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Artificial neural networks for ion beam analysis

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Artificial neural networks for ion beam analysis

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Instituto Tecnológico e Nuclear

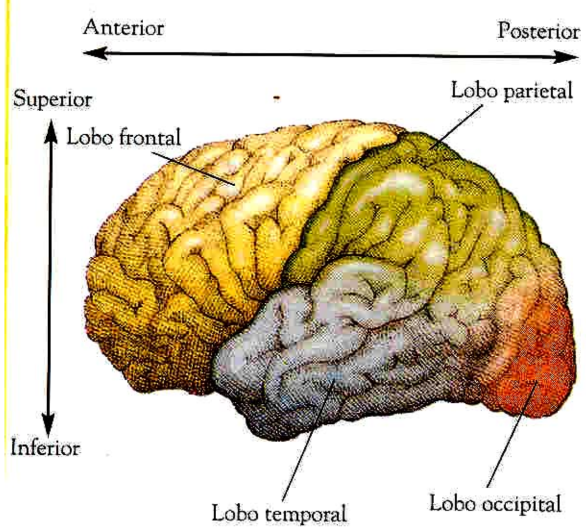
- Introduction
- Biological neural networks
- Artificial neural networks
- RBS data analysis with ANNs
- Automation of experiments
- Outlook

Introduction

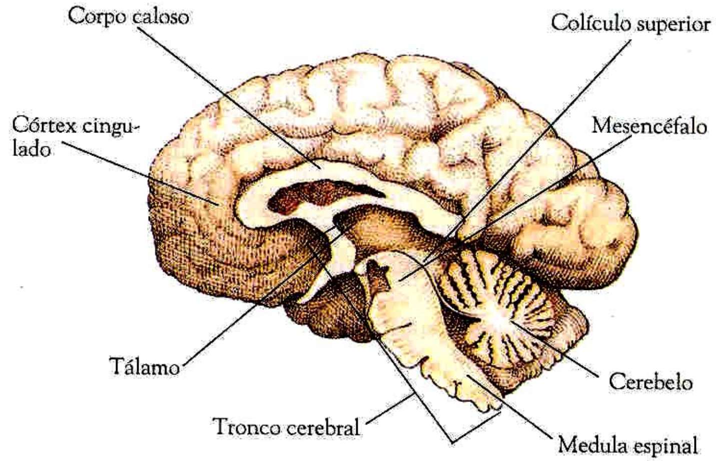
- **Simple problems:**
  “What is the emission of a black body?”
  “How do two charged particles interact?”
  “How do two massive particles interact?”
  “How does a system composed of 1e23 similar particles evolve?”
  “What are things made of?”

- **Complicated problems:**
  “What happens when a butterfly flies?”
  “How can Moore’s law be fulfilled?”
  “WIll it rain tomorrow? And in 10 years’ time?”
  “What is this sample made of?”

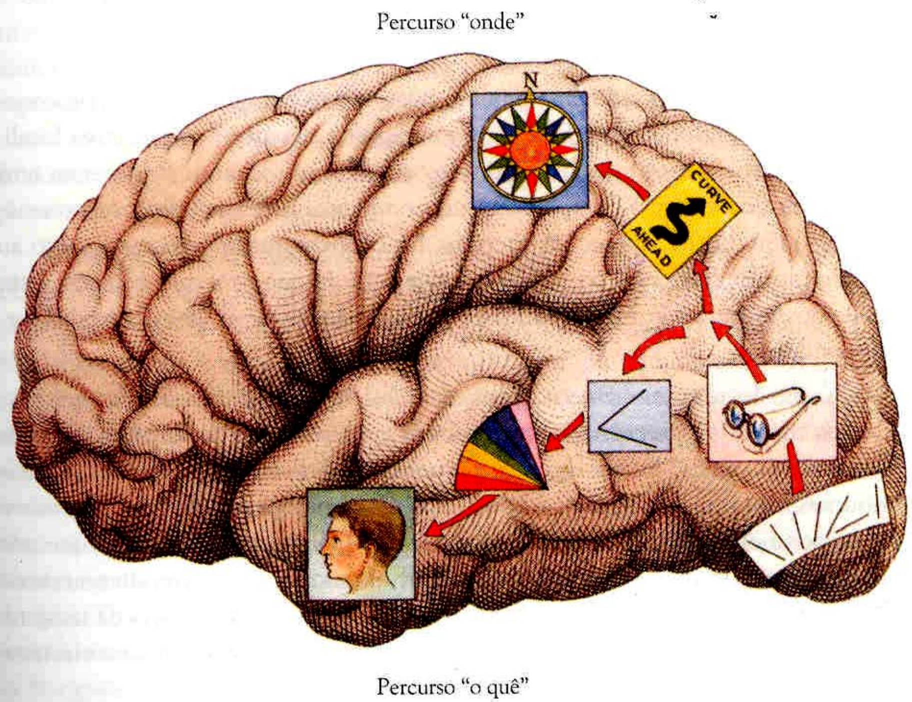
- **An emergent paradigm of problem solving?**
  Artificial neural networks
  Genetic algorithms
  Simulated annealing



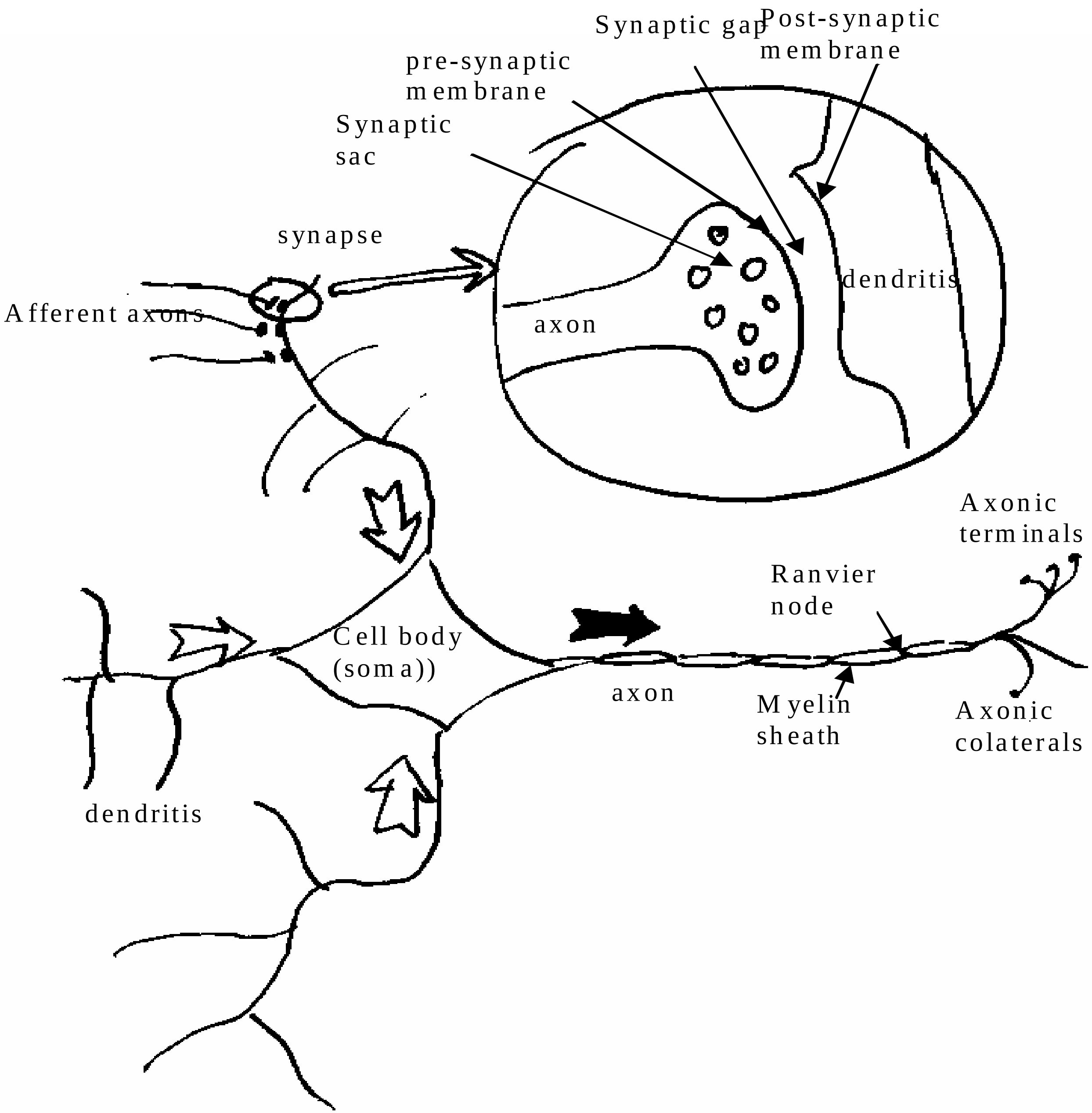
Esta perspectiva lateral do cérebro mostra os quatro lobos do hemisfério cerebral esquerdo.



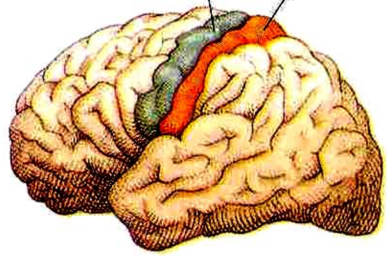
Esta perspectiva mediana do cérebro mostra várias estruturas relacionadas com este livro.

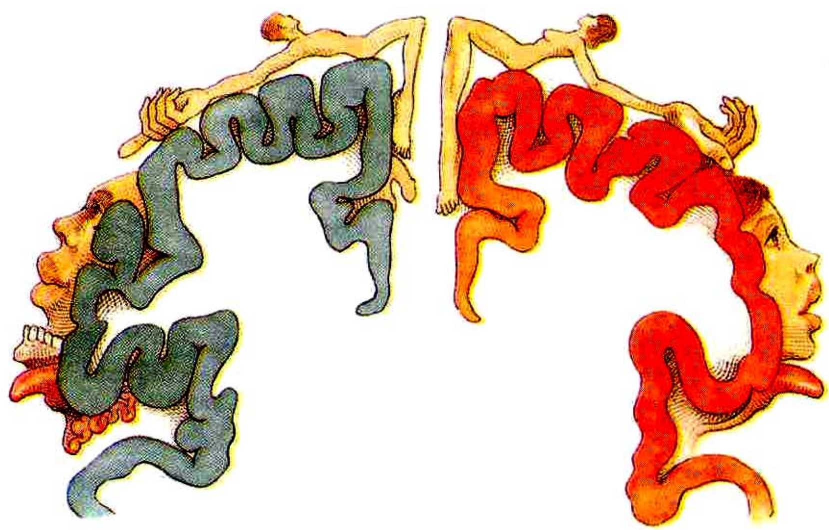


Os percursos "o quê" e "onde" do sistema visual incluem áreas especializadas no processamento da percepção da profundidade (simbolizada por um par de óculos), da forma (um ângulo), da cor e da direcção (sinal de aproximação de curva). O resultado é o reconhecimento do objecto (percurso "o quê") ou a localização do objecto (percurso "onde").

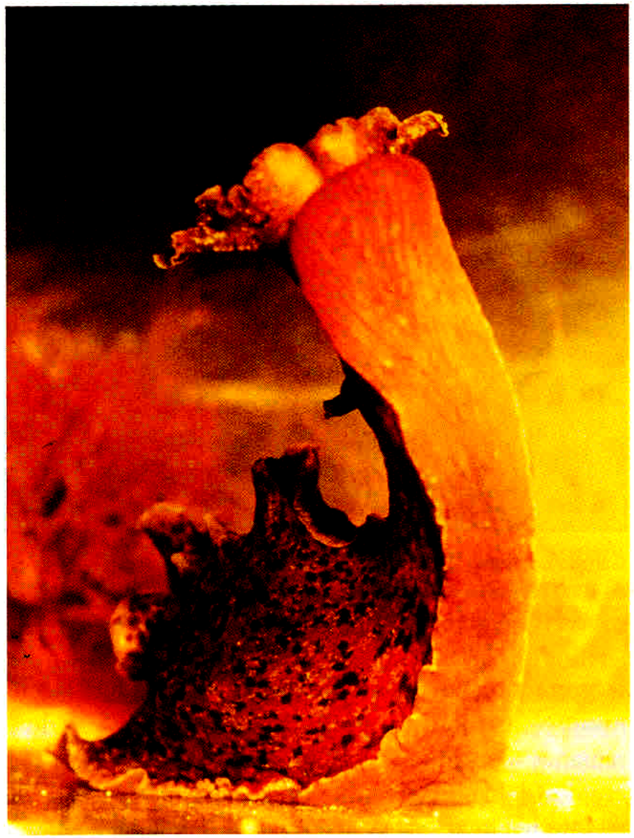

Synaptic gap
Post-synaptic membrane
pre-synaptic membrane
Synaptic sac
synapse
Afferent axons
axon
dendritis
Axonic terminals
Ranvier node
Cell body (soma))
axon
Myelin sheath
Axonic colaterals
dendritis

Os receptores sensoriais de cada parte do corpo projectam-se numa área específica do córtex (o córtex somatossensorial) e, de igual maneira, uma área específica do córtex (o córtex motor) controla os movimentos de cada parte do corpo. Deste modo, o córtex forma um mapa da superfície corporal, representado pelas partes desproporcionadas do corpo. Estão distorcidas porque a área do córtex dedicada a cada parte do corpo é proporcional não ao tamanho da parte mas à precisão com a qual é sentida ou controlada.





Aplysia Californica 1



Caracol marinho *(Aplysia californica)*. O sistema nervoso relativamente simples deste animal torna-o indicado para estudos moleculares e celulares da aprendizagem e da memória.

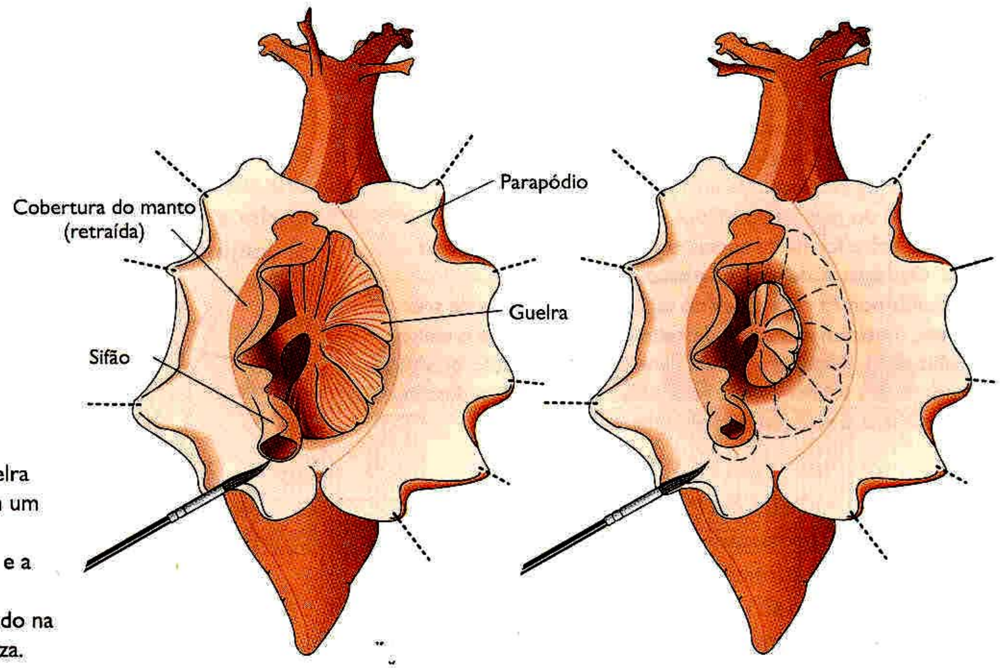
20000 nerve cells:

- Several very large (1 mm)
- Several identifiable, similar in all specimens

Gill withdrawall reflex:

- controlled by roughly 100 nerve cells
- individual cells can be studied

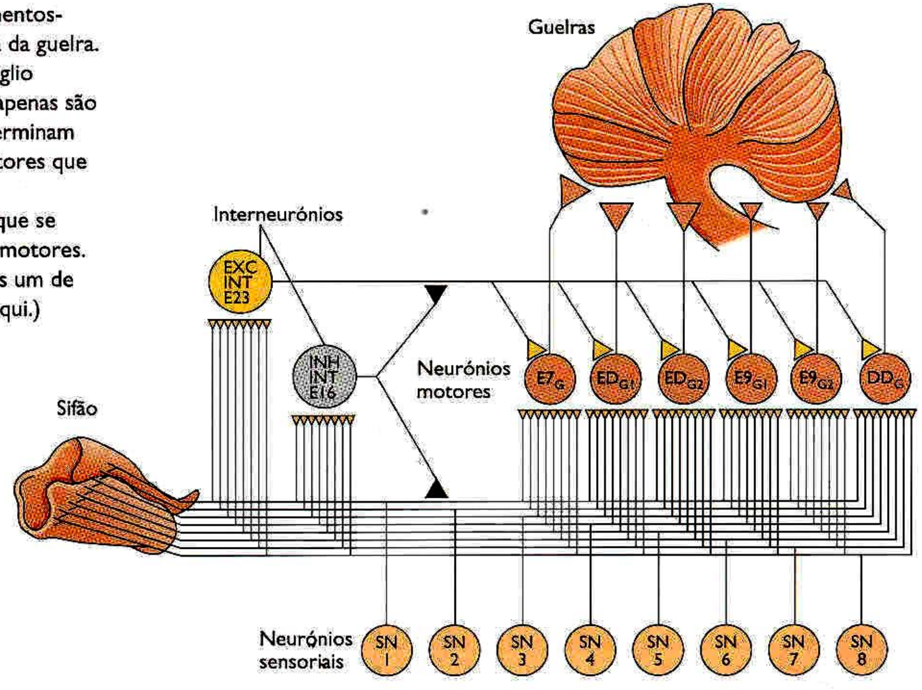
Aplysia Californica 2

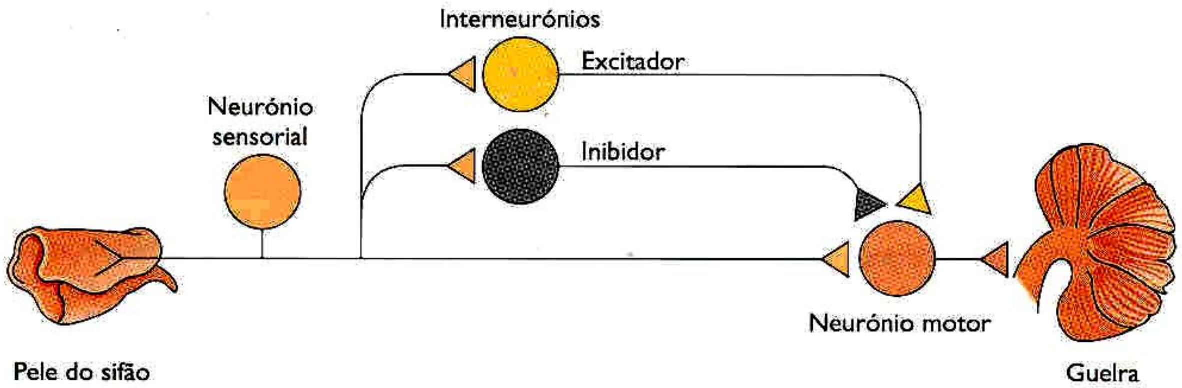


Reflexo de retirada do sifão e guelra no Aplysia. Um toque ligeiro com um pincel fino no sifão (à esquerda) provoca a contracção do mesmo e a retirada da guelra para baixo da cobertura do manto, aqui mostrado na posição retraída para maior clareza.

Aplysia Californica 3

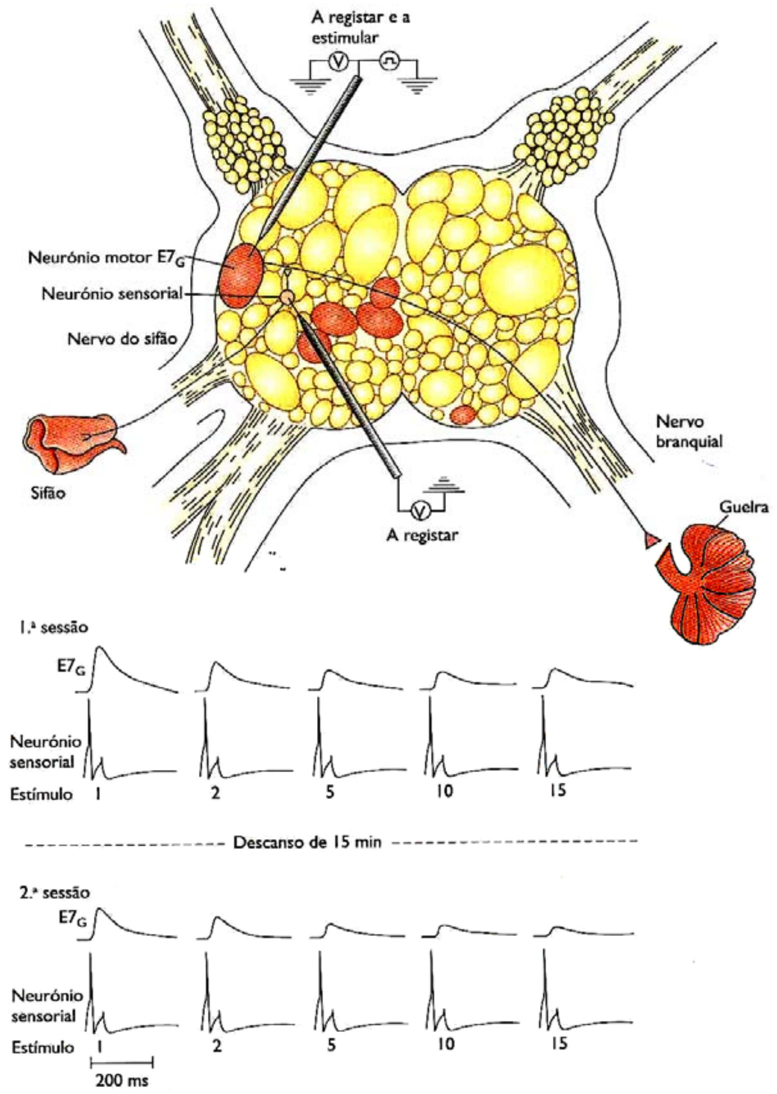
Este circuito simplificado mostra os elementos-
-chave envolvidos no circuito de retirada da guelra. Cerca de 40 neurónios sensoriais no gânglio abdominal cobrem a pele do sifão. Aqui apenas são ilustrados oito. Estas células sensoriais terminam num agrupamento de seis neurónios motores que cobrem a guelra e em vários grupos de interneurónios excitadores e inibidores que se unem através de sinapses aos neurónios motores. (Por uma questão de simplicidade, apenas um de cada tipo de interneurónios é ilustrado aqui.)





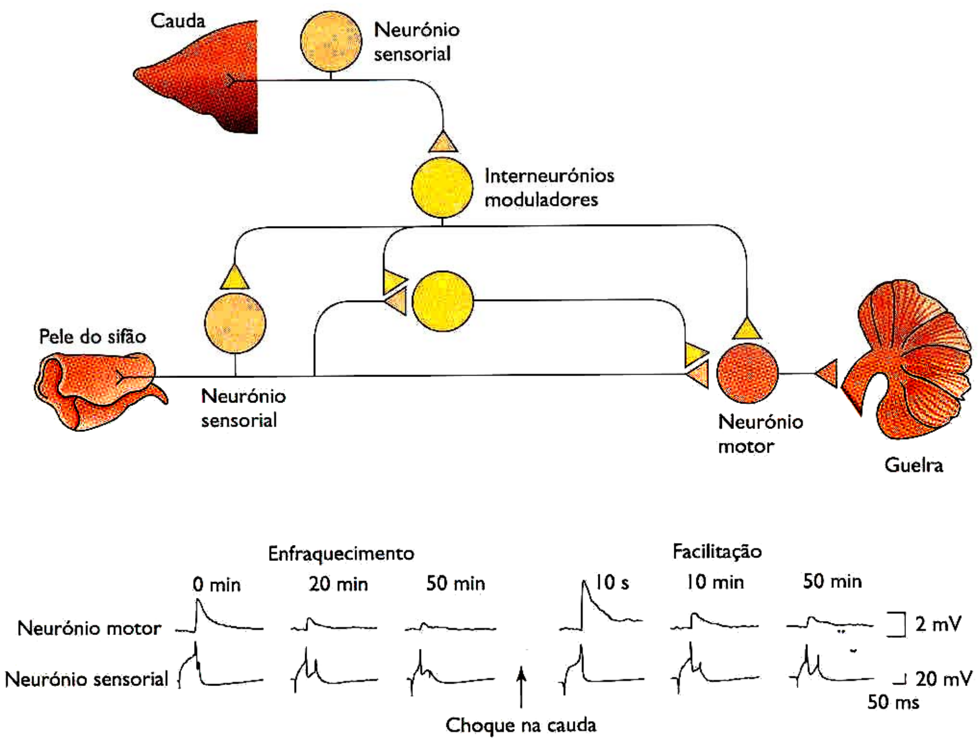
Circuito altamente esquematizado do reflexo de retirada da guelra, mostrando apenas um de cada tipo de neurónios envolvidos.

Aplysia Californica 4

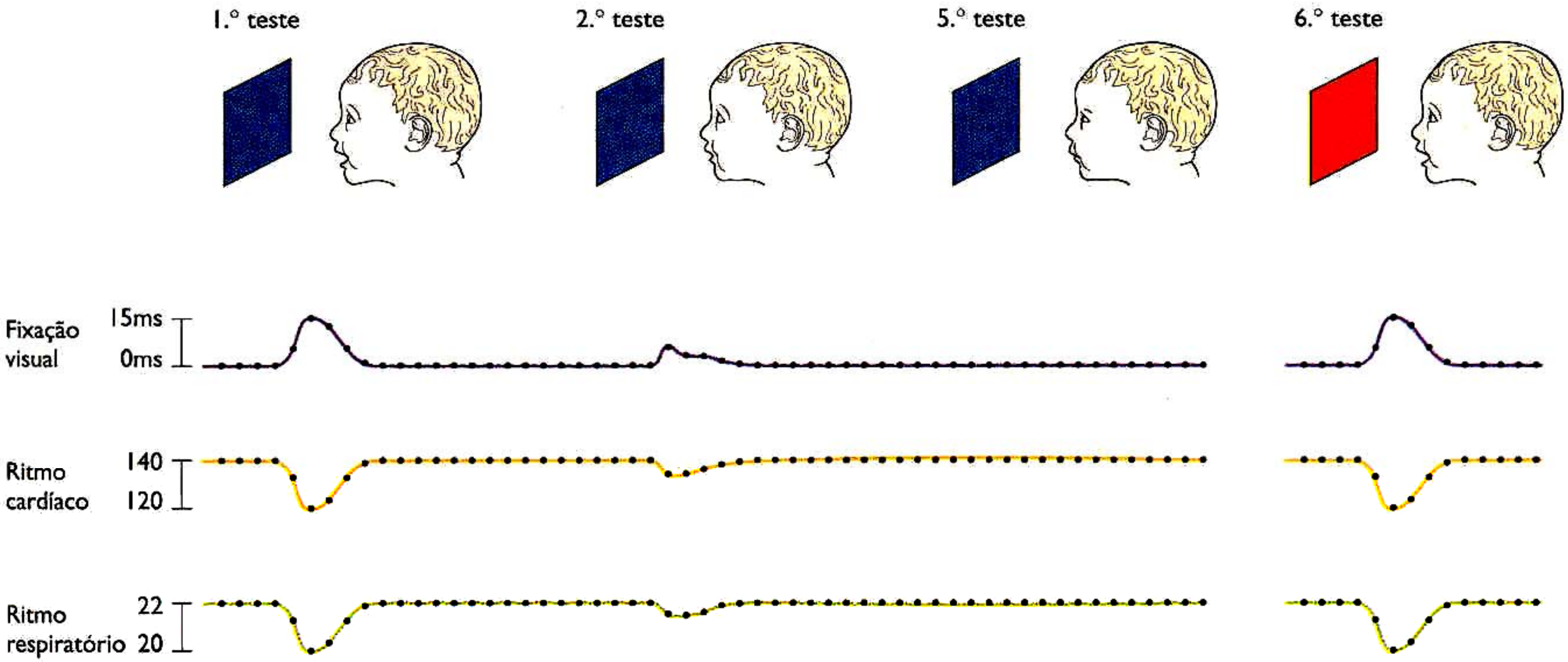


A linha temporal da habituação de curto prazo pode ser estudada registando-se a actividade das células motoras da guelra e de células sensoriais individuais. Em cima: um neurónio sensorial que se une através de uma sinapse ao neurónio motor da guelra E7G é electricamente estimulado de 10 em 10 segundos; um microeléctrodo regista os potenciais pós-sinápticos produzidos nesse neurónio motor. Em baixo: registos de duas sessões de treino consecutivas de 15 estímulos, separadas por 15 minutos, mostram que a reacção do E7G diminui durante a primeira sessão, é parcialmente restaurada após um descanso e diminui ainda mais acentuadamente, quase desaparecendo, com a segunda sessão de treino.

Aplysia Californica 5



Em cima: Circuito neural de sensitização do reflexo de retirada da guelra no *Aplysia* (é mostrado apenas um neurónio de cada um dos tipos por uma questão de simplicidade). Um estímulo perigoso na cauda activa os neurónios sensoriais, que excitam os interneurónios moduladores. Os respectivos sinais para os neurónios sensoriais do sifão incentivam a libertação de transmissores.
Em baixo: Uma só ligação sináptica pode participar em duas formas diferentes de armazenamento em memória: habituação e sensitização. O potencial sináptico produzido na guelra por um só neurónio sensorial do sifão passa por um enfraquecimento, à medida que o animal se habitua, até um choque na cauda sensitizar o animal e a reacção ser restaurada.

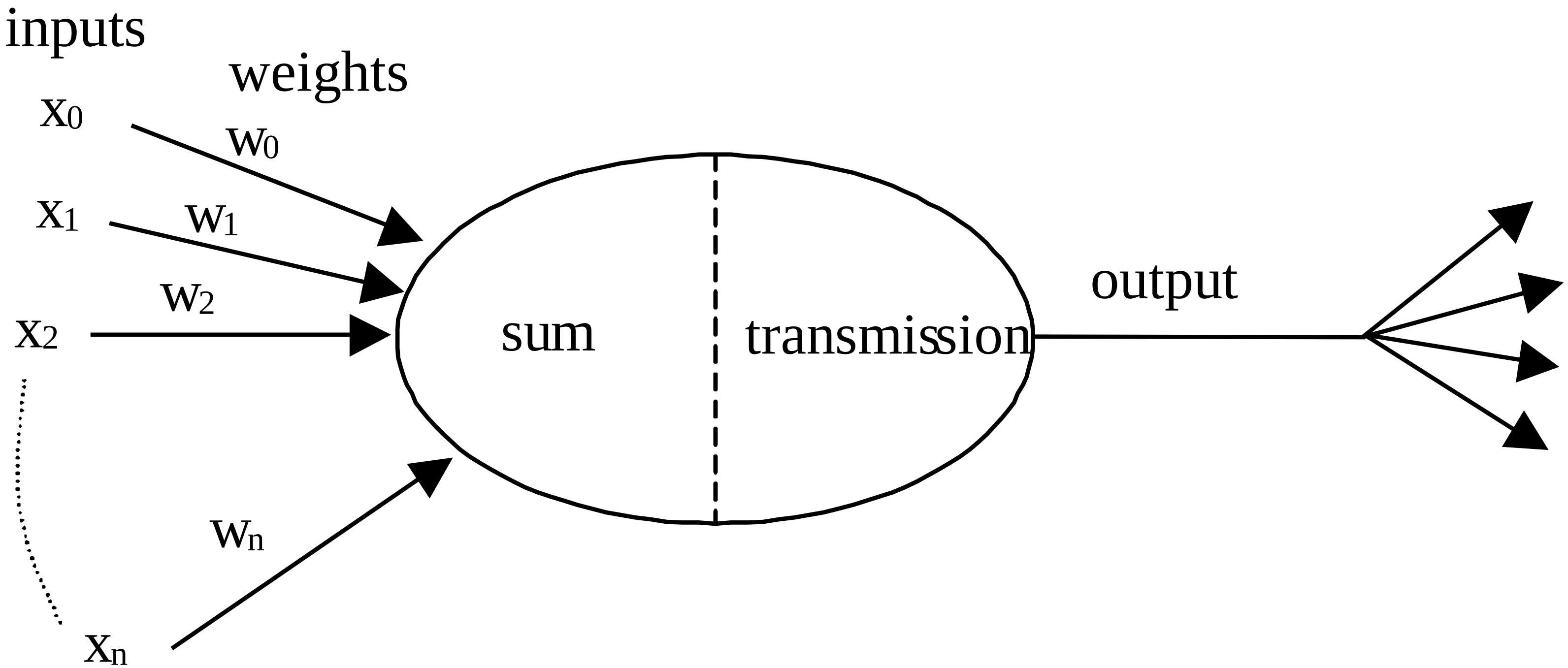


A habituação pode ser usada para estudar a percepção nos recém-nascidos. Quando é mostrado pela primeira vez a um recém-nascido um quadrado azul, a sua atenção visual é captada pelo estímulo e os seus ritmos cardíaco e respiratório diminuem. À medida que o quadrado azul é repetidamente mostrado, o bebé aprende a ignorar o estímulo familiar e as suas reacções sofrem uma habituação. No entanto, quando lhe é mostrado um novo quadrado vermelho, o estímulo novo volta imediatamente a captar a atenção visual do bebé e os seus ritmos cardíaco e respiratório diminuem novamente. Desta maneira, os cientistas determinaram que um bebé consegue distinguir uma cor de outra.

Neurons – some characteristics

- Inputs: many, coming from many afferent neurons. Take continuous values
- Outputs: only one, to many neurons. Yes/no
- Synaptic connections: where the output of one neuron leads to the input in another one, with efficiency depending on the connection
- Each neuron has a reduced, but non-linear, processing ability
- The overall processing ability is distributed amongst the connected set of neurons
- Learning is done through experience, coded in changes in connection strength

Artificial neuron

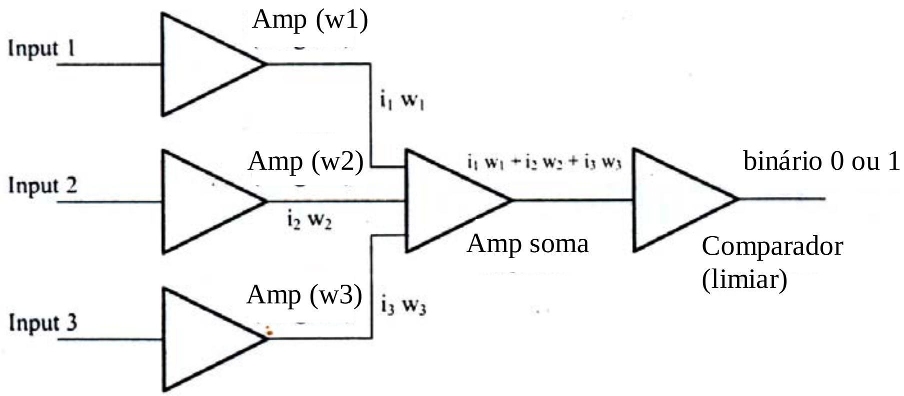


TLU (threshold logic unit)

activation a = **x** · **w**
output y(a) = 1 if a ≥ θ, 0 if a < θ

w = (0,1), θ =0.5					**w** = (0.2,0.8), θ =0.5					**w** = (0.2,0.8), θ =0.5			
					Degraded weights					Degraded inputs			
x_1	x_2	a	output		x_1	x_2	a	output		x_1	x_2	a	output
0	0	0	0		0	0	0.2	0		0.2	0.2	0.2	0
0	1	1	1		0	1	0.8	1		0.2	0.8	0.8	1
1	0	0	0		1	0	0.2	0		0.8	0.2	0.2	0
1	1	1	1		1	1	0.8	1		0.8	0.8	0.8	1

Hardware implementation:

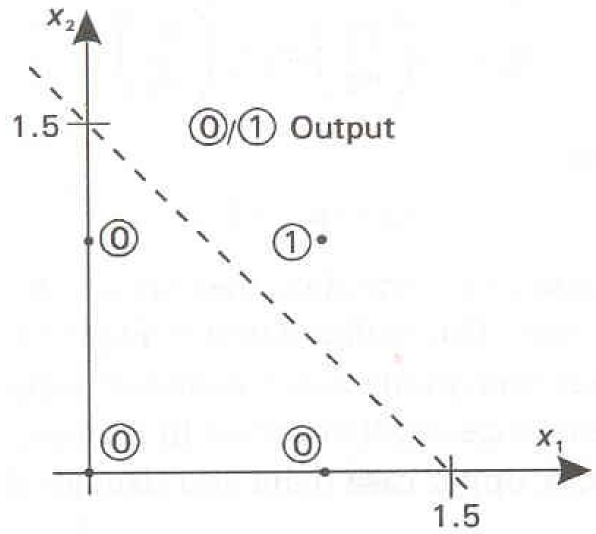


Decision hiperplanes

$a=\theta$ leads to $\mathbf{w}\cdot\mathbf{x}=\theta$, which, for fixed **w** and θ, defines an hiperplane normal to the weight vector **w**, with position defined by the threshold θ .

Let e.g. **w** =(1,1) and θ =1.5

$\mathbf{w}$ = (1,1), θ =1.5			
x_1	x_2	a	output
0	0	0	0
0	1	1	0
1	0	1	0
1	1	2	1



Decision hiperplanes 2

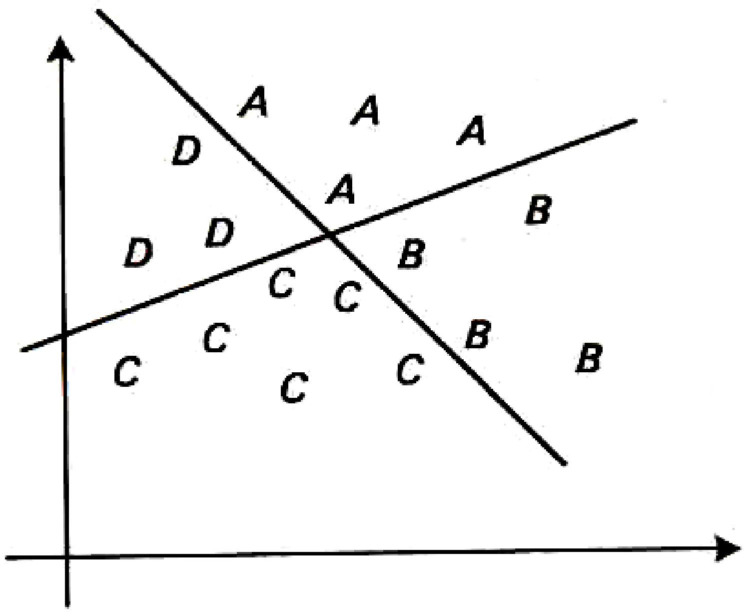
In general, in a TLU defines an hiperplane that separates two linearly separable classes, i.e., defines a decision surface

For non linearly separable classes, e.g. XOR, a multilayer network must be used

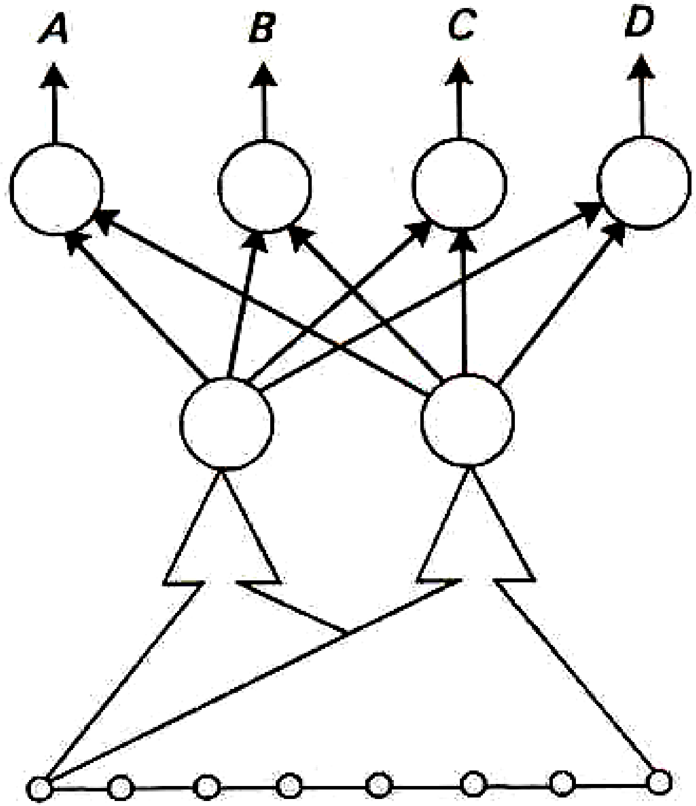
U_1: w = (1,1), θ =0.5					**U_2: w** = (-1,-1), θ =-1.5					**U_3: w** = (1,1), θ =1.5			
x_1	x_2	a	output		x_1	x_2	a	output		x_1	x_2	a	output
0	0	0	0		0	0	0	1		0	0	0	0
0	1	1	1		0	1	-1	1		0	1	1	0
1	0	1	1		1	0	-1	1		1	0	1	0
1	1	2	1		1	1	-2	0		1	1	2	1

XOR					
		U_1	**U_2**	**U_3**	
x_1	x_2	output	output	a	output
0	0	0	1	1	0
0	1	1	1	2	1
1	0	1	1	2	1
1	1	1	0	1	0

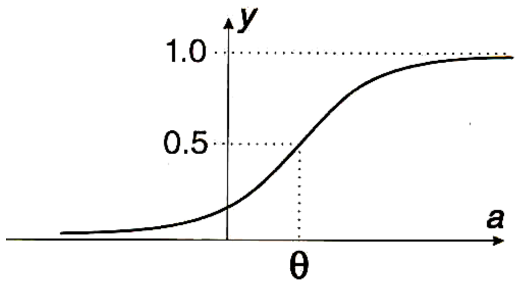
Decision hiperplanes 3 – non linearly separable classes

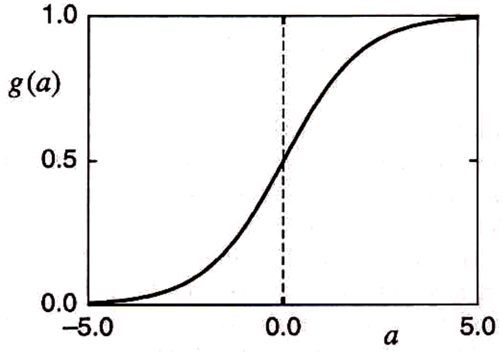


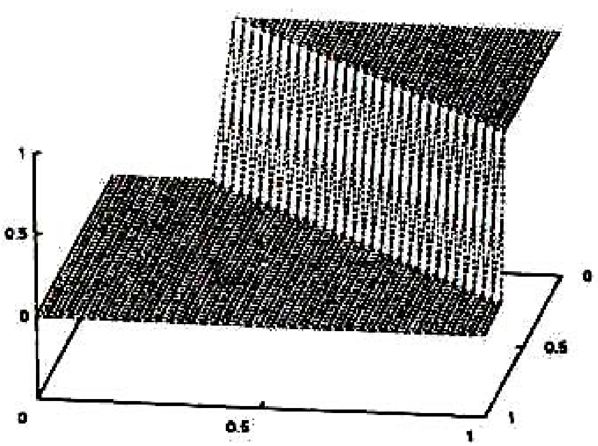
Final classification



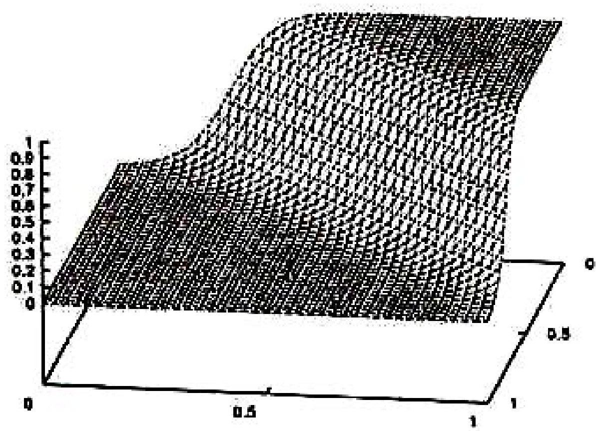
Transmission function: sigmoid, allows continuous output





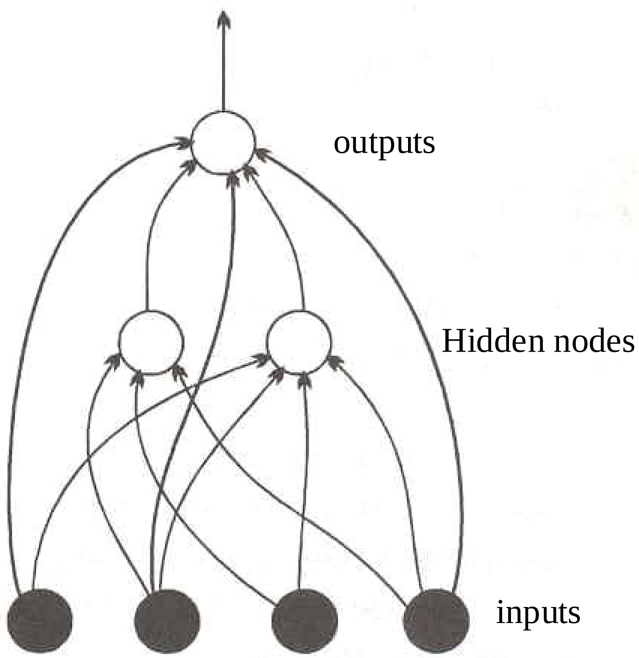


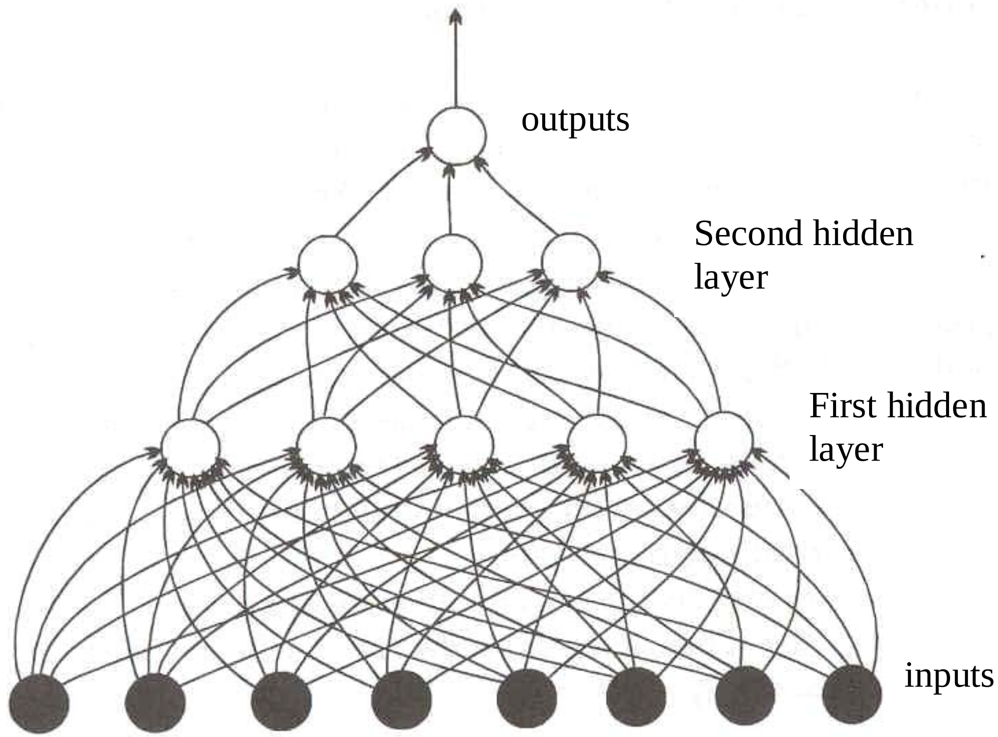
TLU



Sigmóide

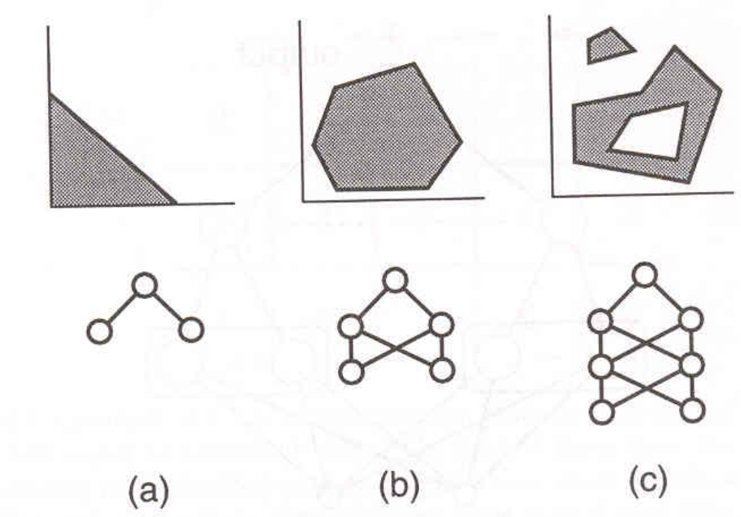
Multilayer perceptron (MLP) 1





MLP 2

A feedforward ANN based on TLUs may generate arbitrarily complex decision hipersurfaces



In principle, a MLP with a single hidden layer and sigmoidal activation functions can approximate wiht any required precision any functional relationship between two sets of vectors of finite dimension

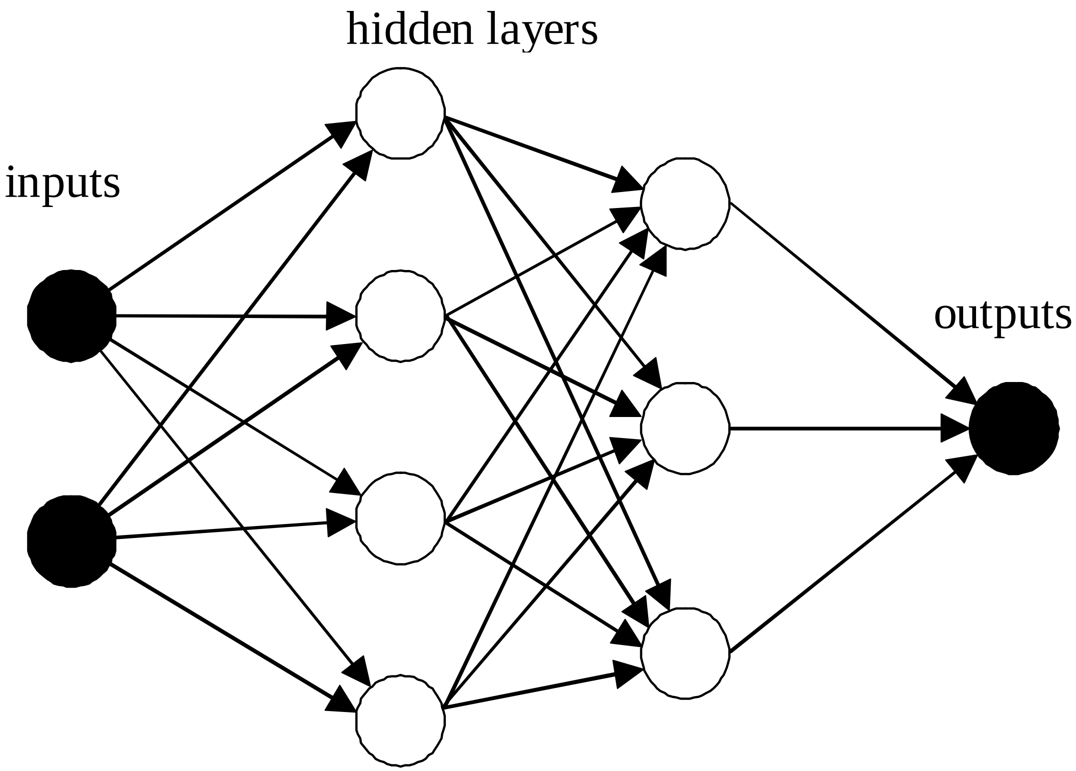
Where is the “knowledge” about the function?

In the weights (for a given architecture)

How does the ANN know what are “good” weights for a given problem?

Natural born talent and years of training

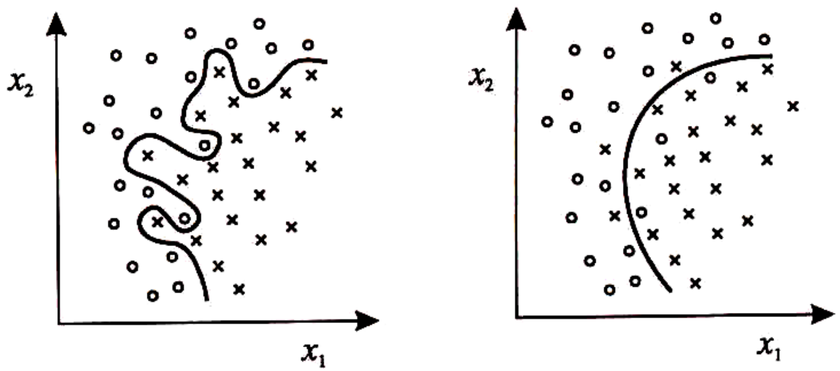
Learning - backpropagation



- Each connection has a given weight, initially random;
- A known set of inputs with corresponding known outputs is given;
- The weights are adjusted to minimise the diference between the calculated and known outputs

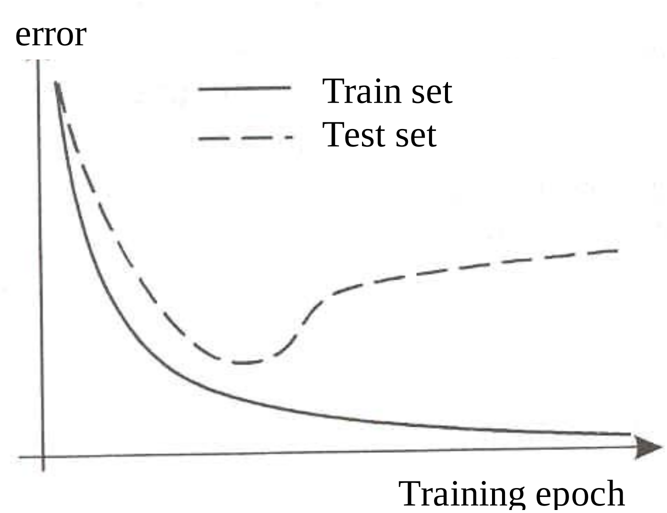
Generalisation and overtraining

generalisation consists in building a statistical model of the process that generates the data



An independent set of data, the test set, is used to control the amount of training required

Noise in the training data also helps generalisation



Biological neural systems		Artificial neural networks
Functioning of each unit (limited capacity)		
PSP: continuous (excitatory or inibitory)		$w_i \times x_i$ take continuous values, positive or negative
Membrane potential at the axon entry (Soma) is the sum of the different PSPs that reach it within a certain time period		$a = \mathbf{w} \cdot \mathbf{x}$
That sum determines whether an action potential is generated or not		output = f(a)
Potencial de acção: sim ou não, sempre igual		output: 0 ou 1 num TLU; existem outras funções de resposta (sigmóide)
Conexionism (distributed “computation”)		
Certain groups of neurons connect in complex ways, with well-defined architecture, that may change with learning		Pre-defined layered architecture
Synapses: action potential synapse strength		Connections between nodes: inputs x weigthts w
Plasticity through strengthening or weakening of connections between neurons		Plasticity through change of the weights w

Biological neural systems		Artificial neural networks
Pre-processing		
In general, the first areas of the brain to process a given input (e.g. visual) recognise low-level characteristics (e.g. lines). Further structures integrate and process signals of succesively higher level		Pre-processing, generally accompanied by a dimensionality reduction, leads to better and more efficient generalisation. Non-supervised layers may extract relevant low-level characteristics
Distributed representation of knowledge		
Each neuron learns in a basically local way		Local learning in most algorithms; non-local algorithms exist
When recalling a given event, the same neural groups are activated that were involved in the originalk event. The control is given by the medial temporal lobe.		In MLPs the entire net is activated. In Hopfield nets an input pattern similar to a stored pattern leads to “recalling” the original pattern, which is located in well defined nodes.
Structures are organised in pre-determined configurations, specialised and optimised in given tasks. Training may be very fast.		Coupling and interference between hidden units leads to highly non-linear learning, with problems involving local minima and planar error regions. Training is very slow.

Characteristics of ANNs

Characteristic	Traditional methods (Von Neumann)	Artificial neural networks
logics	Deductive	Inductive
Processing principle	Logical	Gestalt
Processing style	Sequential	Distributed (parallel)
Functions realised through	concepts, rules, calculations	Concepts, images, categories, maps
Connections between concepts	Programmed a priori	Dynamic, evolving
Programming	Through a limited set of rigid rules	Self-programmable (given an appropriate architecture)
Learning	By rules	By examples (analogies)
Self-learning	Through internal algorithmic parameters	Continuously adaptable
Tolerance to errors	Mostly none	Inerent

ANNs – some properties

- The mean square error of an ANN decreases with the number of parameters much faster than in a series expansion, particularly in high dimensional spaces. The price to pay is the non-linearity in relation to the parameters to optimise.
- Minising the mean square error of an ANN leads to the fact that the outputs can be interpreted as probabilities.
- Pre- and post-processing normally increase the effciency of ANNS, by reducing dimensionality, incorporating previous knowledge, and making up for incomplete data.
- The role of the hidden layers is to reorganise the results of previous layers into a more separable or classifiable form, and to establish relevant characteristics
- Nodes may be added or eliminated during training, providing a degree of flexibility to the architecture.

ANNs and Ion Beam Analysis

- Objective: automated data analysis
  - Simulated annealing: IBA DataFurnace
    general (RBS, EBS, ERDA, NRA, NDP)
    not optimised for specific systems
  - ANNs: (Ge)Si, (Er)$\underline{Al_2O_3}$, Si/NiTaC
    for specific systems
    instantaneous
- Objective: automated optimisation of experiments
  - For automated control
- Integrated set of ANNs (and other code)

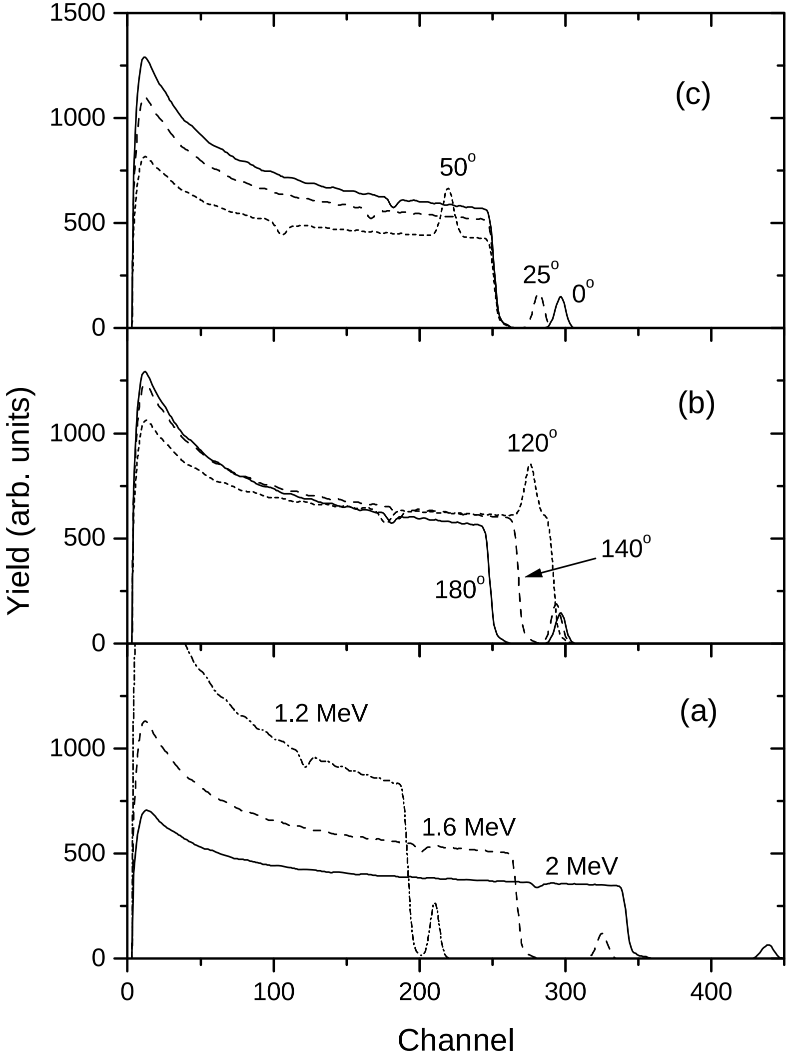
ANNs and Ion Beam Analysis

- ANNs recognize recurring patterns in the input data, without knowledge of the causes. ANNs are then an ideal candidate to do automatically what RBS analysts have long done:

  to relate specific features of the data to specific properties of the sample.

- …because RBS spectra can be treated as just pictures

Rutherford backscattering: where is the pattern?



