Continuous neural networks

Nicolas Le Roux
joint work with Yoshua Bengio

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Usual Neural Networks

\[ f(x_t) = \sum_j w_j g(v_j \cdot x_t) + b \]

\[ g(v_1 \cdot x_t) \quad \ldots \quad g(v_n \cdot x_t) \]

\[ x_{t,1} \quad \ldots \quad x_{t,d} \]

\( g \) is the **transfer function**: tanh, sigmoid, sign, ...
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.
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Neural Networks with an infinite number of hidden units should be able to approximate every function arbitrarily well.
A nice picture before the Maths

\[ \ldots h_{v_1} \ldots h_{v_2} \ldots h_{v_k} \ldots \]

\[ O_{1} \ldots O_{p} \]

\[ x_{t,1} \quad x_{t,2} \ldots x_{t,d} \]
Going to infinity

\[ \hat{f}(x) = \sum_j w_j g(v_j \cdot x) + b \rightarrow \hat{f}(x) = \int_j w(j) g(v(j) \cdot x) \, dj + b \]
Hornik’s theorem tells us that any function $f$ from $\mathbb{R}^d$ to $\mathbb{R}$ can be approximated arbitrarily well by:
Going to infinity

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2. a function from \( \mathbb{R} \) to \( \mathbb{R}^{d+1} \): \( v \) the “input weights function”
A new vision of neural networks
The input weights function
Properties of continuous neural networks
Another vision

Introduction
Going to infinity
Conclusion
Questions

Going to infinity

\[ \hat{f}(x) = \sum_{j} w_j \ g(v_j \cdot x) + b \quad \longrightarrow \quad \hat{f}(x) = \int w(j) \ g(v(j) \cdot x) \ dj + b \]

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3. a scalar: \( b \) the output bias.
Going to infinity

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But a function from \( \mathbb{R} \) to \( \mathbb{R}^{d+1} \) is \( d + 1 \) functions from \( \mathbb{R} \) to \( \mathbb{R} \).
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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.
n for usual neural networks

\[ \hat{f}(x) = \int_u g(v(u) \cdot x) \, du + b = \sum_j w_j g(v_j \cdot x) + b \]
A new vision of neural networks

The input weights function

Properties of continuous neural networks

Another vision

For usual neural networks, we have:

$$v_j = w_j \cdot f(x)$$

Neural networks approximate $v$ with a piecewise constant function.
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1. The function \( \mathcal{V} \) is a trajectory in the space of all possible input weights.
2. Each point corresponds to an input weight associated to an infinitesimal output weight.
3. A piecewise constant trajectory only crosses a finite number of points in the space of input weights.
4. We could imagine trajectories that "fill" the space a bit more.
Piecewise affine approximations

\[ v(j) \]
A new vision of neural networks
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Piecewise affine approximations

\[
\hat{f}(x) = \sum_j \frac{w_j}{(v_j - v_{j-1}) \cdot x} \ln \left( \frac{\cosh(v_j \cdot x)}{\cosh(v_{j-1} \cdot x)} \right) + b
\]

Nicolas Le Roux  
Snowbird 2006
Piecewise affine approximations

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Seeing \( v \) as a function, we could introduce smoothness wrt \( j \) using constraints on successive values of \( v \).
Rate of convergence

\[ |f(x) - \hat{f}(x)| \leq 2a \int_0^1 |(v(t) - \hat{v}(t)) \cdot x| \, dt \]
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**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).
A new vision of neural networks
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Piecewise affine approximations (again)
A few remarks on the optimization on the input weights

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A few remarks on the optimization on the input weights

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

\[ v(j) = \sum_{k} w_{v,k} g(v_{v,k} \cdot j + b_{v,k}) \]
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2. Such priors include the Gaussian prior commonly used.
3. The prior over \( v_{v,k} \) and \( b_{v,k} \) determines the level of dependence between the \( j \)'s.
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4. The prior over \( v_{v,k} \) and \( b_{v,k} \) determines the level of dependence between the \( j \)'s.

