

Overfitting?

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The small number of data points could be a problem.

If there is a clear and consistent simple rule that works well for the training set –

- e.g. "All and only those who got over 60% on Non-Sym Al become millionaires, forget all the other courses as they are irrelevant"
- -- then it might be reasonable to trust this.

But if the Black Box generates really complex rules involving scores on many courses, this may well be over-fitting the data.

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Training and Test data

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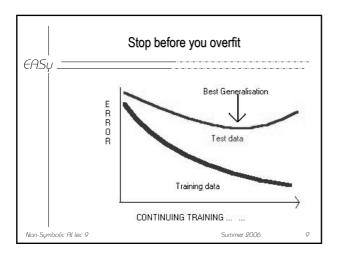
The standard way to check for overfitting is to split the data into a training set and a test set.

Train the Black Box (... whatever method this may be ...) on the training set, and then see how well it generalises to the unseen test data.

If there is a risk of overfitting, then the longer you train on the training data, the better the fit on the training data will be – but very likely at some stage the generalisation to test data will get worse.

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Calculating the errors

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Errors, on either training or test data, depend on the difference between predictions (the actual output of the Black Box prediction machine, the ANN) and te known Target values.

Guessing 1.2 too high, or 1.2 too low usually counts as equally bad.

So the usual measure of errors is Sum Squared Errors

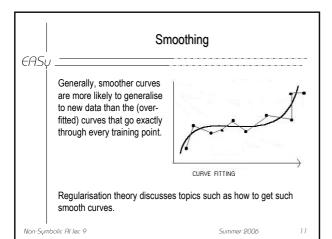
So over all the M members of a test set, the error measure will be

$$SSE = \sum_{i=1}^{i=M} (T_i - O_i)^2$$

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Regularisation

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One method of 'encouraging' an ANN to produce smoother curves is to avoid lots of big positive or big negative weights – they are the ones that tend to produce jagged, non-smooth curves.

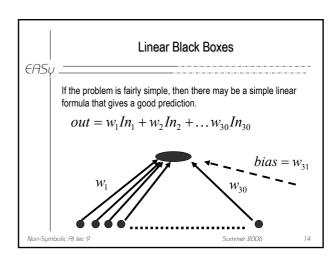
A good trick for doing this is weight-decay.

Introduce an extra routine into your program code, so that after every set of weight changes (through eg backprop) **all** the weights are decreased in (absolute) value by eg just 1%.

Then if the algorithm 'has a choice' between producing jagged curves or smooth ones, it will inevitably tend to opt for the smoother curves.

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Too little data? EASU Back to the train/test approach for avoiding over-fitting. That requires you to keep some part of the dataset back for testing, to check for generalisation. But if you only have 20 items of data anyway, dividing these into 2 parts makes the training data set even smaller. This is often a serious problem.



Linear

So a single-layer perceptron could handle this.

Note that if you have 30 weights to discover (or 31 if you add a bias term), and only 20 data points, then there will be many different possible **exactly accurate** formulae (or Black Boxes).

$$eqn1...1.0 = 0.6w_1 + 0.3w_2 + ... + 0.7w_{30} + w_{31}$$
......

 $eqn20...0.0 = 0.5w_1 + 0.55w_2 + ... + 0.65w_{30} + w_{31}$

20 simultaneous equations in 31 variables, to be solved.

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Linear (ctd)

Basically, if you have **N**=31 parameters to find (weights + bias in a

many of which will not generalise ...)

feedforward ANN, or formula as before), then

If you have less than **N** equations (less than **N** examples in your training set) there are loads of possible 'exact' solutions (...

□ If you have exactly **N** eqns there is 1 'exact' solution (and math techniques can find it, you don't need ANNs)

☐If there are more than **N** eqns (datapoints – CSAI students) then probably there is not an exact linear solution.

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Non-linear Black Boxes

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A linear Black Box is something relatively simple like:

"Chance of becoming a millionaire = 2.0 $^{\circ}$ Non-Sym Al score minus 3.2 $^{\circ}$ Logic Prog score +0.5"

Otherwise rephrased as: $out = 2.0In_{12} - 3.2In_{17} + 0.5$

Non-linear means potentially much more complex formulae, like:-

$$y = 0.2x_1 - 3x_1^2 + 2x_1x_2 - x_3^{4.5} + \frac{x_6}{\sqrt{x_7}} - \log\left[2x_5 - \frac{x_4^3}{x_5}\right] + \dots$$

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But don't worry ...