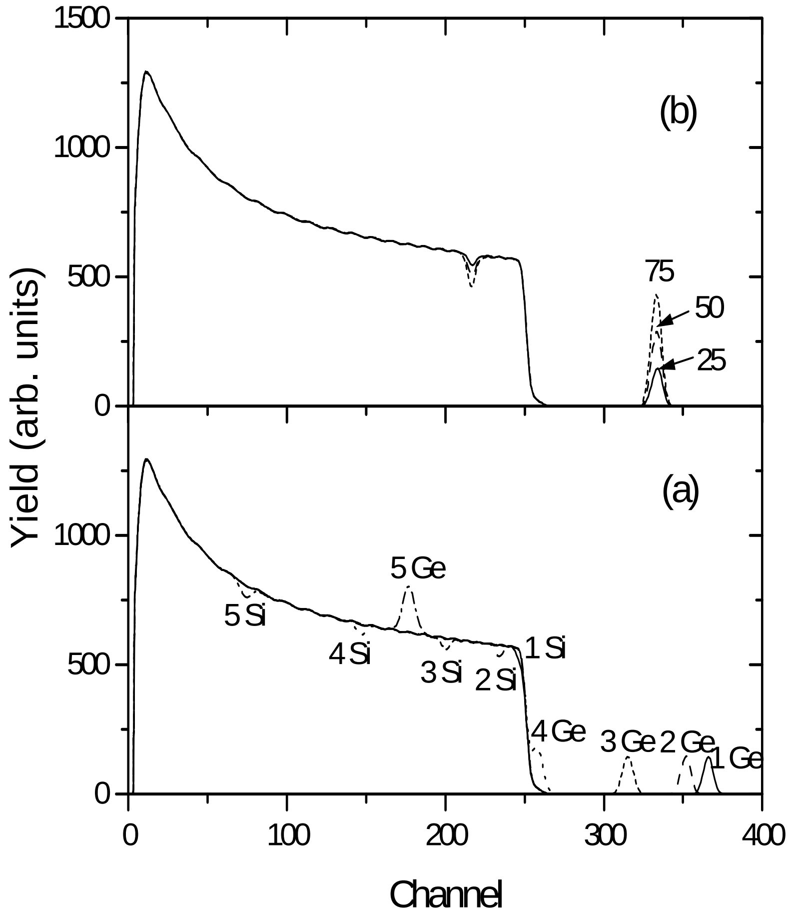
25Å Ge δ-layer under 400 nm Si

Angle of incidence

Scattering angle

Beam energy

Patterns in RBS: Ge δ-layers in Si

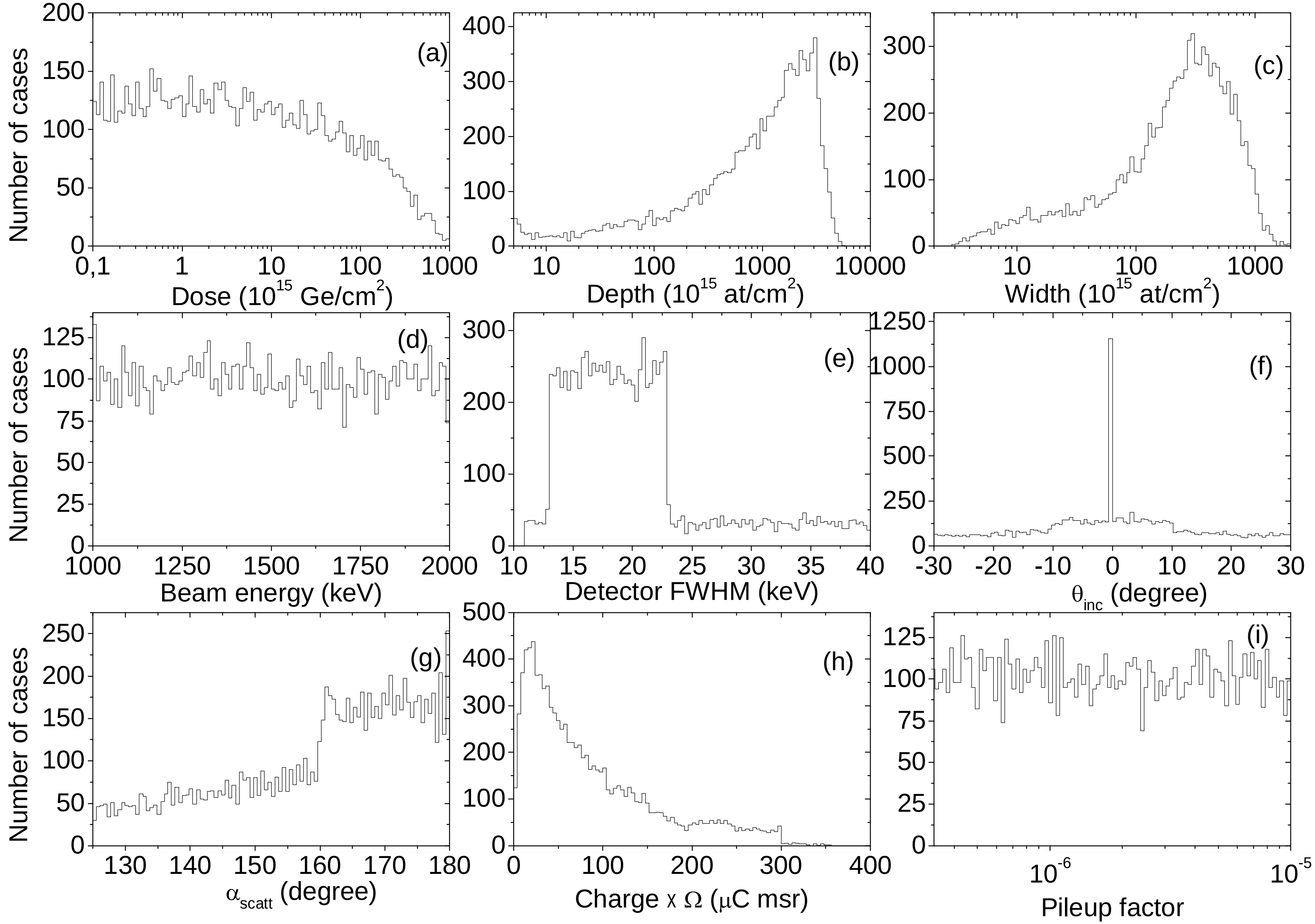


25, 50, 75 Å, under 200 nm Si

25 Å, under 20, 100, 300, 600, 1000 nm Si

…similar with other parameters

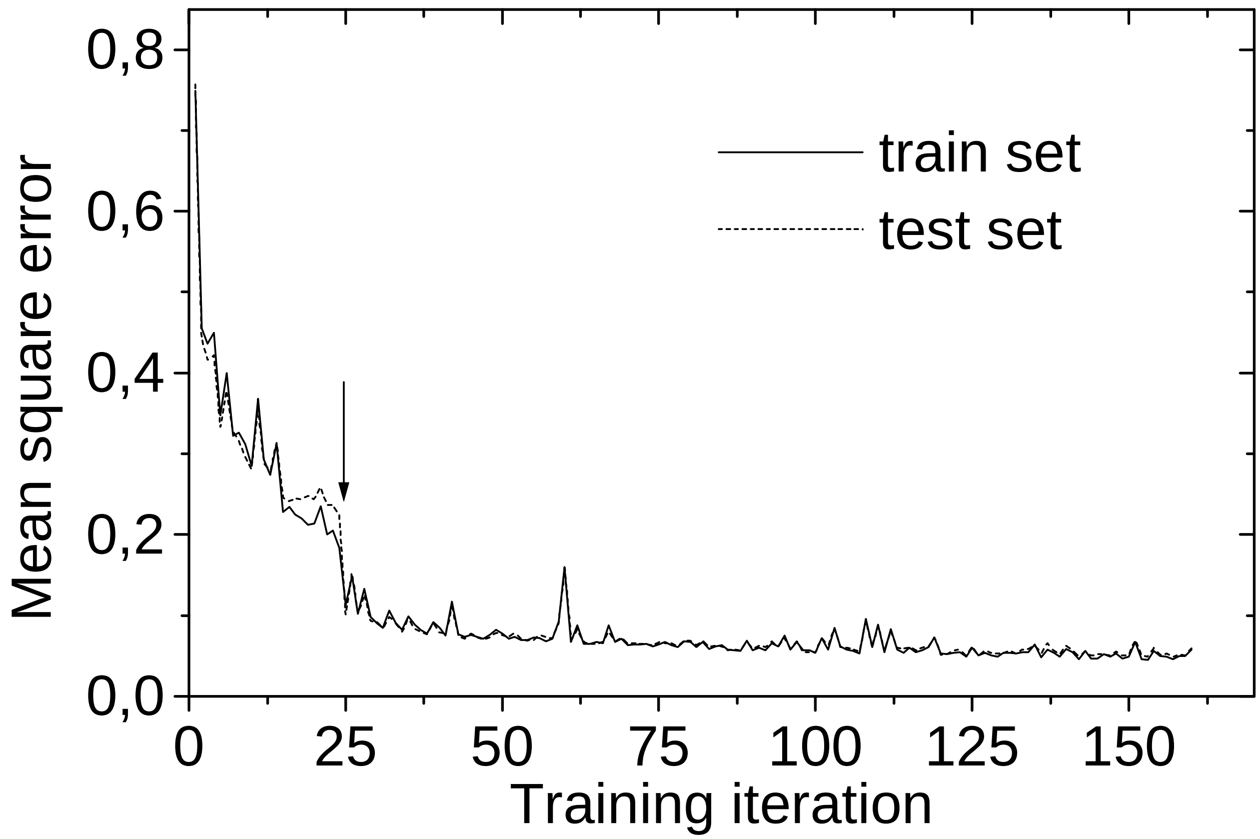
Ge implanted in Si: training data set



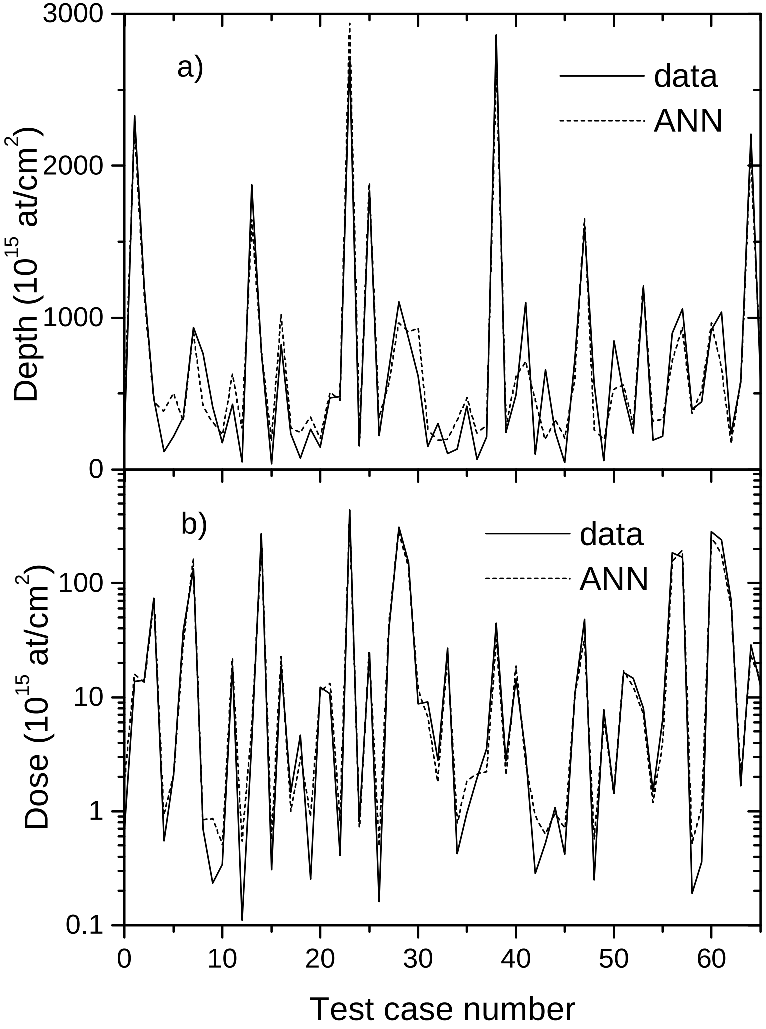
Ge in Si: ANN architecture

architecture	train set error	test set error
(I, 100, O)	6.3	11.7
(I, 250, O)	5.2	10.1
(I, 100, 80, O)	3.6	5.3
(I, 100, 50, 20, O)	4.2	5.1
(I, 100, 80, 50, O)	**3.0**	**4.1**
(I, 100, 80, 80, O)	2.8	4.7
(I, 100, 50, 100, O)	3.0	4.2
(I, 100, 80, 80, 50, O)	3.2	4.1
(I, 100, 80, 50, 30, 20, O)	3.8	5.3

Ge in Si: training

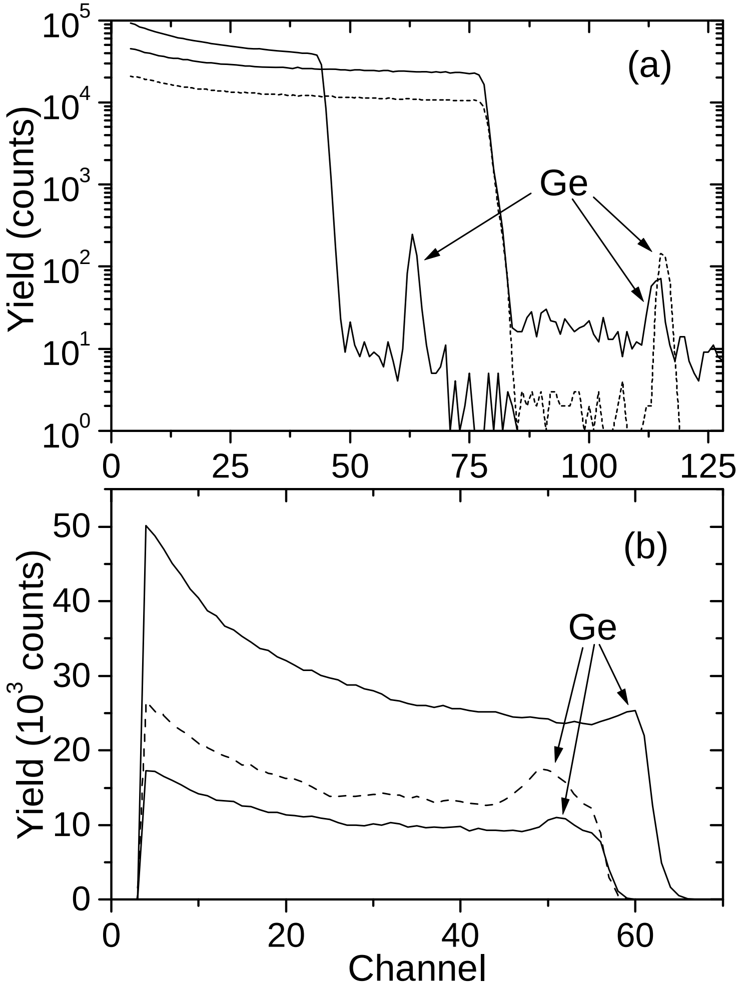


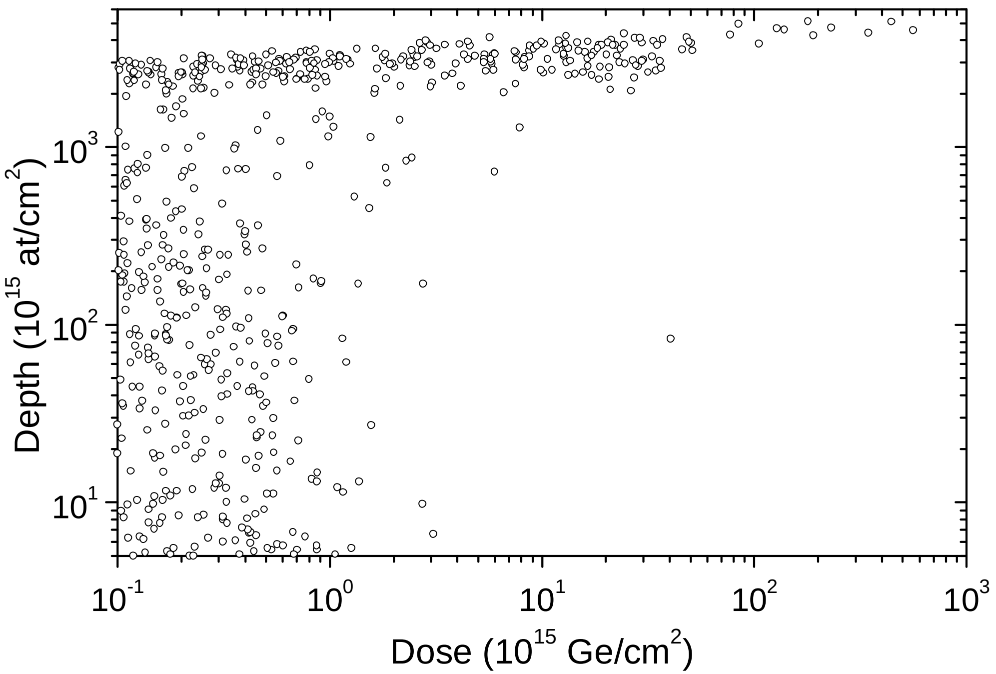
Training: test set



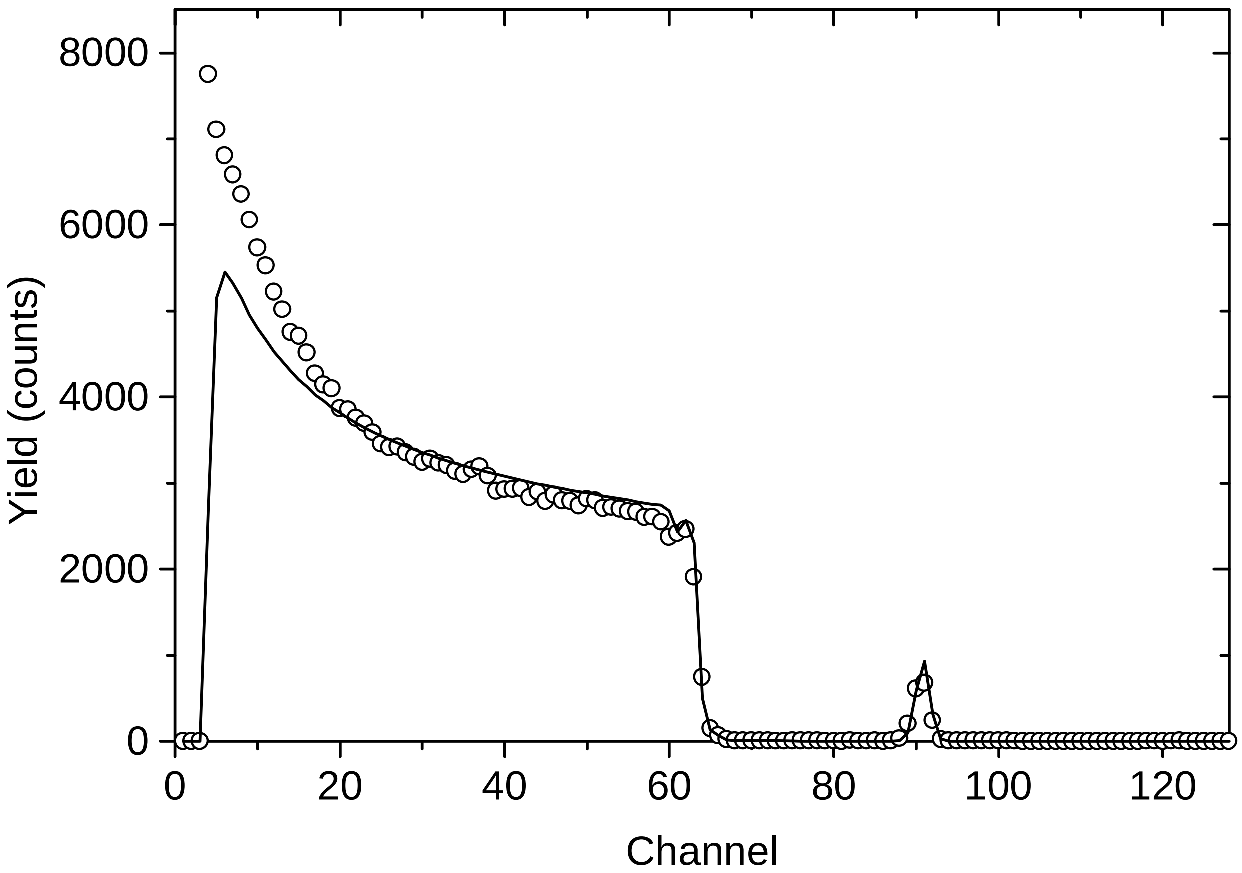
at 17% mse, worst cases eliminated from training