5. The prior over \( w_{v,k} \) determines the amplitude of the \( v(j) \)'s.
A bit of recursion

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\[ v(j) = \sum_k w_{v,k} g(v_{v,k} \cdot j + b_{v,k}) \]

2. What about the \( v_{v,k} \) and the \( b_{v,k} \)?
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1. \[ v(j) = \sum_k w_{v,k} g(v_{v,k} \cdot j + b_{v,k}) \]

2. What about the \(v_{v,k}\) and the \(b_{v,k}\)?

3. We could define them as the output of a neural network.
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4. Let’s stop a bit to rest.
Summary

Input weights can be seen as a function.
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4. Example: handling of sequential data.
Having all possible input neurons at once

Instead of optimizing input weights, we could use all of them:

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and only optimize the output weights \(\rightarrow\) this is convex.
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3. The optimal solution is of the form:
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4. With a sign transfer function, this integral can be computed analytically and yields a kernel machine.
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   \[ f(x) = \int_E w(\nu)g(\nu \cdot x) \, d\nu \]
   and only optimize the output weights \( \longrightarrow \) this is convex.

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5. \( K_{\text{sign}}(x, y) = A - B \|x - y\| \)
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6. \( K_{\text{sign}}(x, y) = A - B \|x - y\| \)

7. This kernel has no hyperparameter.
## Results on USPS with 6000 training samples

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$wd = 10^{-3}$</th>
<th>$wd = 10^{-6}$</th>
<th>$wd = 10^{-12}$</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{\text{sign}}$</td>
<td>2.27±0.13</td>
<td>1.80±0.08</td>
<td>1.80±0.08</td>
<td>4.07</td>
</tr>
<tr>
<td>G. $\sigma = 1$</td>
<td>58.27±0.50</td>
<td>58.54±0.27</td>
<td>58.54±0.27</td>
<td>58.29</td>
</tr>
<tr>
<td>G. $\sigma = 2$</td>
<td>7.71±0.10</td>
<td>7.78±0.21</td>
<td>7.78±0.21</td>
<td>12.31</td>
</tr>
<tr>
<td>G. $\sigma = 4$</td>
<td>1.72±0.11</td>
<td>2.09±0.09</td>
<td>2.10±0.09</td>
<td>4.07</td>
</tr>
<tr>
<td>G. $\sigma = 6$</td>
<td>1.67±0.10</td>
<td>2.78±0.25</td>
<td>3.33±0.35</td>
<td>3.58</td>
</tr>
<tr>
<td>G. $\sigma = 7$</td>
<td>1.72±0.10</td>
<td>3.04±0.26</td>
<td>4.39±0.49</td>
<td>3.77</td>
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</tbody>
</table>
Results on MNIST with 6000 training samples

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$wd = 10^{-3}$</th>
<th>$wd = 10^{-6}, 10^{-9}, 10^{-12}, 0$</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{\text{sign}}$</td>
<td>5.51 ± 0.22</td>
<td>4.54 ± 0.50</td>
<td>4.09</td>
</tr>
<tr>
<td>G. $\sigma = 1$</td>
<td>77.55 ± 0.40</td>
<td>77.55 ± 0.40</td>
<td>80.03</td>
</tr>
<tr>
<td>G. $\sigma = 2$</td>
<td>10.51 ± 0.46</td>
<td>10.51 ± 0.45</td>
<td>12.44</td>
</tr>
<tr>
<td>G. $\sigma = 3$</td>
<td>3.64 ± 0.10</td>
<td>3.64 ± 0.10</td>
<td>4.1</td>
</tr>
<tr>
<td>G. $\sigma = 5$</td>
<td>3.01 ± 0.12</td>
<td>3.01 ± 0.12</td>
<td>3.33</td>
</tr>
<tr>
<td>G. $\sigma = 7$</td>
<td>3.15 ± 0.09</td>
<td>3.18 ± 0.10</td>
<td>3.48</td>
</tr>
</tbody>
</table>
Results on LETTERS with 6000 training samples

