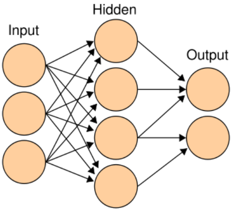
Neural Networks: Architecture Selection

11 March 2020

Architecture Selection

How many layers? How many neurons? How many weights?



- Occam's razor: the simplest network is always the best

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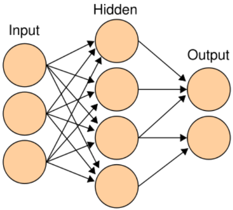

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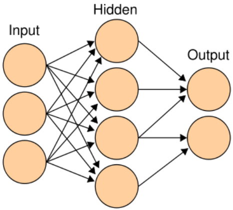

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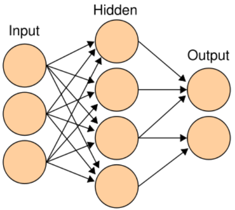

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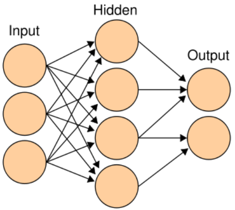

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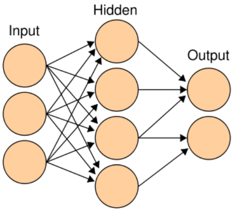

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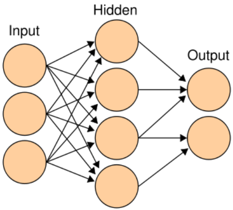

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  - Input/output dimensionality
  - Complexity of input-output relationship (function)

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Making guesstimates based on the number of data patterns

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- If the number of patterns is the same as the number of parameters, we might as well do k-nearest-neighbour classification (no learning)

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   - Pyramidal structures (# neurons reducing from layer to layer) have shown good generalisation performance

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  - Instead of geting out of local minima, gradient descent needs to get over multiple saddle points
  - Saddle points are easier to deal with than local minima!

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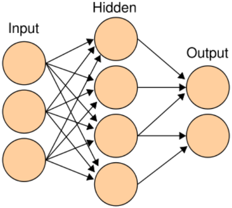

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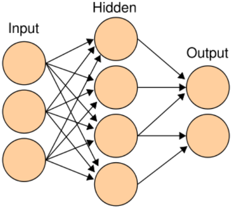

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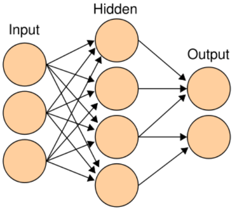

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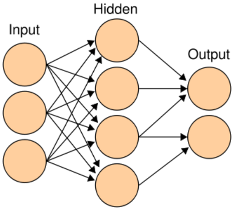

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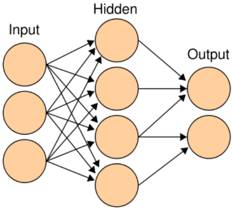

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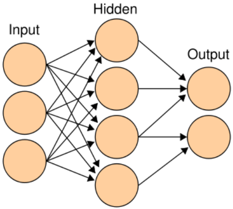

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  - Regularisation: minimise not only the error, but also the complexity

Regularisation

Penalizing complexity

- Add a penalty term to the objective function:
  - $E_{NN} = E + \lambda E_p$
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- Weight elimination:
  - $E_p = \sum_{i=1}^{W} \frac{w_i^2 / w_0^2}{1 + w_i^2 / w_0^2}$
  - w_0 determines the "significance" of weights
  - $|w_i| >> w_0$ => high complexity, penalize more
  - $|w_i| << w_0$ => low complexity, penalize less

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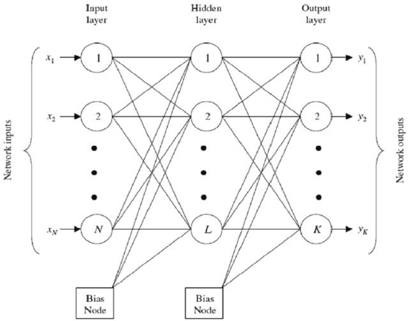
- How do we choose λ?
  - Cross-validation
  - Make it adaptive?

