Deep Learning & Applied AI

Regularization, batchnorm and dropout

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SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2024/2025 · April 14, 2025

Regularization

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

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

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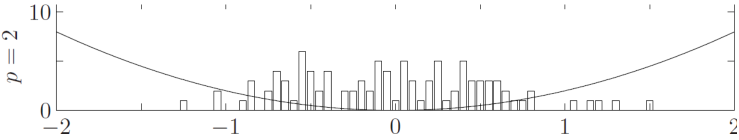
After training, the L_p magnitude of each weight reflects its importance.

L_2 vs L_1 penalties



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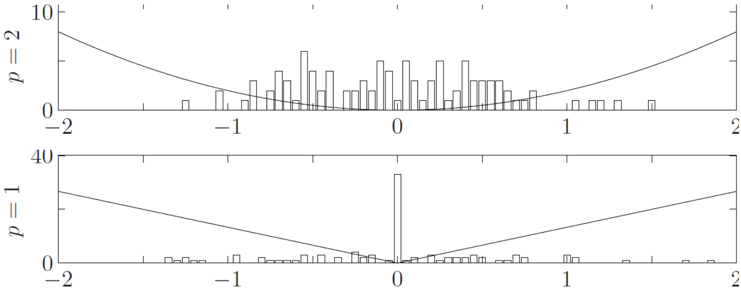

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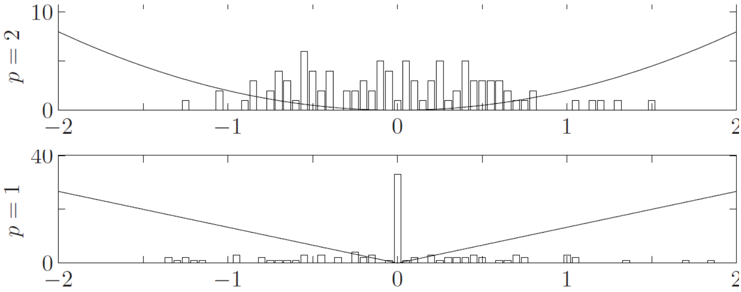

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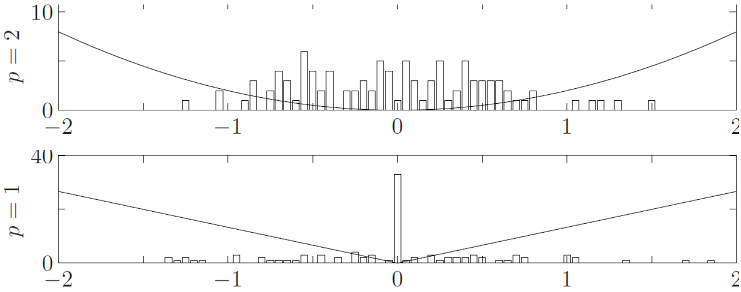

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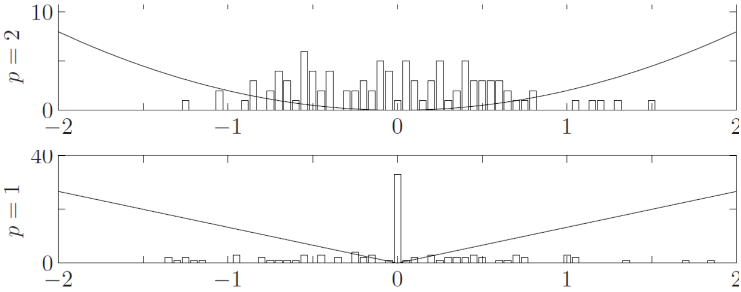
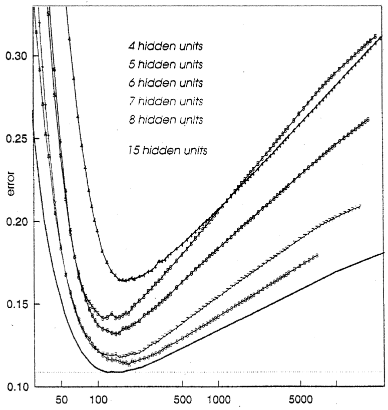


