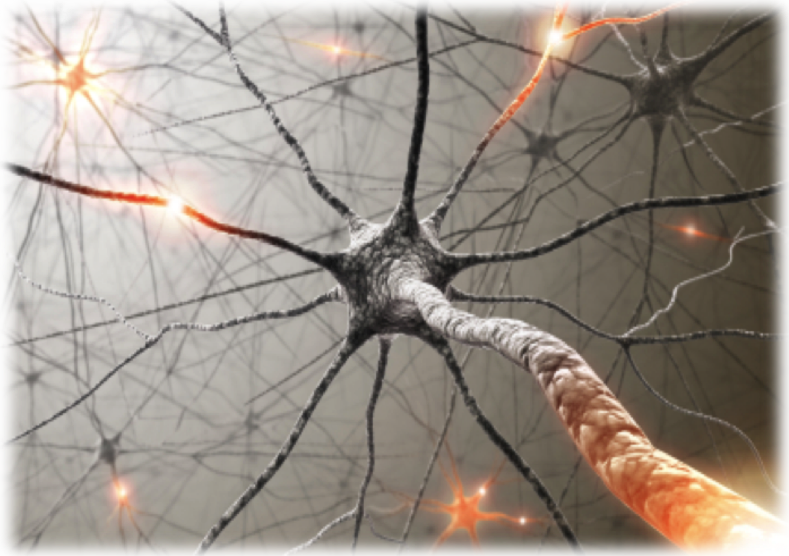
Machine learning: backpropagation



Motivation: regression with four-layer neural networks

Loss on one example:

$$\text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w}) = (\mathbf{w} \cdot \sigma(\mathbf{V}_3 \sigma(\mathbf{V}_2 \sigma(\mathbf{V}_1 \phi(x)))) - y)^2$$

Stochastic gradient descent:

$$\mathbf{V}_1 \leftarrow \mathbf{V}_1 - \eta \nabla_{\mathbf{V}_1} \text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w})$$

$$\mathbf{V}_2 \leftarrow \mathbf{V}_2 - \eta \nabla_{\mathbf{V}_2} \text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w})$$

$$\mathbf{V}_3 \leftarrow \mathbf{V}_3 - \eta \nabla_{\mathbf{V}_3} \text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w})$$

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w})$$

How to get the gradient without doing manual work?

Computation graphs

$$\text{Loss}(x, y, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3, \mathbf{w}) = (\mathbf{w} \cdot \sigma(\mathbf{V}_3 \sigma(\mathbf{V}_2 \sigma(\mathbf{V}_1 \phi(x)))) - y)^2$$

Definition: computation graph

A directed acyclic graph whose root node represents the final mathematical expression and each node represents intermediate subexpressions.

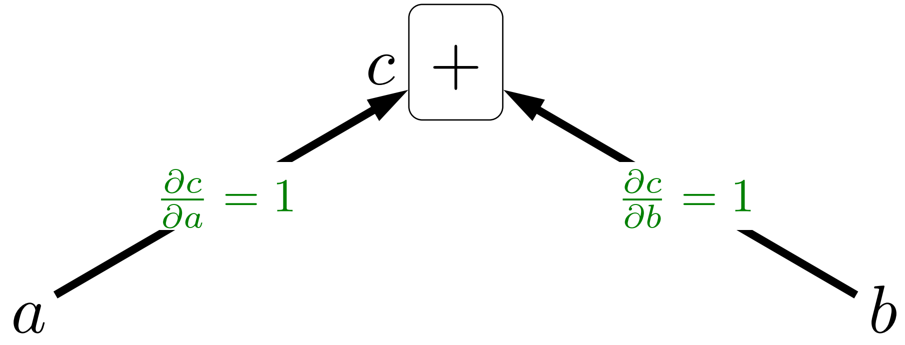
Upshot: compute gradients via general **backpropagation** algorithm

Purposes:

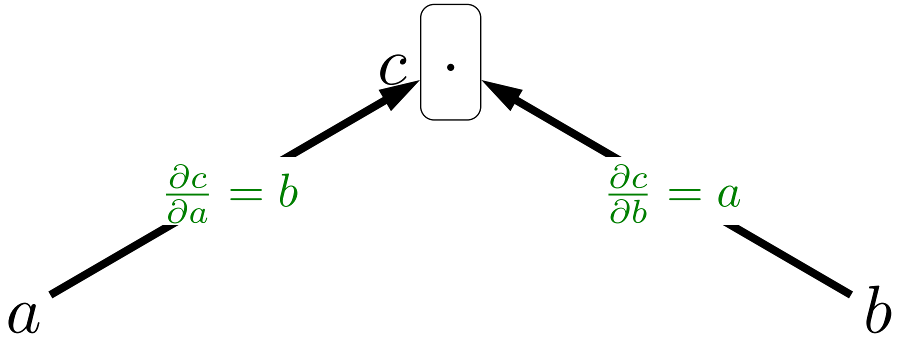
- Automatically compute gradients (how TensorFlow and PyTorch work)
- Gain insight into modular structure of gradient computations

Functions as boxes

$$c = a + b$$



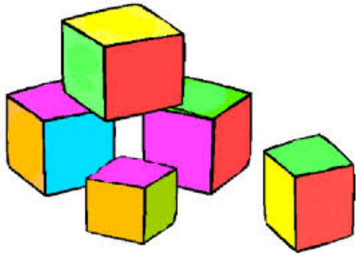
$$c = a \cdot b$$



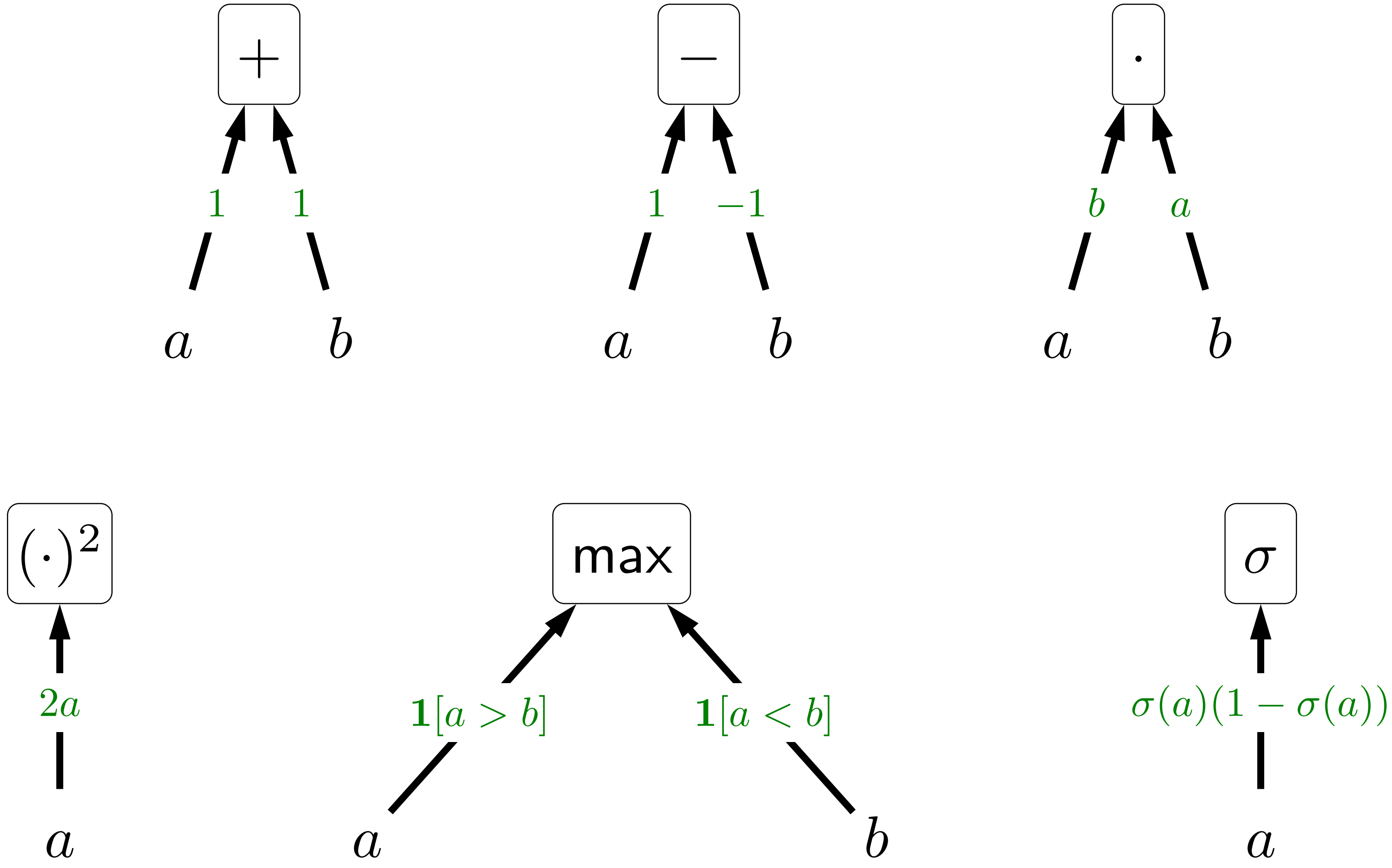
$$(a + \epsilon) + b = c + 1\epsilon$$
$$a + (b + \epsilon) = c + 1\epsilon$$