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>( wd = 10^{-3} )</th>
<th>( wd = 10^{-6} )</th>
<th>( wd = 10^{-9} )</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K_{\text{sign}} )</td>
<td>5.36 ± 0.10</td>
<td>5.22 ± 0.09</td>
<td>5.22 ± 0.09</td>
<td>5.5</td>
</tr>
<tr>
<td>G. ( \sigma = 2 )</td>
<td>5.47 ± 0.14</td>
<td>5.93 ± 0.15</td>
<td>5.92 ± 0.14</td>
<td>5.8</td>
</tr>
<tr>
<td>G. ( \sigma = 4 )</td>
<td>4.97 ± 0.10</td>
<td>11.06 ± 0.29</td>
<td>12.50 ± 0.35</td>
<td>5.3</td>
</tr>
<tr>
<td>G. ( \sigma = 6 )</td>
<td>6.27 ± 0.17</td>
<td>8.47 ± 0.20</td>
<td>17.61 ± 0.40</td>
<td>6.63</td>
</tr>
<tr>
<td>G. ( \sigma = 8 )</td>
<td>8.45 ± 0.19</td>
<td>6.11 ± 0.15</td>
<td>18.69 ± 0.34</td>
<td>9.25</td>
</tr>
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</table>
We showed that training a neural network can be seen as learning an input weight function.
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We introduced an affine-by-part parametrization of that function which corresponds to a continuous number of hidden units.
Summary

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

2. We introduced an affine-by-part parametrization of that function which corresponds to a continuous number of hidden units.

3. 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.
Future work

Learning the transfer function using a neural network.
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1. Learning the transfer function using a neural network.
2. Find other (and better) parametrizations of the input weight function.
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1. Learning the transfer function using a neural network.
2. Find other (and better) parametrizations of the input weight function.
3. Recursively define the input weight function as the output of a neural network.
Now is the time for ...
Computing $\int_E \text{sign}(\mathbf{v} \cdot \mathbf{x} + b)\text{sign}(\mathbf{v} \cdot \mathbf{y} + b) \, dvdb$

1. \(\text{sign}(x)\) function is invariant with respect to the norm of \(x\).
2. \(\text{sign}(\mathbf{v} \cdot \mathbf{x} + b)\text{sign}(\mathbf{v} \cdot \mathbf{y} + b) = \text{sign}(\mathbf{v} \cdot \mathbf{x} + b)(\mathbf{v} \cdot \mathbf{y} + b)\).
3. When \(b\) ranges from \(-M\) to \(+M\), for \(M\) large enough, \(x'\mathbf{v}v'y + b\) is negative on an interval of size \(|\mathbf{v} \cdot (x - y)|\).
4. \(\int_{b=-M}^{+M} \text{sign}(x'\mathbf{v}v'y + b) \, db = 2M - 2|\mathbf{v} \cdot (x - y)|\).
5. Integrating this term on the unit hypersphere yields a kernel of the form \(K(x, y) = A - B\|x - y\|\).
Additive and multiplicative invariance of the covariance matrix

1. In SVM and kernel regression, the elements of the weights vector $\alpha$ sum to 0.
2. The final solution involves $K\alpha$.
3. Thus, adding a term $\frac{\delta}{n}ee'$ to every element of the covariance matrix yields the solution
   \[(K + \frac{\delta}{n}ee')\alpha = K\alpha + \frac{\delta}{n}e(e'\alpha) = K\alpha.\]
4. 
   \[
   C(K, \alpha, b, \lambda) = \mathcal{L}(K\alpha + b, Y) + \lambda\alpha'K\alpha \\
   C\left(\frac{K}{c}, c\alpha, b, \frac{\lambda}{c}\right) = \mathcal{L}\left(\frac{K}{c}c\alpha + b, Y\right) + \frac{\lambda}{c}c\alpha'\frac{K}{c}c\alpha \\
   = C(K, c\alpha, b, \lambda)
   \]