# Lecture 2: A dynamic view on universal interpolation and gradient descent 

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## Part I

# Deep neural networks, generic universal interpolation, and controlled ODEs 

based on joint work with M. Larsson and J. Teichmann

## Goal

Analysis of deep feedforward neural networks from an optimal control theory point of view:

- deep neural networks as discretizations of certain controlled ODEs
- expressiveness and generic universal interpolation
- randomly generated generic expressiveness $\Rightarrow$ large numbers of parameters can be left untrained, and be chosen randomly


## Definition of a deep feedfoward neural network

- Feedfoward neural networks are maps obtained by composing layers consisting of an affine map and a componentwise nonlinearity $\sigma$ :

$$
x(0) \xrightarrow{\ell_{1}} x(1) \xrightarrow{\ell_{2}} x(2) \longrightarrow x(t) \cdots \xrightarrow{\ell_{n}} x(n)
$$

where $x(t) \in \mathbb{R}^{m}$ and

$$
\ell_{t}(x)=\left(\sigma\left(\left\langle A_{t, 1}, x\right\rangle+b_{t, 1}\right), \ldots, \sigma\left(\left\langle A_{t, m}, x\right\rangle+b_{t, m}\right)\right) .
$$

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There is usually a (linear) readout map $R$ such that

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x(n) \longrightarrow R x(n)=y
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- For a given training data set $\left\{\left(x_{i}, y_{i}\right), i=1, \ldots N\right\}$, supervised learning means selecting the parameters of $\left(A_{t}, b_{t}\right)_{t \in\{1, \ldots, n\}}$ and $R$ such that

$$
y_{i} \approx R \circ \ell_{n} \circ \cdots \circ \ell_{1}\left(x_{i}\right), \quad \forall i
$$

## Residual networks

- Define $V\left(x, \theta_{t}\right):=\ell_{t}(x)-x$, where $\theta_{t}$ collects all the parameters of $\ell_{t}$.
- Then $x(t)=x(t-1)+V\left(x(t-1), \theta_{t}\right)$, which is sometimes called residual network (see, e.g. He et al. ('15)).
- This is nothing else than a discretization of an ODE

$$
d X_{t}^{\times}=V\left(X_{t}^{\times}, \theta_{t}\right) d t, \quad X_{0}^{\times}=x .
$$

- The feedforward neural network is then modeled by

$$
x \mapsto R\left(X_{1}^{x}\right)
$$

and can be interpreted as a network of continuous depth. The discrete parameter counting the layers is replaced by $t \in[0,1]$.

- This perspective on neural networks can also be found in e.g. E('17); Chang et al.('17); Chen et al.('18); Grathwohl et al.('18); Dupont et al.('19), Liu and Markowich('19).


## Supervised learning as a control problem

- For a given training data set $\left\{\left(x_{i}, y_{i}\right), i=1, \ldots N\right\}$ supervised learning now means selecting $V\left(\cdot, \theta_{t}\right)$ and $R$ so that

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y_{i} \approx R\left(X_{1}^{x_{i}}\right) \quad \forall i
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- We view this training task as a (deterministic) control problem: the $N$ inputs $x_{i}$ should be directed to their respective outputs $y_{i}$, all using the same vector fields.


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- We view this training task as a (deterministic) control problem: the $N$ inputs $x_{i}$ should be directed to their respective outputs $y_{i}$, all using the same vector fields.
- Indeed, recognize $d X_{t}^{\times}=V\left(X_{t}^{x}, \theta_{t}\right) d t$ as controlled ordinary differential equation (CODE) by supposing that

$$
V(x, \theta)=u^{1} V_{1}(x)++u^{d} V_{d}(x)
$$

where $u^{1}, \ldots, u^{d}$ are scalars and $V_{1}, \ldots, V_{d}$ are smooth vector fields on $\mathbb{R}^{m}$.

- We think of $u^{1}, \cdots, u^{d}$ as the only $d$ trainable parameters (part of $\theta$ ) that will be $t$-dependent. The vector fields $V_{1}, \ldots, V_{d}$ are specified by the remaining parameters in $\theta$, which will be non-trainable and constant in $t$.


## The role of randomness and few trainable parameters

- Recall that $V(x, \theta)$ was initially specifed by $V\left(x, \theta_{t}\right)=\ell_{t}(x)-x$ with $\ell_{t}(x)=\left(\sigma\left(\left\langle A_{t, 1}, x\right\rangle+b_{t, 1}\right), \ldots, \sigma\left(\left\langle A_{t, m}, x\right\rangle+b_{t, m}\right)\right)=\sigma\left(A_{t} x+b_{t}\right)$.
- For each layer $t$, a $m \times m$ matrix $A_{t}$ and a vector $b_{t} \in \mathbb{R}^{m}$ has to be trained.
- Our results imply training of very few parameters: for instance we can specify

$$
V\left(x, \theta_{t}\right)=\sum_{i=1}^{7} u_{t}^{i} \sigma_{i}\left(C_{i} x+d_{i}\right)
$$

where $C_{i}$ is a random matrix, $d_{i}$ a random vector and $\sigma_{i}$ polynomials with random coefficients. Only $u_{t}^{i}$ are subject to training to achieve what we call generic expressiveness.

## Universal approximation

One form of expressiveness of neural networks is the universal approximation property.

## Universal approximation (meta)-theorem

Any continuous (say) function $f:[0,1]^{m} \rightarrow \mathbb{R}$ can be uniformly approximated to arbitrary accuracy by a neural network of sufficient depth and/or width.

- This is a very important part of the theory of deep and shallow learning.
- Prominent contributions include Cybenko ('89), Hornik ('91), Barron ('93), Shaham et al. ('16), Bölcskei et al. ('16), etc.


## Universal interpolation

- Another form is what we shall call universal interpolation.
- The system

$$
\begin{equation*}
d X_{t}^{\times}=u_{t}^{1} V_{1}\left(X_{t}^{\times}\right)+\cdots u_{t}^{d} V_{d}\left(X_{t}\right) d t \tag{}
\end{equation*}
$$

turns out to be expressive in the following sense if $V_{1}, \ldots, V_{d}$ are chosen appropriately.

## Universal interpolation

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## Definition

The control system $\left(^{*}\right)$, specified by $V_{1}, \ldots, V_{d}$, is called a universal $N$-point interpolator on $\Omega \subseteq \mathbb{R}^{m}$ if, for any training set $\left\{\left(x_{i}, y_{i}\right) \in \Omega \times \Omega: i=1, \ldots, N\right\}$, there exist controls $u_{t}^{1}, \ldots, u_{t}^{d}$ that achieve the exact matching

$$
X_{1}^{x_{i}}=y_{i} \quad \forall i=1, \ldots, N .
$$

Here it is required that the training inputs and outputs are both pairwise distinct.

- Perfect interpolation is not necessarily a desirable training goal, but here it serves as a measure of expressiveness. The readout $R$ is here the identity.


## 1-point controllability

## Toy training data set $N=1$

- Can we control any input $x \in \mathbb{R}^{m}$ to any output $y \in \mathbb{R}^{m}$ ?


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## Notation

- Lie brackets of vector fields $V$ and $W$ :

$$
[V, W](x)=D W(x) V(x)-D V(x) W(x)
$$

Example: For linear vector fields $V(x)=A x, W(x)=B x$, this is $[V, W](x)=(A B-B A) x$.

- Lie algebra of all vector fields generated by $V_{1}, \ldots, V_{d}$ :

$$
\operatorname{Lie}\left(V_{1}, \ldots, V_{d}\right)=\operatorname{span}\left\{V_{1}, \ldots, V_{d} \text { and their iterated Lie brackets }\right\}
$$

- Evaluation of Lie algebra at $x \in \mathbb{R}^{m}$

$$
\left.\operatorname{Lie}\left(V_{1}, \ldots, V_{d}\right)\right|_{x}=\left\{W(x): W \in \operatorname{Lie}\left(V_{1}, \ldots, V_{d}\right)\right\} \subseteq \mathbb{R}^{m}
$$

## Chow-Rashevskii for 1-point controllability

Theorem (Chow - Rashevsky)
If the Hörmander condition

$$
\left.\operatorname{Lie}\left(V_{1}, \ldots, V_{d}\right)\right|_{x}=\mathbb{R}^{m}
$$

holds at every point $x \in \mathbb{R}^{m}$, then controllability holds: for every input/output pair $(x, y)$ there exist smooth scalar controls $u_{t}^{1}, \ldots, u_{t}^{d}$ that achieve $X_{1}^{x}=y$, where $X_{t}$ is the solution of (*).

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Why Lie brackets?

- Consider linear vector fields $V(x)=A x$ and $W(x)=B x$.
- Flowing along $V$ for a time t gives $x \mapsto e^{t A} x$.
- Alternating between $W, V,-W$, and $-V$ :

$$
e^{-t A} e^{-t B} e^{t A} e^{t B} x=x+t^{2}(A B-B A) x+O\left(t^{3}\right)
$$

This produces motion in the direction $[V, W](x)=(A B-B A) x$.

## Universal $N$-point interpolation

## Training data set of size $N$

- Can we simultanously control inputs $\bar{x}=\left(x_{1}, \ldots, x_{N}\right) \in\left(\mathbb{R}^{m}\right)^{N}$ to outputs $\bar{y}=\left(y_{1}, \ldots, y_{N}\right) \in\left(\mathbb{R}^{m}\right)^{N}$ using a common set of vector fields and controls?
- If yes, how many and which vector fields do we need?
- Consider the "stacked" system

$$
\frac{d}{d t} \underbrace{\left(\begin{array}{c}
X_{t}^{x_{1}} \\
\vdots \\
X_{t}^{x_{N}}
\end{array}\right)}_{\bar{X}_{t}^{\bar{区}}}=u_{t}^{1} \underbrace{\left(\begin{array}{c}
V_{1}\left(X_{t}^{x_{1}}\right) \\
\vdots \\
V_{1}\left(X_{t}^{\times_{N}}\right)
\end{array}\right)}_{V_{1}^{\oplus N}\left(\bar{X}_{t}^{\overline{\overline{ }}}\right)}+\cdots+u_{t}^{d} \underbrace{\left(\begin{array}{c}
V_{d}\left(X_{t}^{x_{1}}\right) \\
\vdots \\
V_{d}\left(X_{t}^{x_{N}}\right)
\end{array}\right)}_{V_{d}^{\oplus N}\left(\bar{X}_{t}^{\overline{\bar{x}})}\right.} .
$$

with initial values in the space of pairwise distinct $N$-tuples: $\bar{\Omega}=\Omega^{N} \backslash \Delta$ with $\Delta=\left\{\left(x_{1}, \ldots, x_{N}\right) \in \Omega^{N}: x_{i}=x_{j}\right.$ for some $\left.i \neq j\right\}$.

- By the Chow-Rashevskii theorem, controllability holds true provided that the $N$-point Hörmander condition, $\operatorname{Lie}\left(V_{1}^{\oplus N}(\bar{x}), \ldots, \ldots V_{d}^{\oplus N}(\bar{x})\right)=\left(\mathbb{R}^{m}\right)^{N}$ holds at every $\bar{x}=\left(x_{1}, \ldots, x_{N}\right) \in \bar{\Omega}$.


## First result

## Theorem

Fix $m \geq 2$ and a bounded open connected subset $\Omega \subseteq \mathbb{R}^{m}$. There exist $d=5$ smooth bounded vector fields $V_{1}, \ldots, V_{5}$ on $\mathbb{R}^{m}$ such that

$$
\begin{equation*}
d X_{t}^{\times}=u_{t}^{1} V_{1}\left(X_{t}^{\times}\right)+\cdots u_{t}^{d} V_{d}\left(X_{t}\right) d t \tag{}
\end{equation*}
$$

is a universal $N$-point interpolator in $\Omega$, for every $N$.

## Remarks

- $m=1$ is not covered (on the real line inputs cannot be directed to outputs if they are differently ordered)
- Note that $d=5$ is independent of both $N$ and $m$, and the same vector fields (but not the same controls) work for any $N$.
- 5 is probably not optimal.


## Sketch of the proof

- Let $V_{1}(x)=A x, V_{2}(x)=B x$, where $A$ and $B$ are suitable traceless $m \times m$ matrices and

$$
V_{3}(x)=\left(\begin{array}{c}
0 \\
\vdots \\
0 \\
1
\end{array}\right), \quad V_{4}(x)=\left(\begin{array}{c}
\left(x^{m}\right)^{2} \\
0 \\
\vdots \\
0
\end{array}\right), \quad V_{5}(x)=\left(\begin{array}{c}
x^{1} x^{m} \\
x^{2} x^{m} \\
\vdots \\
\left(x^{m}\right)^{2}
\end{array}\right) .
$$

Then $\operatorname{Lie}\left(V_{1}, \ldots, V_{5}\right)$ contains all polynomial vector fields.

- The set of all polynomial vector fields on $\mathbb{R}^{m}$ interpolates at every $\bar{x} \in \bar{\Omega}$, i.e. for every $\bar{x} \in \bar{\Omega}$ and $\bar{y} \in\left(\mathbb{R}^{m}\right)^{N}$ there exists some polynomial vector field $V$ s.t. $V\left(x_{i}\right)=y_{i}$ for all $i$. The same property thus holds for $\operatorname{Lie}\left(V_{1}, \ldots, V_{5}\right)$.
- This implies the $N$-point Hörmander condition for these five vector fields at every $\bar{x}$ and in turn the $N$-point interpolator property.


## Generic expressiveness

- So far: universal interpolators can be constructed using just five vector fields.
- Our next goal is to prove that such expressive systems are generic.
- Appropriately randomly chosen nonlinear polynomial vector fields allow to generate controlled $\operatorname{ODEs}\left(^{*}\right)$ that are sufficiently expressive to interpolate almost every training set.
- Instead of using the identity as final read out, we relate here the input $x$ and output $y$ via

$$
\begin{aligned}
y & =\lambda\left(X_{1}^{x}-x\right), \text { with } X_{1}^{x} \text { solving } \\
d X_{t}^{x} & =u_{t}^{1} V_{1}\left(X_{t}^{x}\right)+\cdots u_{t}^{d} V_{d}\left(X_{t}^{x}\right)
\end{aligned}
$$

where $\lambda$ is some scalar parameter which has to be trained.

## Main result - Ingredients

- Bounded open connected subset $\Omega \subset \mathbb{R}^{m}, m \geq 2$
- A polynomial vector field $V$ of degree at most $k$ has components of the form

$$
V^{j}(x)=\sum_{|\alpha|=0}^{k} c_{\alpha}^{j} x^{\alpha}
$$

Coefficient vector: $\mathbf{c}=\left(c_{\alpha}^{j}: j=1, \ldots, m,|\alpha| \leq k\right) \in \mathbb{R}^{D_{k}}$ where $D_{k}=m\binom{m+k}{m}$.

- $d \geq 5$ polynomial vector fields $V_{1}, \ldots, V_{d}$ of degree at most $k \geq 2$ in $\Omega$, with coefficients $\left(\mathbf{c}_{1}, \ldots, \mathbf{c}_{d}\right)$
- For some $I \in \mathbb{N}$, some polynomial map $Q: \mathbb{R}^{\prime} \rightarrow\left(\mathbb{R}^{D_{k}}\right)^{d}$, and some random vector $Z$ in $\mathbb{R}^{\prime}$, we assume the coefficients are drawn randomly in the following way.

$$
\left(\mathbf{c}_{1}, \ldots, \mathbf{c}_{d}\right)=Q(Z)
$$

## Main result

Theorem (C., M. Larsson and J. Teichmann)
Assume that
(1) the law of $Z$ admits a probability density on $\mathbb{R}^{\prime}$;
(2) for some $\hat{z} \in \mathbb{R}^{\prime}$, the Lie algebra generated by the vector fields with coefficients $\left(\widehat{\mathbf{c}}_{1}, \ldots, \widehat{\mathbf{c}}_{d}\right)=Q(\widehat{z})$ contains all polynomial vector fields;
(3) the training data set is generic: inputs $x_{i}$ of $\left\{\left(x_{i}, y_{i}\right) \in \Omega \times \Omega: i=1, \ldots, N\right\}$ are drawn from some density on $(\Omega)^{N}$; outputs $y_{i}$ are just pairwise distinct.

Then, with probability one, (**) forms a universal interpolator, i.e. there exist controls $u_{t}^{1}, \ldots, u_{t}^{d}$ and a constant $\lambda>0$ such that $y_{i}=\lambda\left(X_{1}^{x_{i}}-x_{i}\right)$ for all $i$.

Example

- Let $I=\left(D_{k}\right)^{5}$ and $Q$ be the identity map.
- Draw $\left(\mathbf{c}_{1}, \ldots, \mathbf{c}_{d}\right)$ from any density on $\left(\mathbb{R}^{D_{k}}\right)^{5}$.
- Take $\widehat{z}=\left(\widehat{\mathbf{c}}_{1}, \ldots, \widehat{\mathbf{c}}_{5}\right)$, where $\left(\widehat{\mathbf{c}}_{1}, \ldots, \widehat{\mathbf{c}}_{5}\right)$ are the coefficients of the specific 5 polynomial vector fields from above.


## Idea of the proof

- Let $\vec{V}=\left(V_{1}, \ldots, V_{5}\right)$ be polynomial vector fields parameterized by coefficients $\left(\mathbf{c}_{1}, \ldots, \mathbf{c}_{5}\right) \in\left(\mathbb{R}^{D_{k}}\right)^{5}$ such that $\left(\mathbf{c}_{1}, \ldots, \mathbf{c}_{5}\right)=Q(Z)$ for $Q: \mathbb{R}^{\prime} \rightarrow\left(\mathbb{R}^{D_{k}}\right)^{5}$.
- Let $\left(\widehat{\mathbf{c}}_{1}, \ldots, \widehat{\mathbf{c}}_{5}\right)=Q(\widehat{z})$ are the coefficients of the specific 5 polynomial vector fields $\widehat{V}_{1}, \ldots, \widehat{V}_{5}$ from the previous theorem.
- $\operatorname{Lie}\left(\widehat{V}_{1}, \ldots, \widehat{V}_{5}\right)$ contains a basis $E_{1}(\overrightarrow{\widehat{V}}, x), \ldots, E_{D_{n}}(\vec{V}, x)$ for the space of polynomial vector fields of degree at most $n$.
- To guarantee that $\left\langle E_{1}(\vec{V}, \cdot), \ldots E_{D_{n}}(\vec{V}, \cdot)\right\rangle$ interpolates at $\left(x_{1}, \ldots, x_{N}\right) \in \Omega^{N}$, the $m N \times D_{n}$ matrix

$$
\left(\begin{array}{ccc}
E_{1}\left(\vec{V}, x_{1}\right) & \cdots & E_{D_{n}}\left(\vec{V}, x_{1}\right) \\
\vdots & & \vdots \\
E_{1}\left(\vec{V}, x_{N}\right) & \cdots & E_{D_{n}}\left(\overrightarrow{\vec{V}}, x_{N}\right)
\end{array}\right)
$$

has to have columns that span $\left(\mathbb{R}^{m}\right)^{N}$, i.e. the determinant of at least one $m N \times m N$ matrix has to be nonzero.

## Idea of the proof

- $E_{j}$ are polynomials in $x$, but also in $Z$ (seen as function in $Z$ generating $V$ ). The same holds for the squared determinant $\Gamma_{n}\left(x_{1}, \ldots, x_{N}, Z\right)$.
- Since for $n$ big enough the squared determinant $\Gamma_{n}\left(x_{1}, \ldots, x_{N}, \widehat{z}\right)>0$ for every pairwise distinct data set, we can conclude that

$$
\left(x_{1}, \ldots, x_{N}, Z\right) \mapsto \Gamma_{n}\left(x_{1}, \ldots, x_{N}, Z\right)
$$

it is not identically zero. Here Condition (2) is needed.

- The density condition on the data set and $Z$ is used to avoid zeros which can exist, but which only constitute a nullset.


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- The density condition on the data set and $Z$ is used to avoid zeros which can exist, but which only constitute a nullset.
- With probability 1 , $\operatorname{Lie}\left(V_{1}, \ldots, V_{5}\right)$ interpolates at $\bar{x}$. $\Rightarrow N$-point Hörmander condition holds at $\bar{x}$.
- By continuity, there is an open connected neighborhood $\mathcal{U} \subset \Omega^{N}$ of $\bar{x}$ where the Hörmander condition holds. $\Rightarrow$ Choose $\lambda>0$ large enough so that $\bar{x}+\lambda^{-1} \bar{y} \in \mathcal{U}$.
- The Chow - Rashevskii theorem then implies that $x_{i}+\lambda^{-1} y_{i}$ can be reached $X_{1}^{x_{i}}$ for all $i=1, \ldots, N$.


## Concrete example of neural network typ

## Corollary

Consider $d=7$ vector fields of the form $V_{i}(x)=\sigma_{i}\left(C_{i} x+b_{i}\right), i=1, \ldots, 7$, where

- $C_{i}$ is a random matrix in $\mathbb{R}^{m \times m}, b_{i}$ a random vector in $\mathbb{R}^{m}$, and
- $\sigma_{i}(\cdot)$ a polynomial nonlinearity, whose coefficients depend polynomially on some random vector $Z_{0}$.

Assume that
(1) the random elements $Z=\left(Z_{0}, C_{1}, \ldots, C_{7}, b_{1}, \ldots, b_{7}\right)$ admit a joint density;
(2) for some value $\hat{z}_{0}$ of $\operatorname{supp}\left(\operatorname{law}\left(Z_{0}\right)\right)$, we have $\sigma_{i}(r)=r$ for $i=1,2,3$, and $\sigma_{i}(r)=r^{2}$ for $i=4,5,6,7$;
(3) the training data set is generic.

Then with probability one, $\left({ }^{* *}\right)$ forms a universal interpolator in the sense of the above Theorem.

## Consequences for training

- Universal interpolation is a generic property.
- In practice, the $\operatorname{CODE}\left({ }^{*}\right)$ is replaced by a discretization, say with $M$ steps.
- This yields a network of depth $M$. After randomly choosing $d$ vector fields, the number of trainable parameters (including $\lambda$ ) becomes $M d+1$.
- This tends to be much smaller than the total number of parameters needed to specify the vector fields, and can potentially simplify the training task significantly.
- The fact that most parameters are chosen randomly reinforces the view that randomness is a crucial ingredient for training.


## Conclusion

- Deep feedforward neural networks can be modeled as controlled dynamical systems.
- Expressiveness can be proved in this formulation using classical results on controllability.
- Expressiveness is generic since $\operatorname{Lie}\left(V_{1}^{\oplus N}, \ldots V_{d}^{\oplus N}\right)$ generically spans $\left(\mathbb{R}^{m}\right)^{N}$.
- Many parameters can be chosen randomly, which truely works in applications.
- We illustrate this with the MNIST data set by training a generic network with much less trainable parameters than in the standard implementation.


## Part II

## Gradient descent and backpropagation

## Supervised learning task with neural networks

## Supervised learning

Given training data $\left\{\left(x_{i}, y_{i}\right), i=1, \ldots N\right\}$ with $x_{i} \in \mathbb{R}^{m}$ and $y_{i} \in \mathbb{R}^{d}$, find a neural network $g$ within a class of neural networks $N N_{\Theta}$ with a certain architecture characterized by parameters $\theta \in \Theta$, such that

$$
g \in \underset{N N_{\ominus}}{\operatorname{argmin}} \sum_{i=1}^{N} \mathcal{L}\left(g\left(x_{i}\right), y_{i}\right),
$$

where $\mathcal{L}$ is a loss function: $C\left(\mathbb{R}^{m}, \mathbb{R}^{\widetilde{d}}\right) \times \mathbb{R}^{d} \rightarrow \mathbb{R}_{+}$. Note that the input dimension of the neural network is $m$ and the output dimension $\widetilde{d}$.

Since $g$ is determined by the parameters $\theta$, the above optimization corresponds to searching the minimum in the parameter space $\Theta$ which is nothing else than the collection of $\left(A_{t}, b_{t}\right)_{t=1, \ldots, n}$ (if we have $n$ hidden layers) and the readout map $R$.

## Examples

- Example MNIST classification: $x_{i} \in \mathbb{R}^{28 \times 28}$, i.e. $m=28 \times 28$ and $\underset{\sim}{y} \in \mathbb{R}$, i.e. $d=1$. The output dimension of the neural network is $d=10$. The loss function is given by

$$
\mathcal{L}(g(x), y)=\sum_{k=1}^{10} 1_{\{y=k-1\}} \log \left((g(x))_{k}\right)
$$

- Example classical regression with $L^{2}$ loss:

$$
\mathcal{L}(g(x), y)=\|g(x)-y\|^{2} .
$$

Here the output dimension of the neural network $\widetilde{d}$ is equal to $d$.

## But how...?

- ... to deal with a non-linear, non-convex optimization problem and with around 600000 parameters, as it is the case for the MNIST data set?


## Gradient descent: the simplest method

- The gradient of a function $F(\theta): \mathbb{R}^{M} \rightarrow \mathbb{R}$ is given by

$$
\nabla F(\theta)=\left(\partial_{\theta_{1}} F(\theta), \ldots, \partial_{\theta_{M}} F(\theta)\right)
$$

- Gradient descent:
starting with an initial guess $\theta^{(0)}$, one iteratively defines for some learning rate $\eta_{k}$

$$
\theta^{(k+1)}=\theta^{(k)}-\eta_{k} \nabla F\left(\theta^{(k)}\right)
$$

## Gradient descent: the simplest method



## Classical convergence result

## Theorem

Suppose the function $F: \mathbb{R}^{M} \rightarrow \mathbb{R}$ is convex and differentiable, and that its gradient is Lipschitz continuous with constant $L>0$, i.e. we have that $\|\nabla F(\theta)-\nabla F(\beta)\| \leq L\|\theta-\beta\|$ for any $\theta, \beta \in \mathbb{R}^{M}$. Then if we run gradient descent for $k$ iterations with a fixed step size $\eta \leq 1 / L$, it will yield a solution $F\left(\theta^{(k)}\right)$ which satisfies

$$
F\left(\theta^{(k)}\right)-F\left(\theta^{*}\right) \leq \frac{\left\|\theta^{(0)}-\theta^{*}\right\|^{2}}{2 \eta k},
$$

where $F\left(\theta^{*}\right)$ is the optimal value. Intuitively, this means that gradient descent is guaranteed to converge and that it converges with rate $O(1 / k)$.

In practice, the convexity condition is often not satisfied. Moreover, the solution depends crucially on the inital value.

## How to compute the gradient

- Nevertheless all optimization algorithms build on the classical idea of gradient descent usually in its enhanced form of stochastic gradient descent.
- How to compute the gradient in our case of supervised learning, where

$$
F(\theta)=\sum_{i=1}^{N} \mathcal{L}\left(g\left(x_{i} \mid \theta\right), y_{i}\right)
$$

and $\theta$ corresponds to $\left(A_{t}, b_{t}\right)_{t=1, \ldots, n}$ (if we have $n$ hidden layers) and the readout map $R$ ? We here indicate the dependence of the neural network on $\theta$.

- We suppose here for simplicity that the readout map $R$ is linear, i.e.

$$
R(x)=A_{n+1} x+b
$$

where $A_{n+1}$ has $\widetilde{d}$ rows and $b \in \mathbb{R}^{\widetilde{d}}$, so that $\theta=\left\{\left(A_{t}, b_{t}\right)_{t=1, \ldots, n+1}\right\}$.

## Backpropagation

- Since

$$
\nabla_{\theta} F(\theta)=\sum_{i=1}^{N} \nabla_{\theta} \mathcal{L}\left(g\left(x_{i} \mid \theta\right), y_{i}\right)
$$

we need to determine $\partial_{A_{t}, k l} \mathcal{L}(g(x \mid \theta), y)$ and $\partial_{b_{t}, k} \mathcal{L}(g(x \mid \theta), y)$.

- By the chain rule this is given by

$$
\begin{aligned}
\partial_{A_{t}, k l} \mathcal{L}(g(x \mid \theta), y) & =\left\langle\partial_{g} \mathcal{L}(g(x \mid \theta), y), \partial_{A_{t}, k l} g(x \mid \theta)\right\rangle \\
\partial_{b_{t}, k} \mathcal{L}(g(x \mid \theta), y) & =\left\langle\partial_{g} \mathcal{L}(g(x \mid \theta), y), \partial_{b_{t}, k} g(x \mid \theta)\right\rangle .
\end{aligned}
$$

- Output Layer:

$$
\begin{aligned}
& \partial_{A_{n+1}, k \mathcal{L}} \mathcal{L}(g(x \mid \theta), y)=\left(\partial_{g} \mathcal{L}(g(x \mid \theta)) y\right)_{k}(\underbrace{\sigma\left(A_{n}(\cdots)+b_{n}\right)}_{x(n)}) \\
& \partial_{b_{n+1}, k} \mathcal{L}(g(x \mid \theta), y)=\left(\partial_{g} \mathcal{L}(g(x \mid \theta)) y\right)_{k}
\end{aligned}
$$

## Backpropagation: second last layer

- Recall $x(t+1)=\sigma\left(z_{t+1}\right)$ where $z_{t+1}=A_{t+1} x(t)+b_{t+1}$ and $g=z_{n+1}=A_{n+1} \times(n)+b_{n+1}$.
- To continue with the second last layer, we use the chain rule again Note that $\mathcal{L}(g, y)=\mathcal{L}\left(z_{n+1}, y\right)=\mathcal{L}\left(A_{n+1} x(n)+b_{n}, y\right)$. Hence..

$$
\begin{aligned}
\partial_{A_{n}, k \mid} \mathcal{L} & =\left\langle\partial_{x(n)} \mathcal{L}, \partial_{A_{n}, k \mid x}(n)\right\rangle=\left\langle A_{n+1} \partial_{g} \mathcal{L}, \partial_{A_{n}, k \mid} x(n)\right\rangle \\
& =\langle A_{n+1} \partial_{g} \mathcal{L}, \operatorname{diag}\left(\sigma^{\prime}\left(z_{n}\right)\right) \underbrace{}_{\text {similar as in the last layer }} \underbrace{\partial_{A_{2}}}_{A_{n}, k \mid z_{n}}\rangle
\end{aligned}
$$

