Deep Learning & Applied AI

Regularization

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2nd semester a.y. 2019/2020 · April 15, 2020

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- Implicit regularization.

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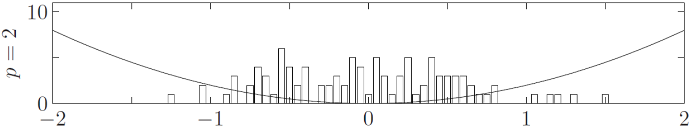
- Tikhonov (L_2) regularization



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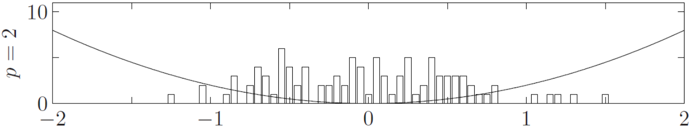

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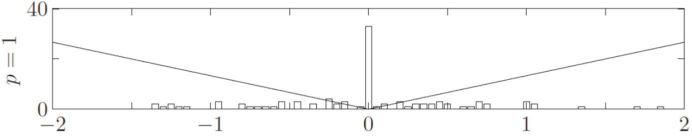

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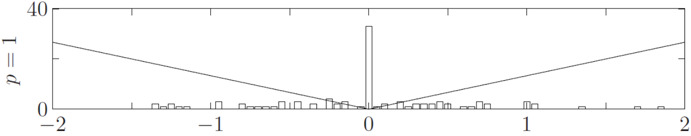

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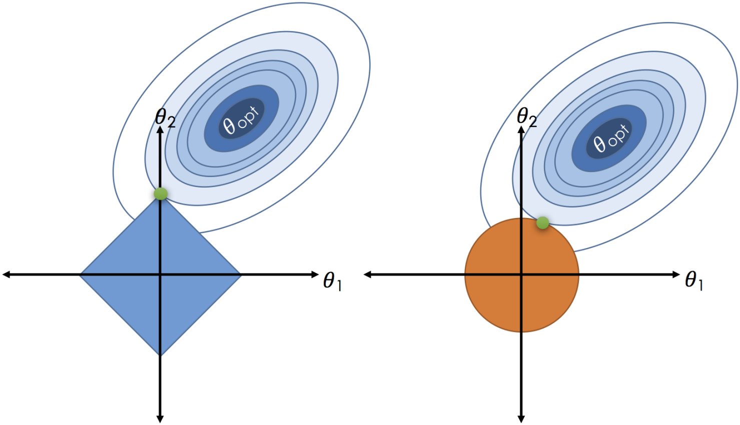
After training, the L_p magnitude of each weight reflects its importance.

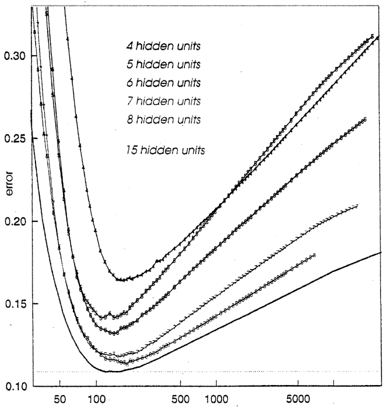
Sparsity



L_1 penalty $\qquad\qquad$ L_2 penalty

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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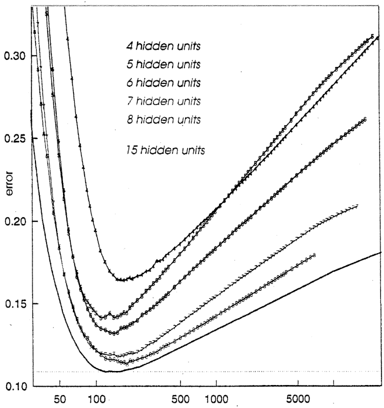
- Small networks can also overfit.



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Detecting overfitting

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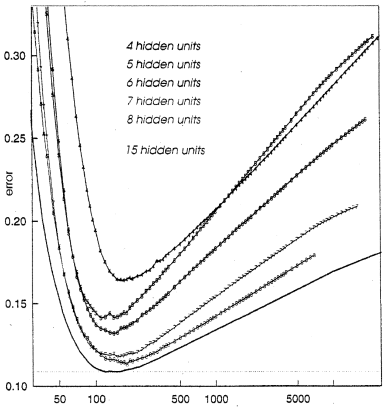
- Small networks can also overfit.
- Large networks have best performance if they stop early.



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Early stopping: Overview

Large network $\approx$ superposition of small networks.

In the first epochs of training, large nets tend to learn models similar to those learned by smaller nets.

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However:

- This ability depends on the optimization algorithm.
- Not always true that more parameters lead to overfitting.

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However:

- This ability depends on the optimization algorithm.
- Not always true that more parameters lead to overfitting.

Early stopping: Stop training as soon as performance on a validation set decreases. This is where the network starts to overfit the training set.

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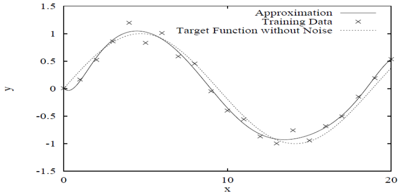
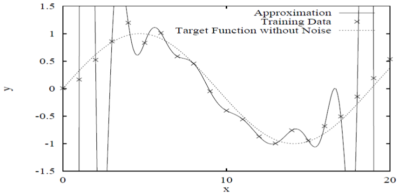
Many parameters $\neq$ overfitting



Order 10

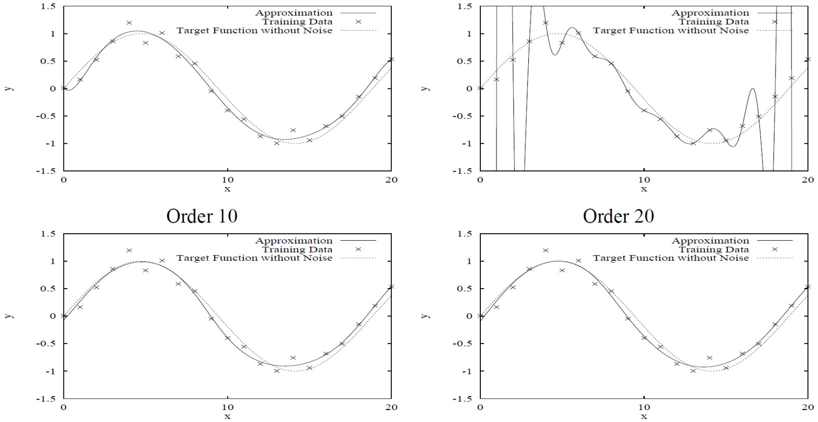


Order 20

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

Many parameters ≠ overfitting

More MLP parameters not leading to overfitting:



Order 10 | Order 20

10 Hidden Nodes | 50 Hidden Nodes

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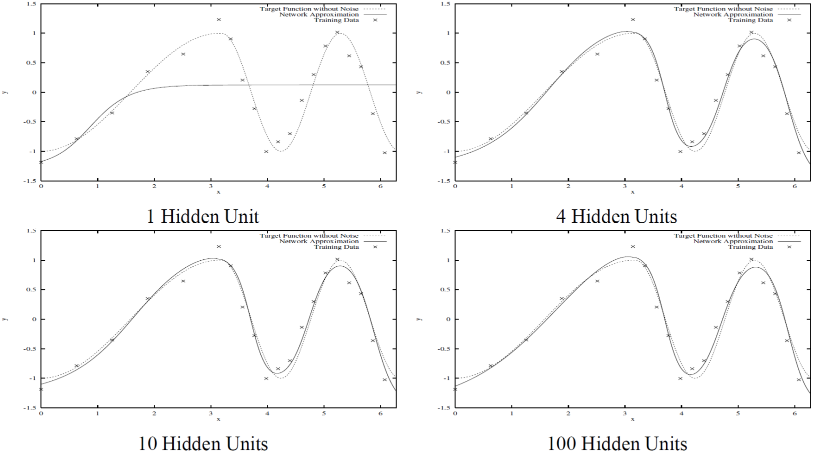
Good fit over all the different data regions:



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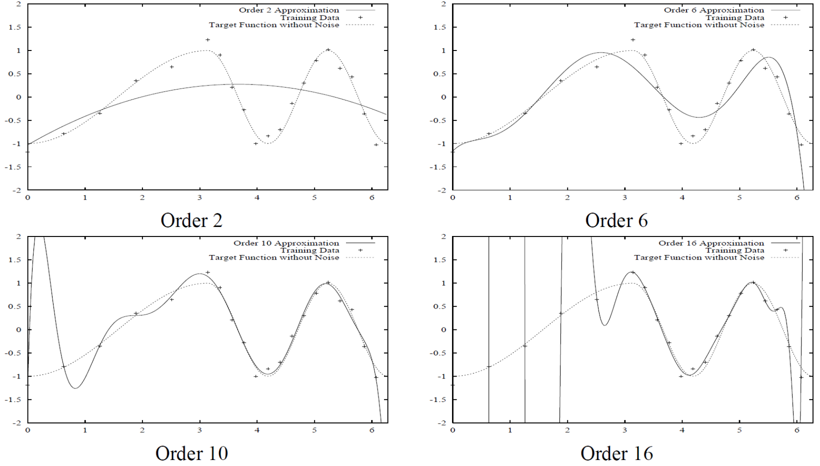
Overfitting as a local phenomenon

Overfitting is local and can vary significantly in different regions:



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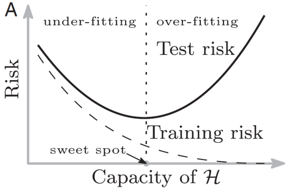
Double descent

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



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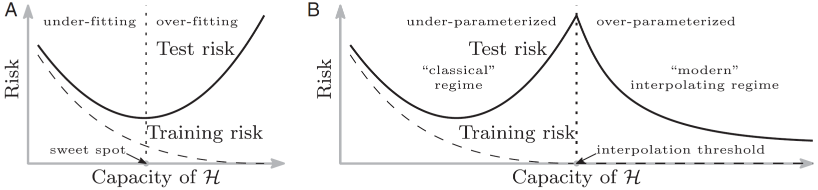

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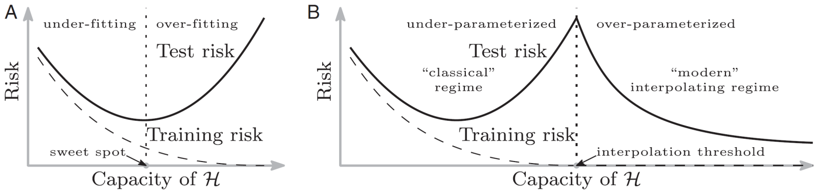

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"By considering larger function classes, which contain more candidate predictors compatible with the data, we are able to find interpolating functions that have smaller norm and are thus "simpler." Thus, increasing function class capacity improves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

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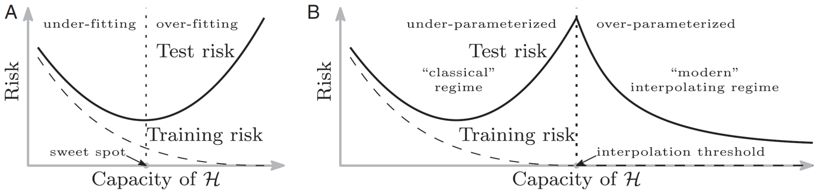

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The surprising fact is that SGD is able to find such good models.

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Early stopping

Our requirements:

- Avoid underfitting regions of high nonlinearity.
- Avoid overfitting regions of low nonlinearity.

Better optimization methods (e.g. conjugate gradient) yield worse generalization because they tend to overfit regions of low non-linearity.

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Epoch-wise double descent

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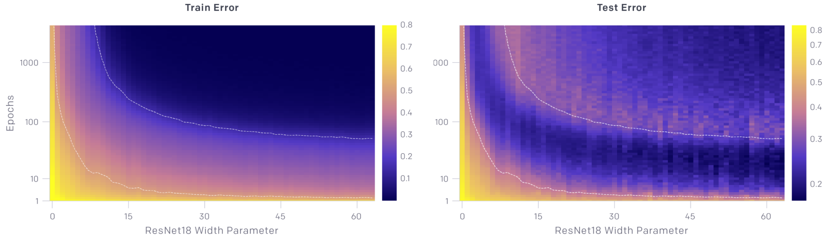

