Deep Learning & Applied AI

Regularization, batchnorm and dropout

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2022/2023 · April 12, 2023

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- Explicit penalties.

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tuttavia questo succede quasi sempre

Regularization is a general mechanism to reduce overfitting and thus improve generalization.

General idea: reduce the number of free parameters.

i free parameters sono tutti quei parametri che possono essere allenati

- Eliminate network weights.

  e.g. estimate network sensitivity w.r.t. each weight.

- Weight sharing (i.e. $\#$ weights $< \#$ connections).

  lo abbiamo già visto

- Explicit penalties.
- Implicit regularization.

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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

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

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

quindi il regolarizzatore è una funzione
dipendente dai parametri della loss

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Typical penalties:

- Tikhonov (L_2) regularization $\Rightarrow$ promotes shrinkage riduce la grandezza dei pesi
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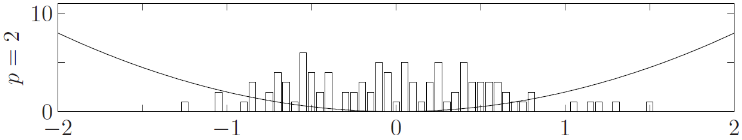
After training, the L_p magnitude of each weight reflects its importance.

L_2 vs L_1 penalties



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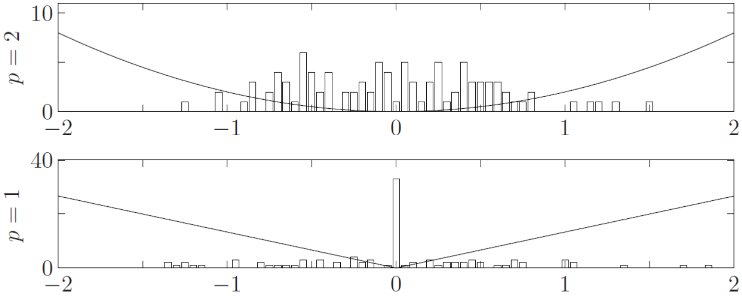

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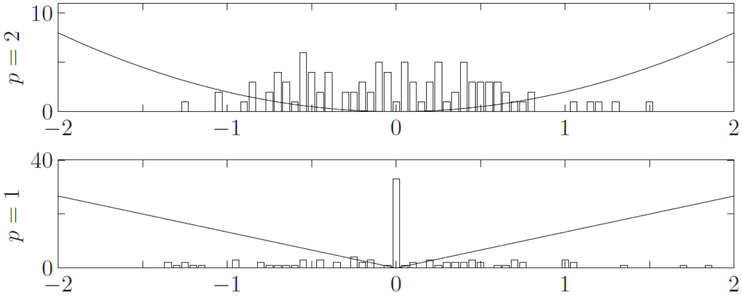

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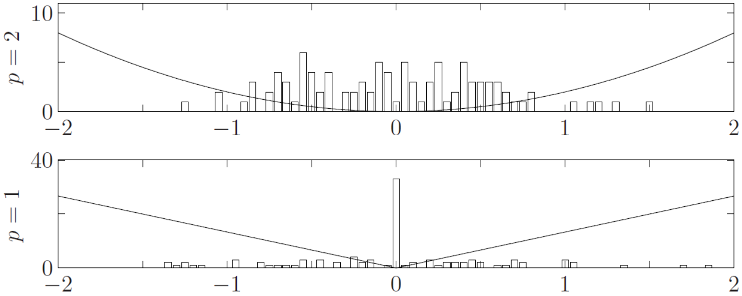

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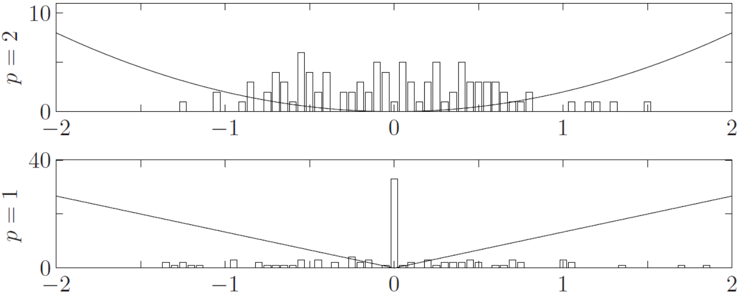
- Almost no reduction in $\|\mathbf{\Theta}\|_2$ for values < 1. Sparsity is discouraged!

