A Formal Proof of the Expressiveness of Deep Learning

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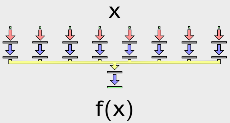
Motivation

- Case study of proof assistance in the field of machine learning
- Development of general-purpose libraries
- Study of the mathematics behind deep learning

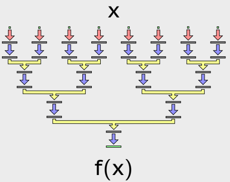
Fundamental Theorem of Network Capacity
(Cohen, Sharir & Shashua, 2015)

Shallow network



needs exponentially more nodes to express the same function as

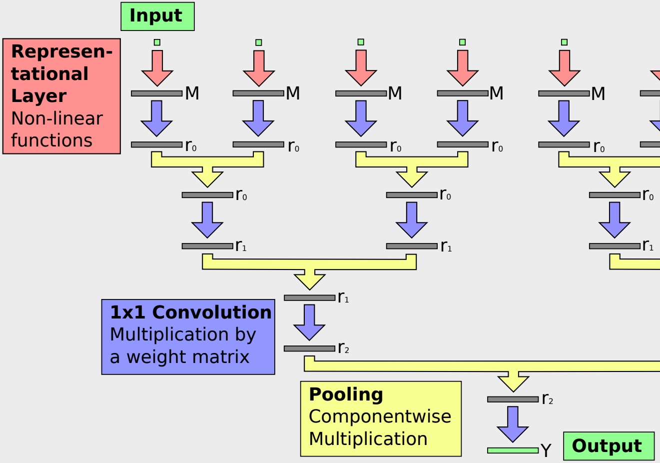
deep network



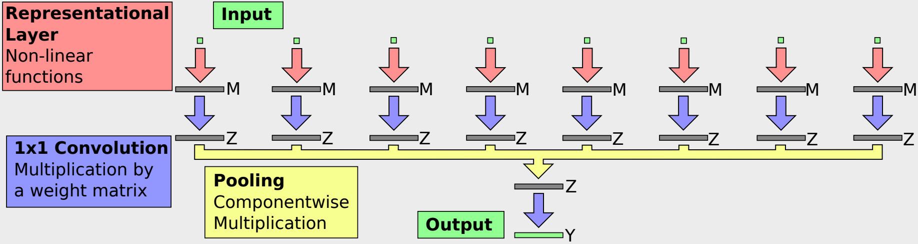
for the vast majority of functions*

* except for a Lebesgue null set of functions

Deep convolutional arithmetic circuit



Shallow convolutional arithmetic circuit



Convolutional arithmetic circuits $\neq$ CNNs

- CACs are not quite the standard architecture

But:

- Easier to analyze
- Allow to prove similar results for CNNs
- Perform better than CNNs when computational resources are limited

The proof on one slide

- **Def1** Define a tensor $\mathcal{A}(\mathrm{w})$ that describes the function expressed by the deep network with weights w
- **Lem1** The CP-rank of $\mathcal{A}(\mathrm{w})$ tells how many nodes the shallow network needs to express the same function
- **Def2** Define a polynomial p with the deep network weights w as variables
- **Lem2** If $\mathrm{p}(\mathrm{w}) \neq 0$, then $\mathcal{A}(\mathrm{w})$ has a high CP-rank
- **Lem3** $\mathrm{p}(\mathrm{w}) \neq 0$ almost everywhere

Restructuring the proof

Before

Def1	Tensors
Lem1	Tensors, shallow network
Induction over the deep network	
Lem2	Polynomials, Matrices
Def2	Polynomials, Tensors
Lem3a	Matrices, Tensors
Lem3b	Measures, Polynomials

After

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Def2	Polynomials, Tensors

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Induction over the deep network

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* except for a zero set of a polynomial

Lebesgue measure

definition lborel :: (α :: euclidean_space) measure

Isabelle's standard probability library

Lebesgue measure

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Isabelle's standard probability library

Solution:

My new definition

definition $\mathsf{lborel_f}$ :: nat $\Rightarrow$ (nat $\Rightarrow$ real) measure **where**
$\mathsf{lborel_f}\ \mathsf{n} = \prod_{\mathsf{M}} \mathsf{b} \in \{..< \mathsf{n}\}.\ (\mathsf{lborel} :: \mathsf{real\ measure})$

Matrices

- Isabelle's multivariate analysis library
- Sternagel & Thiemann's matrix library
  (Archive of Formal Proofs, 2010)
- Thiemann & Yamada's matrix library
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I added definitions and lemmas for

- matrix rank
- submatrices

Multivariate polynomials

Lochbihler & Haftmann's polynomial library

I added various definitions, lemmas, and the theorem

- "Zero sets of polynomials $\not\equiv 0$ are Lebesgue null sets."

theorem
  fixes p :: real mpoly
  assumes $\mathsf{p} \neq 0$ **and** vars $\mathsf{p} \subseteq \{..<\mathsf{n}\}$
  shows $\{\mathsf{x} \in \mathsf{space}\ (\mathsf{lborel}_\mathsf{f}\ \mathsf{n}).\ \mathsf{insertion}\ \mathsf{x}\ \mathsf{p} = 0\}$
  $\in \mathsf{null\_sets}\ (\mathsf{lborel}_\mathsf{f}\ \mathsf{n})$

My tensor library

typedef α tensor $=$
$\{(\mathsf{ds} :: \mathsf{nat\ list}, \mathsf{as} :: \alpha\ \mathsf{list}).\ |\mathsf{as}| = \prod \mathsf{ds}\}$

- addition, multiplication by scalars, tensor product, matricization, CP-rank
- Powerful induction principle uses subtensors:
  - Slices a $d_1 \times d_2 \times \cdots \times d_N$ tensor into d_1 subtensors of dimension $d_2 \times \cdots \times d_N$

Type for convolutional arithmetic circuits

datatype α cac $=$

$\boxed{\text{Input nat}}$ | $\boxed{\text{Conv } \alpha \ (\alpha \text{ cac})}$ | $\boxed{\text{Pool } (\alpha \text{ cac}) \ (\alpha \text{ cac})}$

Type for convolutional arithmetic circuits

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$$\textbf{fun}\ \mathsf{insert\_weights} :: \underbrace{(\mathsf{nat} \times \mathsf{nat})\ \mathsf{cac}}_{\text{network without weights}} \Rightarrow \underbrace{(\mathsf{nat} \Rightarrow \mathsf{real})}_{\text{weights}} \Rightarrow \underbrace{\mathsf{real\ mat\ cac}}_{\text{network with weights}}$$

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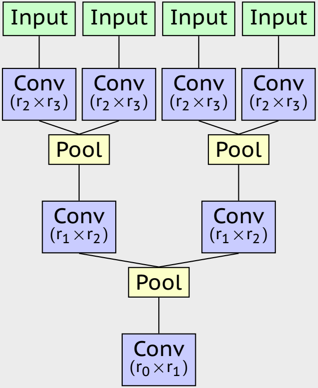
fun evaluate_net :: $\underbrace{\text{real mat cac}}_{\text{network}} \Rightarrow \underbrace{\text{real vec list}}_{\text{input}} \Rightarrow \underbrace{\text{real vec}}_{\text{output}}$

Deep network parameters

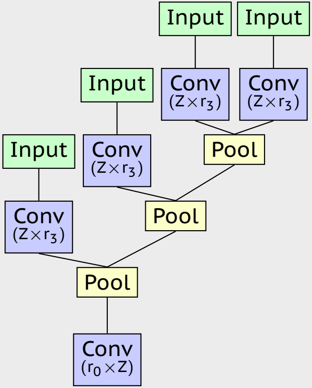
locale deep_net_params =
  fixes rs :: nat list
  assumes length rs $\geq$ 3
  and $\forall$r $\in$ set rs. 0 $<$ r

Deep and shallow networks

deep_net $=$



shallow_net Z $=$



Def1 Define a tensor $\mathcal{A}(\mathrm{w})$ that describes the function expressed by the deep network with weights w

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$\mathcal{A}$ w = tensor_from_net (insert_weights deep_net w)

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fun tensor_from_net :: real mat cac $\Rightarrow$ real tensor

If two networks express the same function, the representing tensors are the same

Lem1 The CP-rank of $\mathcal{A}(\mathrm{w})$ tells how many nodes the shallow network needs to express the same function

```
lemma
  cprank (tensor_from_net
                (insert_weights w (shallow_net Z))) ≤ Z
```

- by definition of CP-rank

Def2 Define a polynomial p with the deep network weights w as variables

Easy to define as a function:

definition $\mathsf{p}_{\mathsf{func}} :: (\mathsf{nat} \Rightarrow \mathsf{real}) \Rightarrow \mathsf{real}$ **where**

$\mathsf{p}_{\mathsf{func}}\ \mathsf{w} = \mathsf{det}\ (\mathsf{submatrix}\ [\mathcal{A}\ \mathsf{w}]\ \mathsf{rows\_with\_1}\ \mathsf{rows\_with\_1})$

But:

We must prove that $\mathsf{p}_{\mathsf{func}}$ corresponds to a polynomial

Lem2 If $p(w) \neq 0$, then $\mathcal{A}(w)$ has a high CP-rank

lemma
assumes $p_{func}\ w \neq 0$
shows $r^{N\_half} \leq \text{cprank}\ (\mathcal{A}\ w)$

- Follows directly from definition of p_{func} using properties of matricization and of matrix rank

Lem3 $p(w) \neq 0$ almost everywhere

Theorem:
Zero sets of polynomials $\not\equiv 0$ are Lebesgue null sets

Hence it suffices to show that $p \not\equiv 0$

So we need a weight configuration w with $p(w) \neq 0$

Final theorem

theorem

$\forall_{\mathrm{ae}}\, \mathsf{w_d}$ w.r.t. $\mathsf{lborel_f}$ weight_space_dim. $\nexists \mathsf{w_s}\ \mathsf{Z}$.

$\mathsf{Z} < \mathsf{r}^{\mathsf{N\_half}} \wedge$

$\forall$is. input_correct is $\longrightarrow$

evaluate_net (insert_weights deep_net $\mathsf{w_d}$) is $=$

evaluate_net (insert_weights (shallow_net Z) $\mathsf{w_s}$) is

Conclusion

Outcome

- First formalization on deep learning
  Substantial development ($\sim$ 7000 lines including developed libraries)
- Development of libraries
  New tensor library and extension of other libraries
- Generalization of the theorem
  Proof restructuring led to a more precise result

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More information:

http://www.cs.vu.nl/~abp290/

Archive of Formal Proofs entry

ITP paper

M.Sc. thesis