

Preventing Overfitting in Neural Networks



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Overfitting

- The training data contains information about the regularities in the mapping from input to output. But it also contains noise
 - The target values may be unreliable.
 - There is **sampling error**. There will be accidental regularities just because of the particular training cases that were chosen.
- When we fit the model, it cannot tell which regularities are real and which are caused by sampling error.
 - So it fits both kinds of regularity.
 - If the model is very flexible it can model the sampling error really well. **This is a disaster.**

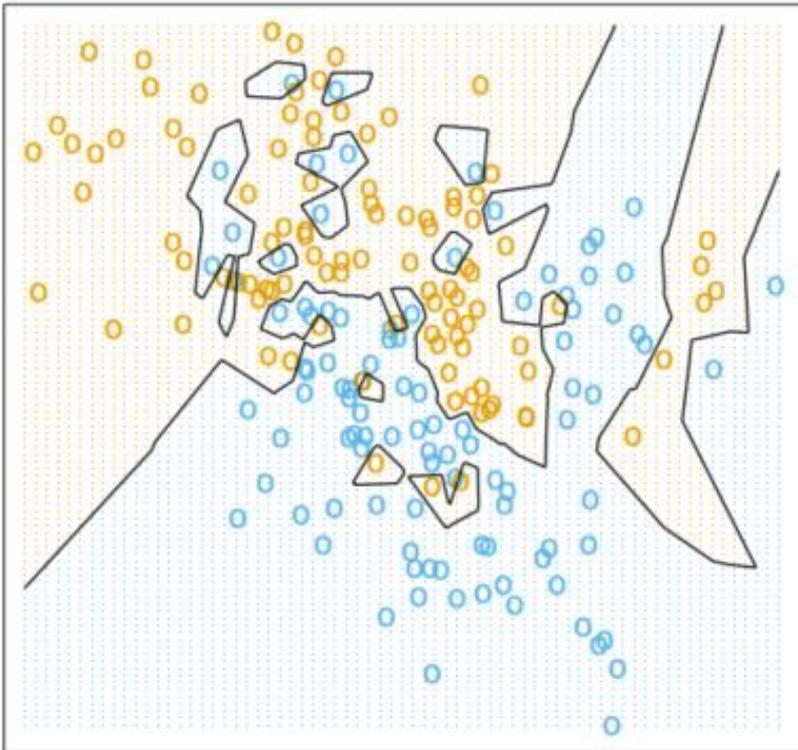
Preventing overfitting

- Use a model that has the right capacity:
 - enough to model the true regularities
 - not enough to also model the spurious regularities (assuming they are weaker)
- Fitting curves in 2D:
 - Only fit lines, not higher-degree polynomials (example on the board)
 - Only fit quadratics, not higher degree polynomials