L_2 vs L_1 penalties

istogrammi che indicano il numero di parametri che hanno uno specifico valore

Tikhonov



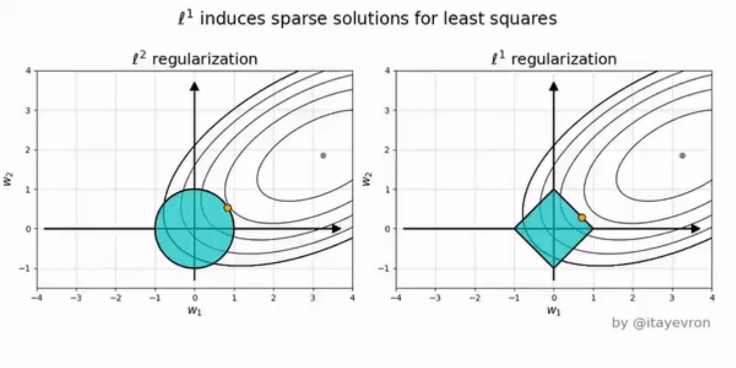
Lasso

le linee indicano l'impatto della penalità

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

perché la L_1 riduzione ha così tanti valori pari a 0? Vedi prossima slide...

l'ellissi che gira è la energy function
che dobbiamo minimizzare

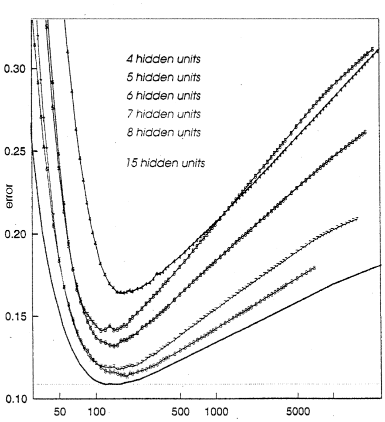


nel caso della L_1, la soluzione (il valore ottimo per i parametri) è un punto che si trova molto frequentemente sulle assi delle coordinate, mentre nel caso di L_2 la soluzione si muove spesso. In pratica la capacità di regolarizzazione con L_1 è meno precisa rispetto ad L_2, risultando nell'azzeramento di molti parametri con un valore basso

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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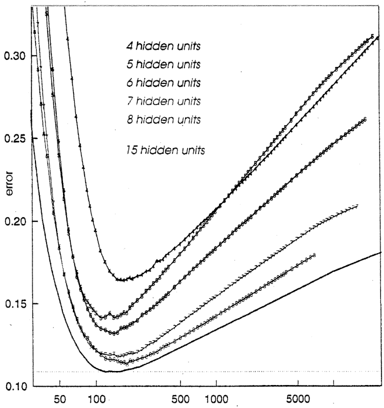
- Small networks can also overfit.



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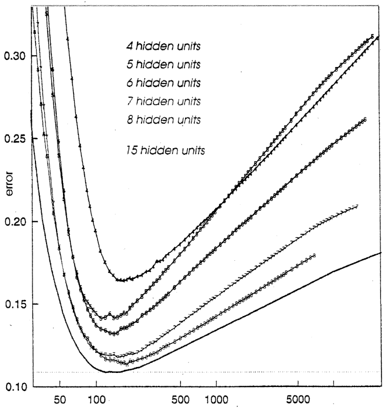

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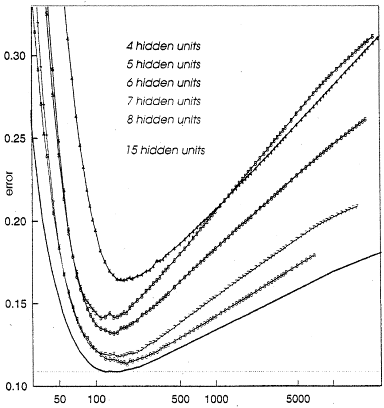
Detecting overfitting: Early stopping