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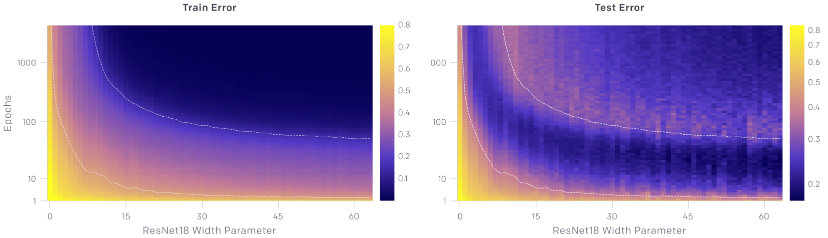

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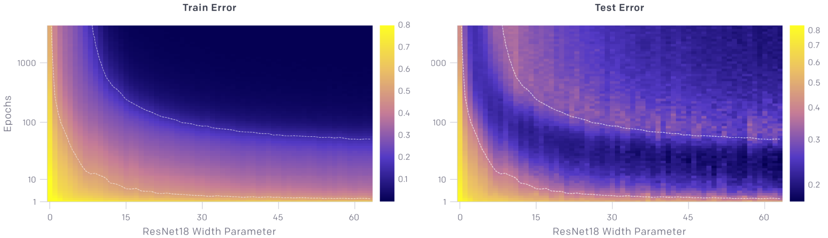

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For a fixed number of parameters, we observe double descent as a function of training time.

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

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

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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Beneficial properties include:

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

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Beneficial properties include:

- 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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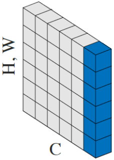

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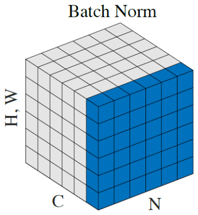
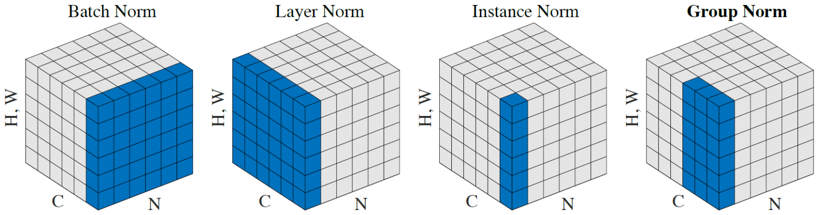


Normalization variants

Normalizing along the batch dimension can lead to inconsistency:

- Bad transfer across different data distributions.
- The stats must be reliable; reducing the mini-batch size increases the model error dramatically.

Several variants have been proposed:



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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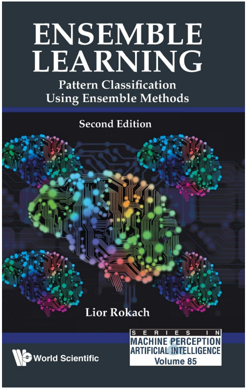

Neal, "Bayesian Learning for Neural Networks", 1996

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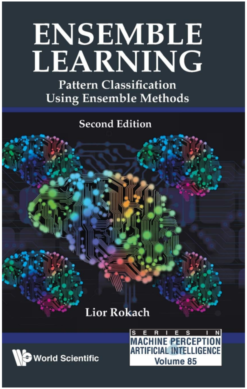
However, for deep nets this would come at a high computational cost.



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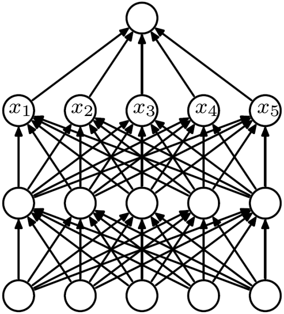
Dropout