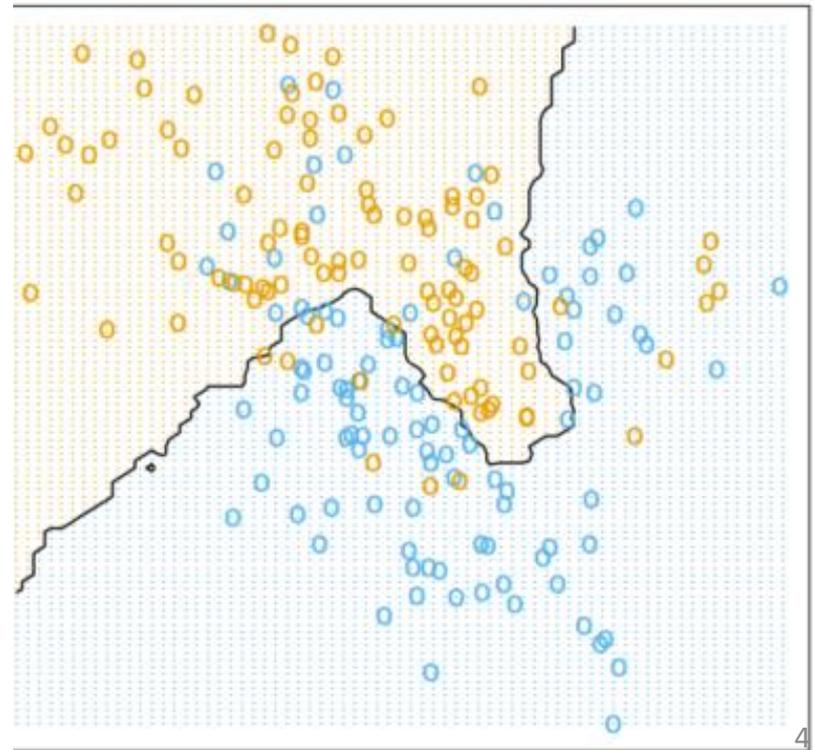
Reminder: Nearest Neighbours

- More nearest-neighbours \rightarrow less capacity
 - More complicated decision surfaces are not possible

1-Nearest Neighbor Classifier



15-Nearest Neighbor Classifier



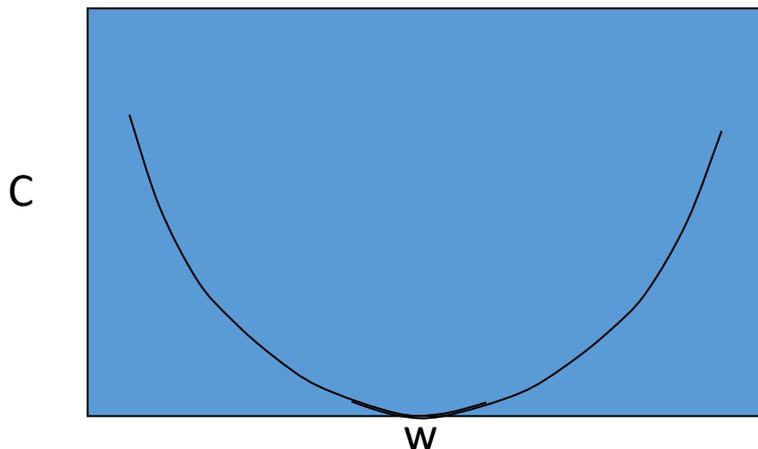
Limiting the Capacity of a Neural Network

- Limit the number of hidden units.
- Limit the size of the weights.
- Stop the learning before it has time to overfit.

Weight Decay: Limiting the size of the weights

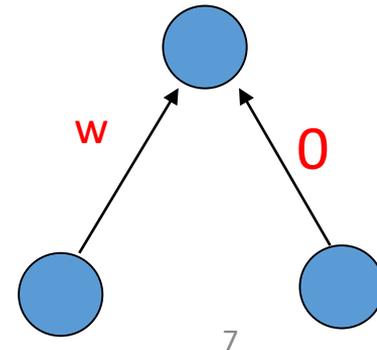
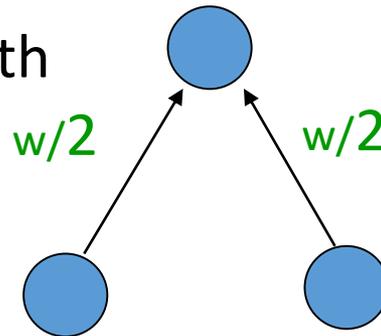
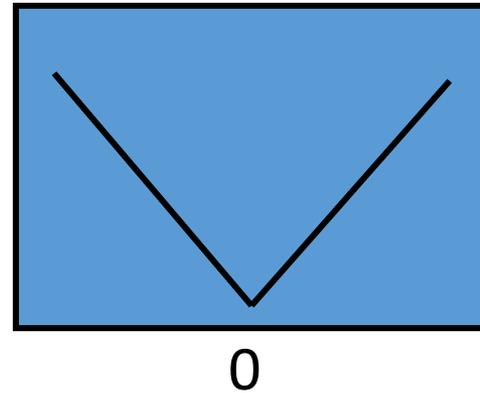
- Weight-decay involves adding an extra term to the cost function that penalizes the squared weights.
 - Keeps weights small unless they have big error derivatives.