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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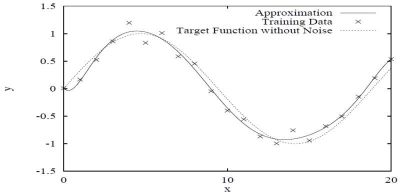
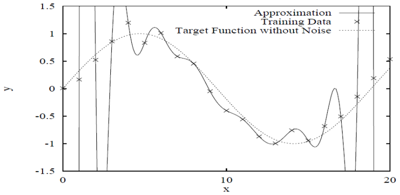
Many parameters $\neq$ overfitting

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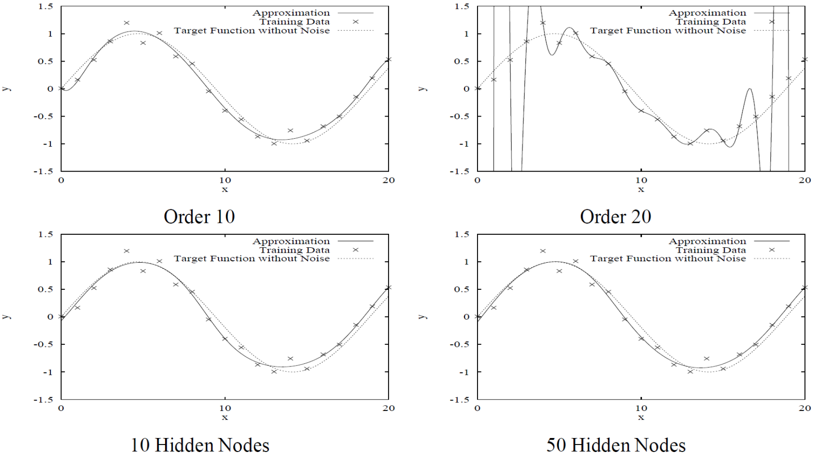
...but more MLP parameters not always lead to overfitting:



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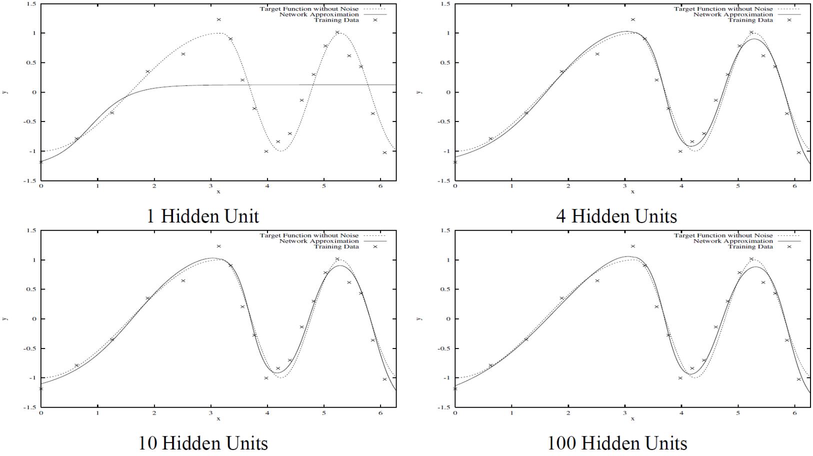
Good fit over all the different data regions:



1 Hidden Unit

4 Hidden Units

10 Hidden Units

100 Hidden Units

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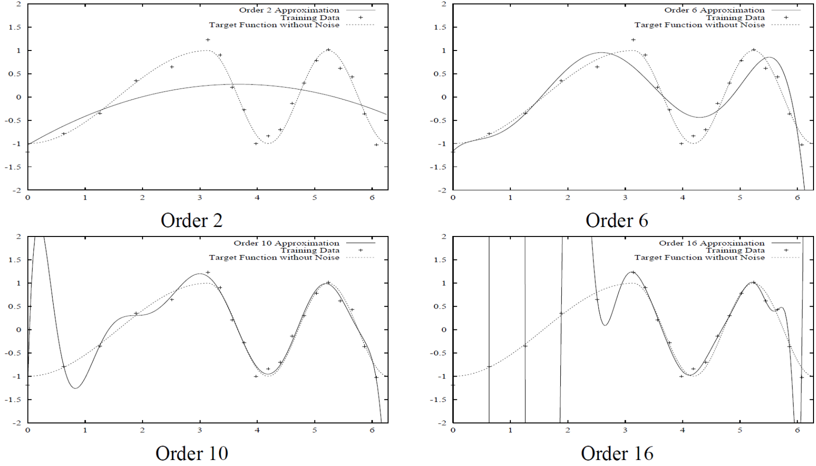
Overfitting as a local phenomenon

Overfitting is local and can vary significantly in different regions:



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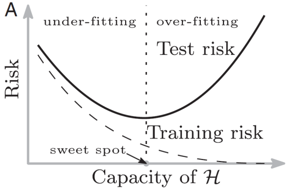
Double descent

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



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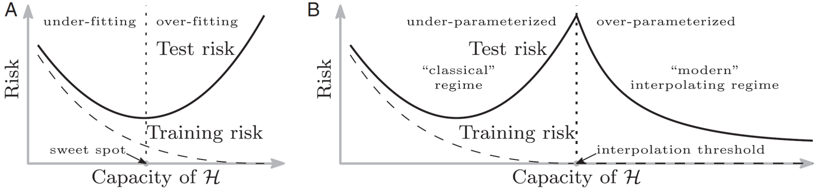

Interpolation: perfect fit on the training data.

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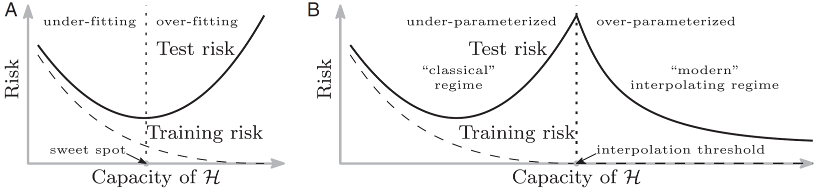

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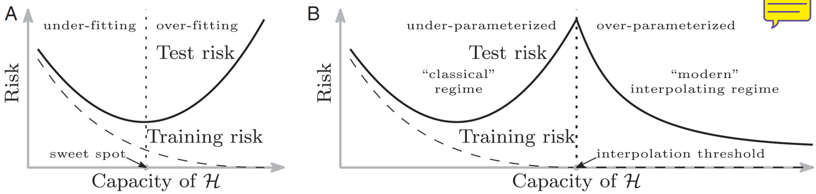

H = rete neurale

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

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Early stopping

Early stopping is based on the "smoothness" heuristic:

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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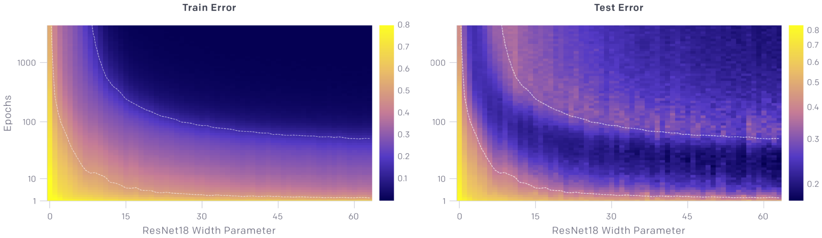
Epoch-wise double descent

There is a regime where training longer reverses overfitting.



