ETH
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inf | Informatik
Computer Science

Introduction to Machine Learning

Neural networks / “feature learning”

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Importance of features

- Success in learning crucially depends on the quality of features
- Hand-designing features requires domain-knowledge
- What about kernel methods?
  - Rich set of feature maps
  - Can fit „any function“ with infinite data*
  - Choosing the „right“ kernel can be challenging
  - Computational complexity grows with size of data
- Can we learn good features from data directly??

Learning features

- Learning with *m* hand-designed features

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_{i=1}^{n} \ell\left(y_i; \sum_{j=1}^{m} w_j \phi_j(\mathbf{x}_i)\right)$$

- **Key Idea**: Parameterize the feature maps, and optimize over the parameters!

$$\mathbf{w}^* = \arg\min_{\mathbf{w},\theta} \sum_{i=1}^{n} \ell\left(y_i; \sum_{j=1}^{m} w_j \phi(\mathbf{x}_i, \theta_j)\right)$$

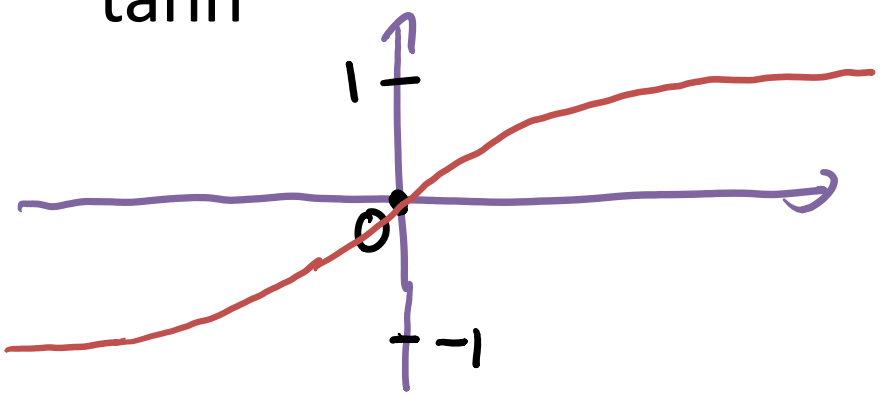
Parameterizing feature maps

- One possibility:

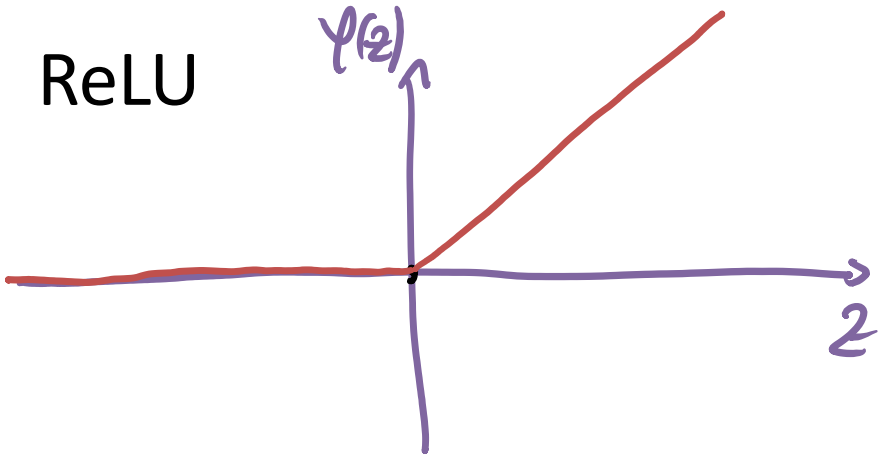
$$\phi(\mathbf{x}, \theta) = \varphi(\theta^T \mathbf{x})$$

- Hereby, $\theta \in \mathbb{R}^d$ and $\varphi : \mathbb{R} \to \mathbb{R}$ is a nonlinear function, called „activation function“

tanh



ReLU



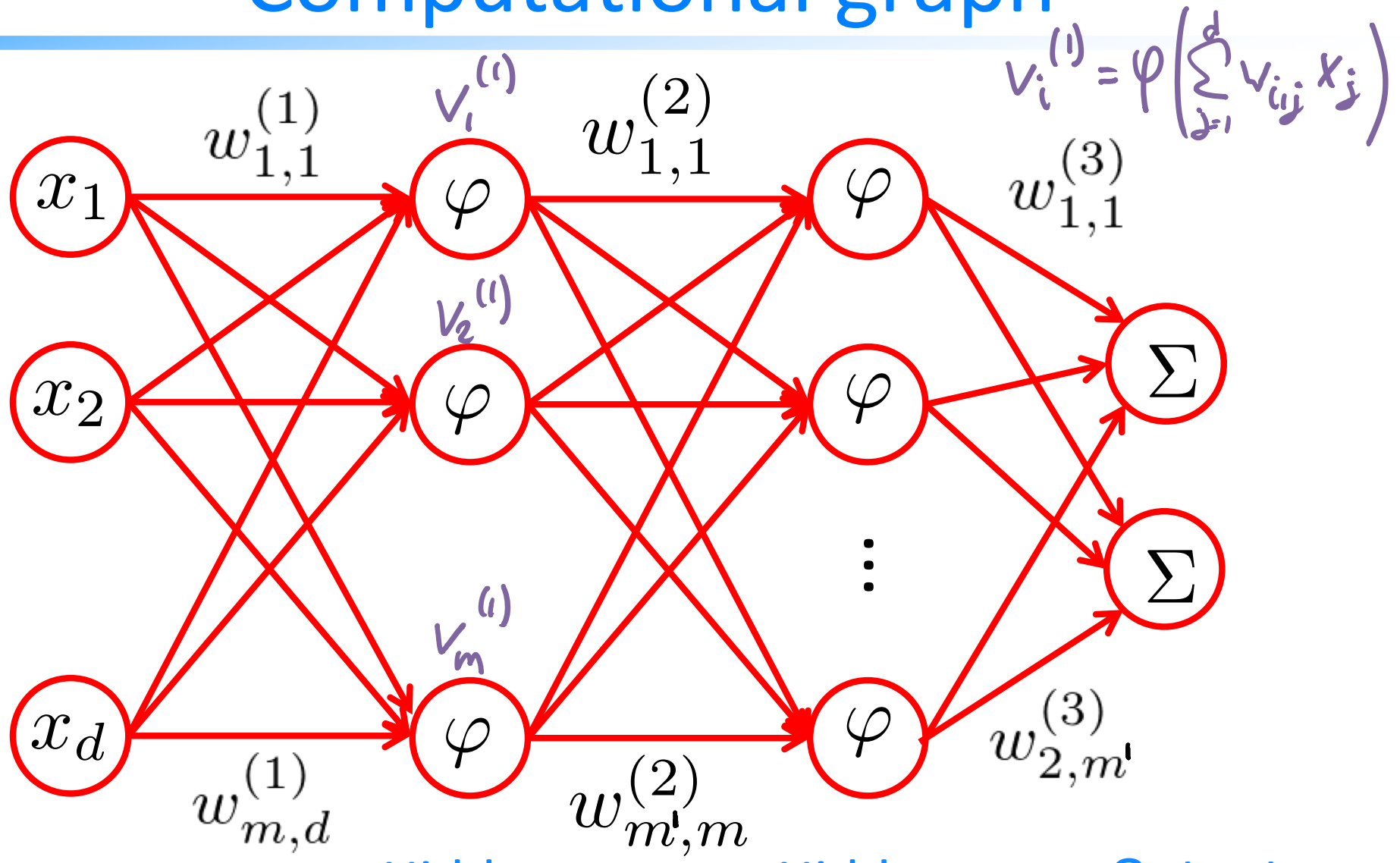
Artificial Neural networks (ANNs)

- Functions of this form

$$f(\mathbf{x}; \mathbf{w}, \theta_{1:d}) = \sum_{j=1}^{m} w_j \varphi(\theta_j^T \mathbf{x}) = \mathbf{w}^T \varphi(\Theta \mathbf{x})$$

- are (examples of) artificial neural networks (ANNs) (also called Multi-layer Perceptrons)
- More generally, the term artificial neural network refers to nonlinear functions which are nested compositions of (variable) linear functions composed with (fixed) nonlinearities

Computational graph



Forward propagation (short notation)

- For input layer: $\mathbf{v}^{(0)} = \mathbf{x}$
- For each hidden layer $\ell = 1 : L-1$

$$\mathbf{z}^{(\ell)} = \mathbf{W}^{(\ell)}\mathbf{v}^{(\ell-1)}$$

$$\mathbf{v}^{(\ell)} = \varphi(\mathbf{z}^{(\ell)})$$

$\varphi([z_1 \dots z_m]) = [\varphi(z_1) \dots \varphi(z_m)]$

- For output layer: $f = \mathbf{W}^{(L)}\mathbf{v}^{(L-1)}$

- Predict: $\mathbf{y} = \mathbf{f}$ (regression)

  or $\mathbf{y} = \text{sign}(\mathbf{f})$ or $y = \arg\max_i f_i$ (class.)

Universal Approximation Theorem

Theorem 2. *Let σ be any continuous sigmoidal function. Then finite sums of the form*

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j^T x + \theta_j)$$

are dense in $C(I_n)$. In other words, given any $f \in C(I_n)$ and $\varepsilon > 0$, there is a sum, $G(x)$, of the above form, for which

$$|G(x) - f(x)| < \varepsilon \qquad \text{for all} \quad x \in I_n.$$

- Cybenko., G. (1989) "Approximations by superpositions of sigmoidal functions", Mathematics of Control, Signals, and Systems, 2 (4), 303-314

➔ demo

How can we train the weights?

- Given data set $D = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n)\}$

  want to optimize weights $\mathbf{W} = (\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)})$
- How do we measure and optimize goodness of fit?

➔ Apply loss function (e.g., Perceptron loss, multi-class hinge loss, square loss, etc.) to output

$$\ell(\mathbf{W}; \mathbf{y}, \mathbf{x}) = \ell\big(\mathbf{y} - f(\mathbf{x}, \mathbf{W})\big)$$

➔ Then optimize the weights to minimize loss over D

$$\hat{\mathbf{W}} = \arg\min_{\mathbf{W}} \sum_{i=1}^{n} \ell(\mathbf{W}; \mathbf{x}_i, y_i)$$

Side note: Losses for multi-outputs

- When predicting multiple outputs at the same time, usually define loss as sum of per-output losses:

$$\ell(\mathbf{W}; \mathbf{y}, \mathbf{x}) = \sum_{i=1}^{p} \ell_i(\mathbf{W}; y_i, \mathbf{x})$$

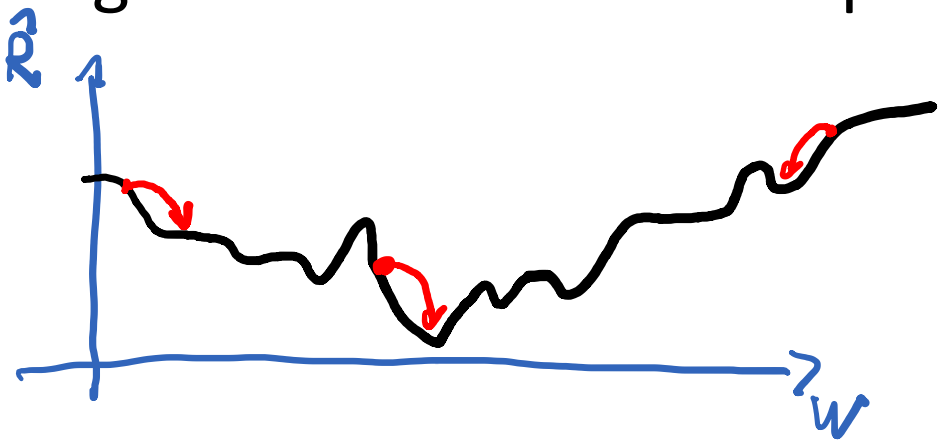
- Examples
  - For regression tasks, i.e., $y_i \in \mathbb{R}$ may use squared loss
  - For classification, may use multiclass Perceptron or hinge loss

How do we optimize over weights?

- Want to do Empirical Risk Minimization

$$\hat{\mathbf{W}} = \arg\min_{\mathbf{W}} \sum_{i=1}^{n} \ell(\mathbf{W}; \mathbf{x}_i, y_i)$$

- I.e., jointly optimize over all weights for all layers to minimize loss over the training data
- This is in general a non-convex optimization problem



- Nevertheless, can try to find a local optimum

Stochastic gradient descent for ANNs

$$\hat{\mathbf{W}} = \arg\min_{\mathbf{W}} \sum_{i=1}^{n} \ell(\mathbf{W}; \mathbf{x}_i, y_i)$$

- Initialize weights $\mathbf{W}$
- For t = 1,2,...
  - Pick data point $(\mathbf{x}, \mathbf{y}) \in D$ uniformly at random
  - Take step in negative gradient direction

$$\mathbf{W} \leftarrow \mathbf{W} - \eta_t \nabla_{\mathbf{W}} \ell(\mathbf{W}; \mathbf{y}, \mathbf{x})$$

ANN Demo

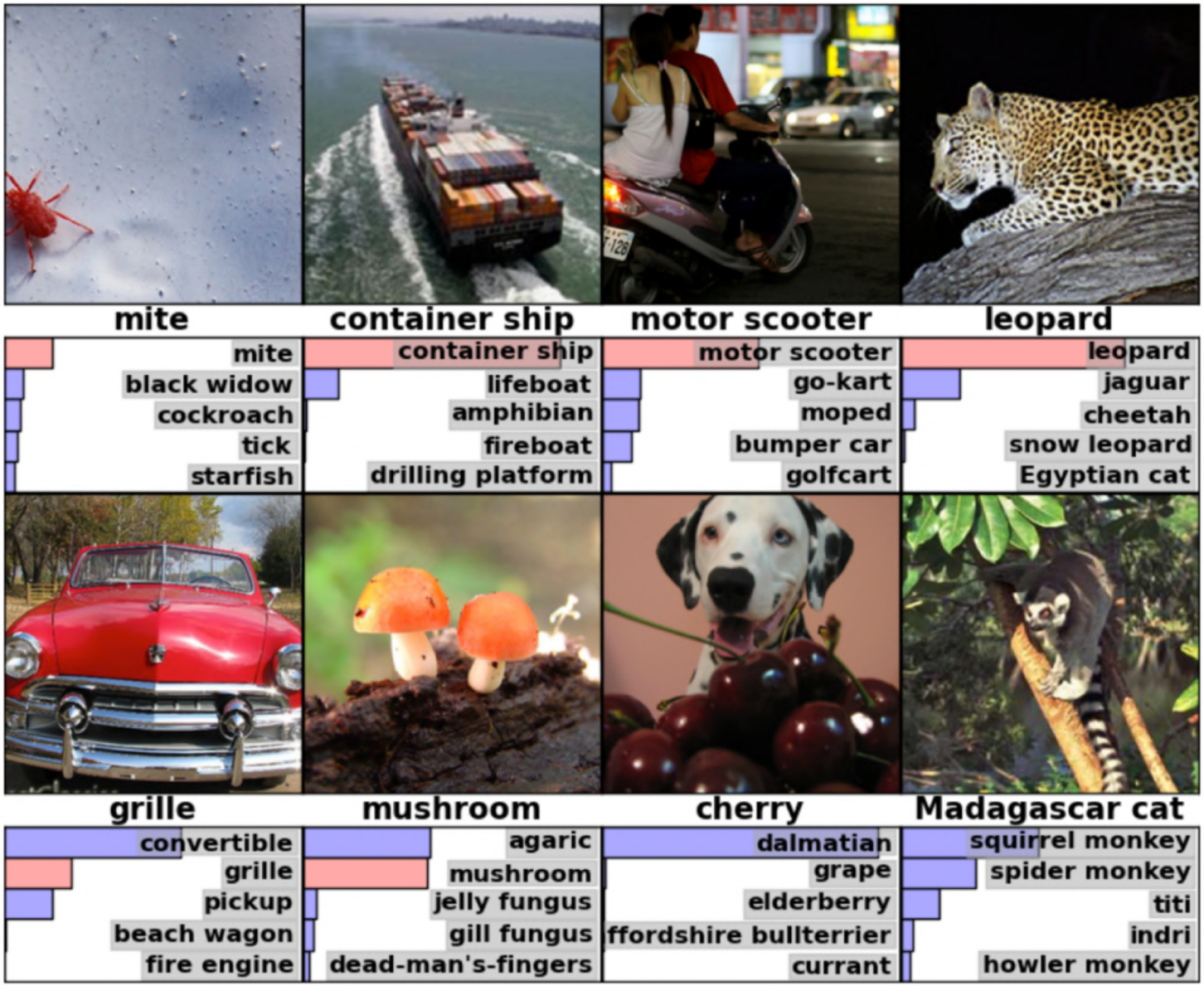
Deep Learning

- Generally refers to models with nested, layered non-linearities
- Common example:
  - Classical ANNs with multiple (many) hidden layers
  - Trained via SGD and variants
  - Some new algorithmic insights (e.g., dropout regularization) and extensions (Convnets, Resnets, RNNs, LSTMs, GRUs...)

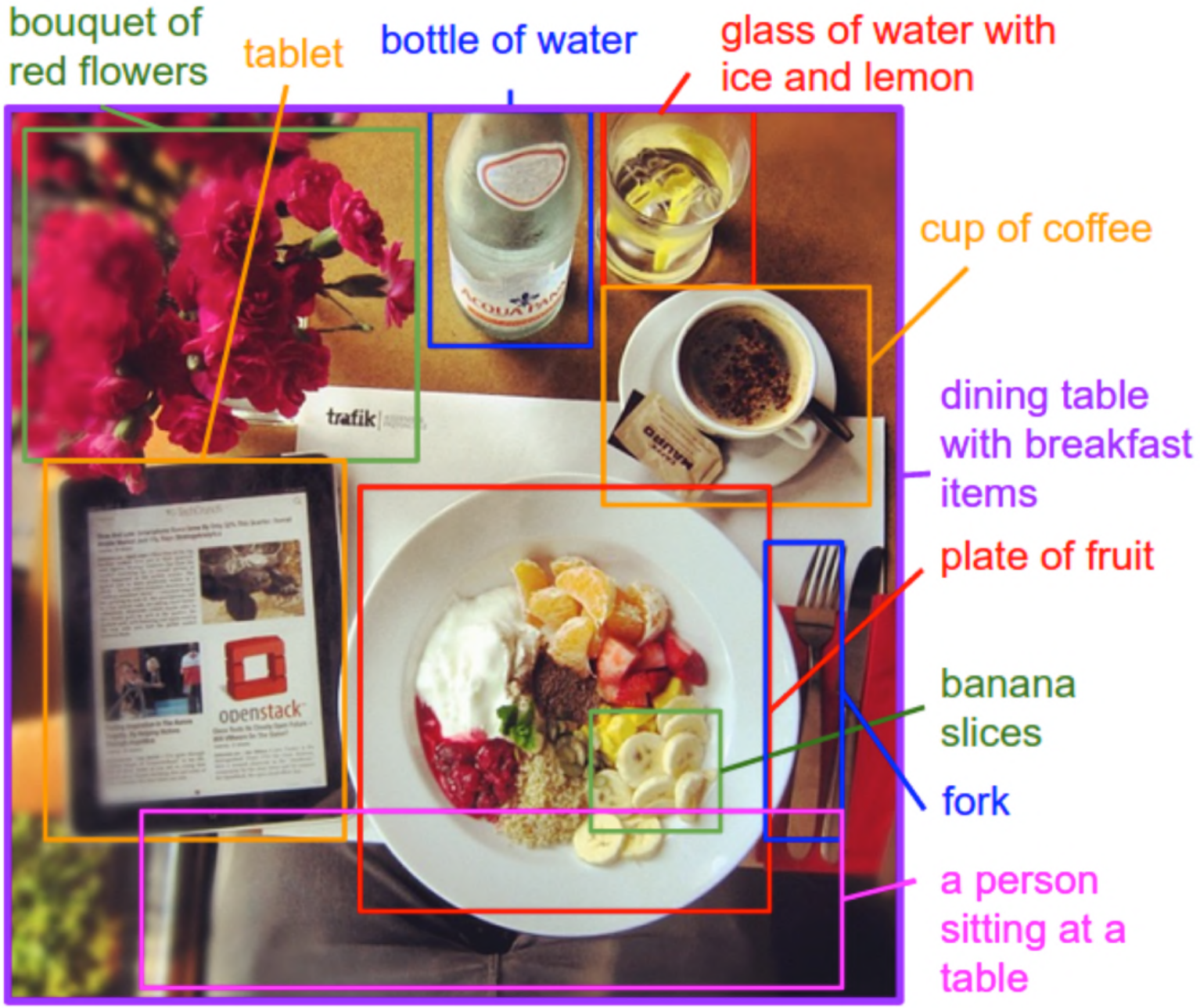
Some deep learning success stories

- State of the art performance on some difficult classification tasks
  - Speech recognition (TIMIT)
  - Image recognition (MNIST, ImageNet)
  - Natural language processing (semantic word embeddings)
  - Speech translation
- A lot of recent work on sequential models (Recurrent Neural Networks, LSTMs, GRUs, …)

Example: Image Classification



Krizhevsky et al. ImageNet Classification with Deep Convolutional Neural Networks ‘12



[Karpathy, Li '14]

Example: Image captioning

Y

X

A person riding a motorcycle on a dirt road.

Two dogs play in the grass.

A skateboarder does a trick on a ramp.

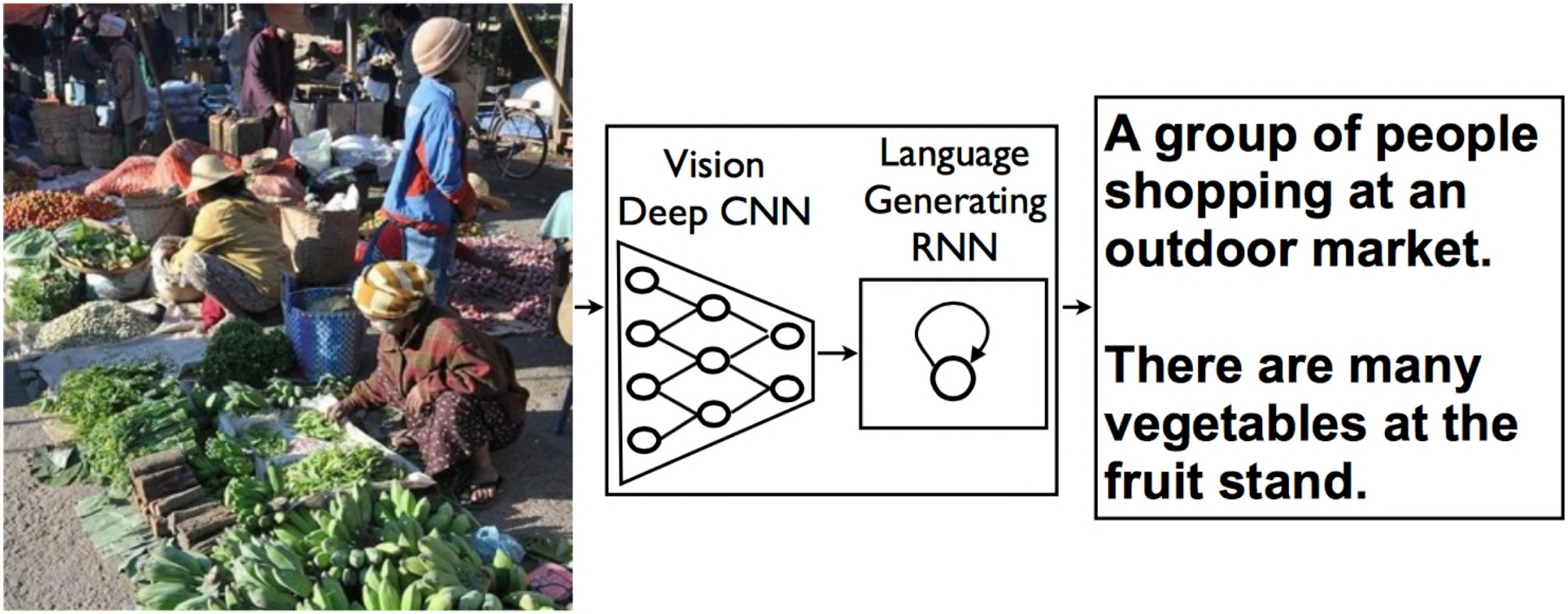
A group of young people playing a game of frisbee.

Two hockey players are fighting over the puck.

A little girl in a pink hat is blowing bubbles.

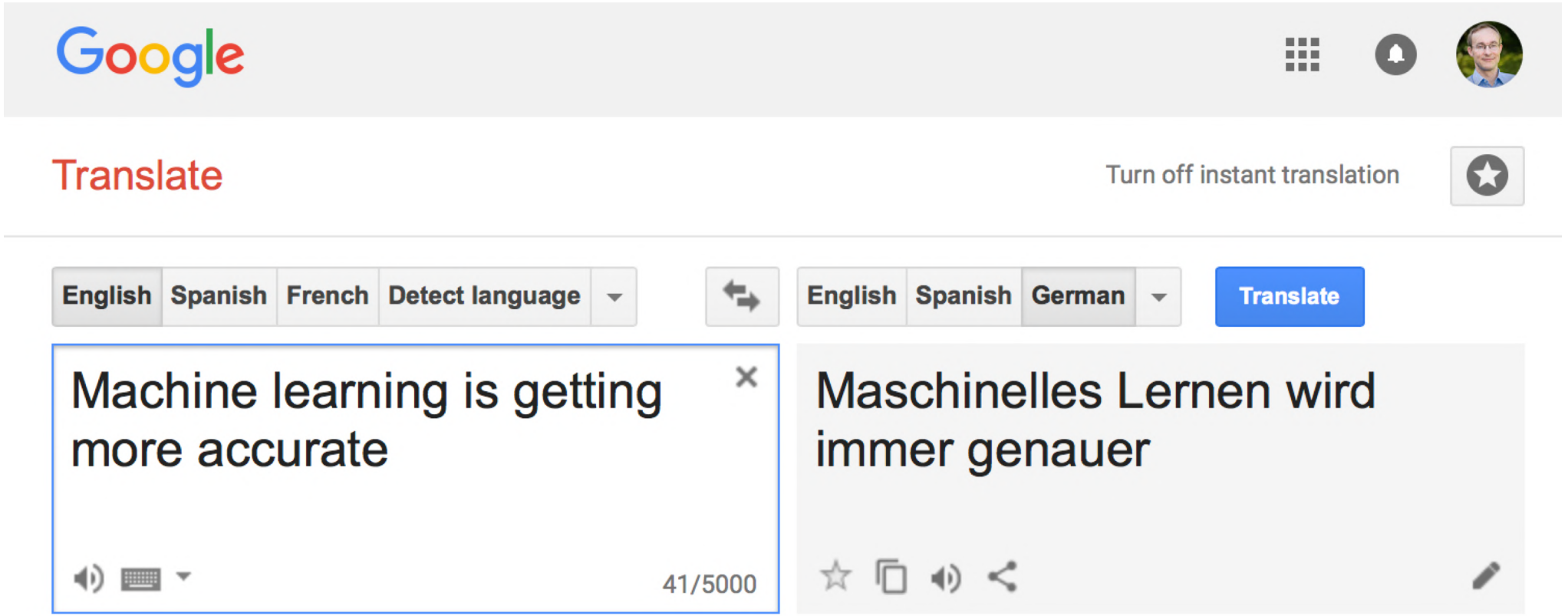
Vinyals et al. *Show and Tell: A Neural Image Caption Generator* '14

Image captioning



[Vinyals et al ‘14]

Example: Translation



X **Y**

Some questions

- How can we compute the gradient?
- How should we initialize the weights?
- When should we terminate?
- How do we choose parameters (number of units/layers/activation functions/learning rate/ ...)?
- What about overfitting?

Computing the gradient

- In order to apply SGD, need to compute

$$\nabla_{\mathbf{W}} \ell(\mathbf{W}; \mathbf{y}, \mathbf{x})$$

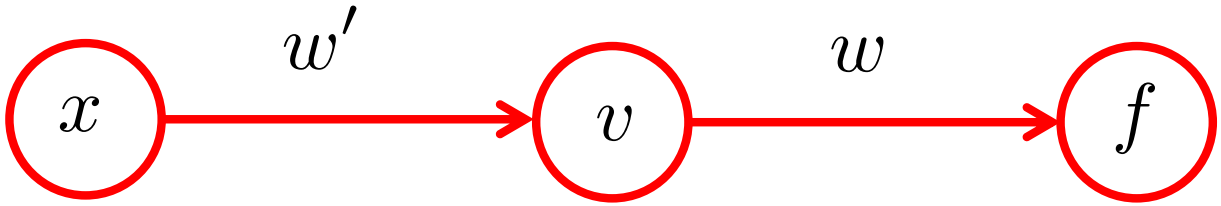
- I.e., for each weight between any two connected units *i* and *j* need

$$\frac{\partial}{\partial w_{i,j}} \ell(\mathbf{W}; \mathbf{y}, \mathbf{x})$$

Simple example

- ANN with 1 output, 1 hidden and 1 input unit

$W = [w, w']$



- Here, $f(x, \mathbf{W}) = w\varphi(w'x)$

$D = \{(x, y)\}$

$L(w', w) := L = \ell(f, y) = \ell_y(f)$

Computed by forward prop.

E.g.: $\ell_y(f) = (f-y)^2$

$\Rightarrow \ell_y'(f) = 2(f-y)$

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial f}\frac{\partial f}{\partial w} = \ell_y'(f) \cdot v$$

$$\frac{\partial L}{\partial w'} = \frac{\partial L}{\partial f}\frac{\partial f}{\partial v}\frac{\partial v}{\partial w'} = \delta \cdot w \cdot \varphi'(z) \cdot x$$

δ — already computed

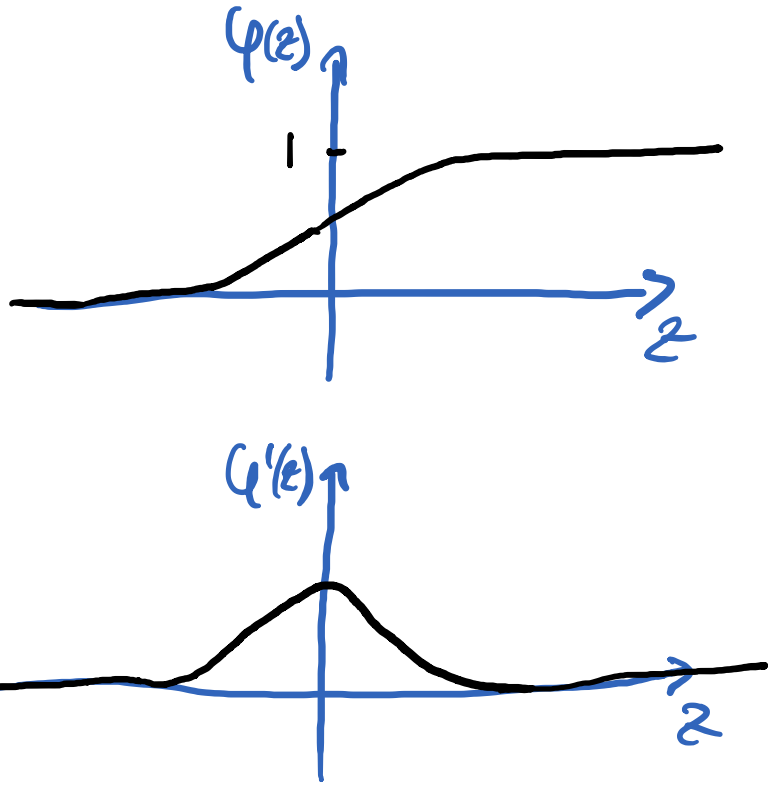
v

δ'

Derivatives of activation functions

- Sigmoid: $$\varphi(z) = \frac{1}{1 + \exp(-z)}$$

$$\varphi'(z) = \frac{-1}{(1+e^{-z})^2} \cdot e^{-z} \cdot (-1) = \underbrace{\frac{e^{-z}}{1+e^{-z}}}_{1-\varphi(z)} \cdot \underbrace{\frac{1}{1+e^{-z}}}_{\varphi(z)} = \varphi(z)(1-\varphi(z))$$



+ diff'able everywhere

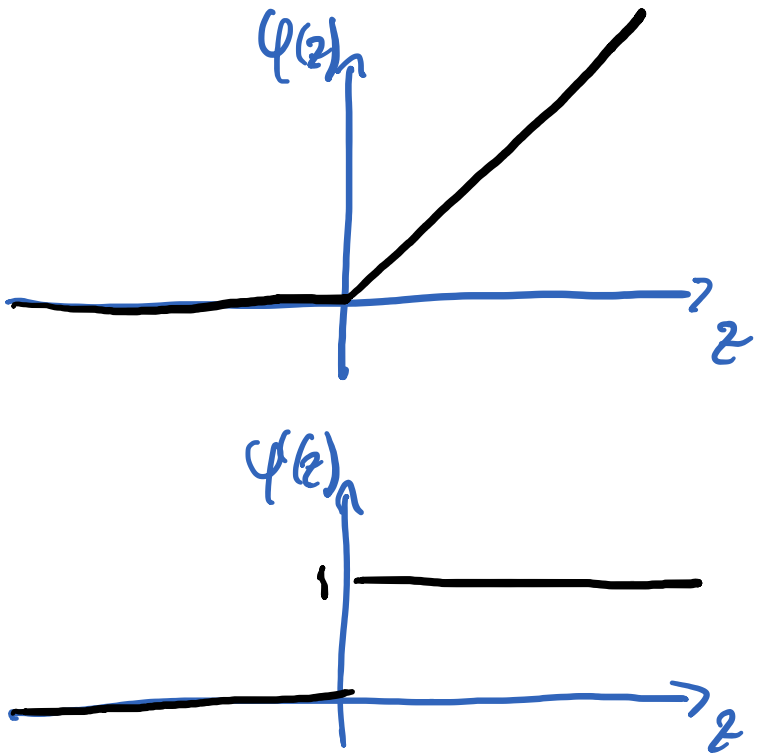
$\rightarrow \varphi' \approx 0$ unless $z \approx 0$

$\Rightarrow$ often lead to vanishing gradients for deep models

Derivatives of activation functions

- Rectified Linear Unit (ReLU): $\varphi(z) = \max(z, 0)$

$$\varphi'(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otw.} \end{cases}$$

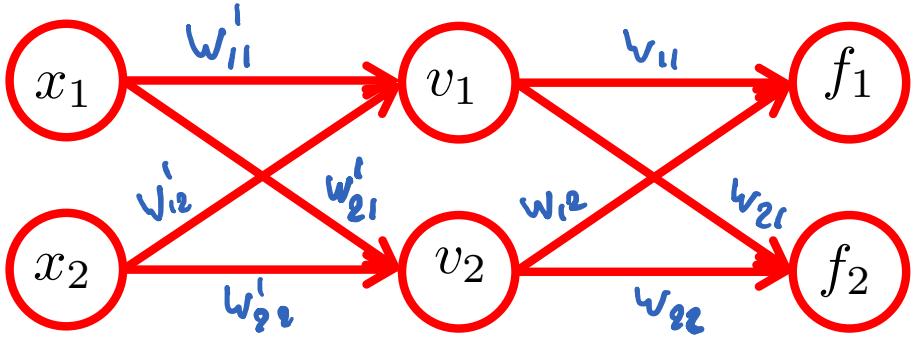


- not diff'able at 0
  (in practice not a problem)

+ $\varphi' = 1$ for all $z > 0$

⇒ helps with avoiding vanishing gradients

Slightly more complicated example



$$L = \sum_{i=1}^{2} \ell_i \left(\sum_j w_{i,j} \varphi \left(\sum_k w'_{j,k} x_k \right) \right)$$

$W = [(w_{ij})_{ij}, (w'_{ij})_{ij}]$

$$\frac{\partial L}{\partial w_{ij}} = \frac{\partial L}{\partial f_i} \frac{\partial f_i}{\partial w_{ij}} = \underbrace{\ell_i'(f_i)}_{\delta_i} \cdot v_j$$

compute' by forward prop.

$$\frac{\partial L}{\partial w'_{jk}} = \sum_{i=1}^{2} \underbrace{\frac{\partial L}{\partial f_i}}_{\delta_i} \frac{\partial f_i}{\partial v_j} \frac{\partial v_j}{\partial w'_{jk}} = \underbrace{\sum_{i=1}^{2} \delta_i \, w_{ij}}_{\delta'_j} \varphi'(z_j) \cdot x_k$$

δ_i ← already computed

Backpropagation

- For each unit j on the output layer
  - Compute error signal $\delta_j = \ell'_j(f_j)$
  - For each unit i on layer L, $\frac{\partial}{\partial w_{j,i}} = \delta_j v_i$
- For each unit j on hidden layer $\ell = L-1 : -1 : 1$
  - Compute error signal $\delta_j = \varphi'(z_j) \sum_{i \in \text{Layer}_{\ell+1}} w_{i,j}\delta_i$
  - For each unit i on layer $\ell - 1$, $\frac{\partial}{\partial w_{j,i}} = \delta_j v_i$

Backpropagation: Matrix form

- For the output layer
  - Compute „error“ $\delta^{(L)} = \mathbf{l}'(\mathbf{f}) = [l'(f_1), \ldots, l'(f_p)]$
  - Gradient: $\nabla_{\mathbf{W}^{(L)}} \ell(\mathbf{W}; \mathbf{y}, \mathbf{x}) = \delta^{(L)} \mathbf{v}^{(L-1)T}$
- For each hidden layer $\ell = L-1 : -1 : 1$
  - Compute „error“ $\delta^{(\ell)} = \varphi'(\mathbf{z}^{(\ell)}) \odot (\mathbf{W}^{(\ell+1)T} \delta^{(\ell+1)})$

    pointwise multiplication
  - Gradient $\nabla_{\mathbf{W}^{(\ell)}} \ell(\mathbf{W}; \mathbf{y}, \mathbf{x}) = \delta^{(\ell)} \mathbf{v}^{(\ell-1)T}$