$$(a + \epsilon)b = c + b\epsilon$$
$$a(b + \epsilon) = c + a\epsilon$$

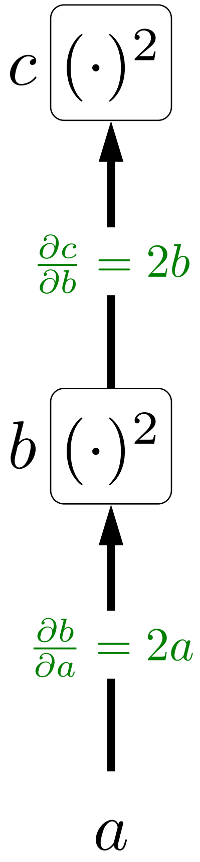
Gradients: how much does c change if a or b changes?



Basic building blocks



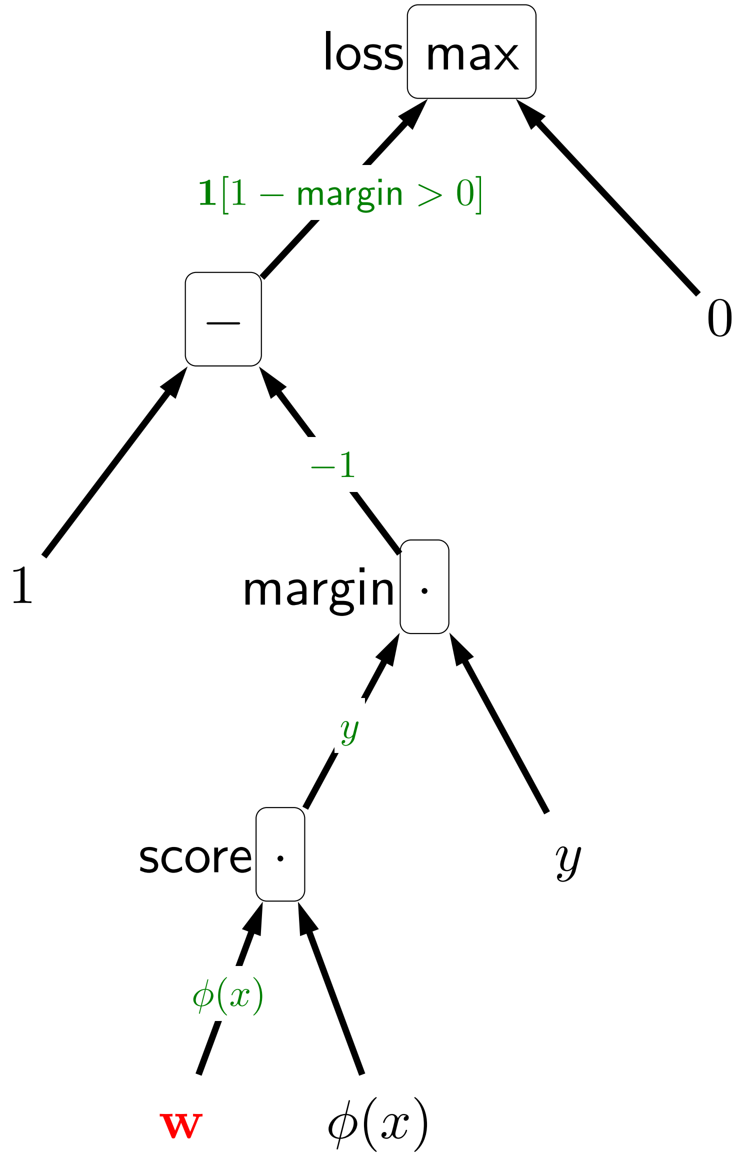
Function composition



Chain rule:

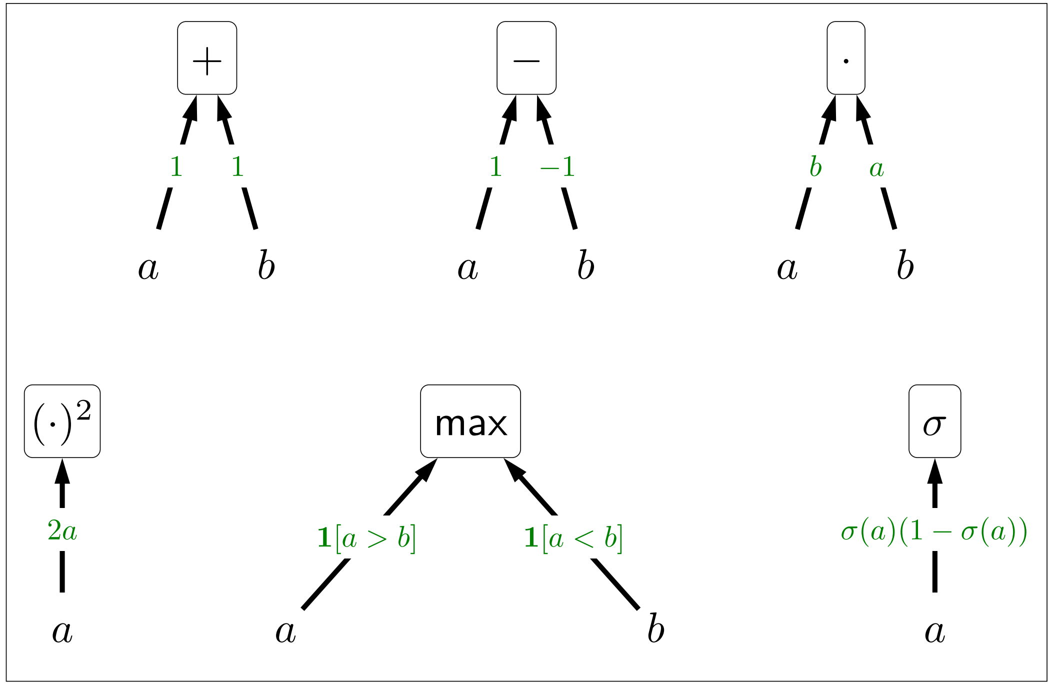
$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b}\frac{\partial b}{\partial a} = (2b)(2a) = 4a^3$$

Linear classification with hinge loss

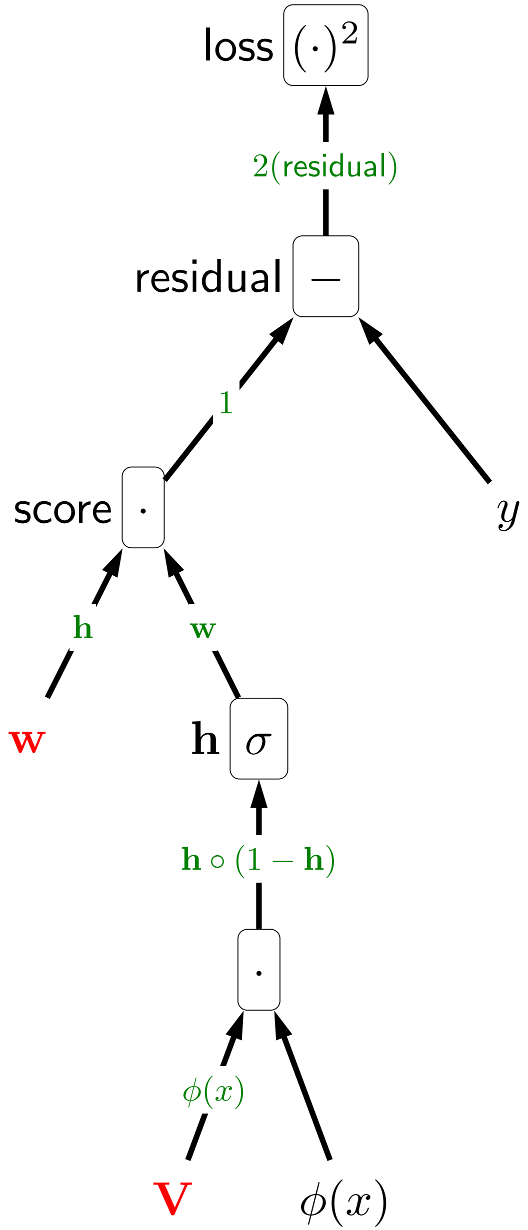


$$\text{Loss}(x, y, \mathbf{w}) = \max\{1 - \mathbf{w} \cdot \phi(x) y, 0\}$$

$$\nabla_{\mathbf{w}} \text{Loss}(x, y, \mathbf{w}) = -\mathbf{1}[\text{margin} < 1] \phi(x) y$$