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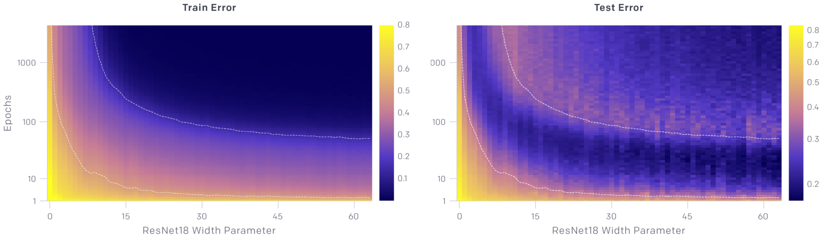

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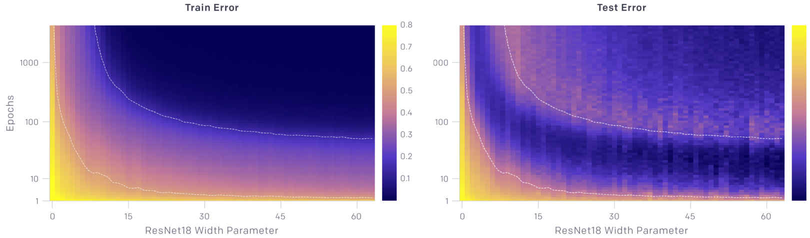

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For a fixed number of parameters, we observe double descent as a function of training time.

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Batch normalization

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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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Batch normalization

k indica il livello
della rete

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sigma è sempre
l'activation function

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training set

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.

Ioffe and Szegedy, "Batch normalization: Accelerating deep network training by reducing internal covariate shift", ICML 2015

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.

questa proprietà aggiunge potere di generalizzazione

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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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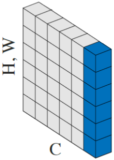

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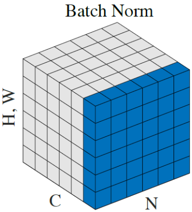

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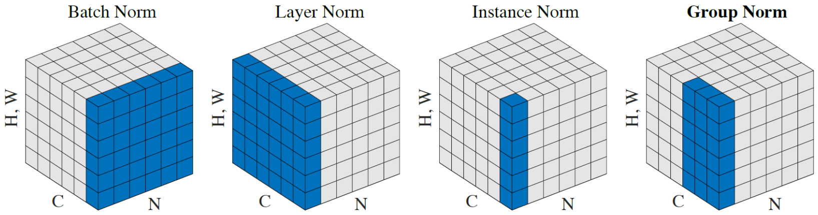
Several variants:



In questi esempi, una colonna corrisponde
ad un sample del dataset

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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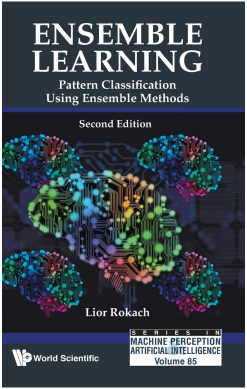

Neal, "Bayesian Learning for Neural Networks", 1996

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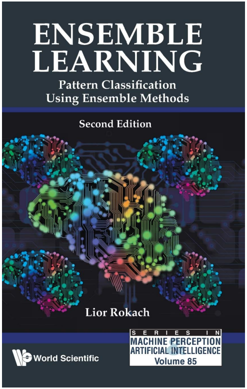
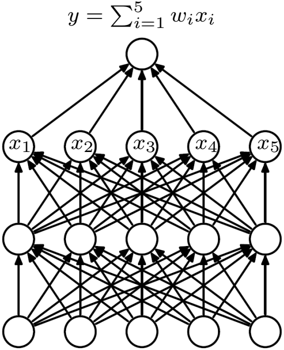
However, for deep nets this would come at a high computational cost.



c'è una tecnica che permette di fare ensable learning.
Vedi prossima slide...

Neal, "Bayesian Learning for Neural Networks", 1996

Dropout

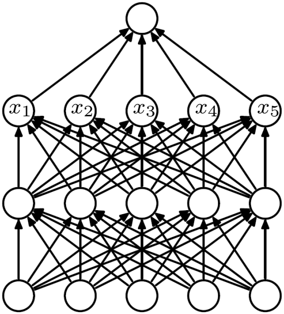


2-layer fully connected

Dropout

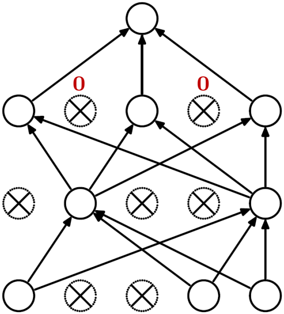
Main idea: Parametrize each model in the ensemble by dropping random units (i.e. nodes with their input/output connections):

