Deep Learning & Applied AI

Regularization, batchnorm and dropout

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- Explicit penalties.

- Implicit regularization.

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Any modification that is intended to reduce the generalization error but not the training error.

Goodfellow et al., "Deep Learning", MIT Press 2016

Weight penalties

$$\underbrace{\ell(\boldsymbol{\Theta})}_{\text{loss}} + \lambda \underbrace{\rho(\boldsymbol{\Theta})}_{\text{regularizer}}$$

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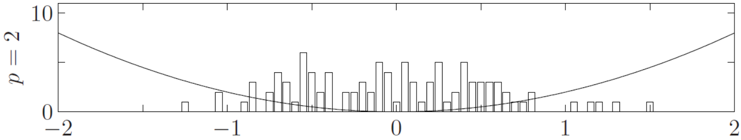
After training, the L_p magnitude of each weight reflects its importance.

L_2 vs L_1 penalties



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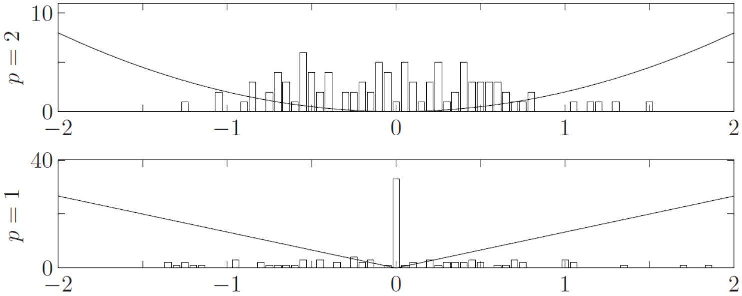

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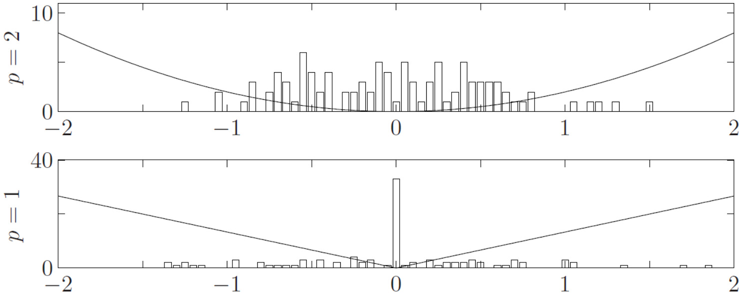

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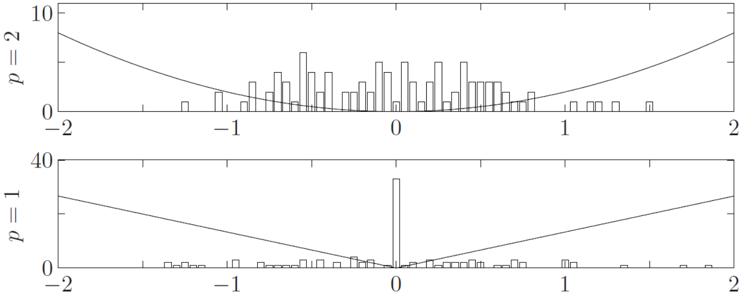