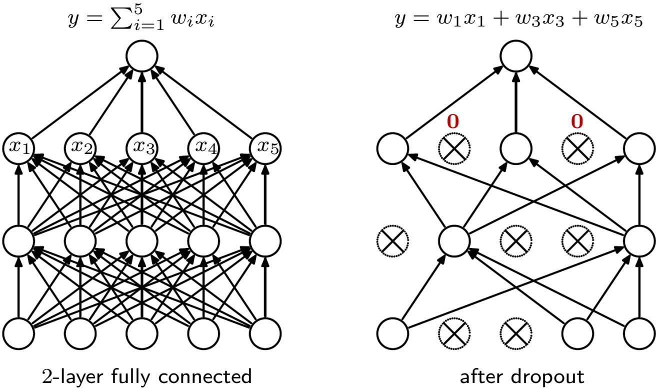
$y = \sum_{i=1}^{5} w_i x_i$



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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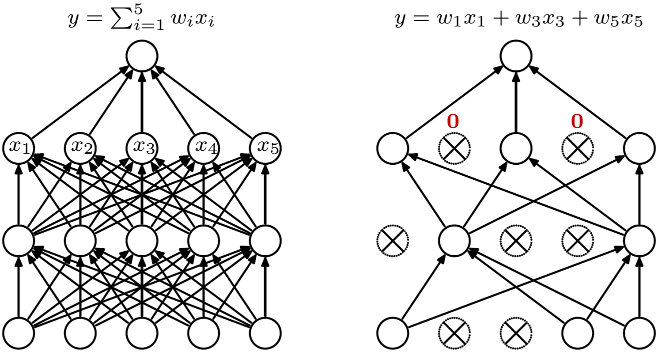

2-layer fully connected

after dropout

Crucially, all networks share the same parameters.

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

Dropout

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

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

  The individual models are not trained to convergence.

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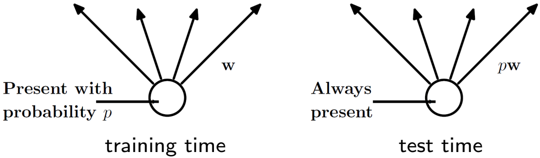

If a unit is retained with probability p during training (chosen by hand, even per layer), its outgoing weights are multiplied by p.

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Dropout as an ensemble method

Dropout has two key features:

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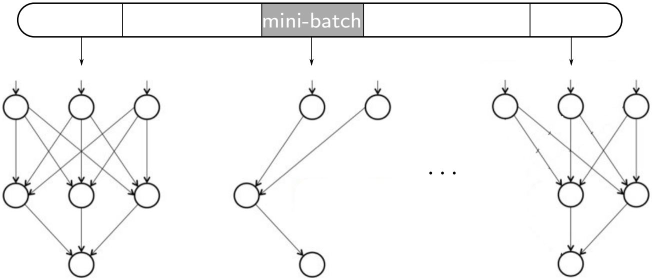

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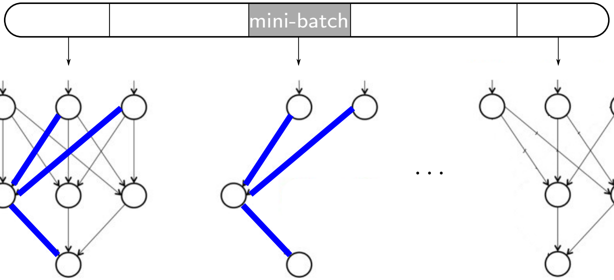

At each training step, the weight update is applied to all members of the ensemble simultaneously.

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

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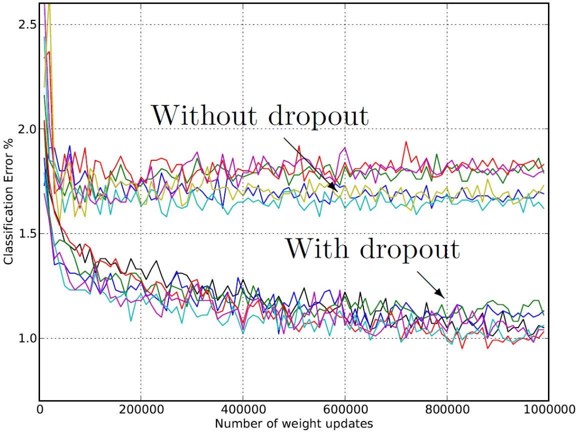

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Dropout: Implicit bias

In a 2-layer network (input $\mathbf{U}$ + hidden $\mathbf{V}$) dropout is equivalent to:

$$\ell(\mathbf{U}, \mathbf{V}) + \frac{1-p}{p} \sum_{i=1}^{r} \|\mathbf{u}_i\|^2 \|\mathbf{v}_i\|^2$$

where the vectors are the columns of $\mathbf{U}$ and $\mathbf{V}$.

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It equalizes the norms $\|\mathbf{u}_i\|^2, \|\mathbf{v}_i\|^2$ for all i, which is conjectured to reduce co-adaptation.

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For small enough dropout rate, all minima are global.

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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`
- Talk by René Vidal on the implicit bias of dropout:
  `https://ipam.wistia.com/medias/30h1ay475i`