$$cost_{WD} = cost + \frac{\lambda}{2} \sum_{i,j,k} (W^{(k,i,j)})^2$$
$$\frac{\partial cost_{WD}}{\partial W^{(k,i,j)}} = \frac{\partial cost_{WD}}{\partial W^{(k,i,j)}} + \lambda W^{(k,i,j)}$$



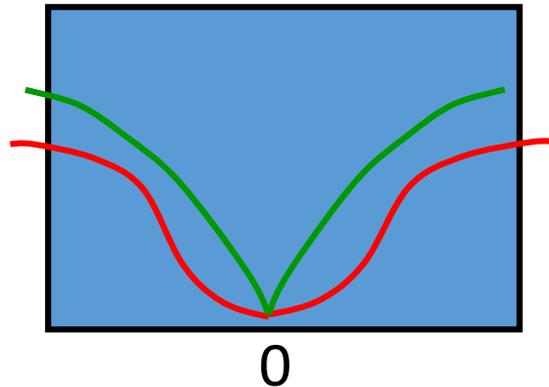
Other kinds of weight penalty

- Sometimes it works better to penalize the absolute values of the weights. (I.e., we penalized the L1 norm of the weights rather than the L2 norm)
- Sometimes leads to smaller test errors
- Makes some weights zero
- Compared to the square penalty, which would not tend to do that
- This is sometimes helpful with interpreting the features

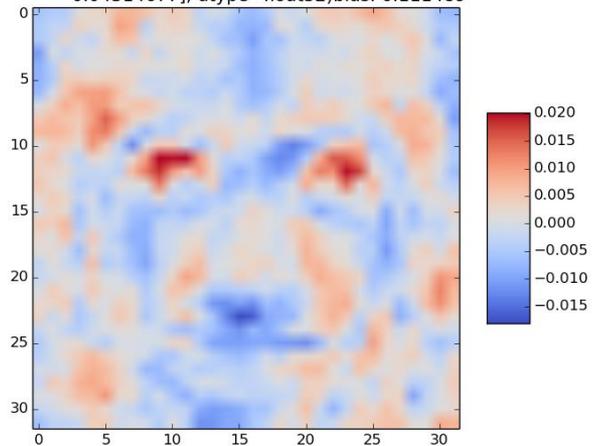


Another kind of Weight penalty

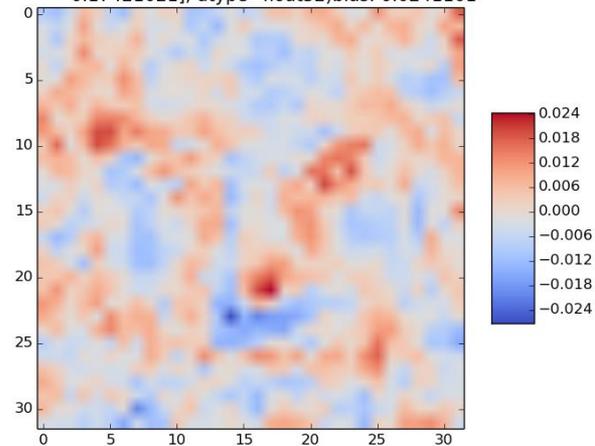
- Sometimes it works better to use a weight penalty that has negligible effect on **large** weights.
 - Some weights *need* to be large for the neural network to work correctly!