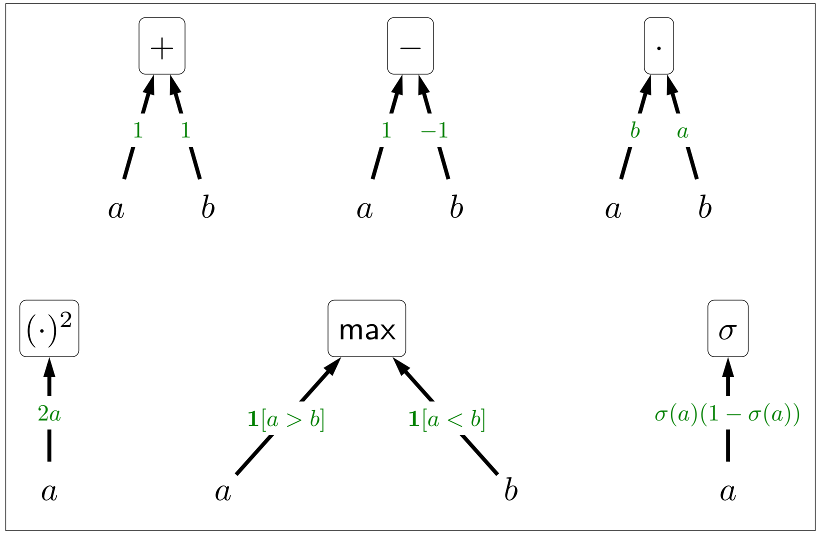
Two-layer neural networks



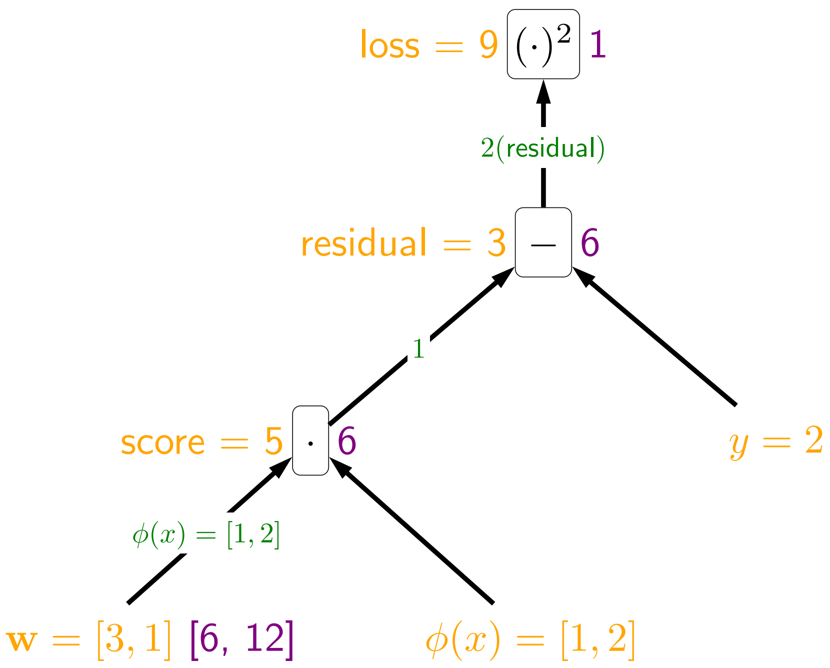
$$\text{Loss}(x, y, \mathbf{V}, \mathbf{w}) = (\mathbf{w} \cdot \sigma(\mathbf{V}\phi(x)) - y)^2$$

$$\nabla_{\mathbf{w}} \text{Loss}(x, y, \mathbf{V}, \mathbf{w}) = 2(\text{residual})\mathbf{h}$$

$$\nabla_{\mathbf{V}} \text{Loss}(x, y, \mathbf{V}, \mathbf{w}) = 2(\text{residual})\mathbf{w} \circ \mathbf{h} \circ (1 - \mathbf{h})\phi(x)^\top$$



Backpropagation



$$\text{Loss}(x, y, \mathbf{w}) = (\mathbf{w} \cdot \phi(x) - y)^2$$

$$\mathbf{w} = [3, 1], \phi(x) = [1, 2], y = 2$$

backpropagation

$$\nabla_{\mathbf{w}} \text{Loss}(x, y, \mathbf{w}) = [6, 12]$$

Definition: Forward/backward values

Forward: f_i is value for subexpression rooted at i

Backward: $g_i = \frac{\partial \text{loss}}{\partial f_i}$ is how f_i influences loss

Algorithm: backpropagation algorithm

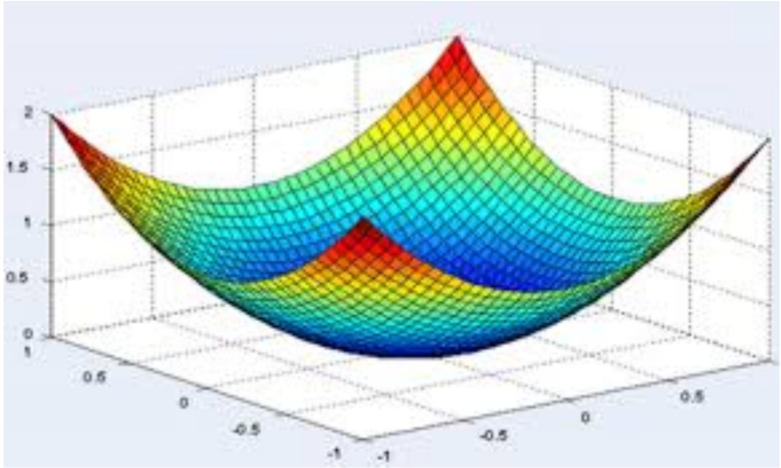
Forward pass: compute each f_i (from leaves to root)

Backward pass: compute each g_i (from root to leaves)

A note on optimization

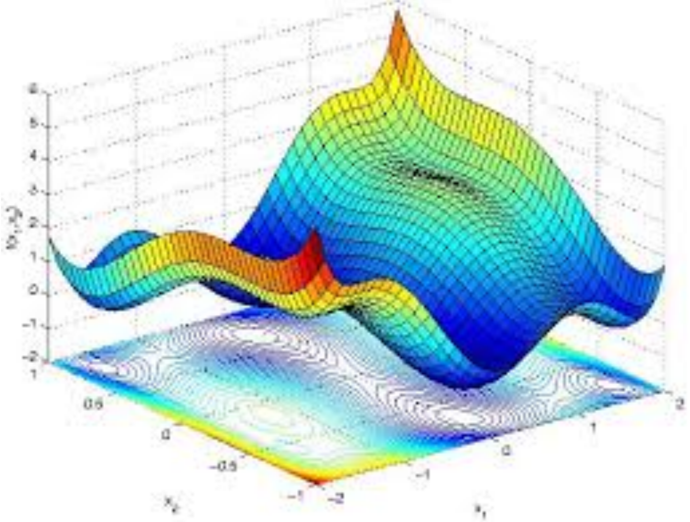
$$\min_{\mathbf{V},\mathbf{w}} \text{TrainLoss}(\mathbf{V},\mathbf{w})$$

Linear predictors



(convex)

Neural networks

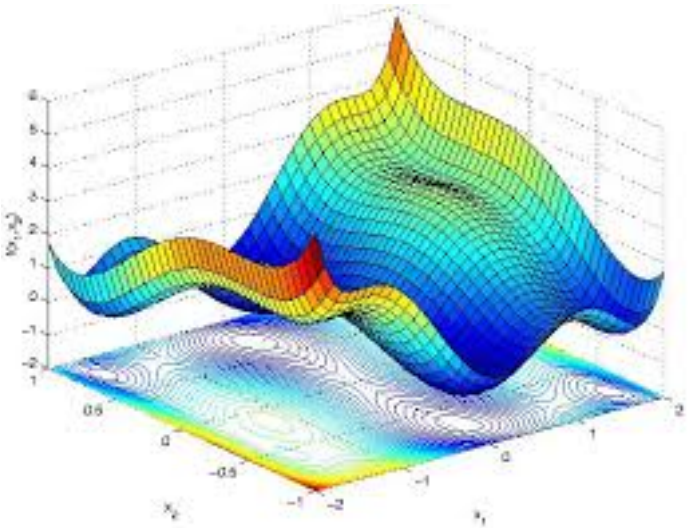


(non-convex)

Optimization of neural networks is in principle hard

How to train neural networks

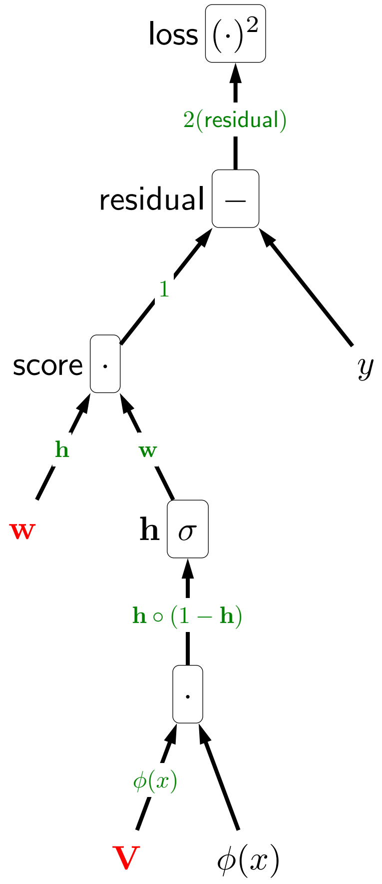
$$\text{score} = \mathbf{w} \cdot \sigma(\mathbf{V}\,\phi(x))$$



- Careful initialization (random noise, pre-training)
- Overparameterization (more hidden units than needed)
- Adaptive step sizes (AdaGrad, Adam)

Don't let gradients vanish or explode!

Summary



- Computation graphs: visualize and understand gradients
- Backpropagation: general-purpose algorithm for computing gradients