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



2-layer fully connected

$y = w_1 x_1 + w_3 x_3 + w_5 x_5$



after dropout

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

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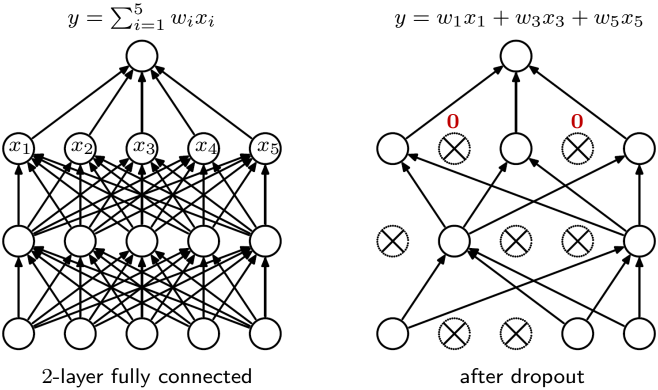

Crucially, all networks share the same parameters.

quindi in teoria si fanno tante prove con configurazioni diverse e si confrontano i risultati...

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

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

Dropout

... ma c'è un problema

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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. perché la configurazione cambia ad ogni iterazione

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

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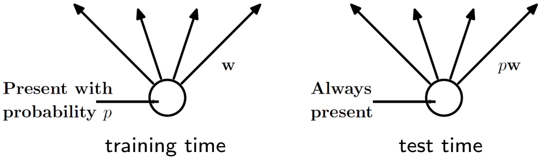

If a unit is retained with probability p during training (chosen by hand, even per layer), its outgoing weights are multiplied by p.

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:

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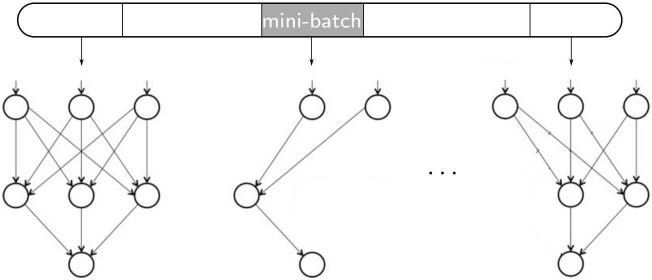

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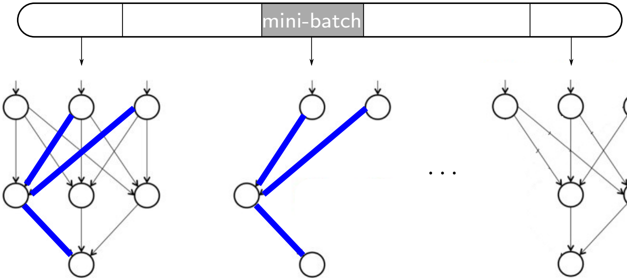

At each training step, the weight update is applied to all members of the ensemble simultaneously.

solo i pesi dei nodi attivi durante l'iterazione vengono aggiornati

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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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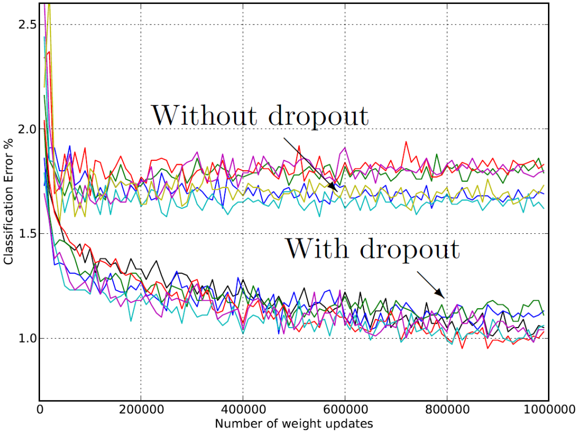

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Suggested reading

- 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`