- Big reduction in $\|\mathbf{\Theta}\|_2$ if you scale down the values > 1
- Almost no reduction in $\|\mathbf{\Theta}\|_2$ for values < 1. Sparsity is discouraged!
- All the values are treated the same in $\|\mathbf{\Theta}\|_1$, no matter if they are > 1 or < 1. Any value can be set to zero, leading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

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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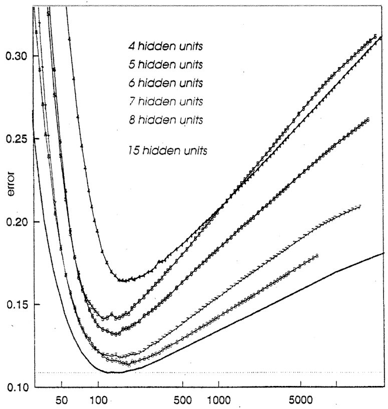

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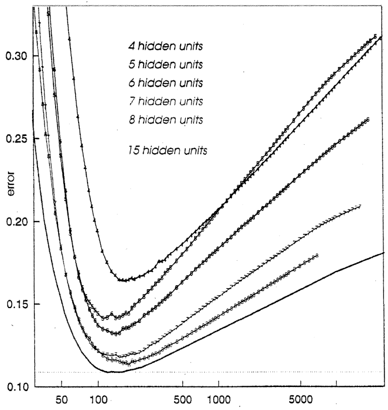

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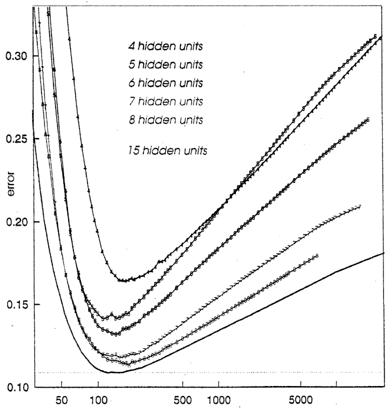
Detecting overfitting: Early stopping

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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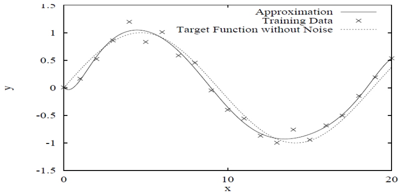
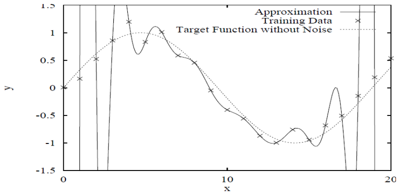
Many parameters $\neq$ overfitting

Typical overfitting with polynomial regression:



Order 10

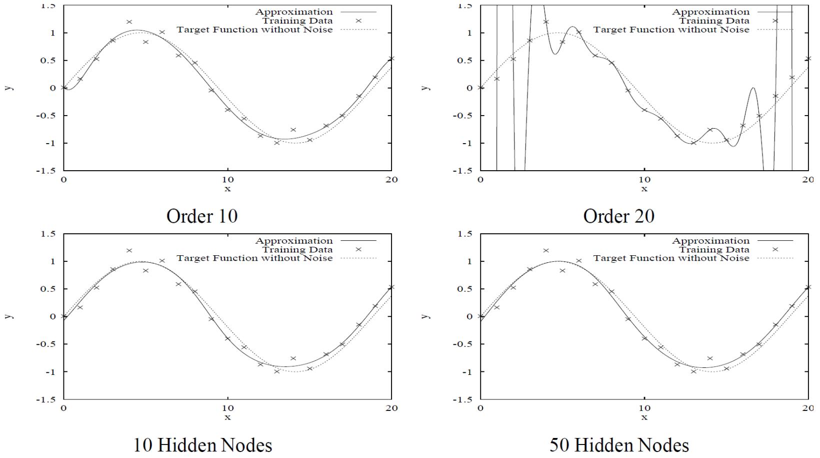


Order 20

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

Many parameters ≠ overfitting

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



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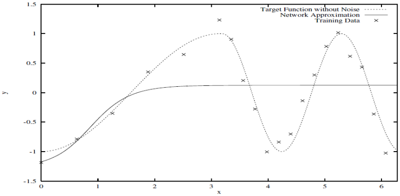
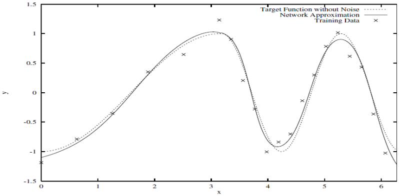
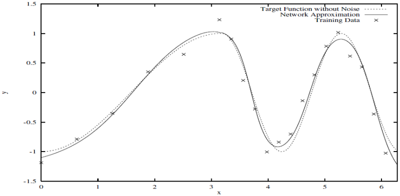
Good fit over all the different data regions:



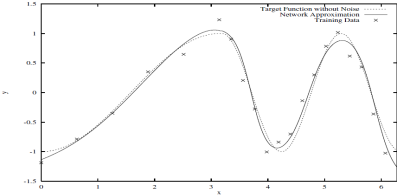
1 Hidden Unit



4 Hidden Units



10 Hidden Units



100 Hidden Units

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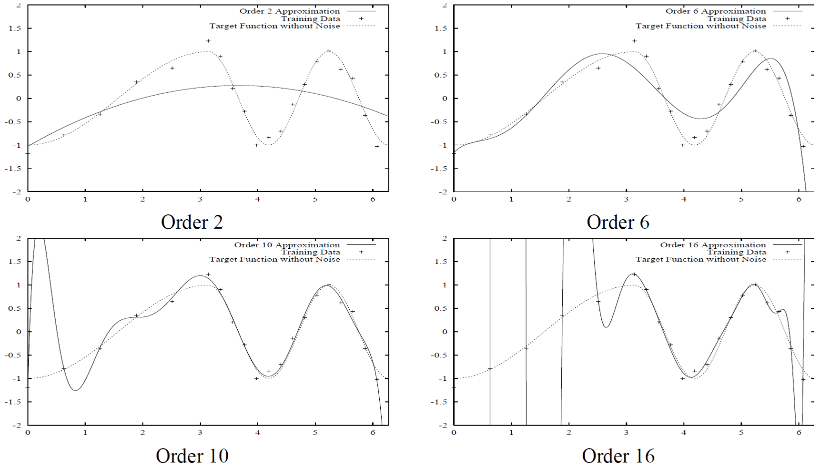
Overfitting as a local phenomenon

Overfitting is local and can vary significantly in different regions:



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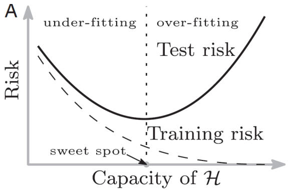
Double descent

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



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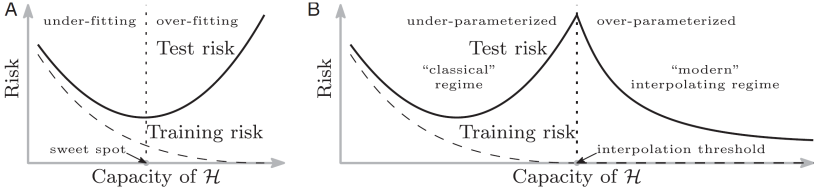

Interpolation: perfect fit on the training data.