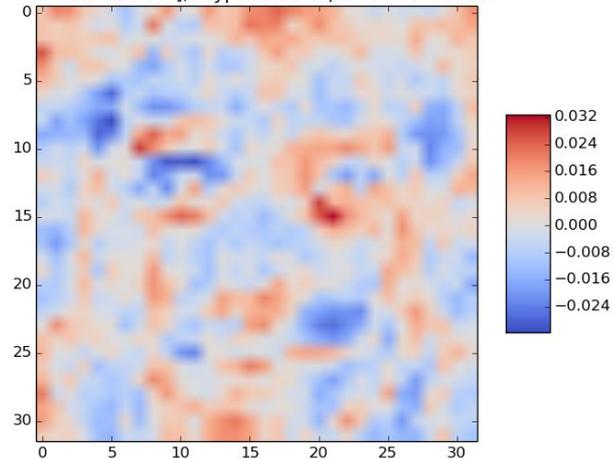
s: array([-0.1032981, -0.02623156, -0.04492124, 0.04031333, 0.09555781, 0.04314677], dtype=float32) bias: 0.111489



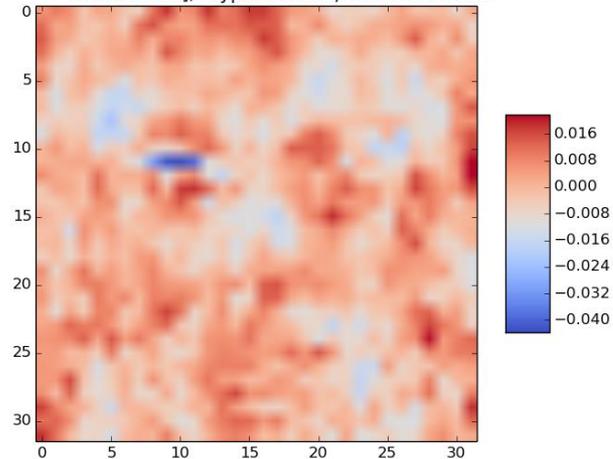
s: array([-0.05847707, 0.02304747, -0.04514949, -0.06355965, 0.02980999, 0.17421021], dtype=float32) bias: 0.0241101



s: array([0.03922304, 0.05484759, 0.06025519, 0.02333124, -0.26381665, 0.05690645], dtype=float32) bias: 0.00307018

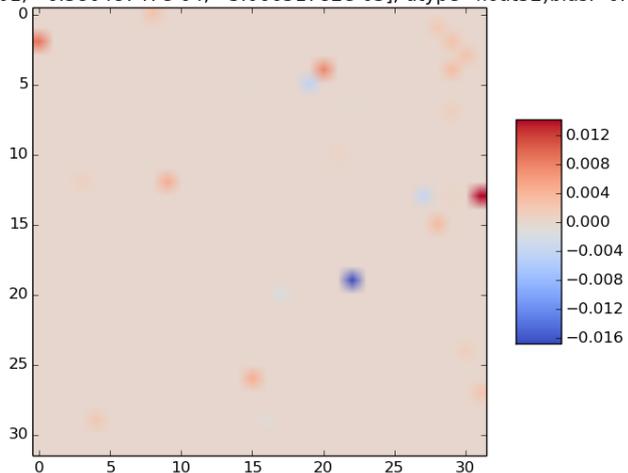


s: array([0.06559545, -0.14167207, 0.06504502, 0.01543506, -0.14153987, 0.06434423], dtype=float32) bias: 0.0287023

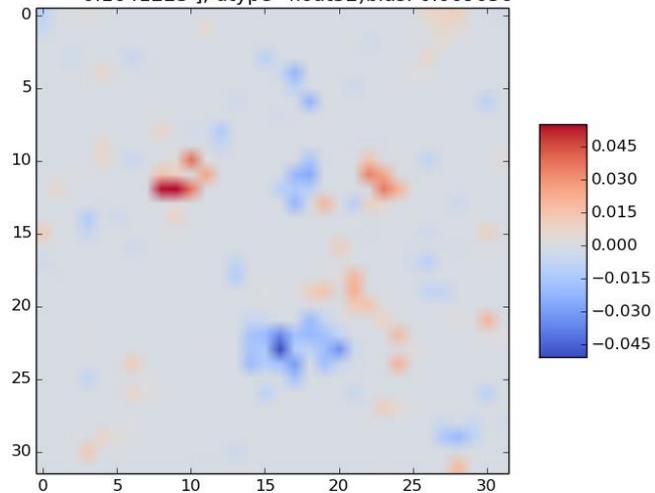


act = ['Gerard Butler', 'Daniel Radcliffe', 'Michael Vartan', 'Lorraine Bracco', 'Peri Gilpin', 'Angie Harmon']

