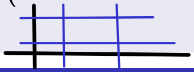
Just give an example with $\mathbb{R}^2$ and explain

separable: we can find a suitable f On est capable de trouver la fontion f qui classe les donnée

linearly separable: among all the suitable f, there is an hyperplan (a line in $\mathbb{R}^2$)

Give a circle and a line as examples

Example of a rectangle as separator (i.e. the normal patients for medical data)



A first simple algorithm (perceptron)

to start...

- Look for $h(a, b)(x) = a.x + b = a_1 x_1 + a_2 x_2 + ::: + a_n x_n + b$
- init: $a \leftarrow (0, \dots, 0)$; $b \leftarrow 0$; done $\leftarrow$ false;
  while not done
  done $\leftarrow$ true;
  for each $(x, y) \in TS$, if $(a.x + b).y \leq 0$ //disagreement
  then
  $a \leftarrow a + \tau.y.x$
  $b \leftarrow b + \tau.y$; done $\leftarrow$ false
  return (a, b)
  $\tau > 0$ (convergence speed tuning)

A first simple algorithm (perceptron)

On commence par admettre que les données sont linéairement séparables.

to start...

- Look for $h(a,b)(x) = a.x + b = a_1 x_1 + a_2 x_2 + ::: + a_n x_n + b$
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  done $\leftarrow$ true;
  for each $(x, y) \in TS$, if $(a.x + b).y \leq 0$ //disagreement
  then
  $\vec{a} \leftarrow \vec{a} + \tau.y.\vec{x}$ On avance dans le sens de la dérivé pour a
  $b \leftarrow b + \tau.y$; done $\leftarrow$ false puis pour b
  return (a, b)
  $\tau > 0$ (convergence speed tuning) Pas de l'algo

properties

1. simple...
2. incremental
3. convergence iff linearly separable

Proba de faire une erreur sur le Training Set : $\frac{1}{m}\sum_{i=1}^{m} |\, yi - h(a,b)(xi) \,|$

Using Gradient Descent: a better algorithm

Chercher exemple sur le net

to start again

- Again $h(a,b)(x) = a.x + b = a_1x_1 + a_2x_2 + ::: + a_nx_n + b$
- Minimize empirical error on TS: $e_{emp} = \frac{1}{m}\Sigma|(h(a,b)(x) - y)|$
- Simpler to minimize on TS, $E(a,b)(TS) = \frac{1}{2}\Sigma_{(x,y)\in TS}(h(a,b)(x) - y)^2$
- init: $a \leftarrow (0,\ldots,0)$; $b \leftarrow 0$; ϵ (precision) τ (step size)
  while $\Delta e_{emp} > \epsilon$ (or $\Delta E > \epsilon$) tant que l'écart entre les erreurs entre x et x+1 > epsilone on continu
  for each $(x,y) \in TS$,
  $a \leftarrow a + \tau.(y - (a.x + b)).x$ $(i.e. \frac{\delta E(a,b)(TS)}{\delta a})$
  $b \leftarrow b + \tau.(y - (a.x + b))$ $(i.e. \frac{\delta E(a,b)(x)}{\delta b})$;
  end while return (a,b)

Question application essai exo

Using Gradient Descent: a better algorithm

to start again

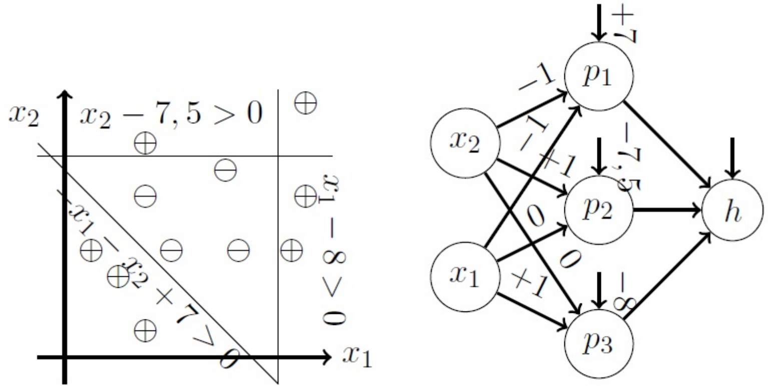
- Again $h(a,b)(x) = a.x + b = a_1x_1 + a_2x_2 + ::: + a_nx_n + b$
- Minimize empirical error on TS: $e_{emp} = \frac{1}{n}\Sigma|(h(a,b)(x) - y)|$
- Simpler to minimize on TS,
  $E(a,b)(TS) = \frac{1}{2}\Sigma_{(x,y)\in TS}(h(a,b)(x) - y)^2$
- init: $a \leftarrow (0,\dots,0); b \leftarrow 0; \epsilon$ (precision) τ (step size)
  while $\Delta e_{emp} > \epsilon$ (or $\Delta E > \epsilon$)
  for each $(x,y) \in TS$,
  $a \leftarrow a + \tau.(y - (a.x + b)).x$ $(i.e. \frac{\delta E(a,b)(TS)}{\delta a})$
  $b \leftarrow b + \tau.(y - (a.x + b))$ $(i.e. \frac{\delta E(a,b)(x)}{\delta b})$;
  end while return (a, b)

properties

1. convergence whatever the situation
2. convergence can be very very slow !
3. other minimization functions (log, etc.)

Neural Networks howto

The big idea...



Neural Networks ... propagate

One node per function

- a finite set $\mathcal{N}$ of nodes
- n variables then n input nodes: they do not classify - 1 output node h
- Each internal node m provides a classifier
- Combining the classifiers provides the resulting hypothesis h
- $\forall l \in \mathcal{N}$, (except input nodes - recursive definition)

  $$l(x) = sign(\Sigma \alpha_{ml} m(x) + \beta_l)$$

  where β_l is the weight of node l and α_{ml} the weight of the edge from node m to node l (i.e. m is a parent of l)
- Propagate the answer (the class) from input to output h
- Retro-propagate the error $y - h(x)$ from output h to input

Neural Networks ... retro-propagate

Learning the weight !

- for all $(x, y) \in TS$
- for all $l \in \mathcal{N}$, compute $l(x)$ (then $h(x)$ is computed)
- $\delta h \leftarrow \tau(y - h(x))$
- //retro-propagate the final error
  For each hidden node l, (recursive definition)
  $\delta l = \Sigma \alpha_{lm} \delta m$ for m child of l where β_l is the weight of node l and α_{ml} the weight of the edge from node m to node l
- //update the weight coefficients
  $\forall l \in \mathcal{N}, \alpha l \leftarrow \alpha_l + \delta_l$
  $\beta_l \leftarrow \beta_l + \delta_l$
-

Neural Networks pro/cons

Pro

- Very successfull for diverse tasks
- Can use other "neuronal" functions (i.e. non linear classifiers)
  Ex.: sigmoid $sigm(a) = \frac{1}{1+e^{-\lambda a}}$ and replace *sign* with *sigm*
- On the shelves product (weka for instance!)
- Revival with "deep learning"

recherche net

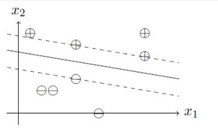
Cons

- Empirical init of the nodes and structure (done by human experts...)
- Empirical init of the weights and very long training time
- Tuning very difficult
- Halting condition

Chercher la démarche machine learning.

Support Vector Machines (V. Vapnik - 1979, etc.)

Another clever idea !



If linearly separable, there is a kind of "separating PIPE"

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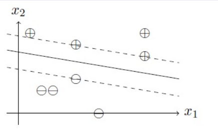

If linearly separable, there is a kind of "separating PIPE"

Let us think about it

- Infinite number of separating hyperplans
- The "best" one could be the one maximizing the margin !
- Support vectors = the examples on the pipe limits!
- We don't care about the other examples...

SVM: some facts

The problem...

- Notion of margin associated to a separating hyperplan H
- Ultimately find the hyperplan with the biggest margin...
- Hyperplan H with equation $a.x + b = 0$ with normalized normal vector $w = \frac{a}{||a||}$
- Given $z \in TS$, distance $d(z, H)$ to be computed
- Let $y \in H$ such that $d(z, H) = d(z, y)$ i.e. $y = z - d(z, H).\frac{a}{||a||}$
- Then $a.y + b = 0$ i.e. $a.(z - d(z, H).\frac{a}{||a||}) + b = 0$ i.e. $d(z, H) = \frac{a.z+b}{||a||}$
- geometric margin for z : $marg(z, H) = cl(z).(\frac{a.z+b}{||a||})$
  geometric margin for H : $min\{marg(z, H) | z \in TS\}$
- Maximizing $marg(H)$ equivalent to maximize $\frac{1}{||a||}$ i.e. minimize $\frac{1}{2}||a||^2$

SVM: the algorithm

The problem...

- Initial pb.: unknown a and b ($n+1$ variables) - then minimize $||a||^2$
- Constraints: $\forall (x,y) \in TS, y \times (a.x+b) \geq 1$
- Classical math exercise... can be solve in $\mathcal{O}(n^3)$ and unique solution
- On the shelve software to do the job !
- Convergence if linearly separable... STUNNING PERFORMANCES...
- and ... IF NOT ????????????????????????

SVM for non linerarly separable data: how to ?

The problem...

- $TS = \{1, +1), (2, +1), (4, -1), (5, -1), (8, +1), (9, +1)\}$
- Projection in $\mathbb{R}$ with $\phi(x) = (x, x^2)$... linearly separable
- The main idea...

New optimization problem to be solved!

- Find $\phi : \mathbb{R}^n \to \mathbb{R}^m$ such that
  - $\exists (a, b) \in \mathbb{R}^m \times \mathbb{R}$ with
  - $\forall (x, y) \in TS, y.(a.\phi(x) + b) \geq 1$
- But only $K(x, x') = \phi(x).\phi(x')$ needed (. is the scalar product also denoted $\phi(x)^T\phi(x')$)
- K kernel function (kernel trick)

SVM on the shelves

Usual kernels

- Gaussian kernel $K(x, y) = \frac{e^{-||x-y||^2}}{2\sigma^2}$
- Polynomial kernel $K(x, y) = (x.y + 1)^p$
- Combination of kernels $K + K', K \times K', exp(K(x, x')), \dots$
- "Magic" extension of SVM...

Applications

- Weka has SVM included (LibSVM weka)
- K kernel function representing "similarity" between examples...
- Example outside $\mathbb{R}^n$: A a subset of a finite universe $\mathcal{A} : K(A, B) = 2^{|A \cap A'|}$

Concluding remarks

- A lot of other options and methods (SMO, Ridge regression, etc.)
- Generally black box approach
- Parameter tuning: highly difficult and empirical task
- A lot of commercial implementations as well