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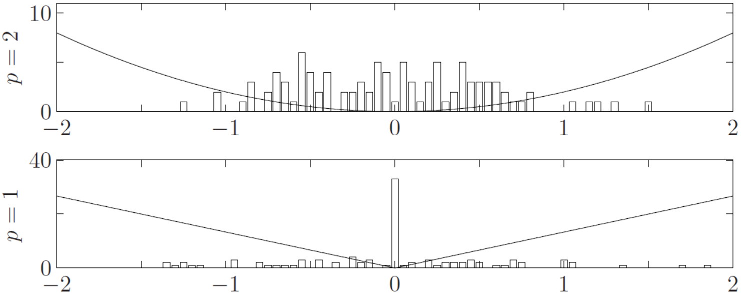
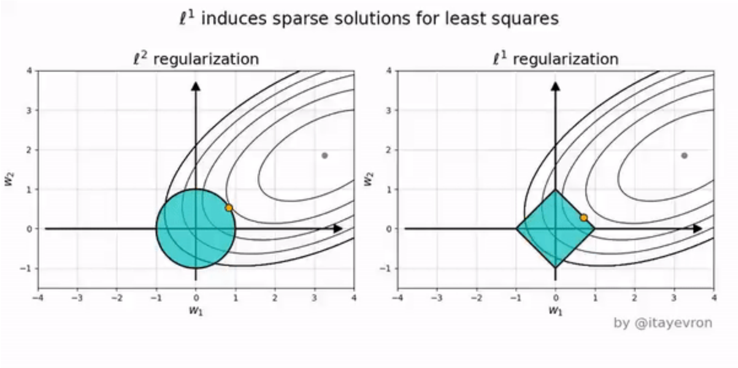


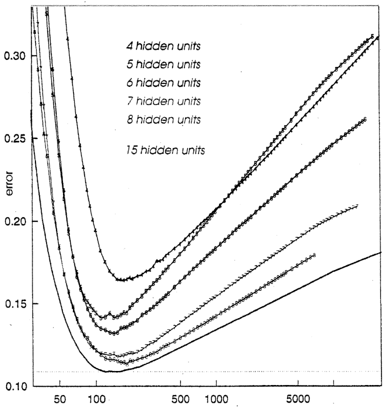
- Big reduction in $\|\mathbf{\Theta}\|_2$ if you scale down the values > 1
- Almost no reduction in $\|\mathbf{\Theta}\|_2$ for values < 1. Sparsity is discouraged!
- All the values are treated the same in $\|\mathbf{\Theta}\|_1$, no matter if they are > 1 or < 1. Any value can be set to zero, leading to sparse solutions.



Source code: `https://github.com/ievron/RegularizationAnimation/`

Detecting overfitting

Overfitting can be recognized by looking at the validation error:



Weigend, "On overfitting and the effective number of hidden units", 1993

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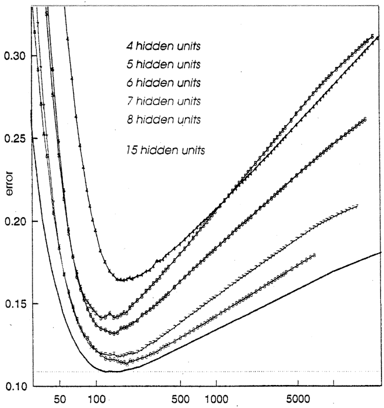
Overfitting can be recognized by looking at the validation error:

- Small networks can also overfit.



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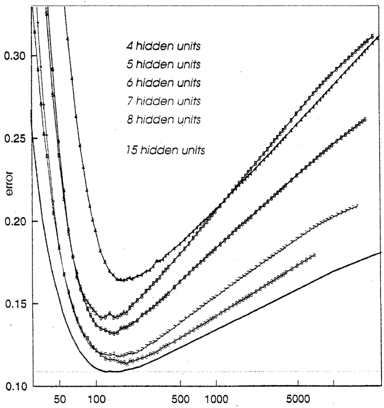

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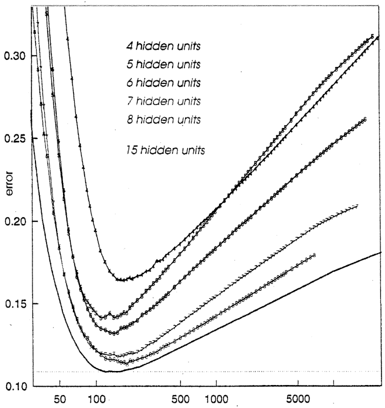
Detecting overfitting: Early stopping

Overfitting can be recognized by looking at the validation error:

- Small networks can also overfit.
- Large networks have best performance if they stop early.
- Early stopping: Stop training as soon as performance on a validation set decreases.