Regularisation and the Bias Weights



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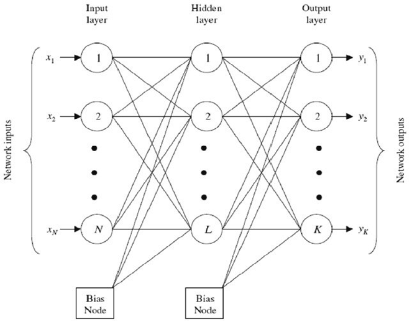

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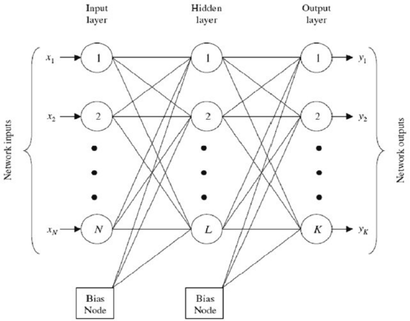

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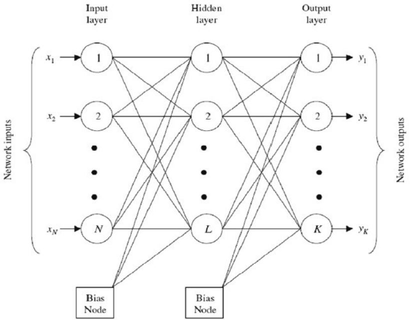

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- In practice, we usually **do not** regularise the bias weights
- Regularising biases may cause underfitting

Regularisation

"Dropout: A Simple Way to Prevent Neural Networks from Overfitting", Srivastava et al. 2012

Dropout: a new form of regularization

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- Can be combined with other regularisation methods

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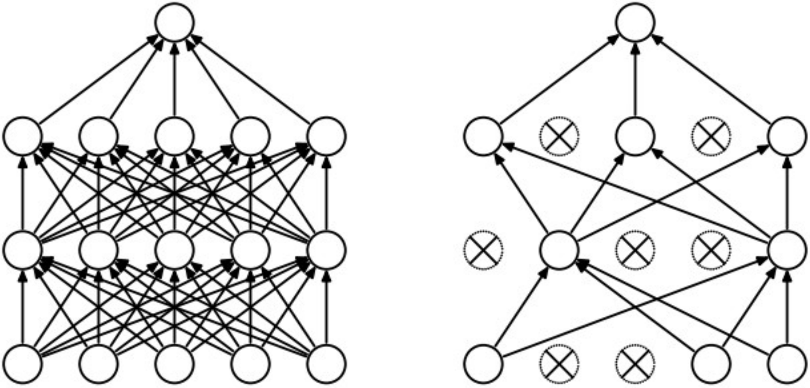

(a) Standard Neural Net (b) After applying dropout.

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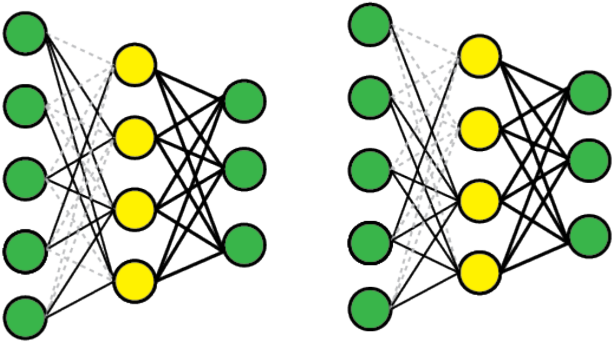
"A motivation for dropout comes from a theory of the role of sex in evolution (Livnat et al., 2010). Sexual reproduction involves taking half the genes of one parent and half of the other, adding a very small amount of random mutation, and combining them to produce an offspring. The asexual alternative is to create an offspring with a slightly mutated copy of the parent's genes. It seems plausible that asexual reproduction should be a better way to optimize individual fitness because a good set of genes that have come to work well together can be passed on directly to the offspring. On the other hand, sexual reproduction is likely to break up these co-adapted sets of genes, especially if these sets are large and, intuitively, this should decrease the fitness of organisms that have already evolved complicated coadaptations. However, sexual reproduction is the way most advanced organisms evolved."