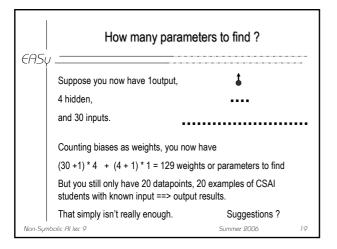
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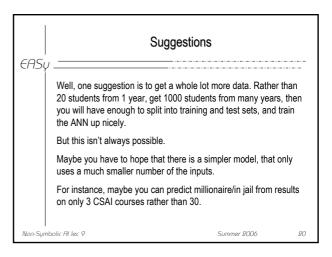
... because a multi-layer perceptron or ANN – and normally adding just 1 hidden layer will do --- with non-linear transfer functions (the sigmoids) can do a pretty good job of making a Black Box that reproduces **any** such complex formula.

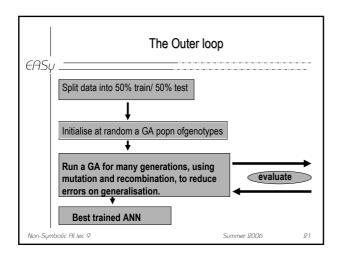
Provided that you have enough hidden nodes, and can find the right weights through a learning algorithm such as backprop.

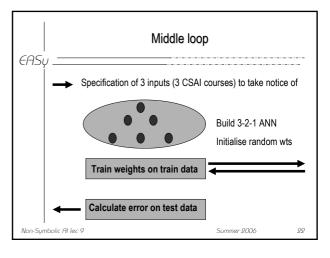
Still a few problems, though.

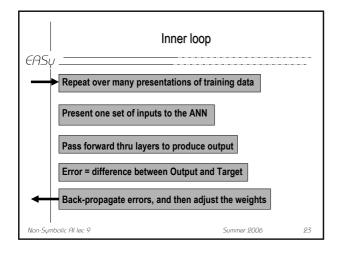
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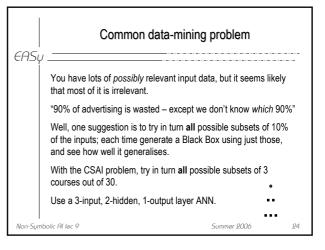












Smaller ANN This smaller ANN now has only (3+1)*2 +(2+1)*1 = 10 weights to learn, so we might have a chance even with only 20 or so training data. We could split this into 10 training data, 10 test data. Then for each selection of 3 courses (from 30): Build a 3-2-1 ANN Train on the training data Test on the test data

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Compare all the possibilities So now we will find that for many subsets-of-3 courses, we get lousy predictions of millionaire/in jail (for the previously unseen test data). But hopefully some of them will generalise well – and we can pick out the best generaliser. Then we will have two successes: Then most relevant 3 courses to consider (ignore the rest!) And the non-linear combination of the scores on those 3 courses, that combine to give a good prediction.

A problem

There is at least one problem with all this method – anyone spot it?

We are going to have to do lots of choices of 3 subsets out of 30, and then do a whole neural network training routine each time.

How many of these will there be?

30*29*28/6 = 4,060 = rather a lot

Can we cut this down? -- Yes!

Use a Genetic Algorithm

There is a search space of thousands of subsets-of-3, and a ready-made fitness function for any one of them –
--- namely the Error on trying to generalise to test data.
(This is the kind of fitness-function one tries to make as small as possible).

So why not use a Genetic Algorithm to search through various possible sets-of-3 – and hopefully we can find the ideal set-of-3 with much less than exhaustive search of all the possibilities.

Genetic encoding

There are several different possible ways to genetically encode possible solutions.

A genotype must specify 3 out of the 30 possibilities. One simple way would be this:

Genotype[0] = 5 13 27

Genotype[1] = 11 17 29 etc etc

Then a mutation would change any selection to a new number in range 1-30

But problems ...

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Firstly, a mutation might produce a genotype 5 13 13
Secondly, recombination between 2 parents might also produce 5 13 13
Where this is now a selection of 2 different, rather than 3 different numbers. Solutions?
One solution is to put special code in the program, so as to prohibit mutations or crossovers that produce such results.

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