Ge in Si training: eliminated cases





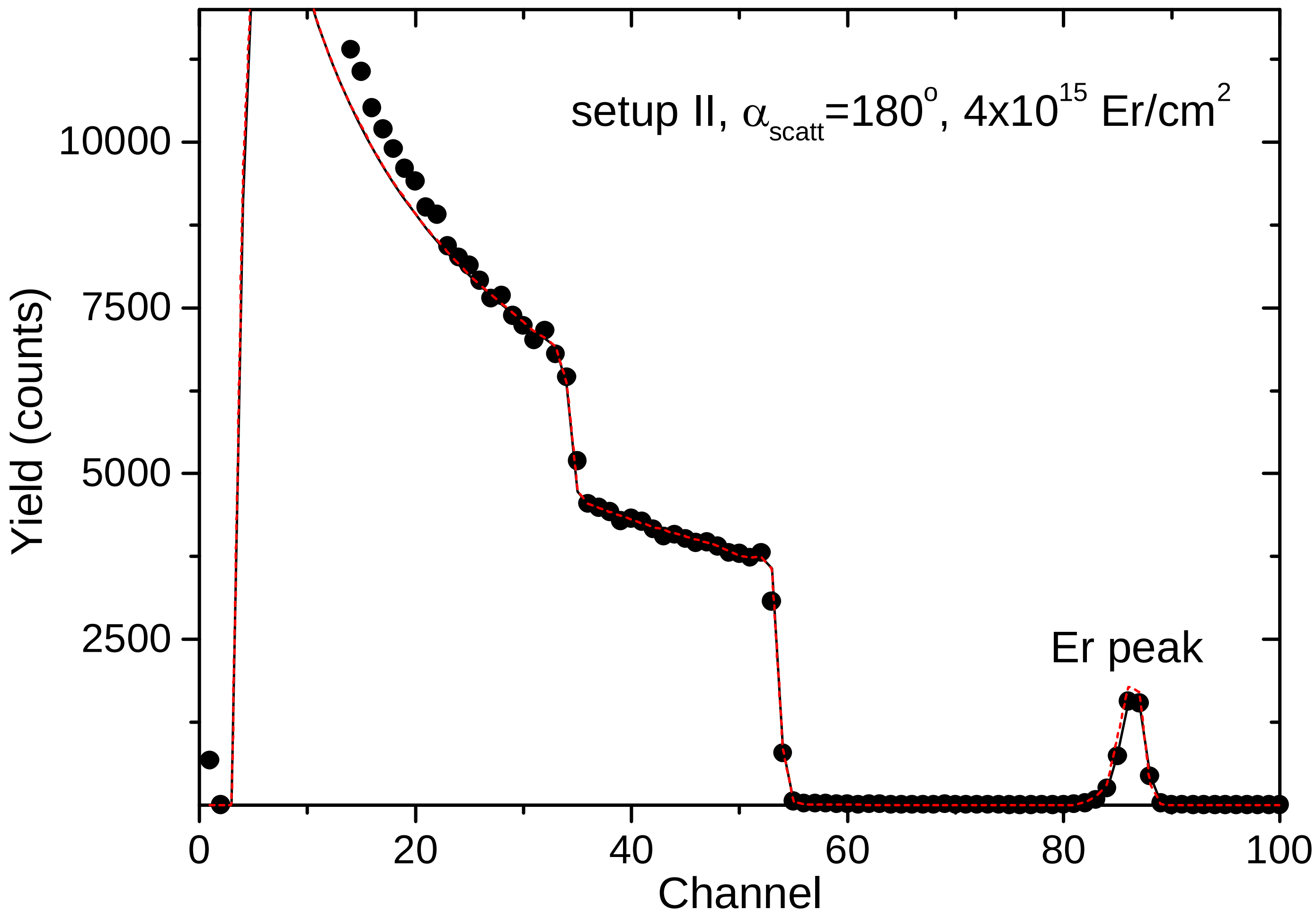
Ge in Si results: real data



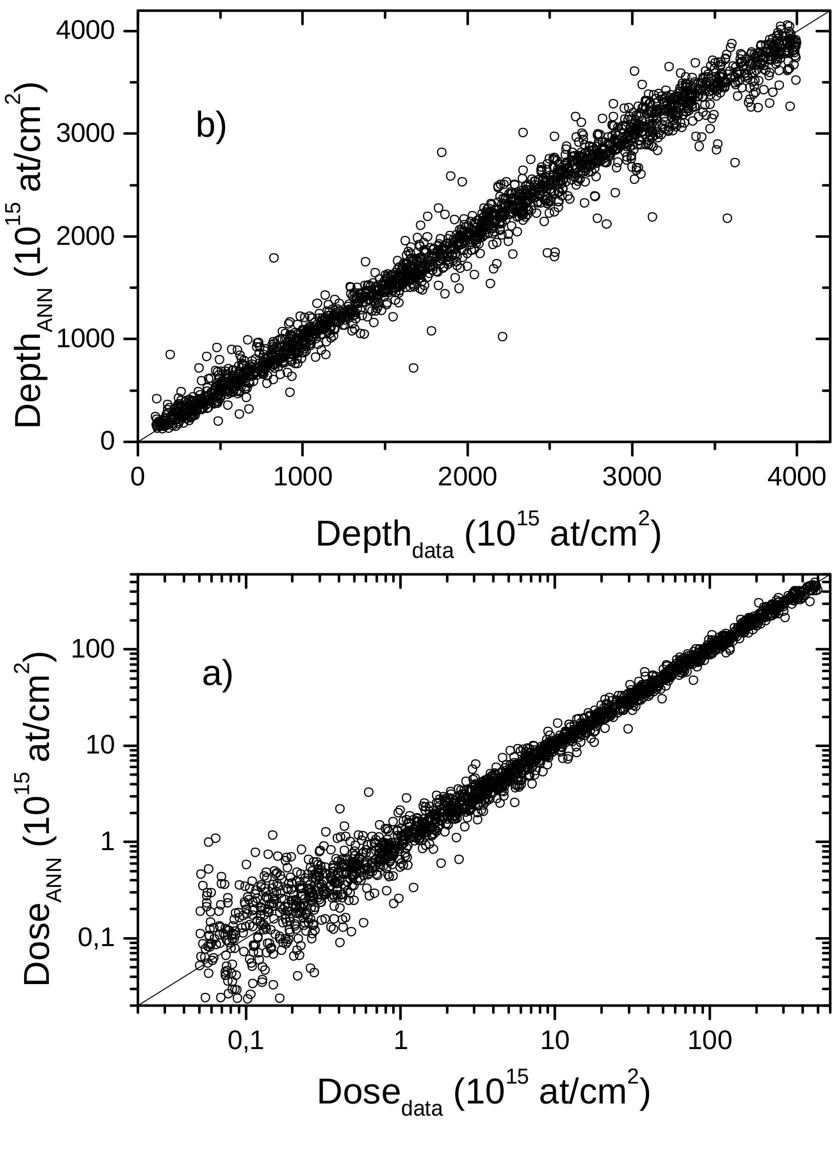
Ge in Si results: real data

	Values derived with NDF		Values obtained with the ANN	
sample	Ge (10^{15} at/cm^2)	depth (10^{15} at/cm^2)	Ge (10^{15} at/cm^2)	depth (10^{15} at/cm^2)
1	16.7	332.8	16.3	267.4
2	14.4	302.3	12.4	223.7
3	13.6	318.2	15.3	307.2
4	14.7	334.5	12.4	236.8
5	15.7	378.0	10.6	245.7
6	9.3	250.7	12.2	308.7
7	26.8	246.3	27.9	214.3
8	9.8	349.1	12.7	359.4
9	9.6	356.8	12.6	384.7
10	9.7	316.3	11.9	329.4

Data analysis: (Er)$\underline{Al_2O_3}$



Anything in Al_2O_3: test set



Anything in Al2O3

	nominal dose (at/cm^2)	implant energy (keV)	beam energy (MeV)	setup / scattering angle	angle of Incidence	solid angle -charge (μC msr)	dose (10^{15} at/cm^2) ANN	NDF	depth (10^{15} at/cm^2) ANN	NDF
28 Ti	1×10^{15}	100	1.6	II/160º	6º	18.0	0.26	1.34	1307	742
32	1×10^{15}	100	1.6	II/180º	6º	104.4	0.65	1.08	1561	706
35	1×10^{17}	100	1.6	II/180º	5º	57.6	75.7	92.4	756	632
36 Fe	1×10^{16}	160	1.6	II/160º	4º	17.55	10.0	10.6	1384	1222
40	1×10^{16}	160	1.6	II/180º	4º	99.0	9.49	10.3	1320	904
43	5×10^{17}	160	1.6	II/180º	4º	55.7	365	407	832	487
21 Co	1×10^{15}	150	2	I/180º	7º	99.2	0.68	0.96	1161	680
22	5×10^{16}	150	2	I/180º	3º	94.8	40.9	48.4	1119	729
24	5×10^{17}	150	2	I/180º	2º	64.3	385	448	632	622
8 Er	8×10^{13}	200	1.6	II/160º	0º	5.83	0.03	0.07	650	770
11	4×10^{15}	200	1.6	II/160º	0º	6.87	3.39	3.75	922	726
15	4×10^{15}	200	1.6	II/180º	0º	20.48	4.89	3.83	861	736
26 Au	6×10^{16}	160	2	II/180º	2º	52.0	69.6	59.3	278	394

Architecture as in Ge in Si

Anything in anything

- Any element, with Z between 18 and 83, into_any target composed of one or two lighter elements .

- Same architecture as before led to very large errors
- Extremely large networks were necessary to obtain train errors around 20%: complexity of ANN expands to meet complexity of problem.

- Pre-processing: reduce complexity of problem.
- Peak recognition routine determines automatically the peak position and area. It fails ocasionally (5-10%).

Anything in anything – inputs and outputs

- Experimental conditions

E0	1 : 2.1 MeV
α_{scatt}	135º : 180º
θ_{inc}	-20º : 20º (IBM geometry)
Q.Ω	1 : 200 μC msr
(FWHM:	10 : 40 keV)

- Sample

Z	18 : 83
M	(redundant)
Z1, Z2	6 : 82
f1, f2	0 : 1

- Pre-processing: P (peak position), A (area)
- Outputs

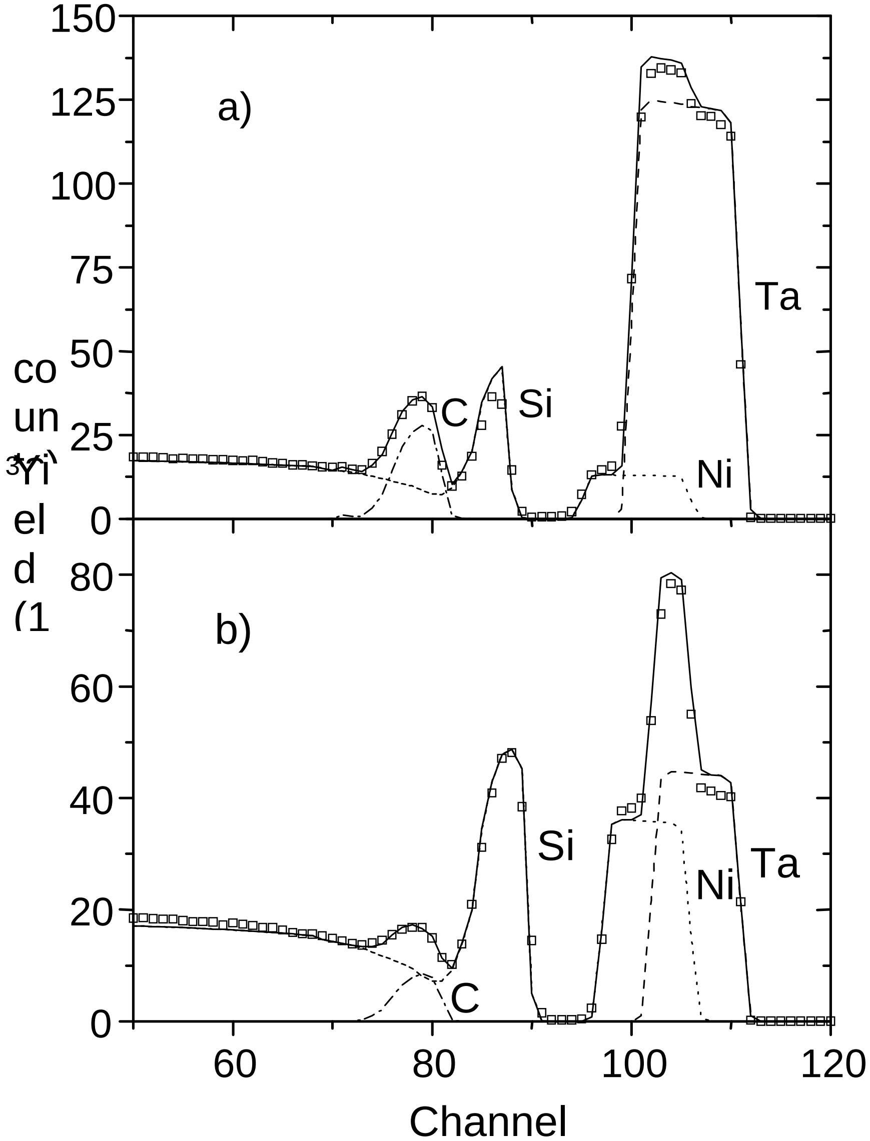
Dose	1 : 100 $\times 10^{15}$ at/cm^2
Depth	100 : 3700 $\times 10^{15}$ at/cm^2

Anything in anything

Network Topology	Train error (%)	Test error (%)	# eliminated cases (%)
(12:30:10:2)	3.15	3.37	19.7
(12:30:20:2)	3.12	3.70	20.7
(12:40:10:2)	3.20	3.25	19.8
(12:40:20:2)	2.98	3.22	20.5

ANN	$Dose_{ANN}/Dose_{NDF}$	$\lvert Depth_{ANN} - Depth_{NDF} \rvert$ (10^{15} at/cm^2)
Ge in Si	1.11	53
Er in Al_2O_3	1.17	106
all in Al_2O_3	1.02	235
all in all	**0.96**	**83**

Data analysis: Si/NiTaC



1.75 MeV protons:
EBS

Simulated RBS spectrum (solid line) for two samples, calculated for the outputs given by the ANN. The dashed lines corresponds to the contribution from each element, squares are the collected data

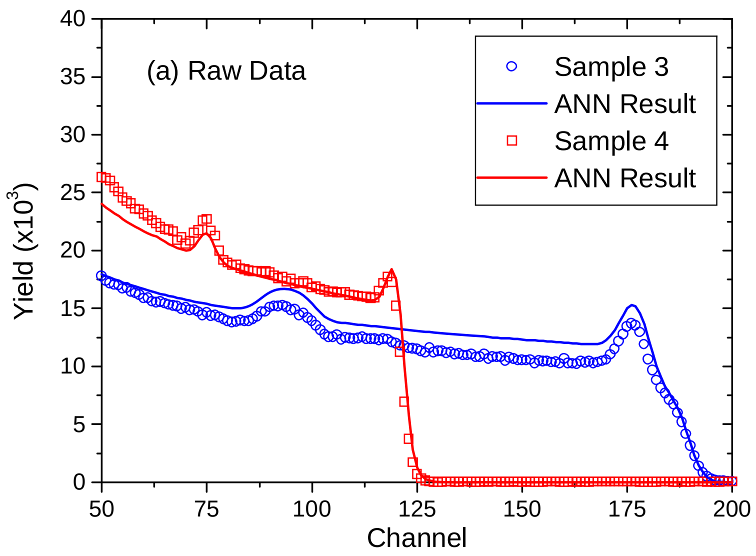
Data analysis: Si/NiTaC

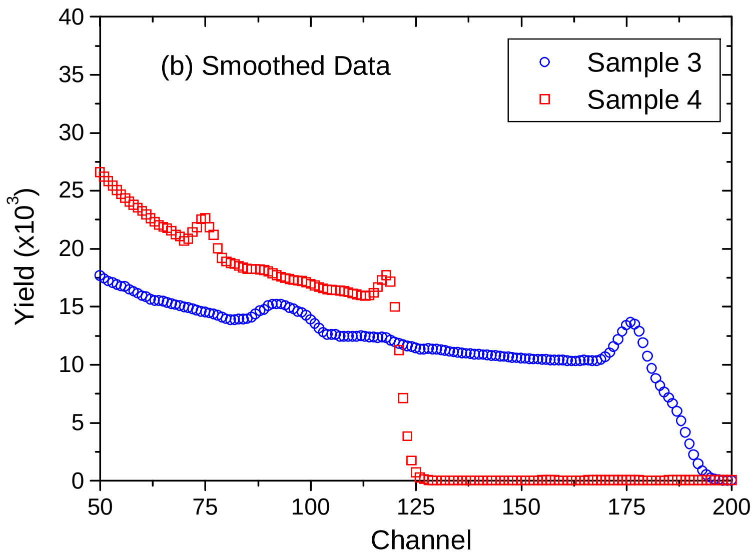
	NDF				ANN			
sample	t (10^{15} at/cm^2)	C (at.%)	Ni (at.%)	Ta (at.%)	t (10^{15} at/cm^2)	C (at.%)	Ni (at.%)	Ta (at.%)
1	6890	7.2	79.4	13.4	6918	7.2	78.2	14.6
2	7286	7.6	78.4	14.0	7387	7.5	77.0	15.5
3	6437	10.7	72.4	16.9	6593	10.8	72.3	16.9
4	7516	7.7	72.1	20.2	7752	8.3	72.0	19.7
5	5975	13.7	62.5	23.8	5858	13.1	64.0	22.9
6	6898	12.5	64.4	23.1	7111	13.0	63.1	23.9
7	5774	16.2	57.6	26.3	5719	17.7	56.0	26.3
8	5984	19.1	50.1	30.8	5993	19.8	49.1	31.1
9	7198	22.6	42.8	34.6	7205	22.9	42.1	35.0
10	8352	18.0	44.4	37.6	8419	20.2	41.4	38.4
11	6866	22.4	36.4	41.2	6904	24.2	33.8	42.0
12	7769	24.2	34.1	41.7	7691	25.3	30.6	44.1
13	7662	14.9	61.7	23.4	7858	14.8	61.4	23.8
14	6868	13.9	64.6	21.5	7025	14.5	64.2	21.3
15	5449	16.3	60.6	23.1	5490	16.6	60.4	23.0
16	4809	15.0	63.3	21.7	5208	16.2	62.3	21.5

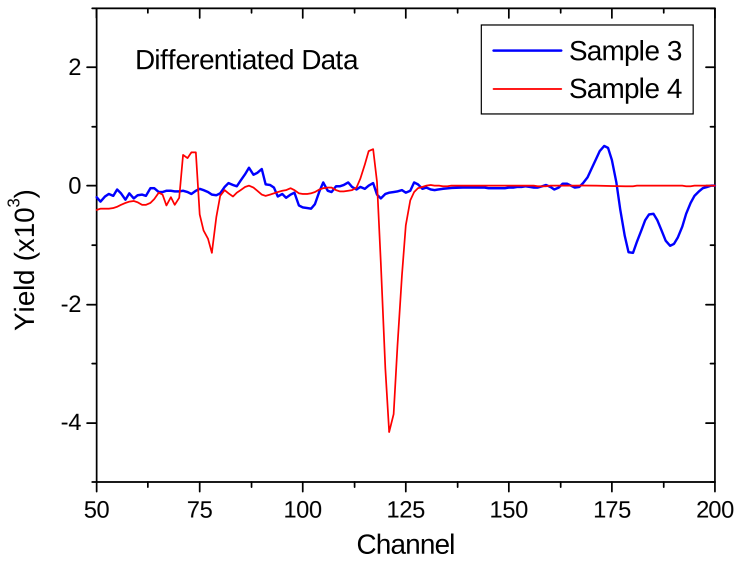
AlN_xO_y t

E = 1 - 2 MeV
angle of incidence = -40º - +40º
Q.Ω = 52.4 - 393 μC msr
t = 150 - 850×10^{15} at/cm^2.