Regularisation

Dropconnect: a generalisation of Dropout

You can also “disable” weights rather than neurons:



Essentially, we train an ensemble that looks like a single NN

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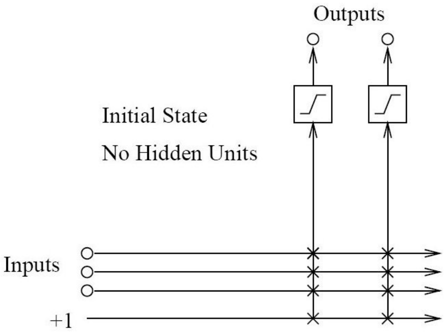
- Start with just a few neurons, add more when stagnation occurs
  - The NN contains a working model when a new neuron is added => integrating the new neuron may slow down training
  - How do we decide when to add a neuron, and when to stop growing?
  - How do we expand this to adding layers?

Cascade Correlation NNs

Goal: Minimial effective architecture, easy training. Fahlman & Lebiere, 1990.



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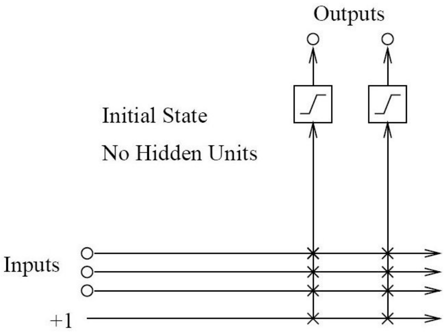

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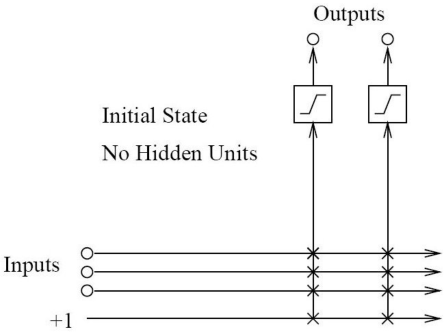

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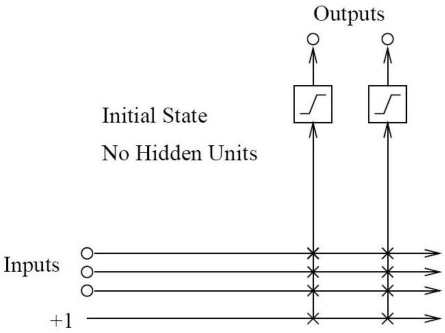

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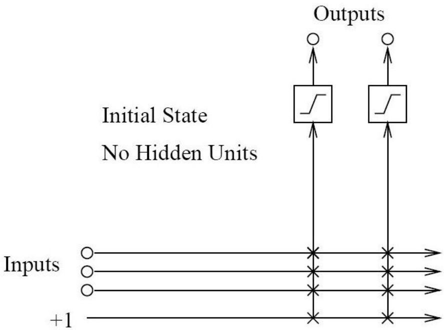

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- If the accuracy after training is unacceptable, a single hidden neuron is added

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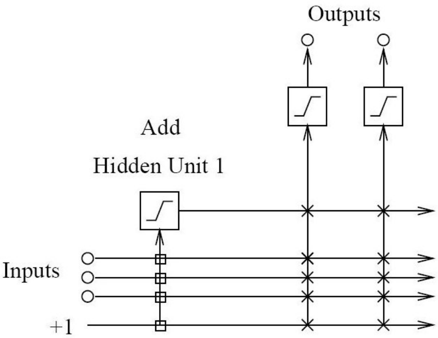

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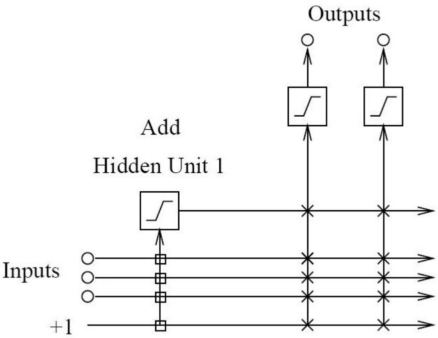

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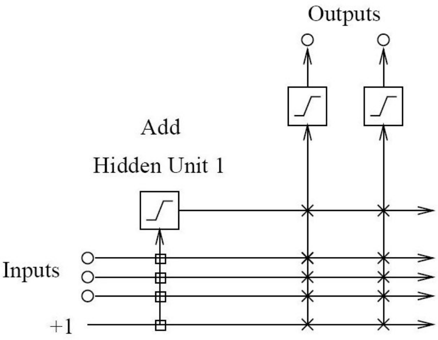
Cascade Correlation NNs