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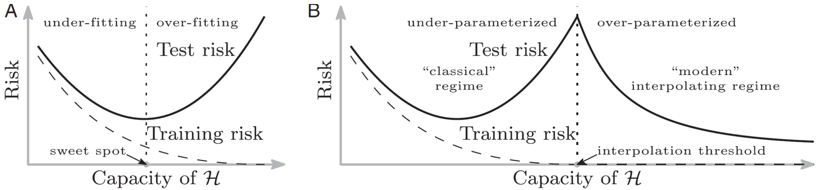

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"By considering larger function classes, which contain more candidate predictors compatible with the data, we are able to find interpolating functions that have smaller norm and are thus "simpler." Thus, increasing function class capacity improves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

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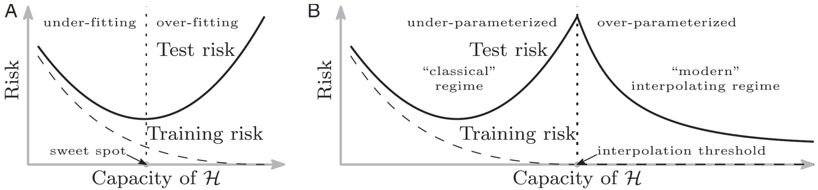

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What's surprising is that SGD finds such good models!

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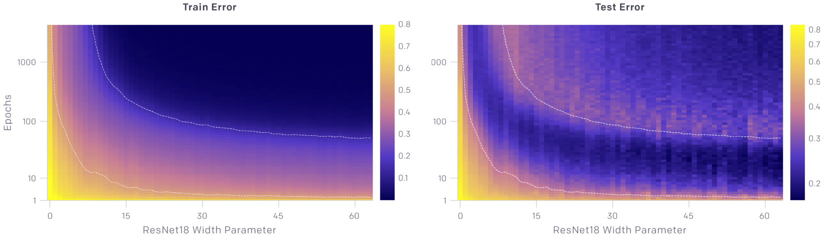
Epoch-wise double descent

There is a regime where training longer reverses overfitting.



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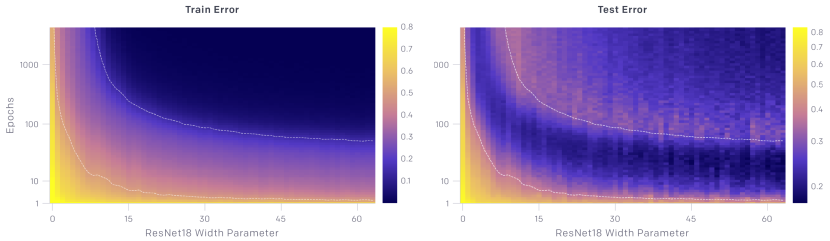

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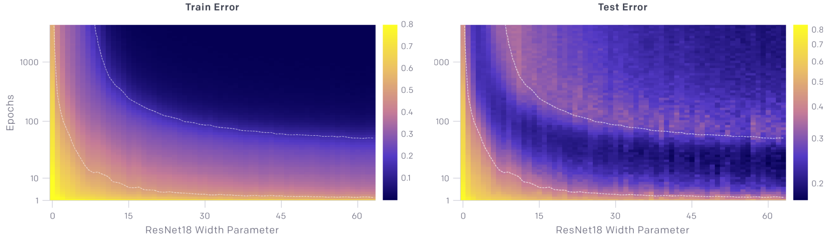

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For a fixed number of parameters, we observe double descent as a function of training time.

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Batch normalization

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Normalize each feature map by the statistics computed within the mini-batch $\mathcal{X}$:

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

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

Backprop will then need the partial derivatives:

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

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Batch normalization: Transformation

Transform each feature map $\mathbf{x}$ as:

$$\mathbf{x} \mapsto \frac{\mathbf{x} - \mathsf{E}[\mathcal{X}]}{\sigma(\mathcal{X})}$$

BN is per feature map, not per feature.

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

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Furthermore, introduce trainable weights:

$$\mathbf{x} \mapsto \gamma \frac{\mathbf{x} - \mathsf{E}[\mathcal{X}]}{\sigma(\mathcal{X})} + \beta$$

These allow to represent the identity $\mathbf{x} \mapsto \mathbf{x}$, if that is the optimal thing to do to solve the task.

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Batch normalization: Using mini-batches

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

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

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

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

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

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

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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 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 absorbed in the mean subtraction.

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Benefits:

- The stochastic uncertainty of the batch stats is a regularizer that can benefit generalization.

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At test time, what μ and σ are used? BN tracks a running average during training, use those!

Benefits:

- The stochastic uncertainty of the batch stats is a regularizer that can benefit generalization.
- BN leads to more stable gradients, thus faster training with higher learning rates.

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Normalization variants

Normalizing along the batch dimension can lead to inconsistency:

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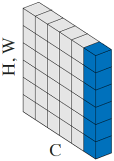

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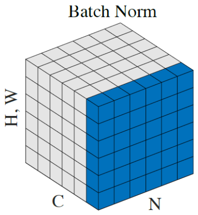

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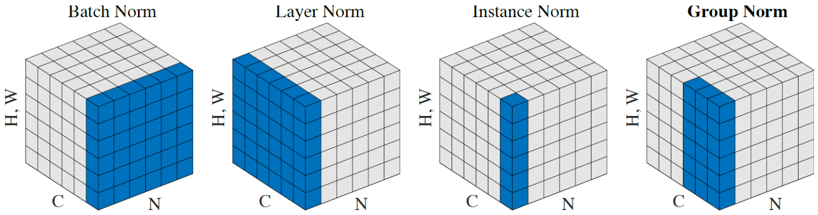

Wu and He, "Group normalization", ECCV 2018

Ensemble deep learning?

Assume you have lots of computational power.

Train an ensemble of deep nets and average their predictions.

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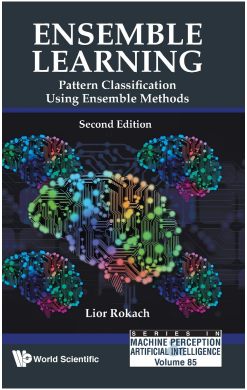
Most successful methods in **Kaggle** are ensemble methods.



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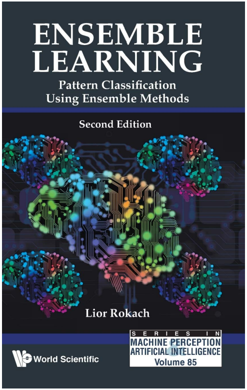
However, for deep nets this would come at a high computational cost.



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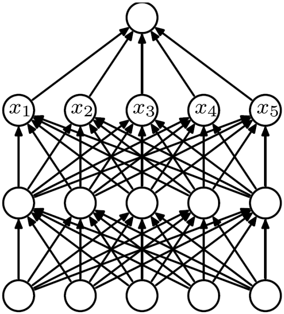
Dropout

