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

Christa Cuchiero based on joint lectures with M. Gambara, J. Teichmann and Hanna Wutte

> Institute of Statistics and Mathematics Vienna University of Economics and Business

# 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 ⇒ 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 *σ*:

$$x(0) \xrightarrow{\ell_1} x(1) \xrightarrow{\ell_2} x(2) \longrightarrow \cdots x(t) \cdots \xrightarrow{\ell_n} x(n),$$

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

$$\ell_t(x) = (\sigma(\langle A_{t,1}, x \rangle + b_{t,1}), \dots, \sigma(\langle A_{t,m}, x \rangle + b_{t,m})).$$

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

 $x(n) \longrightarrow Rx(n) = y.$ 

#### 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 *σ*:

$$x(0) \xrightarrow{\ell_1} x(1) \xrightarrow{\ell_2} x(2) \longrightarrow \cdots x(t) \cdots \xrightarrow{\ell_n} x(n),$$

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

$$\ell_t(x) = (\sigma(\langle A_{t,1}, x \rangle + b_{t,1}), \dots, \sigma(\langle A_{t,m}, x \rangle + b_{t,m})).$$

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

 $x(n) \longrightarrow Rx(n) = y.$ 

For a given training data set {(x<sub>i</sub>, y<sub>i</sub>), i = 1,...,N}, supervised learning means selecting the parameters of (A<sub>t</sub>, b<sub>t</sub>)<sub>t∈{1,...,n}</sub> and R such that

$$y_i \approx R \circ \ell_n \circ \cdots \circ \ell_1(x_i), \quad \forall i$$

## Residual networks

- Define  $V(x, \theta_t) := \ell_t(x) x$ , where  $\theta_t$  collects all the parameters of  $\ell_t$ .
- Then x(t) = x(t-1) + V(x(t-1), θ<sub>t</sub>), which is sometimes called residual network (see, e.g. He et al. ('15)).
- This is nothing else than a discretization of an ODE

 $dX_t^{\times} = V(X_t^{\times}, \theta_t)dt, \quad X_0^{\times} = x.$ 

• The feedforward neural network is then modeled by

 $x \mapsto R(X_1^x)$ 

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 {(x<sub>i</sub>, y<sub>i</sub>), i = 1,...N} supervised learning now means selecting V(·, θ<sub>t</sub>) and R so that

$$y_i \approx R(X_1^{x_i}) \quad \forall i.$$

• We view this training task as a (deterministic) control problem: the N inputs x<sub>i</sub> should be directed to their respective outputs y<sub>i</sub>, all using the same vector fields.

#### Supervised learning as a control problem

For a given training data set {(x<sub>i</sub>, y<sub>i</sub>), i = 1,...N} supervised learning now means selecting V(·, θ<sub>t</sub>) and R so that

$$y_i \approx R(X_1^{x_i}) \quad \forall i.$$

- We view this training task as a (deterministic) control problem: the N inputs x<sub>i</sub> should be directed to their respective outputs y<sub>i</sub>, all using the same vector fields.
- Indeed, recognize  $dX_t^{\times} = V(X_t^{\times}, \theta_t)dt$  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  $u^1, \dots, u^d$  as the only *d* trainable parameters (part of  $\theta$ ) that will be *t*-dependent. The vector fields  $V_1, \dots, V_d$  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  $V(x,\theta_t) = \ell_t(x) x$  with  $\ell_t(x) = (\sigma(\langle A_{t,1}, x \rangle + b_{t,1}), \dots, \sigma(\langle A_{t,m}, x \rangle + b_{t,m})) = \sigma(A_tx + b_t).$
- 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

$$V(x,\theta_t) = \sum_{i=1}^7 u_t^i \sigma_i (C_i x + d_i)$$

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  $f : [0,1]^m \to \mathbb{R}$  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

$$dX_t^{\times} = u_t^1 V_1(X_t^{\times}) + \cdots + u_t^d V_d(X_t) dt \tag{(*)}$$

turns out to be expressive in the following sense if  $V_1, \ldots, V_d$  are chosen appropriately.

## Universal interpolation

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

$$dX_t^{\times} = u_t^1 V_1(X_t^{\times}) + \cdots + u_t^d V_d(X_t) dt \tag{(*)}$$

turns out to be expressive in the following sense if  $V_1, \ldots, V_d$  are chosen appropriately.

#### Definition

The control system (\*), 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  $\{(x_i, y_i) \in \Omega \times \Omega : i = 1, \ldots, N\}$ , there exist controls  $u_t^1, \ldots, u_t^d$  that achieve the exact matching

$$X_1^{x_i} = y_i \quad \forall i = 1, \dots, N.$$

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  $y \in \mathbb{R}^m$ ?

## 1-point controllability

#### Toy training data set N = 1

- Can we control any input  $x \in \mathbb{R}^m$  to any output  $y \in \mathbb{R}^m$ ?
- The answer is given by the classical Chow Rashevskii theorem.

## 1-point controllability

#### Toy training data set N = 1

- Can we control any input  $x \in \mathbb{R}^m$  to any output  $y \in \mathbb{R}^m$ ?
- The answer is given by the classical Chow Rashevskii theorem.

#### Notation

• Lie brackets of vector fields V and W:

$$[V, W](x) = DW(x)V(x) - DV(x)W(x)$$

Example: For linear vector fields V(x) = Ax, W(x) = Bx, this is [V, W](x) = (AB - BA)x.

• Lie algebra of all vector fields generated by  $V_1, \ldots, V_d$ :

 $\text{Lie}(V_1, \ldots, V_d) = \text{span}\{V_1, \ldots, V_d \text{ and their iterated Lie brackets}\}$ 

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

 $\operatorname{Lie}(V_1,\ldots,V_d)|_x = \{W(x): W \in \operatorname{Lie}(V_1,\ldots,V_d)\} \subseteq \mathbb{R}^m$ 

## Chow-Rashevskii for 1-point controllability

Theorem (Chow - Rashevsky)

If the Hörmander condition

 $Lie(V_1,\ldots,V_d)|_x = \mathbb{R}^m$ 

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 (\*).

## Chow-Rashevskii for 1-point controllability

#### Theorem (Chow - Rashevsky)

If the Hörmander condition

$$Lie(V_1,\ldots,V_d)|_x = \mathbb{R}^m$$

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 (\*).

#### Why Lie brackets?

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

$$e^{-tA}e^{-tB}e^{tA}e^{tB}x = x + t^2(AB - BA)x + O(t^3)$$

This produces motion in the direction [V, W](x) = (AB - BA)x.

## Universal N-point interpolation

#### Training data set of size N

- Can we simultanously control inputs  $\bar{x} = (x_1, \dots, x_N) \in (\mathbb{R}^m)^N$  to outputs  $\bar{y} = (y_1, \dots, y_N) \in (\mathbb{R}^m)^N$  using a common set of vector fields and controls?
- If yes, how many and which vector fields do we need?
- Consider the "stacked" system

$$\frac{d}{dt}\underbrace{\begin{pmatrix}X_t^{x_1}\\\vdots\\X_t^{x_N}\\\bar{X}_t^{\bar{x}}\end{pmatrix}}_{\bar{X}_t^{\bar{x}}} = u_t^1\underbrace{\begin{pmatrix}V_1(X_t^{x_1})\\\vdots\\V_1(X_t^{x_N})\end{pmatrix}}_{V_1^{\oplus N}(\bar{X}_t^{\bar{x}})} + \dots + u_t^d\underbrace{\begin{pmatrix}V_d(X_t^{x_1})\\\vdots\\V_d(X_t^{x_N})\end{pmatrix}}_{V_d^{\oplus N}(\bar{X}_t^{\bar{x}})}$$

with initial values in the space of pairwise distinct *N*-tuples:  $\overline{\Omega} = \Omega^N \setminus \Delta$ with  $\Delta = \{(x_1, \dots, x_N) \in \Omega^N : x_i = x_j \text{ for some } i \neq j\}.$ 

 By the Chow-Rashevskii theorem, controllability holds true provided that the N-point Hörmander condition, Lie(V<sub>1</sub><sup>⊕N</sup>(x̄),..., V<sub>d</sub><sup>⊕N</sup>(x̄)) = (ℝ<sup>m</sup>)<sup>N</sup> holds at every x̄ = (x<sub>1</sub>,..., x<sub>N</sub>) ∈ Ω̄.

Christa Cuchiero (WU Wien)

#### First result

#### Theorem

Fix  $m \ge 2$  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

$$dX_t^{\times} = u_t^1 V_1(X_t^{\times}) + \cdots + u_t^d V_d(X_t) dt \qquad (*$$

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  $V_1(x) = Ax$ ,  $V_2(x) = Bx$ , where A and B are suitable traceless  $m \times m$  matrices and

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

Then Lie $(V_1, \ldots, V_5)$  contains all polynomial vector fields.

- The set of all polynomial vector fields on ℝ<sup>m</sup> interpolates at every x̄ ∈ Ω̄, i.e. for every x̄ ∈ Ω̄ and ȳ ∈ (ℝ<sup>m</sup>)<sup>N</sup> there exists some polynomial vector field V s.t. V(x<sub>i</sub>) = y<sub>i</sub> for all i. The same property thus holds for Lie(V<sub>1</sub>,..., V<sub>5</sub>).
- 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 ODEs (\*) 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

$$y = \lambda(X_1^{\times} - x), \text{ with } X_1^{\times} \text{ solving}$$
  
 $dX_t^{\times} = u_t^1 V_1(X_t^{\times}) + \cdots u_t^d V_d(X_t^{\times})$ 

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

$$V^j(x) = \sum_{|lpha|=0}^k c^j_{lpha} x^{lpha}.$$

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

- d ≥ 5 polynomial vector fields V<sub>1</sub>,..., V<sub>d</sub> of degree at most k ≥ 2 in Ω, with coefficients (c<sub>1</sub>,..., c<sub>d</sub>)
- For some  $l \in \mathbb{N}$ , some polynomial map  $Q : \mathbb{R}^{l} \to (\mathbb{R}^{D_{k}})^{d}$ , and some random vector Z in  $\mathbb{R}^{l}$ , we assume the coefficients are drawn randomly in the following way.

$$(\mathbf{c}_1,\ldots,\mathbf{c}_d)=Q(Z).$$

#### Main result

#### Theorem (C., M. Larsson and J. Teichmann)

Assume that

- the law of Z admits a probability density on  $\mathbb{R}^{l}$ ;
- Solution the training data set is generic: inputs x<sub>i</sub> of {(x<sub>i</sub>, y<sub>i</sub>) ∈ Ω × Ω: i = 1,..., N} are drawn from some density on (Ω)<sup>N</sup>; outputs y<sub>i</sub> 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  $y_i = \lambda(X_1^{x_i} - x_i)$  for all *i*.

#### Example

- Let  $I = (D_k)^5$  and Q be the identity map.
- Draw  $(\mathbf{c}_1, \ldots, \mathbf{c}_d)$  from any density on  $(\mathbb{R}^{D_k})^5$ .
- Take  $\hat{z} = (\hat{c}_1, \dots, \hat{c}_5)$ , where  $(\hat{c}_1, \dots, \hat{c}_5)$  are the coefficients of the specific 5 polynomial vector fields from above.

## Idea of the proof

- Let V

   (V<sub>1</sub>,...,V<sub>5</sub>) be polynomial vector fields parameterized by coefficients (c<sub>1</sub>,...,c<sub>5</sub>) ∈ (ℝ<sup>D<sub>k</sub></sup>)<sup>5</sup> such that (c<sub>1</sub>,...,c<sub>5</sub>) = Q(Z) for Q: ℝ<sup>l</sup> → (ℝ<sup>D<sub>k</sub></sup>)<sup>5</sup>.
- Let (\$\hat{c}\_1, \ldots, \hat{c}\_5\$) = Q(\$\hat{z}\$) are the coefficients of the specific 5 polynomial vector fields \$\hat{V}\_1, \ldots, \hat{V}\_5\$ from the previous theorem.
- Lie(\$\hat{V}\_1,...,\$\hat{V}\_5\$) contains a basis \$E\_1(\$\vec{V}\$, \$x\$),...,\$E\_{D\_n}(\$\vec{V}\$, \$x\$) for the space of polynomial vector fields of degree at most \$n\$.
- To guarantee that (E<sub>1</sub>(V, ·), ... E<sub>D<sub>n</sub></sub>(V, ·)) interpolates at (x<sub>1</sub>,..., x<sub>N</sub>) ∈ Ω<sup>N</sup>, the mN × D<sub>n</sub> matrix

$$\begin{pmatrix} E_1(\vec{V}, x_1) & \cdots & E_{D_n}(\vec{V}, x_1) \\ \vdots & & \vdots \\ E_1(\vec{V}, x_N) & \cdots & E_{D_n}(\vec{V}, x_N) \end{pmatrix}$$

has to have columns that span  $(\mathbb{R}^m)^N$ , i.e. the determinant of at least one  $mN \times mN$  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  $\Gamma_n(x_1, \ldots, x_N, Z)$ .
- Since for n big enough the squared determinant Γ<sub>n</sub>(x<sub>1</sub>,..., x<sub>N</sub>, ẑ) > 0 for every pairwise distinct data set, we can conclude that

 $(x_1,\ldots,x_N,Z)\mapsto \Gamma_n(x_1,\ldots,x_N,Z)$ 

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.

## 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  $\Gamma_n(x_1, \ldots, x_N, Z)$ .
- Since for n big enough the squared determinant Γ<sub>n</sub>(x<sub>1</sub>,..., x<sub>N</sub>, ẑ) > 0 for every pairwise distinct data set, we can conclude that

 $(x_1,\ldots,x_N,Z)\mapsto \Gamma_n(x_1,\ldots,x_N,Z)$ 

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.
- With probability 1, Lie(V<sub>1</sub>,..., V<sub>5</sub>) interpolates at x̄.
   ⇒ N-point Hörmander condition holds at x̄.
- By continuity, there is an open connected neighborhood U ⊂ Ω<sup>N</sup> of x̄ where the Hörmander condition holds. ⇒ Choose λ > 0 large enough so that x̄ + λ<sup>-1</sup>ȳ ∈ 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, ..., N.

## Concrete example of neural network typ

#### Corollary

Consider d = 7 vector fields of the form  $V_i(x) = \sigma_i(C_i x + b_i), i = 1, ..., 7$ , where

- $C_i$  is a random matrix in  $\mathbb{R}^{m \times m}$ ,  $b_i$  a random vector in  $\mathbb{R}^m$ , and
- σ<sub>i</sub>(·) a polynomial nonlinearity, whose coefficients depend polynomially on some random vector Z<sub>0</sub>.

#### Assume that

- **1** the random elements  $Z = (Z_0, C_1, \ldots, C_7, b_1, \ldots, b_7)$  admit a joint density;
- **2** for some value  $\hat{z}_0$  of supp(law( $Z_0$ )), we have  $\sigma_i(r) = r$  for i = 1, 2, 3, and  $\sigma_i(r) = r^2$  for i = 4, 5, 6, 7;
- Ithe training data set is generic.

Then with probability one, (\*\*) forms a universal interpolator in the sense of the above Theorem.

## Consequences for training

- Universal interpolation is a generic property.
- In practice, the CODE (\*) 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 Md + 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 Lie $(V_1^{\oplus N}, \dots, V_d^{\oplus N})$  generically spans  $(\mathbb{R}^m)^N$ .
- 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  $\{(x_i, y_i), i = 1, ..., N\}$  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  $NN_{\Theta}$  with a certain architecture characterized by parameters  $\theta \in \Theta$ , such that

$$g \in \operatorname*{argmin}_{NN_{\Theta}} \sum_{i=1}^{N} \mathcal{L}(g(x_i), y_i),$$

where  $\mathcal{L}$  is a loss function:  $C(\mathbb{R}^m, \mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}_+$ . 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  $(A_t, b_t)_{t=1,...,n}$  (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  $y \in \mathbb{R}$ , i.e. d = 1. The output dimension of the neural network is  $\tilde{d} = 10$ . The loss function is given by

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

• Example classical regression with  $L^2$  loss:

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

Here the output dimension of the neural network d is equal to d.

#### But how...?

• ... to deal with a non-linear, non-convex optimization problem and with around 600 000 parameters, as it is the case for the MNIST data set?

## Gradient descent: the simplest method

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

$$\nabla F(\theta) = (\partial_{\theta_1} F(\theta), \dots, \partial_{\theta_M} F(\theta)).$$

• Gradient descent:

starting with an initial guess  $\theta^{(0)}$ , one iteratively defines for some learning rate  $\eta_k$ 

$$\theta^{(k+1)} = \theta^{(k)} - \eta_k \nabla F(\theta^{(k)})$$

#### Gradient descent: the simplest method



## Classical convergence result

#### Theorem

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

$$\mathsf{F}( heta^{(k)})-\mathsf{F}( heta^*)\leq rac{\| heta^{(0)}- heta^*\|^2}{2\eta k},$$

where  $F(\theta^*)$  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 initial 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

$$F(\theta) = \sum_{i=1}^{N} \mathcal{L}(g(x_i|\theta), y_i)$$

and  $\theta$  corresponds to  $(A_t, b_t)_{t=1,...,n}$  (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  $\tilde{d}$  rows and  $b \in \mathbb{R}^{\tilde{d}}$ , so that  $\theta = \{(A_t, b_t)_{t=1,...,n+1}\}$ .

## Backpropagation

Since

$$abla_{ heta} F( heta) = \sum_{i=1}^{N} 
abla_{ heta} \mathcal{L}(g(x_i | m{ heta}), y_i),$$

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

• By the chain rule this is given by

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

• Output Layer:

$$\partial_{A_{n+1},kl}\mathcal{L}(g(x|\theta),y) = (\partial_g \mathcal{L}(g(x|\theta))y)_k(\underbrace{\sigma(A_n(\cdots)+b_n)}_{x(n)})_l$$

$$\partial_{b_{n+1},k}\mathcal{L}(g(x|\theta),y) = (\partial_g\mathcal{L}(g(x|\theta))y)_k$$

#### Backpropagation: second last layer

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

$$\partial_{A_n,kl}\mathcal{L} = \langle \partial_{x(n)}\mathcal{L}, \partial_{A_n,kl}x(n) \rangle = \langle A_{n+1}\partial_g\mathcal{L}, \partial_{A_n,kl}x(n) \rangle$$
$$= \langle A_{n+1}\partial_g\mathcal{L}, \operatorname{diag}(\sigma'(z_n)) \qquad \underbrace{\partial_{A_n,kl}z_n} \rangle$$

similar as in the last layer