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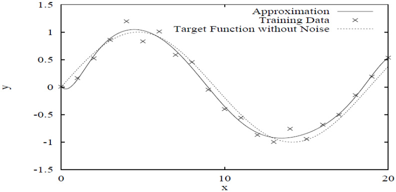
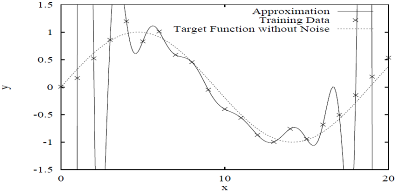
Many parameters $\neq$ overfitting

Typical overfitting with polynomial regression:



Order 10



Order 20

Caruana et al, "Overfitting in Neural Nets: Backpropagation, Conjugate Gradient, and Early Stopping", NIPS 2001

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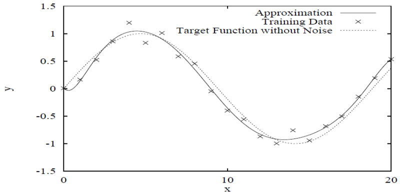
...but more MLP parameters not always lead to overfitting:



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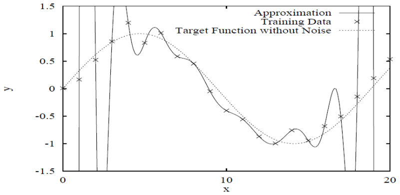

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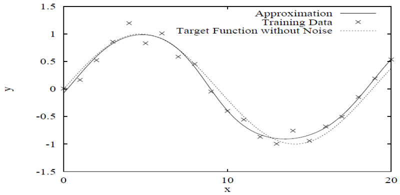
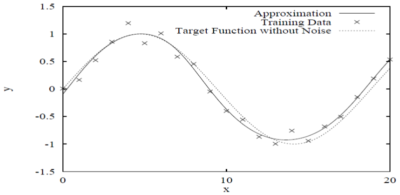


10 Hidden Nodes



50 Hidden Nodes

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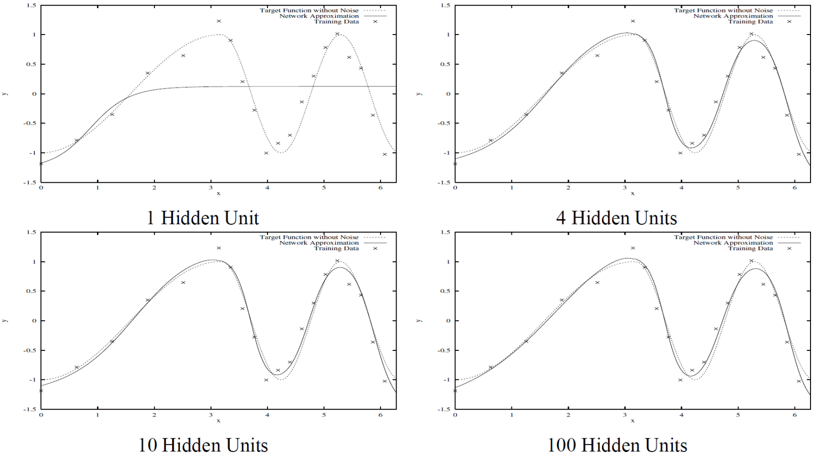
Good fit over all the different data regions:



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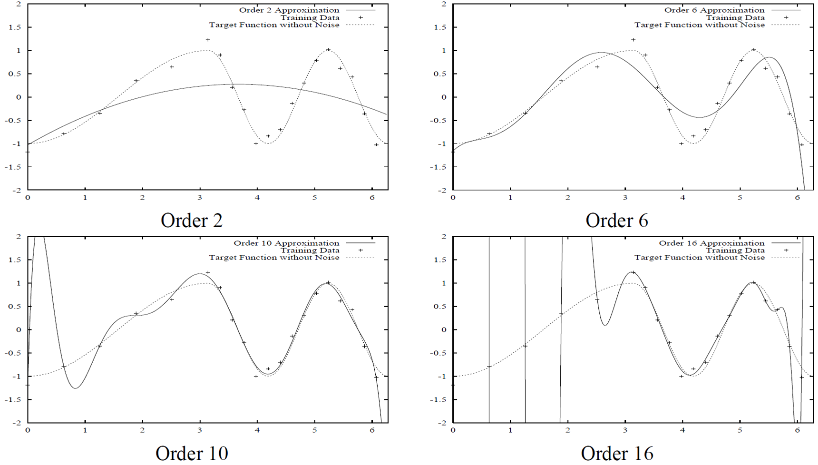
Overfitting as a local phenomenon

Overfitting is local and can vary significantly in different regions:



Order 2

Order 6

Order 10

Order 16

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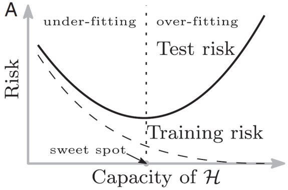
Double descent

U-shaped curve as a function of # network parameters:



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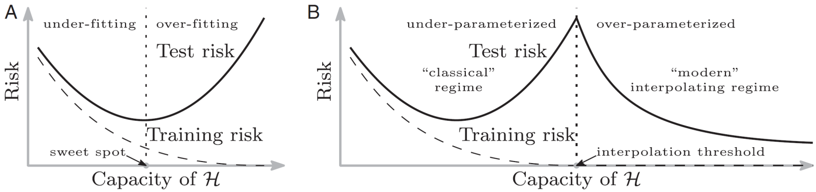

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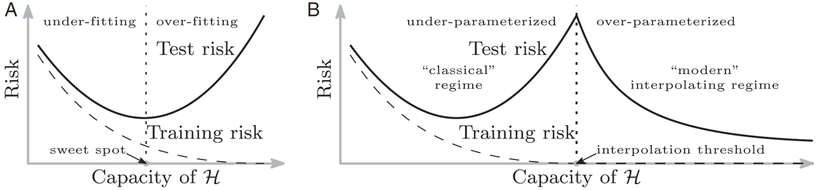

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"By considering larger function classes, which contain more candidate predictors compatible with the data, we are able to find interpolating functions that have smaller norm and are thus "simpler." Thus, increasing function class capacity improves performance of classifiers."

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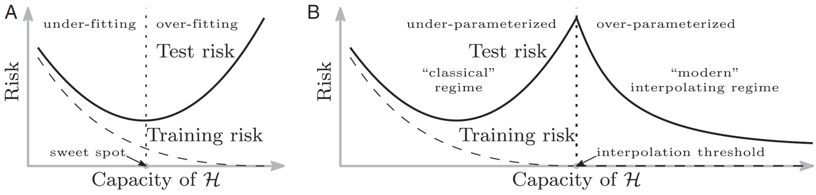

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The surprising fact is that SGD is able to find such good models.

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Early stopping

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Representational power grows with training time

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- Initialize with small weights.
- Simple hypotheses are considered before complex hypotheses.
- Training first explores models similar to what a smaller net of optimal size would have learned.

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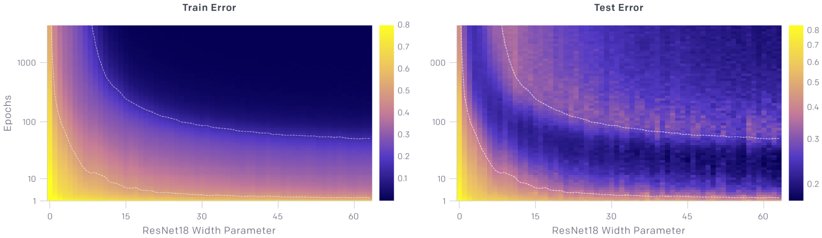
Epoch-wise double descent

There is a regime where training longer reverses overfitting.



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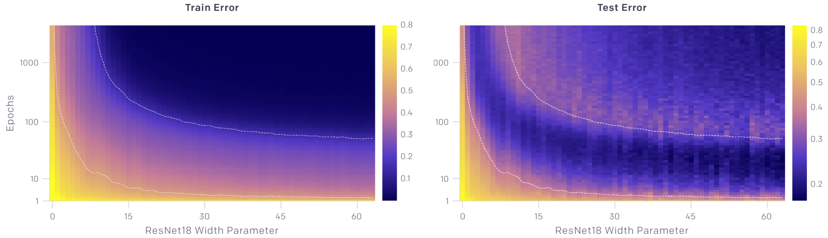

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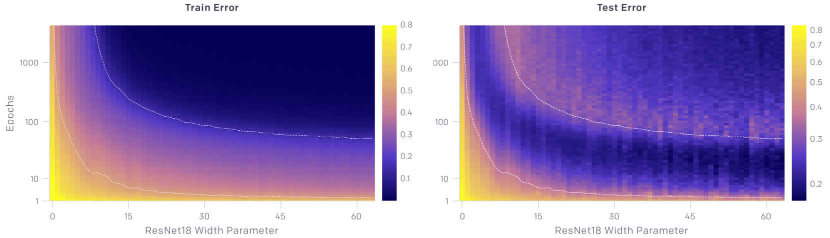

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For a fixed number of parameters, we observe double descent as a function of training time.

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Normalize the features by the statistics computed within the training set:

$$\hat{\mathbf{x}}^{(k)} = \mathrm{normalize}(\mathbf{x}^{(k)}, \mathcal{X})$$

where both $\mathbf{x}$ and $\mathcal{X}$ depend on $\mathbf{W}$.

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In particular, backprop will need the partial derivatives:

$$\frac{\partial}{\partial \mathbf{x}}\mathrm{normalize}(\mathbf{x}, \mathcal{X}), \qquad \frac{\partial}{\partial \mathcal{X}}\mathrm{normalize}(\mathbf{x}, \mathcal{X})$$

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Batch normalization: Transformation

For each dimension of $\mathbf{x}$, transform:

$$x_i \mapsto \frac{x_i - \mathrm{E}[x_i]}{\sqrt{\mathrm{var}(x_i)}}$$

where mean and variance are computed over the training set.

After the transformation, we get mean $= 0$ and var $= 1$.

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Furthermore, introduce trainable weights:

$$x_i \mapsto \gamma_i \frac{x_i - \mathrm{E}[x_i]}{\sqrt{\mathrm{var}(x_i)}} + \beta_i$$

These allow to represent the identity $x_i \mapsto x_i$, if that was the optimal thing to do in the original network.

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Batch normalization: Using mini-batches

Avoid analyzing the entire training set at each parameter update.

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1 \ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

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The batchnorm transformation makes each training example interact with the other examples in each mini-batch.

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Batch normalization: Properties

Typically, batchnorm is applied right before the nonlinearity:

$$\sigma(\mathbf{W}\mathbf{x} + \mathbf{b}) \quad \text{becomes} \quad \sigma \circ \mathrm{BN}_{\gamma,\beta}(\mathbf{W}\mathbf{x})$$

The bias can be removed, since it is ruled out by the mean subtraction.

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- The stochastic uncertainty of the batch statistics acts as a regularizer that can benefit generalization.

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- The stochastic uncertainty of the batch statistics acts as a regularizer that can benefit generalization.
- Batchnorm leads to more stable gradients, thus faster training can be achieved with higher learning rates.

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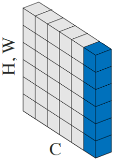

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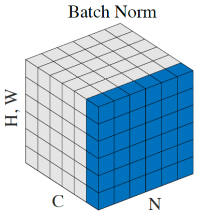

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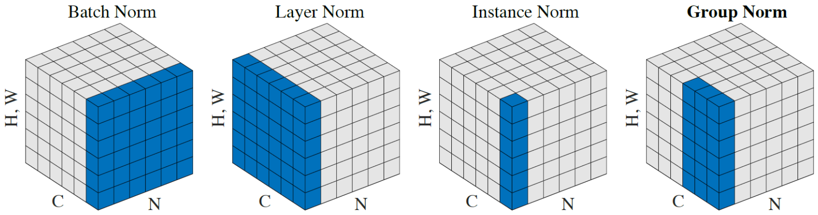

Wu and He, "Group normalization", ECCV 2018

Ensemble deep learning?

Assume you have unlimited computational power.

Train an ensemble of deep nets and average their predictions.

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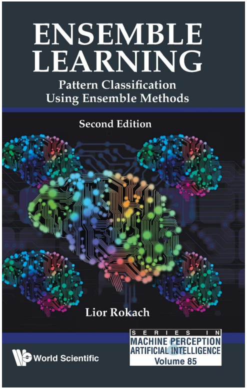
Most successful methods in **Kaggle** are ensemble methods.



Neal, "Bayesian Learning for Neural Networks", 1996

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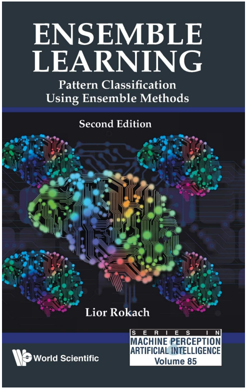
However, for deep nets this would come at a high computational cost.



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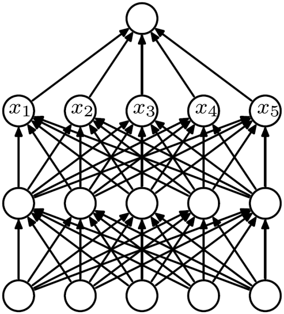
Dropout

$y = \sum_{i=1}^{5} w_i x_i$



2-layer fully connected

Dropout

Main idea: Parametrize each model in the ensemble by dropping random units (i.e. nodes with their input/output connections):

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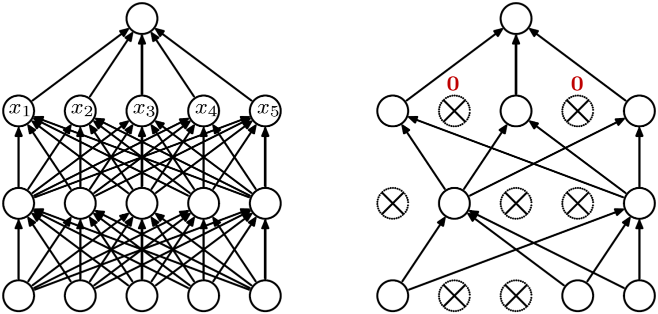

2-layer fully connected $\qquad$ after dropout

Srivastava et al, "Dropout: A Simple Way to Prevent Neural Networks from Overfitting", JMLR 2014

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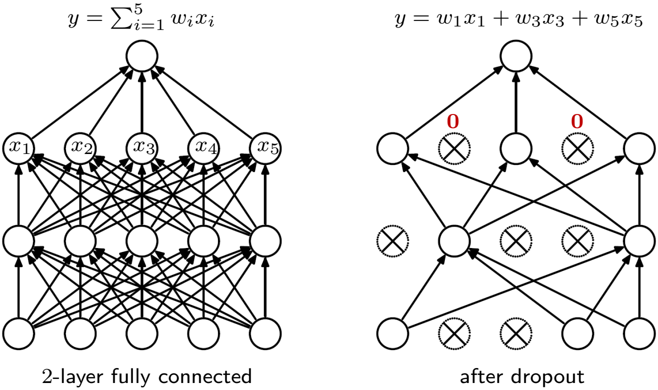

Crucially, all networks share the same parameters.

Srivastava et al, "Dropout: A Simple Way to Prevent Neural Networks from Overfitting", JMLR 2014

Dropout

Can be seen as sampling a network w.r.t. a probability distribution.

n nodes $\Rightarrow$ 2^n possible ways to sample them

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This is way too costly.

- **Training:** All the networks must be trained.
- **Test:** All the predictions must be averaged.

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Make it feasible by keeping one single network:

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  The ensemble is trained to convergence (e.g. with early stopping).

  The individual models are not trained to convergence.

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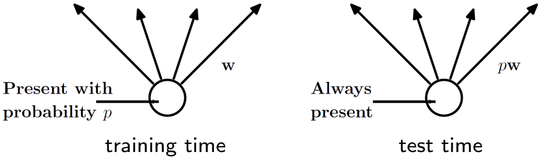

If a unit is retained with probability p during training (chosen by hand, even per layer), its outgoing weights are multiplied by p.

Srivastava et al, "Dropout: A Simple Way to Prevent Neural Networks from Overfitting", JMLR 2014

Dropout as an ensemble method

Dropout has two key features:

- It does bagging, i.e. each model is trained on random data.
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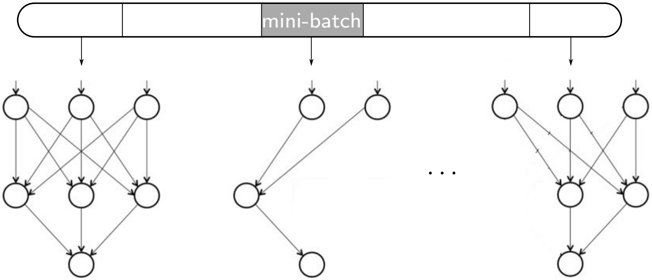

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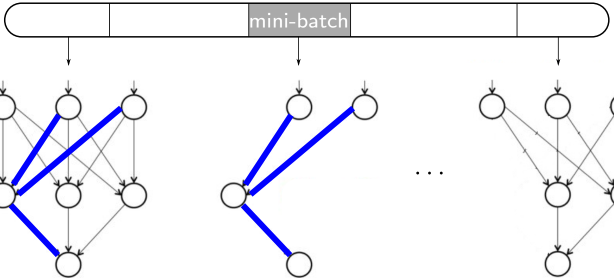

At each training step, the weight update is applied to all members of the ensemble simultaneously.

Dropout: Properties

In a standard neural network, weights are optimized jointly.

Co-adaptation: Small errors in a unit are absorbed by another unit.

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Some properties of dropout as a regularizer:

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- Typical choices: 20% of the input units and 50% of the hidden units.

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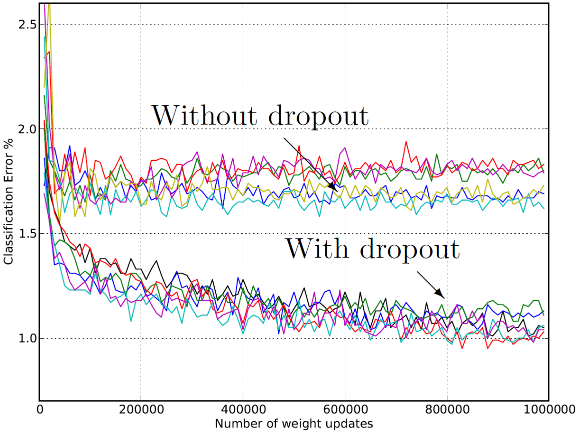

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Suggested reading

- All the references given throughout the slides.
- Interesting thread on the history of double descent:
  https://twitter.com/hippopedoid/status/1243229021921579010
- *Section 4.2.1* is a practical guide for batchnorm by the original authors:
  https://arxiv.org/pdf/1502.03167
- *Appendix A* is a practical guide for dropout by the original authors:
  http://jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf