Continuous neural networks

Nicolas Le Roux joint work with Yoshua Bengio

April 5th, 2006

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Nicolas Le Roux joint work with Yoshua Bengio Snowbird 2006

Structure of Neural Networks Hornik's theorem and its consequences

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Usual Neural Networks



g is the transfer function: tanh, sigmoid, sign, ...

Structure of Neural Networks Hornik's theorem and its consequences

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Neural networks are universal approximators

Hornik et al. (1989)

Multilayer feedforward networks with one hidden layer using arbitrary squashing functions are capable of approximating any function to any desired degree of accuracy, provided sufficiently many hidden units are available.

Structure of Neural Networks Hornik's theorem and its consequences

Neural networks are universal approximators

Hornik et al. (1989)

Multilayer feedforward networks with one hidden layer using arbitrary squashing functions are capable of approximating any function to any desired degree of accuracy, provided sufficiently many hidden units are available.

Neural Networks with an infinite number of hidden units should be able to approximate every function arbitrarily well.

A new vision of neural networks The input weights function Properties of continuous neural networks Another vision

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A nice picture before the Maths



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Going to infinity

$$\widehat{f}(x) = \sum_{j} w_{j} \ g(v_{j} \cdot x) + b \longrightarrow \widehat{f}(x) = \int_{j} w(j) \ g(v(j) \cdot x) \ dj + b$$

Going to infinity

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Hornik's theorem tells us that any function f from \mathbb{R}^d to \mathbb{R} can be approximated arbitrarily well by:

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Hornik's theorem tells us that any function f from \mathbb{R}^d to \mathbb{R} can be approximated arbitrarily well by:

- **①** a function from \mathbb{R} to \mathbb{R} : *w* the "output weights function"
- **②** a function from \mathbb{R} to \mathbb{R}^{d+1} : *v* the "input weights function"

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- **(**) a function from \mathbb{R} to \mathbb{R} : *w* the "output weights function"
- **2** a function from \mathbb{R} to \mathbb{R}^{d+1} : *v* the "input weights function"
- \bigcirc a scalar: *b* the output bias.

$$\widehat{f}(x) = \sum_{j} w_{j} g(v_{j} \cdot x) + b \longrightarrow \widehat{f}(x) = \int_{j} w(j) g(v(j) \cdot x) dj + b$$

Hornik's theorem tells us that any function f from \mathbb{R}^d to \mathbb{R} can be approximated arbitrarily well by:

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But a function from \mathbb{R} to \mathbb{R}^{d+1} is d+1 functions from \mathbb{R} to \mathbb{R} .

$$\widehat{f}(x) = \sum_{j} w_{j} g(v_{j} \cdot x) + b \longrightarrow \widehat{f}(x) = \int_{j} w(j) g(v(j) \cdot x) dj + b$$

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But a function from \mathbb{R} to \mathbb{R}^{d+1} is d+1 functions from \mathbb{R} to \mathbb{R} . This is very similar to Kolmogorov's representation theorem.

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v for usual neural networks



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v for usual neural networks



Neural networks approximate v with a piecewise constant function.

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V is a trajectory in \mathbb{R}^d indexed by t

The function V is a trajectory in the space of all possible input weights.

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- Each point corresponds to an input weight associated to an infinitesimal output weight.

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V is a trajectory in \mathbb{R}^d indexed by t

- The function V is a trajectory in the space of all possible input weights.
- Each point corresponds to an input weight associated to an infinitesimal output weight.
- A piecewise constant trajectory only crosses a finite number of points in the space of input weights.
- We could imagine trajectories that "fill" the space a bit more.

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Piecewise affine approximations



Going to infinity

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Piecewise affine approximations



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Piecewise affine approximations



Seeing v as a function, we could introduce smoothness wrt j using constraints on successive values of v.

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Rate of convergence



 $\left|f(x)-\widehat{f}(x)\right|\leq 2a\int_{0}^{1}\left|\left(v(t)-\widehat{v}(t)\right)\cdot x\right|dt$

Introduction A new vision of neural networks Going to infinity The input weights function Conclusion Questions Another vision

Rate of convergence

0

$$\left|f(x)-\widehat{f}(x)\right|\leq 2a\int_{0}^{1}\left|\left(v(t)-\widehat{v}(t)\right)\cdot x\right|dt$$

2 A good approximation of v yields a good approximation of f.

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Rate of convergence

$$\left|f(x)-\widehat{f}(x)\right|\leq 2a\int_{0}^{1}\left|\left(v(t)-\widehat{v}(t)\right)\cdot x\right|dt$$

A good approximation of v yields a good approximation of f.
Trapezoid rule (continuous piecewise affine functions) has a faster convergence rate than rectangle rule (piecewise constant functions).

Rate of convergence

a

$$\left|f(x)-\widehat{f}(x)\right|\leq 2a\int_{0}^{1}\left|\left(v(t)-\widehat{v}(t)\right)\cdot x\right|dt$$

2 A good approximation of v yields a good approximation of f.

Trapezoid rule (continuous piecewise affine functions) has a faster convergence rate than rectangle rule (piecewise constant functions).

Theorem: rate of convergence of affine neural networks

Affine neural networks converge in $O(n^{-2})$ whereas usual neural networks converge in $O(n^{-1})$ (when *n* grows to infinity).

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Piecewise affine approximations (again)



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A few remarks on the optimization on the input weights

• Having a complex function V requires lots of pieces.

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A few remarks on the optimization on the input weights

- Having a complex function V requires lots of pieces.
- Without constraints, having many pieces will lead us nowhere.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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A few remarks on the optimization on the input weights

- Having a complex function V requires lots of pieces.
- Without constraints, having many pieces will lead us nowhere.
- Maybe we could use other parametrizations inducing constraints on the pieces.

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A few remarks on the optimization on the input weights

- Having a complex function V requires lots of pieces.
- Without constraints, having many pieces will lead us nowhere.
- Maybe we could use other parametrizations inducing constraints on the pieces.
- Instead of optimizing each input weight v(j) independently, we could parametrize them as the output of a neural network.

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Input weights function as the output of a neural network



Nicolas Le Roux

Snowbird 2006

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Input weights function as the output of a neural network

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 $v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Input weights function as the output of a neural network

$$v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$$

Setting a prior on the parameters of that network induces a prior on v.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Input weights function as the output of a neural network

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- Such priors include the Gaussian prior commonly used.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Input weights function as the output of a neural network

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- Such priors include the Gaussian prior commonly used.
- The prior over $v_{v,k}$ and $b_{v,k}$ determines the level of dependence between the *j*'s.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Input weights function as the output of a neural network

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- Setting a prior on the parameters of that network induces a prior on v.
- Such priors include the Gaussian prior commonly used.
- The prior over v_{v,k} and b_{v,k} determines the level of dependence between the j's.
- The prior over $w_{v,k}$ determines the amplitude of the v(j)'s.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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A bit of recursion



 $v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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A bit of recursion

 $v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$

2 What about the $v_{v,k}$ and the $b_{v,k}$?

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We could define them as the output of a neural network.

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A bit of recursion

$$v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$$

- **2** What about the $v_{v,k}$ and the $b_{v,k}$?
- We could define them as the output of a neural network.
- You should be lost by now.

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A bit of recursion

$$v(j) = \sum_{k} w_{v,k} g\left(v_{v,k} \cdot j + b_{v,k}\right)$$

- **2** What about the $v_{v,k}$ and the $b_{v,k}$?
- We could define them as the output of a neural network.
- You should be lost by now.
- Let's stop a bit to rest.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Summary

Input weights can be seen as a function.

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Summary

- Input weights can be seen as a function.
- There are parametrizations of that function that yield theoretically more powerful networks than the usual ones.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Summary

- Input weights can be seen as a function.
- There are parametrizations of that function that yield theoretically more powerful networks than the usual ones.
- Moreover, such parametrizations allow to set different constraints than the common ones.

A new vision of neural networks The input weights function **Properties of continuous neural networks** Another vision

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Summary

- Input weights can be seen as a function.
- There are parametrizations of that function that yield theoretically more powerful networks than the usual ones.
- Moreover, such parametrizations allow to set different constraints than the common ones.
- Example: handling of sequential data.

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Having all possible input neurons at once

• Instead of optimizing input weights, we could use all of them: $f(x) = \int_E w(v)g(v \cdot x) dv$

Having all possible input neurons at once

- Instead of optimizing input weights, we could use all of them: $f(x) = \int_{E} w(v)g(v \cdot x) dv$
- **2** and only optimize the output weights \longrightarrow this is convex.

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- With a sign transfer function, this integral can be computed analytically and yields a kernel machine.

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$$K_{\mathrm{sign}}(x,y) = A - B \|x - y\|$$

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This kernel has no hyperparameter.