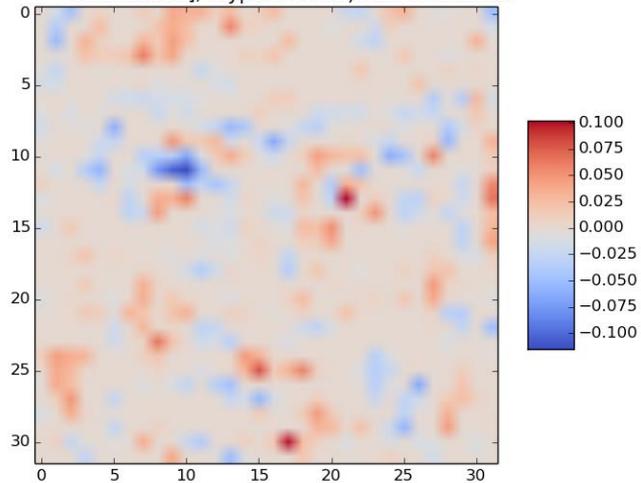
veights: array([3.24537978e-02, 1.03307003e-02, 1.28493230e-06,
50160e-01, -6.38048747e-04, -3.06651782e-05], dtype=float32)bias: -0.0576:



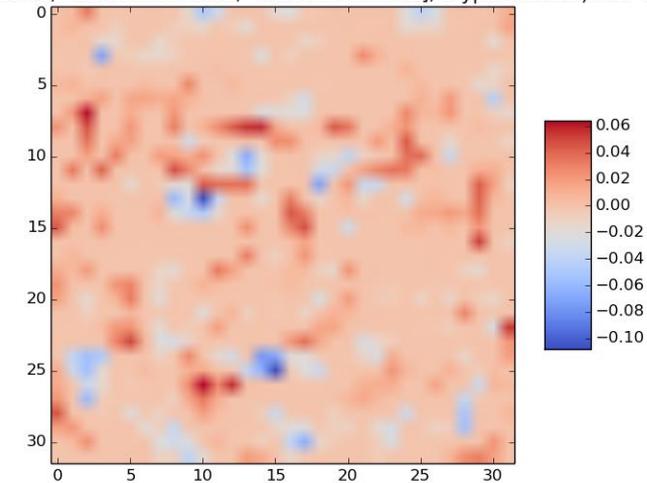
s: array([-0.29401857, -0.01724279, 0.00310232, 0.12068836, 0.0708182 ,
0.1641223], dtype=float32)bias: 0.069056



s: array([0.22145636, -0.6399256 , 0.13758378, 0.03394366, -0.37346393,
0.11635391], dtype=float32)bias: 0.0822999



veights: array([-1.94610730e-01, 3.78219485e-01, -6.13273799e-01,
55651e-04, 2.73087807e-02, -6.53727800e-02], dtype=float32)bias: 0.1243:



Weight decay and Bayesian Inference

- On the board

The effect of weight decay

- It prevents the network from using weights that it does not need (especially the L1 penalty).
 - This can often improve generalization a lot.
 - It helps to stop it from fitting the sampling error.
 - It makes a smoother model in which the output changes more slowly as the input changes. w
- For the L2 penalty, if the network has two very similar inputs it prefers to put half the weight on each rather than all the weight on one.

Deciding how much to restrict the capacity

- How do we decide which limit to use and how strong to make the limit?
 - If we use the test data we get an unfair prediction of the error rate we would get on new test data.
 - Suppose we compared a set of models that gave random results, the best one on a particular dataset would do better than chance. But it won't do better than chance on another test set.
- So use a separate **validation set** to do model selection.

Using a validation set

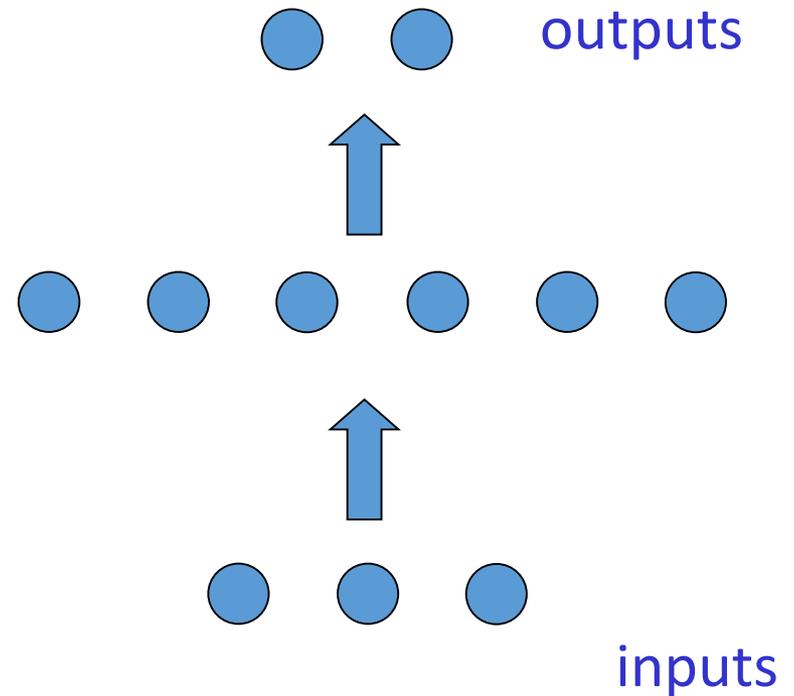
- Divide the total dataset into three subsets:
 - **Training data** is used for learning the parameters of the model.
 - **Validation data** is not used of learning but is used for deciding what type of model and what amount of regularization works best.
 - **Test data** is used to get a final, unbiased estimate of how well the network works. We expect this estimate to be worse than on the validation data.
- We could then re-divide the total dataset to get another unbiased estimate of the true error rate.

Preventing overfitting by early stopping

- If we have lots of data and a big model, its very expensive to keep re-training it with different amounts of weight decay.
- It is much cheaper to start with very small weights and let them grow until the performance on the validation set starts getting worse (but don't get fooled by noise!)
- The capacity of the model is limited because the weights have not had time to grow big.

Why early stopping works

- When the weights are very small, every hidden unit is in its linear range.
 - So a net with a large layer of hidden units is linear.
 - It has no more capacity than a linear net in which the inputs are directly connected to the outputs!
- As the weights grow, the hidden units start using their non-linear ranges so the capacity grows.



Combining networks

- When the amount of training data is limited, we need to avoid overfitting.
 - Averaging the predictions of many different networks is a good way to do this.
 - It works best if the networks are as different as possible.
- If the data is really a mixture of several different “regimes” it is helpful to identify these regimes and use a separate, simple model for each regime.
 - We want to use the desired outputs to help cluster cases into regimes. (But we don’t know how to do that in advance – need to train the network first)

Ways to make predictors differ

- Rely on the learning algorithm getting stuck in a different local optimum on each run.
 - A dubious hack unworthy of a true computer scientist (but definitely worth a try).
- Use lots of different kinds of models:
 - Different architectures
 - Different learning algorithms.
- Use different training data for each model:
 - **Bagging**: Resample (with replacement) from the training set: a,b,c,d,e -> a c c d d
 - **Boosting**: Fit models one at a time. Re-weight each training case by how badly it is predicted by the models already fitted.
 - This makes efficient use of computer time because it does not bother to “back-fit” models that were fitted earlier.