Goal: Minimial effective architecture, easy training



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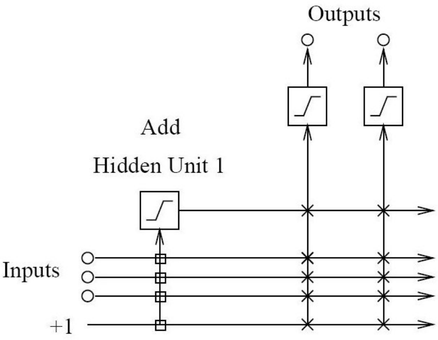

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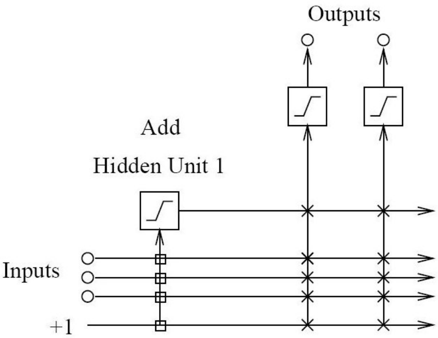
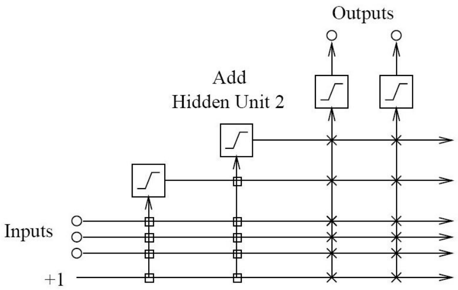


- All previously trained connections remain
- All inputs are connected to the hidden neuron
- Hidden neuron is connected to all output neurons
- Hidden neuron's input weights are adjusted to maximize covariance between the new neuron's output and the NN error
- The input weights are then frozen, and only the output weights are trained

Cascade Correlation NNs
Goal: Minimial effective architecture, easy training



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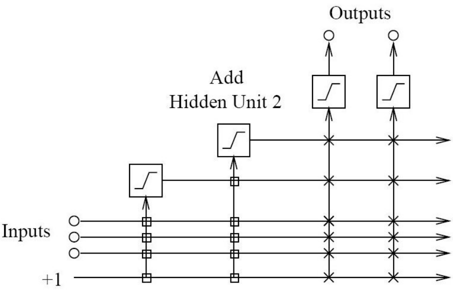

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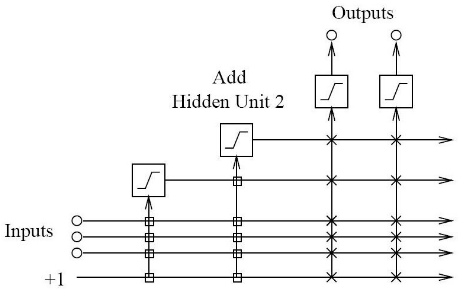

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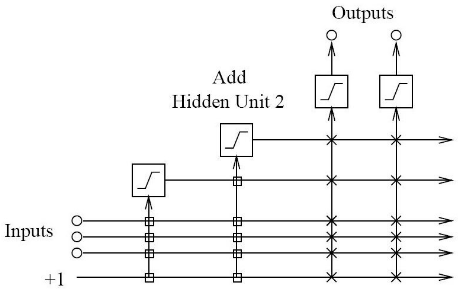

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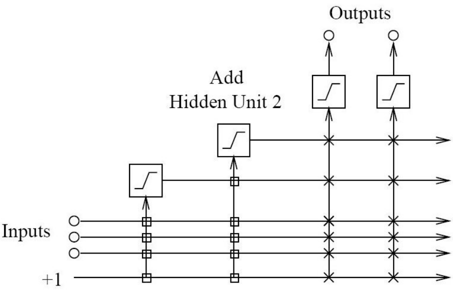

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- We always deal with only a single layer of modifiable weights

Neural Network Construction

Evolutionary approach

- Optimise the weights and/or the architecture using a genetic algorithm

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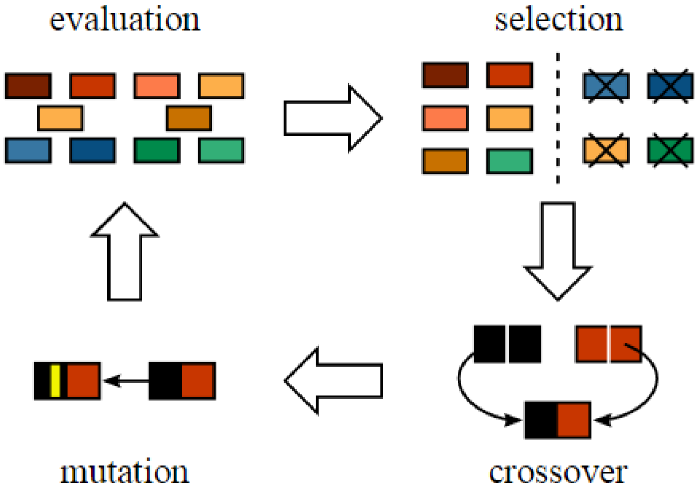
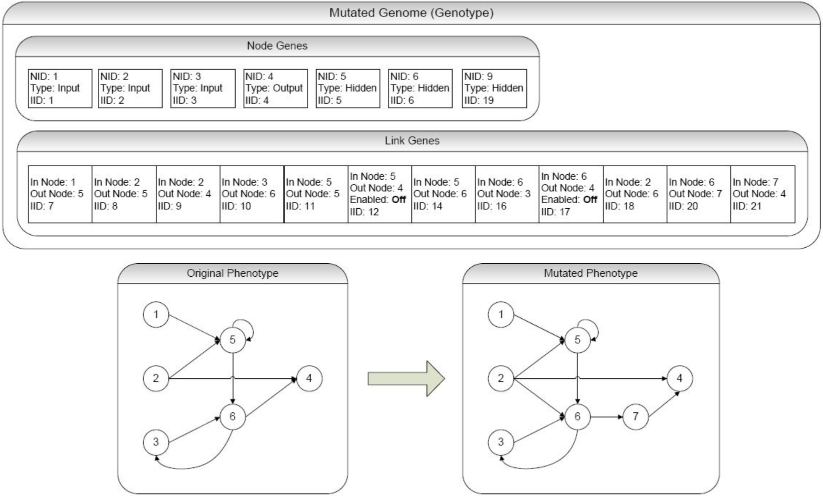
- Make different architectures compete for survival
- Assign higher fitness to smaller architectures

Genetic Algorithms in a Nutshell



Neural Network Construction

NEAT: NeuroEvolution of Augmenting Topologies



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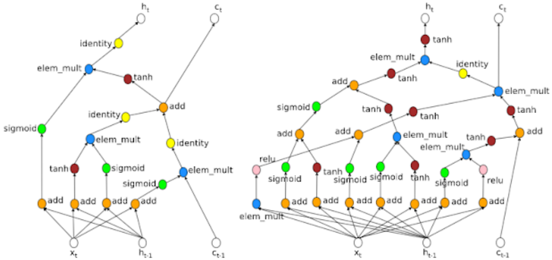
  - The research is ongoing!



Neural Network Pruning

To grow or to prune?

Applying Occam's Razor

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Neural Network Pruning

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Neural Network Pruning

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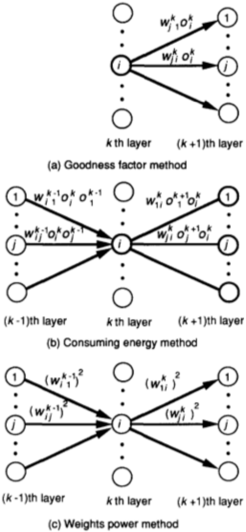
- And a lot of potential for an over-fit?..

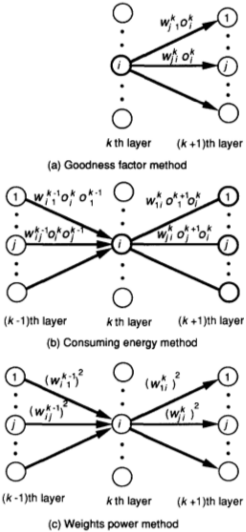
Neural Network Pruning



Intuitive pruning

- Determine the “active” neurons, remove inactive ones

Neural Network Pruning



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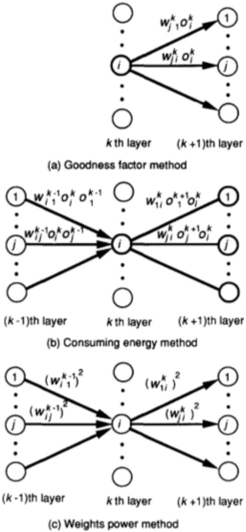

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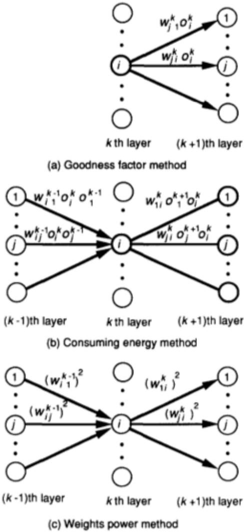

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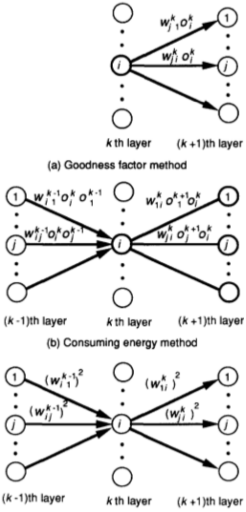

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- Weight magnitude pruning: remove small weights

Neural Network Pruning

Information Matrix pruning

- Fisher information: a way of measuring the amount of information that an observable random variable X carries about an unknown parameter θ upon which the probability of X depends.
  - $I = \frac{1}{P}\sum_{p=1}^{P} \frac{\partial f_{NN}}{\partial w}(\frac{\partial f_{NN}}{\partial w})^T$ - approx. information matrix
  - Calculates the covariance of the weights
  - Captures curvature, just like the Hessian
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- Principal Component Analysis (PCA): prune parameters (weights) that do not account for data variance
- All of these techniques do not scale very well to large NNs

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Hypothesis Testing

- Use statistical tests to calculate the significance of weights/hidden units
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- Assume that weights are $\approx$ normally distributed
  - Remove the weights that are in the distribution tails

Neural Network Pruning

Sensitivity analysis pruning

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  2. Train until a reasonable solution is obtained
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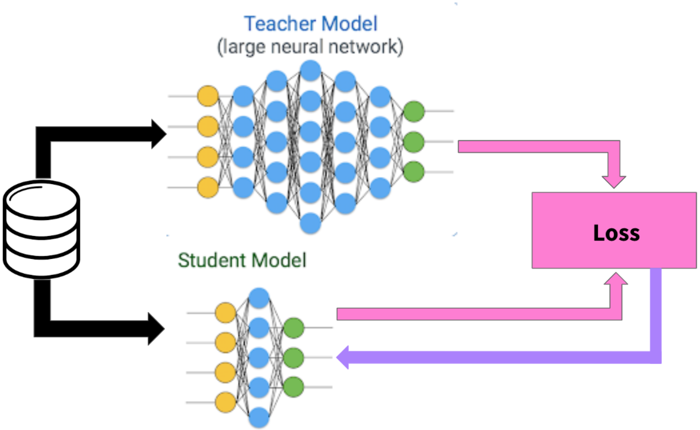
- Hessians are expensive to calculate

Neural Network Knowledge Distillation

Alternative to pruning: use a large NN to train a smaller NN.



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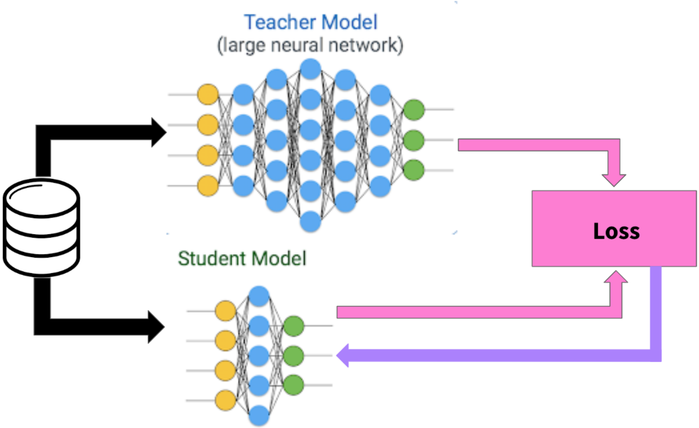

How do we ensure that the students learns from the teacher?

The End

- Questions?
- Next lecture: Deep Learning