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Results on USPS with 6000 training samples

Algorithm	$wd = 10^{-3}$	$wd = 10^{-6}$	$wd = 10^{-12}$	Test
$K_{ m sign}$	2.27±0.13	$1.80{\pm}0.08$	$1.80{\pm}0.08$	4.07
G. $\sigma = 1$	58.27±0.50	58.54±0.27	58.54±0.27	58.29
G. $\sigma = 2$	$7.71 {\pm} 0.10$	7.78±0.21	7.78±0.21	12.31
G. <i>σ</i> = 4	$1.72{\pm}0.11$	$2.09{\pm}0.09$	$2.10{\pm}0.09$	4.07
G. $\sigma = 6$	$1.67{\pm}0.10$	2.78±0.25	3.33±0.35	3.58
G. $\sigma = 7$	$1.72{\pm}0.10$	3.04±0.26	4.39±0.49	3.77

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Results on MNIST with 6000 training samples

Algorithm	$wd = 10^{-3}$	$wd = 10^{-6}, 10^{-9}, 10^{-12}, 0$	Test
$K_{ m sign}$	5.51 ± 0.22	4.54 ± 0.50	4.09
G. $\sigma = 1$	77.55 ± 0.40	77.55 ± 0.40	80.03
G. $\sigma = 2$	10.51 ± 0.46	10.51 ± 0.45	12.44
G. $\sigma = 3$	3.64 ± 0.10	3.64 ± 0.10	4.1
G. $\sigma = 5$	3.01 ± 0.12	3.01 ± 0.12	3.33
G. $\sigma = 7$	3.15 ± 0.09	3.18 ± 0.10	3.48

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Results on LETTERS with 6000 training samples

Algorithm	$wd = 10^{-3}$	$wd = 10^{-6}$	$wd = 10^{-9}$	Test
$K_{ m sign}$	5.36 ± 0.10	5.22 ± 0.09	5.22 ± 0.09	5.5
G. $\sigma = 2$	5.47 ± 0.14	5.93 ± 0.15	5.92 ± 0.14	5.8
G. $\sigma = 4$	4.97 ± 0.10	11.06 ± 0.29	12.50 ± 0.35	5.3
G. $\sigma = 6$	6.27 ± 0.17	8.47 ± 0.20	17.61 ± 0.40	6.63
G. $\sigma = 8$	8.45 ± 0.19	6.11 ± 0.15	18.69 ± 0.34	9.25

Summary Future work

Summary

We showed that training a neural network can be seen as learning an input weight function.

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Summary Future work

Summary

- We showed that training a neural network can be seen as learning an input weight function.
- We introduced an affine-by-part parametrization of that function which corresponds to a continuous number of hidden units.

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Summary Future work

Summary

- We showed that training a neural network can be seen as learning an input weight function.
- We introduced an affine-by-part parametrization of that function which corresponds to a continuous number of hidden units.
- In the extreme case where all the input weights are present, we showed it is a kernel machine whose kernel can be computed analytically and possesses no hyperparameter.

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Summary Future work

Future work

Learning the transfer function using a neural network.

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Summary Future work

Future work

- Learning the transfer function using a neural network.
- Find other (and better) parametrizations of the input weight function.

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Summary Future work

Future work

- Learning the transfer function using a neural network.
- Find other (and better) parametrizations of the input weight function.
- Recursively define the input weight function as the output of a neural network.

Computation of the covariance matrix Additive and multiplicative invariance of the covariance matrix

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Now is the time for ...

Questions?

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Computing $\int_E \operatorname{sign}(v \cdot x + b) \operatorname{sign}(v \cdot y + b) dvdb$

- sign(x) function is invariant with respect to the norm of x.
- $\Im \operatorname{sign}(v \cdot x + b) \operatorname{sign}(v \cdot y + b) = \operatorname{sign}(v \cdot x + b)(v \cdot y + b)].$
- Solution When b ranges from -M to +M, for M large enough, x'vv'y + b is negative on an interval of size $|v \cdot (x - y)|$.
- $\int_{b=-M}^{+M} \operatorname{sign}(x'vv'y+b) \ db = 2M 2|v \cdot (x-y)|.$
- Integrating this term on the unit hypersphere yields a kernel of the form K(x, y) = A − B ||x − y||.

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Additive and multiplicative invariance of the covariance matrix

- In SVM and kernel regression, the elements of the weights vector α sum to 0.
- **2** The final solution involves $K\alpha$.
- Thus, adding a term δ to every element of the covariance matrix yields the solution $(K + \frac{\delta}{n}ee')\alpha = K\alpha + \frac{\delta}{n}e(e'\alpha) = K\alpha.$

$$C(K, \alpha, b, \lambda) = \mathcal{L}(K\alpha + b, Y) + \lambda \alpha' K\alpha$$

$$C\left(\frac{K}{c}, c\alpha, b, \frac{\lambda}{c}\right) = \mathcal{L}\left(\frac{K}{c}c\alpha + b, Y\right) + \frac{\lambda}{c}c\alpha' \frac{K}{c}c\alpha$$

$$= C(K, c\alpha, b, \lambda)$$