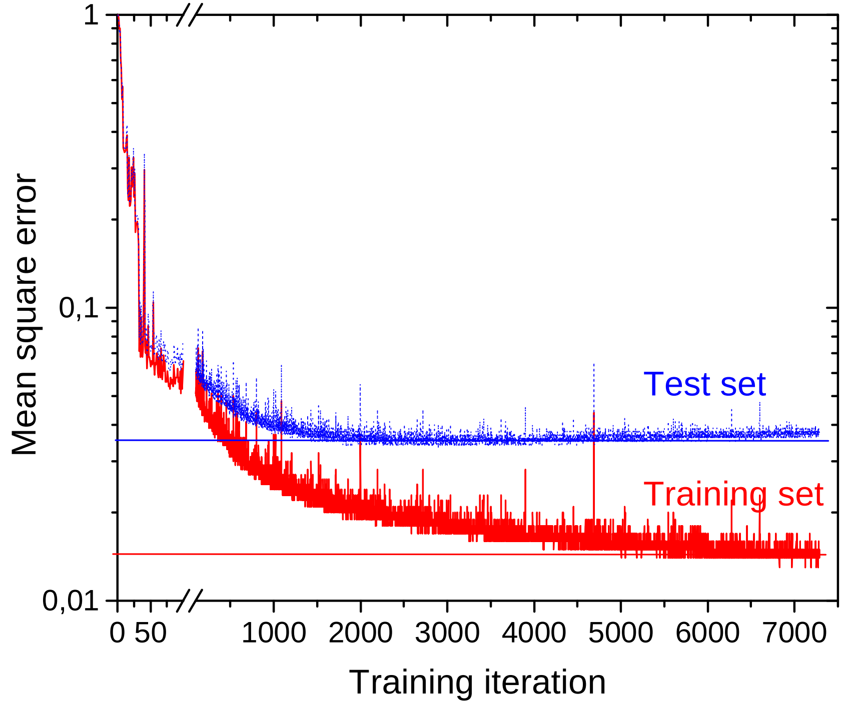
(unintentional channelling)







AlNxOy t - training



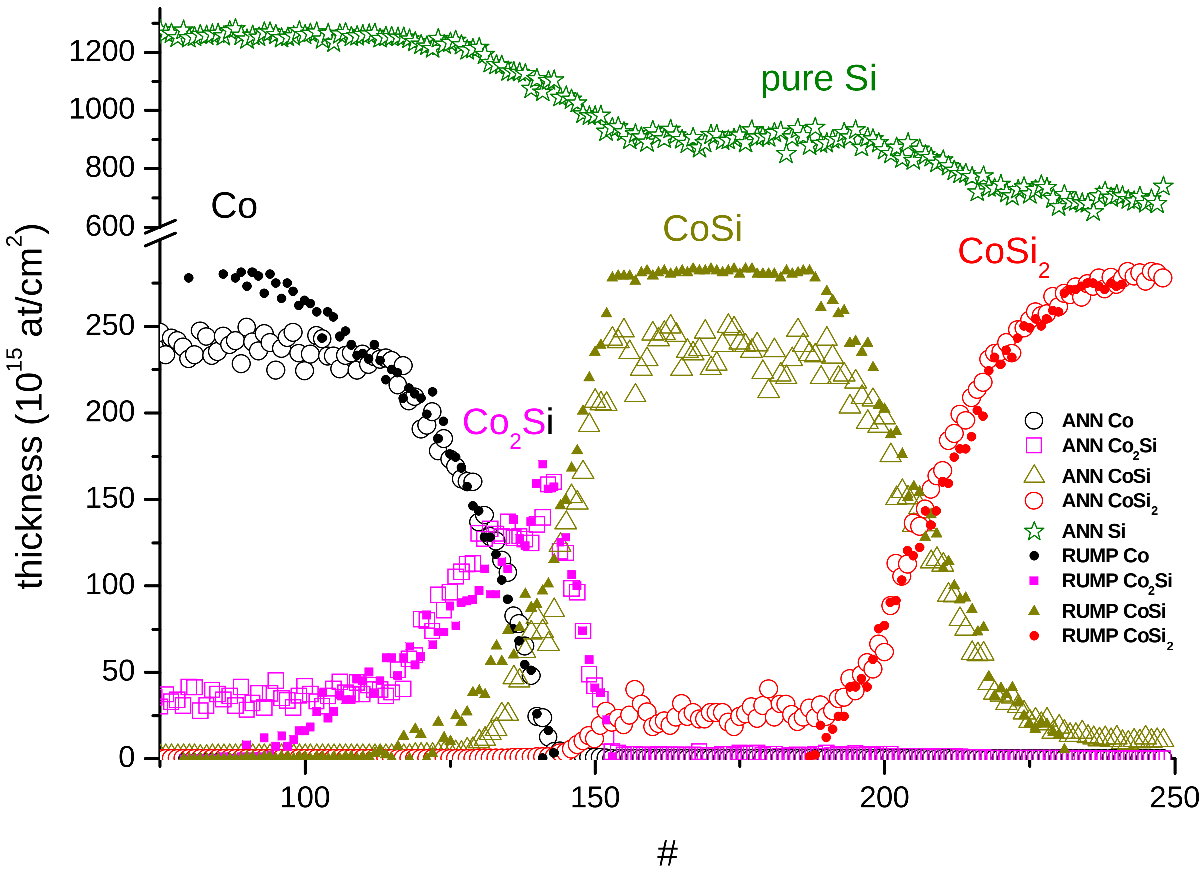
Network	Train set MSE (%)	Test set MSE (%)
ANN-Raw	2,2	2,8
ANN-Smooth	2,9	3,7
ANN-Differentiated	2,4	3,4
ANN-No Exp. Param	3,1	4,3

Sample	ANN	Thickness	[Al]	[N]	[O]
1	Raw	0.92 (0.12)	0.87 (0.08)	1.17 (0.08)	0.75 (0.5)
	Smoothed	0.92 (0.12)	0.85 (0.08)	1.2 (0.08)	0.78 (0.5)
	Differentiated	0.94 (0.16)	0.94 (0.1)	1.07 (0.1)	1.1 (0.3)
	No exp. Param.	0.84 (0.19)	0.83 (0.08)	1.14 (0.09)	1.66 (0.78)
2	Raw	1.14 (0.18)	0.76 (0.17)	1.19 (0.09)	1.5 (1.31)
	Smoothed	1.4 (0.18)	0.77 (0.2)	1.17 (0.07)	1.59 (1.24)
	Differentiated	1.06 (0.08)	1.01 (0.08)	1.02 (0.08)	0.79 (0.34)
	No exp. Param.	1.09 (0.15)	0.98 (0.11)	1.04 (0.11)	0.79 (0.26)
3	Raw	0.91 (0.17)	0.95 (0.13)	1.12 (0.13)	0.51 (0.88)
	Smoothed	0.9 (0.15)	0.93 (0.11)	1.1 (0.15)	0.85 (0.86)
	Differentiated	0.88 (0.15)	0.99 (0.12)	1.04 (0.1)	0.86 (0.3)
	No exp. Param.	0.86 (0.12)	0.93 (0.14)	1.09 (0.11)	0.92 (0.51)
4	Raw	1.14 (0.21)	0.83 (0.09)	7.16 (0.64)	0.75 (0.15)
	Smoothed	1.1 (0.2)	0.89 (0.1)	6.91 (0.63)	0.73 (0.16)
	Differentiated	0.82 (0.17)	1.13 (0.1)	1 (0.27)	0.98 (0.07)
	No exp. Param.	0.82 (0.16)	0.95 (0.09)	1.3 (0.31)	1.09 (0.08)
5	Raw	0.08 (0.03)	1.27 (0.12)	16.82 (1.72)	0.01 (0.04)
	Smoothed	0.11 (0.07)	1.09 (0.1)	19.1 (1.83)	0.01 (0.05)
	Differentiated	0.1 (0.03)	1.38 (0.11)	15.21 (1.64)	0.04 (0.01)
	No exp. Param.	0.1 (0.01)	1.7 (0.19)	10.29 (4.59)	0.09 (0.02)

ANNs for real-time RBS

- Real-time in-situ RBS: to study reaction kinetics
- Sample annealed while being analysed: 2min/spectrum
- Typical runs are 2 weeks beam time, leading to thousands of spectra
- Typically 6 months analysis time with RUMP
- Ideal case for ANNs

- Si / Co
- Si / Co / Co_2Si
- Si / Co / Co_2Si / CoSi
- Si / Co_2Si / CoSi
- Si / CoSi
- Si / CoSi / $CoSi_2$
- Si / $CoSi_2$



Other systems already studied

- Ni(Pt) on Si; Pt as an impurity, 12 parameters
- NiEr on Si, 13 parameters
- Pd on Ge, 3 parameters

- In all cases, many layers, non-fixed phases
- About 1000 spectra each system
- Work continues in other systems
- ANNs make routine real-time work feasible

RBS without humans

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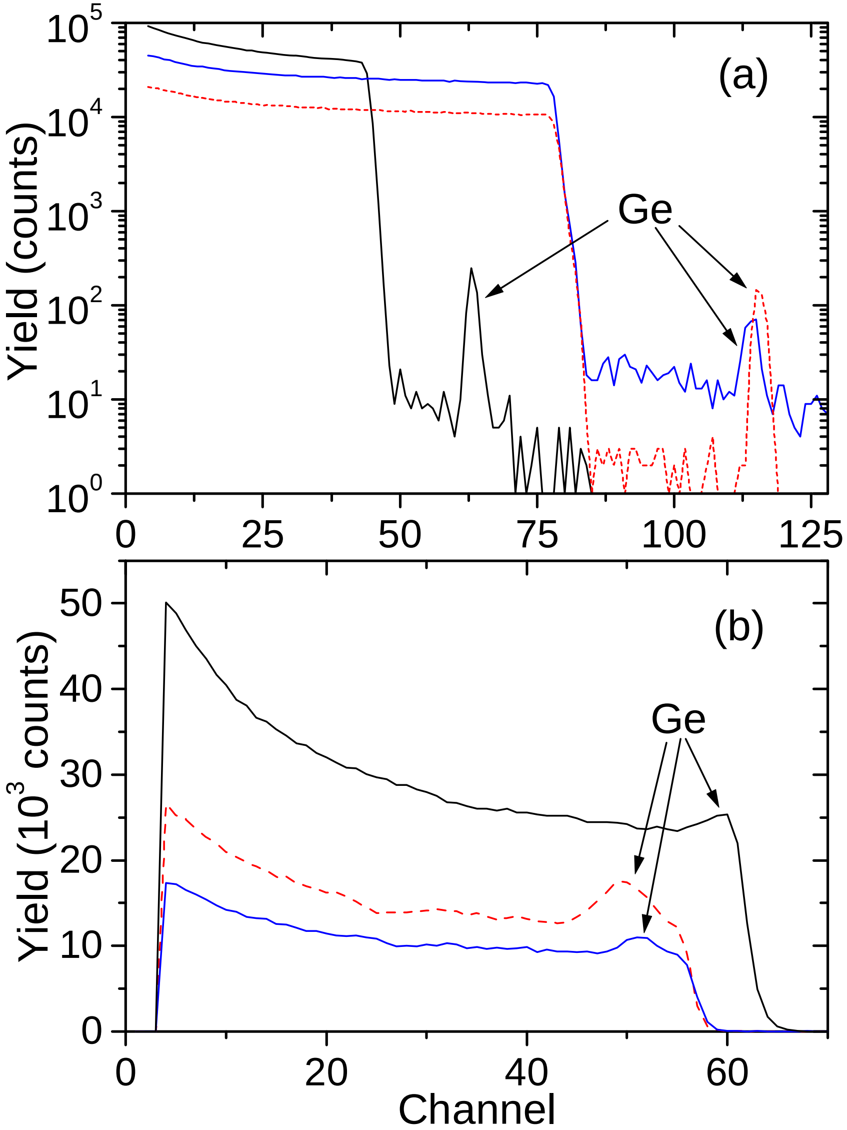
Presented at IBA15 - Cairns

Data classification: (Ge)Si



Three classes:

(1) clean spectra

(2) superimposed signals

(3) separated signals, small doses

There may be class mixing:

(1)+(2): partial superposition

(1)+(3): intermediate doses

(2)+(3): superimposed signals, small doses

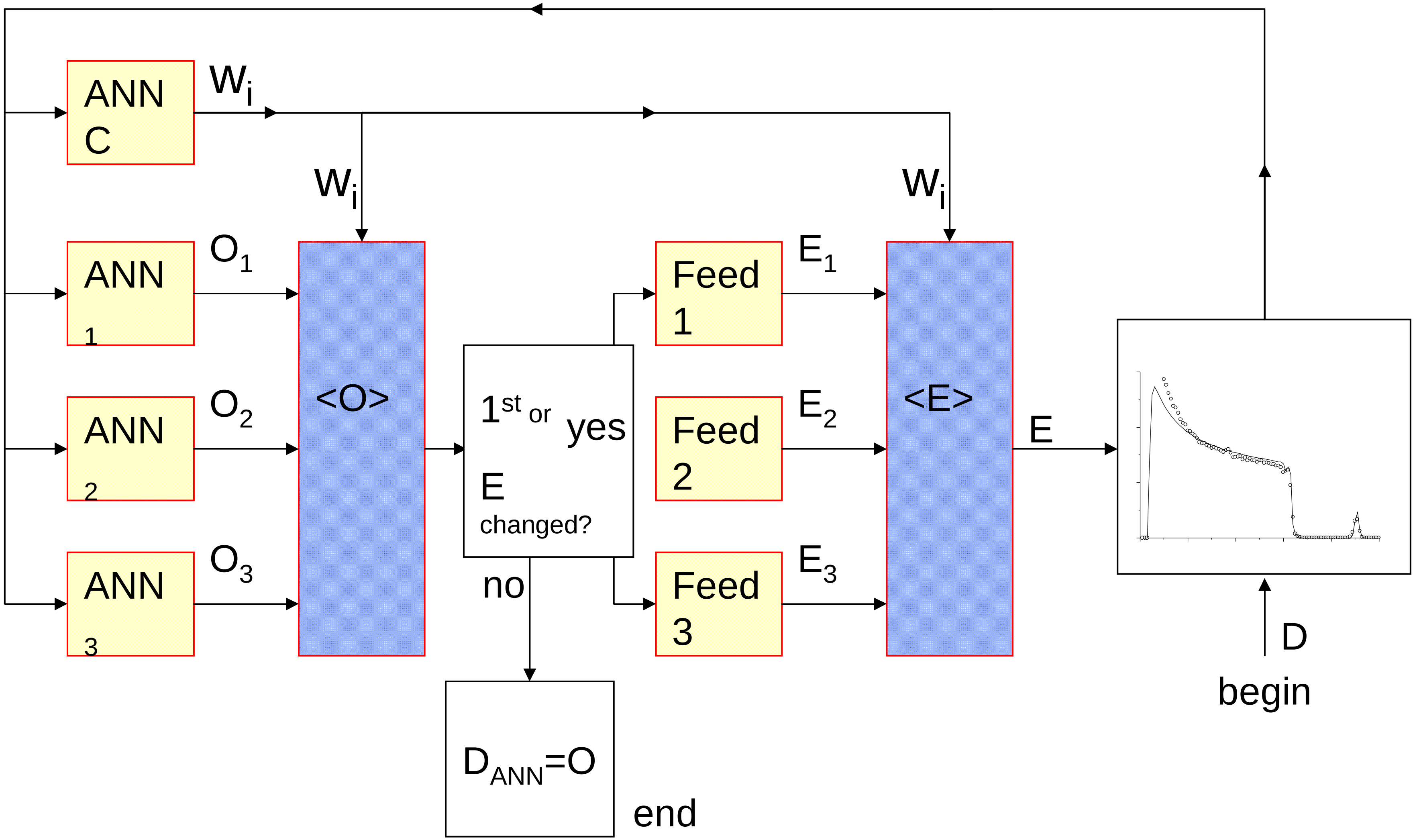
(1)+(2)+(3): partial superposition, small doses

Code required for automation

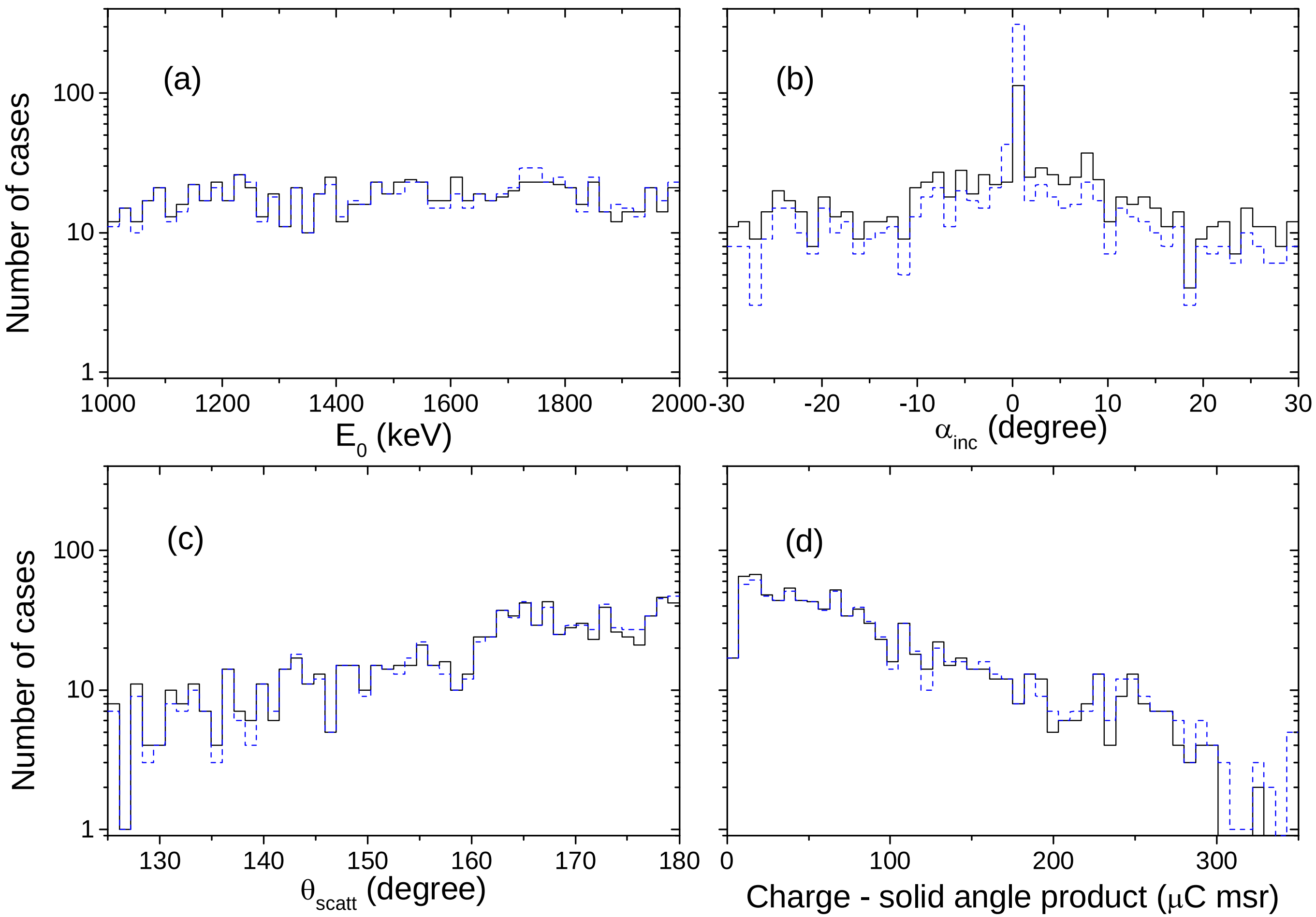
- ANNC: for classification. Output is membership probability
- ANNi: for class (i). Output is Ge dose and depth
- Feed i: feedback algorithm for class (i):

	E	θ_{inc}	α_{scatt}	C
F1	-	0^o if partial superposition	-	$2.25\times F_{old}$ if low Statistics
F2	2 MeV (3rd step)	0^o (1st step)	180^o (2nd step)	-
F3	$1.1\times E_{min\_no\_superp}$ if C > 300 μC msr	-	-	$4\times F_{old}$

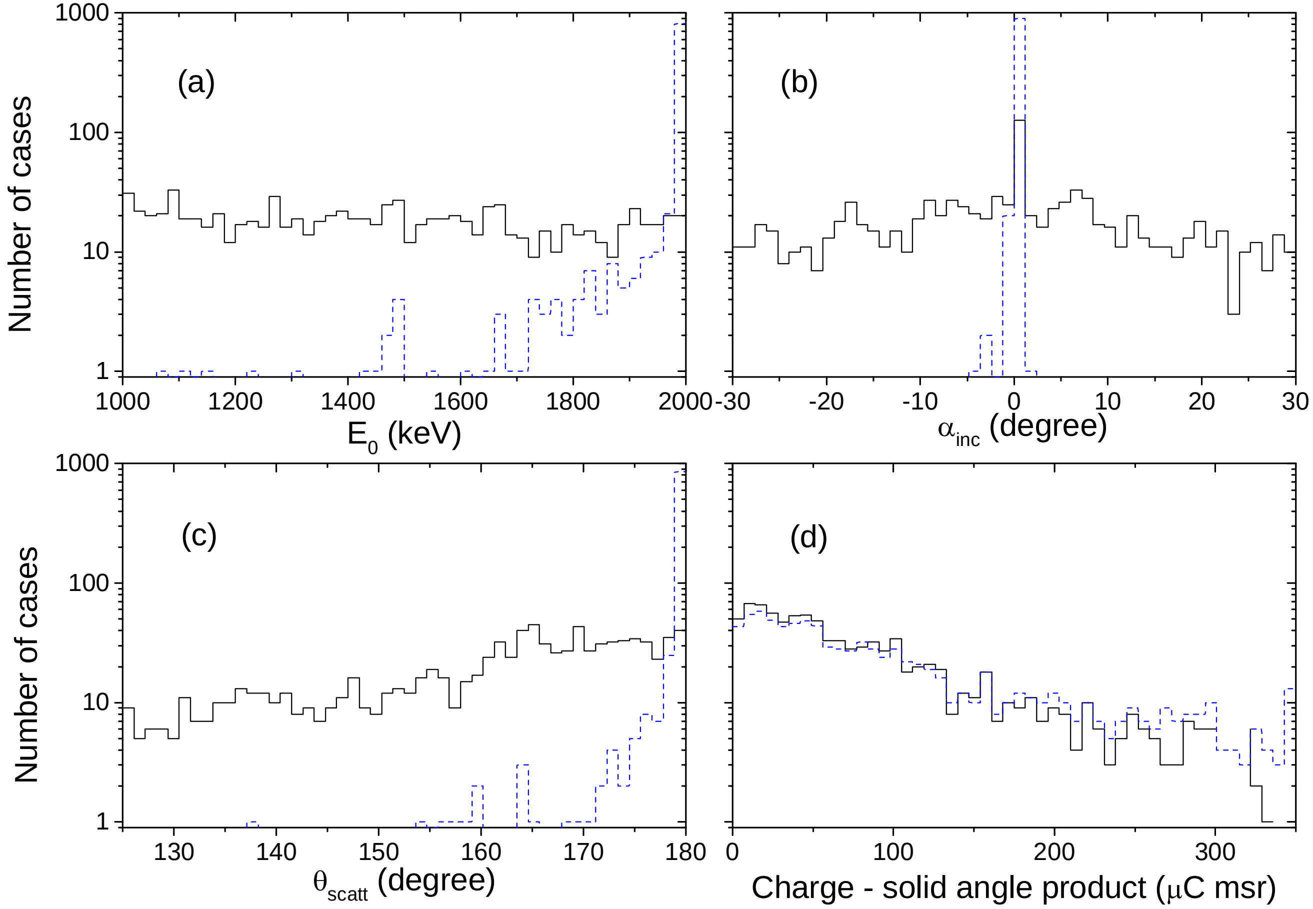
Integrated feedback system



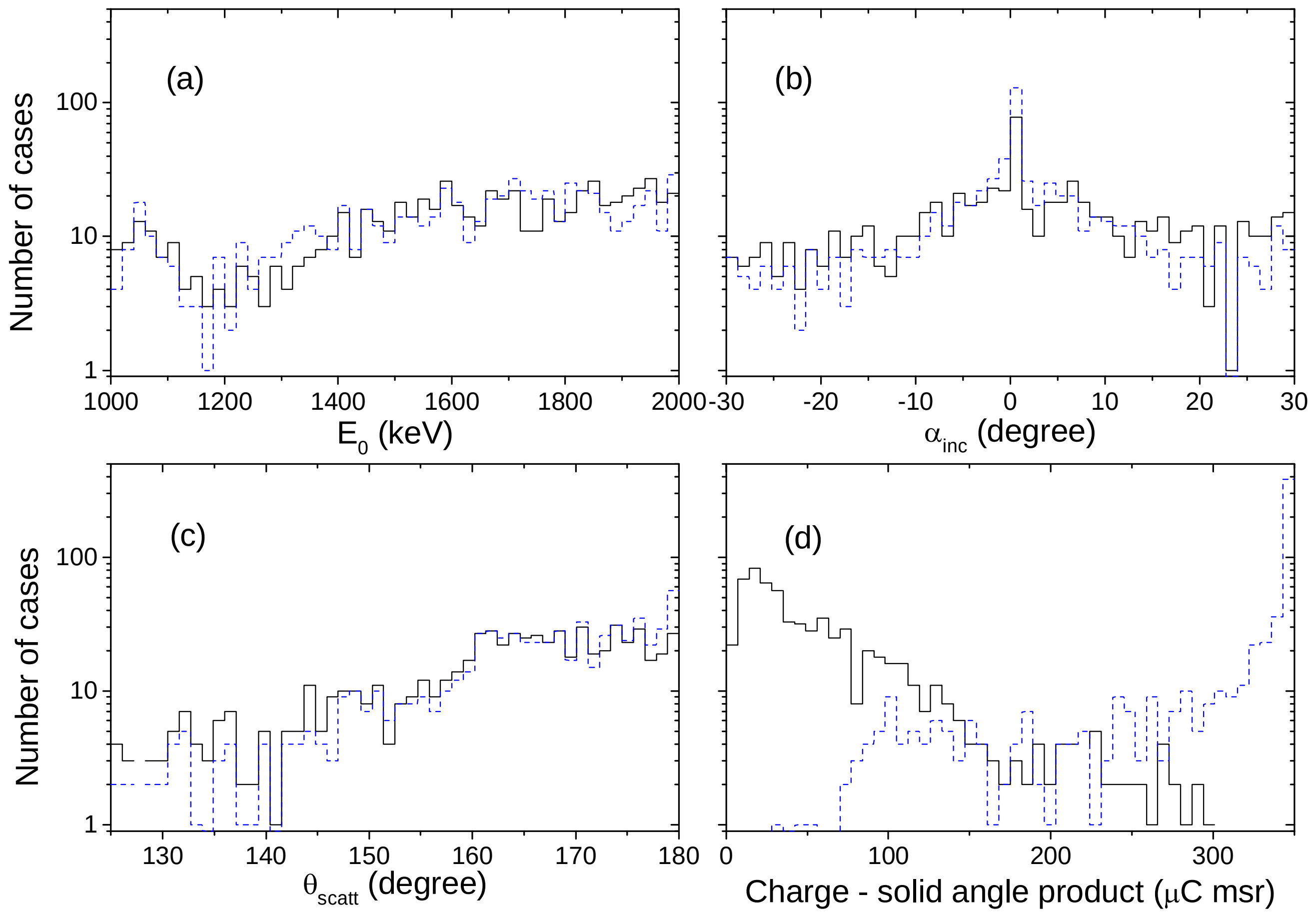
Results: experimental conditions class (1)



Results: experimental conditions class (2)



Results: experimental conditions class (3)



Results: Classes (2) and (3)

a) Initial classif: correct

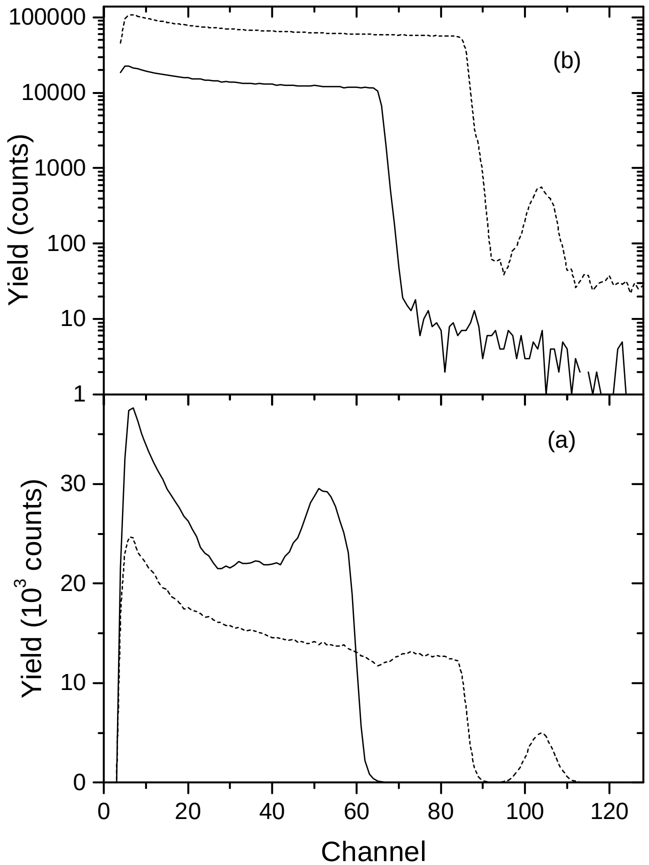
b) Initial classif: (3)

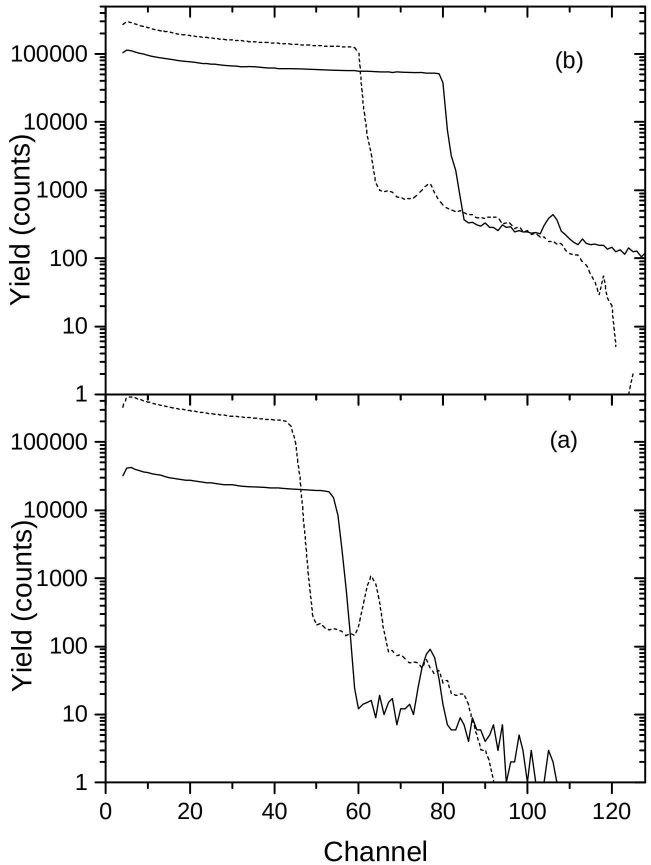
Final class (1) in both

Initial class (3) in both

a) Final class: (1)

b) Final class: (3)





Results of the classification ANN for the spectra before and (after) optimisation of the experimental conditions

ANNC / real	1		2		3	
1	91.7	(98.9)	5.9	(1.1)	2.4	(0)
2	2.7	(30.8)	90.0	(65.2)	7.3	(4.0)
3	1.6	(62.6)	33.1	(7.5)	65.3	(29.9)

			$ANNC_i$: correct		$ANNC_i$: wrong	
real class	final class	analysis	depth	dose	depth	dose
1	1	ANN_i	1.03(13)	0.87(14)	1.07(11)	1.08(12)
		ANN_f	1.01(12)	0.85(14)	0.98(4)	0.81(10)
		NDF	1.00(2)	0.99(2)	1.00(1)	1.00(1)
2	1	ANN_i	1.08(13)	1.17(38)	0.66(35)	0.53(47)
		ANN_f	0.98(3)	0.87(11)	0.72(36)	0.55(35)
		NDF	1.00(1)	0.98(3)	1.00(5)	0.93(17)
	2 or 3	ANN_i	0.98(11)	1.08(56)	0.37(14)	0.14(17)
		ANN_f	0.98(06)	1.22(51)	0.73(33)	0.94(99)
		NDF	0.97(3)	0.96(15)	0.96(13)	0.88(24)
3	1	ANN_i	1.27(65)	1.56(71)	5.80(5.69)	17.1(15.1)
		ANN_f	1.08(54)	1.08(46)	1.35(80)	1.39(47)
		NDF	1.05(31)	0.93(24)	1.05(25)	0.94(18)
	2 or 3	ANN_i	1.37(71)	2.47(1.34)	8.94(8.21)	33.2(21.0)
		ANN_f	2.10(1.91)	3.57(4.75)	4.41(5.06)	7.64(9.55)
		NDF	1.27(82)	0.94(25)	2.67(3.00)	1.03(51)