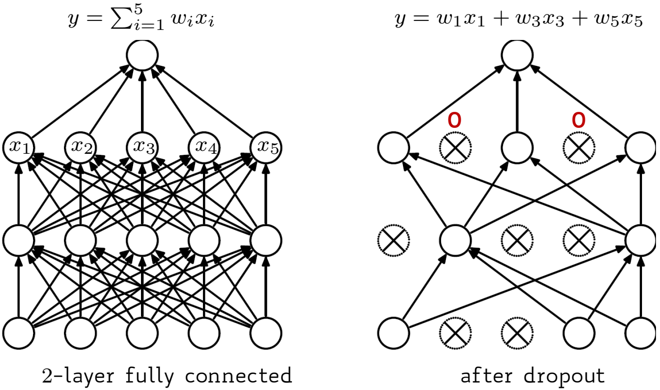
$y = \sum_{i=1}^{5} w_i x_i$



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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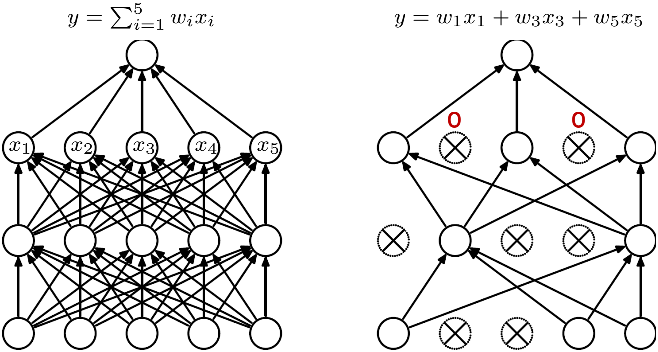

2-layer fully connected after dropout

Crucially, all networks share the same parameters.

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

This is way too costly.

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

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

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

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

Make it feasible by keeping one single network:

- **Training:** Generate a new sampling for each mini-batch in SGD.

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  The ensemble is trained to convergence.

  The individual models are not trained to convergence.

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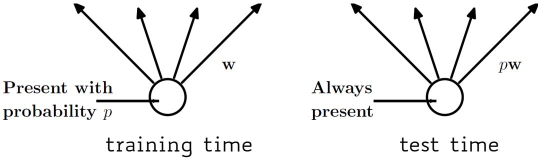

If a unit is retained with probability p during training (chosen by hand for each layer), its outgoing weights are multiplied by p.

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Dropout as an ensemble method

Dropout has two key features:

- Bagging, i.e. each model is trained on random data.
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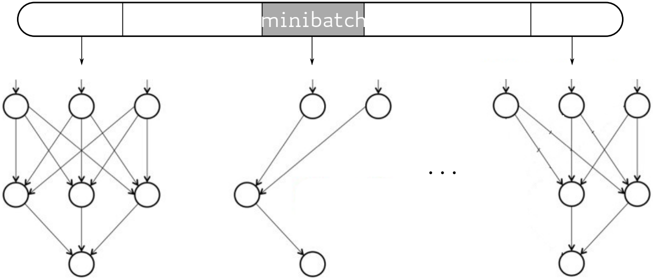

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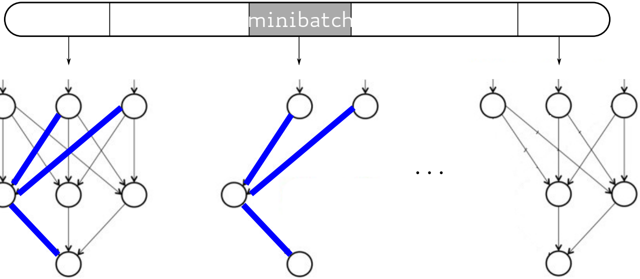

At each training step, the weight update is applied to all members of the ensemble simultaneously.

Dropout: Properties

In neural networks, weights are optimized jointly.

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

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- Longer training times: parameter updates are now noisier.
- Typical choices: 20% of the input units and 50% of the hidden units.

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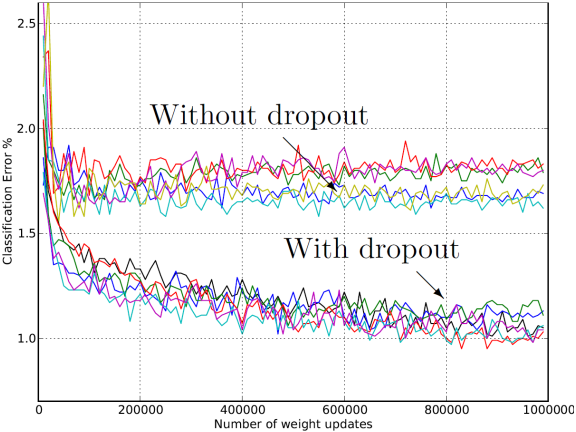

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Suggested reading

- 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/abs/1502.03167
- *Appendix A* is a practical guide for dropout by the original authors:
  http://jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf