Gradient Descent and Backpropagation 1

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Assigned reading: 6.{2,4}, 7.{1,2}, 5.4.4

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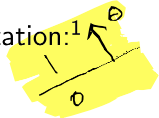
a summary of the previous lecture

- the geometry of θ in the logistic regression given the following parametrization:[1]



$$p(1|x) = \frac{1}{1+\underline{\exp(-\theta^\top x)}} =: p(z(x;\theta)), \text{ where } z(x;\theta) = \theta^\top x$$

$\llcorner\ x = x_\perp + x_\parallel$

  θ is perpendicular to the decision boundary and points to class "1".

- softmax function: generalization of the logistic regression to multiclass ($K > 2$) classification via the generative approach, where we assumed $\underline{X|k \sim \mathcal{N}(\mu_k, \Sigma)}$.
- the negative log-likelihood loss for the logisitic regression and its gradient:

$$\mathcal{L}(\theta) = -y \log p(z(x;\theta)) - (1-y)\log(1-p(z(x;\theta)))$$

$$\nabla_\theta \mathcal{L}(\theta) = \underbrace{(p_z - y)}_{\text{"error"}}\underbrace{\nabla_\theta z}_{x} = (p_z - y)\,x,$$

$$\begin{cases} \theta \leftarrow \theta - \varepsilon x & y = 0 \\ \theta \leftarrow \theta + \varepsilon x & y = 1 \end{cases}$$

  and we interpreted this gradient geometrically in terms of the parameter updates.

- artificial neural networks as simplified models of biological neural networks

[1] Here, I assume the data is "centered", therefore $\theta_0 = 0$.

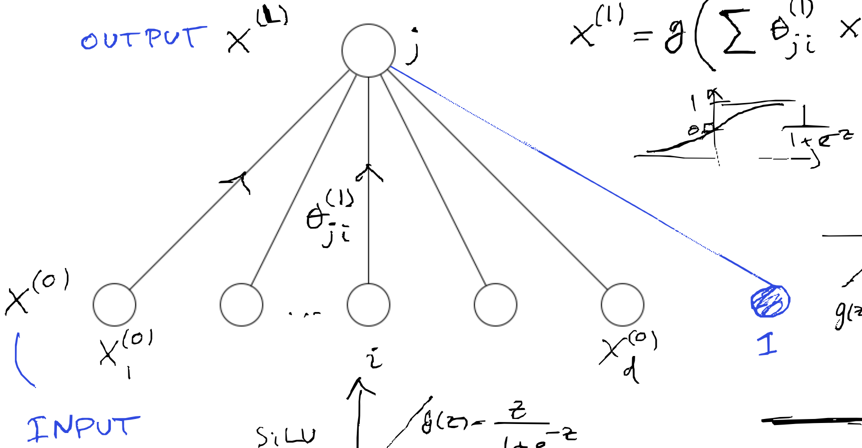
outline

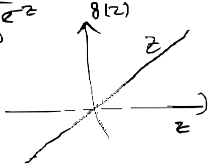
- neural networks as a certain type of nonlinear functions
  - (linear/logisitic regression as single-layer neural network)
  - finish the comparisons with biological neural networks
- training neural networks: stochastic gradient descent
  - gradient of a function
  - the chain rule
  - convex and non-convex functions
  - geometrical interpretation of the gradient
  - stochastic gradient descent (SGD)
- a prelude to backpropagation: the cross-entropy loss for multiclass ($K > 2$) classification and its gradient

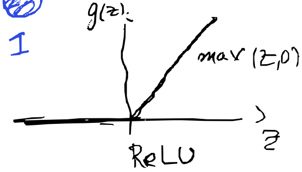
single-layer neural networks

L=1

$$x^{(1)} = g\left(\sum \theta_{ji}^{(1)} x_i^{(0)}\right)$$

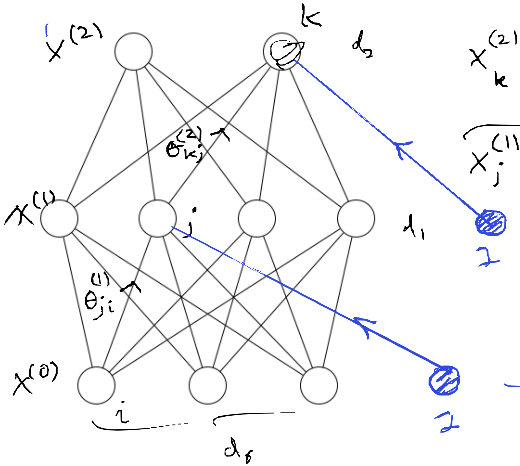






two-layer neural networks

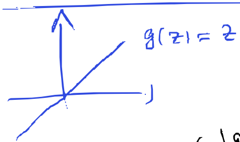
$L = 2$



$$x_k^{(2)} = g\left(\sum_{j=1}^{d_1} \theta_{kj}^{(2)} \left(g\left(\sum_{i=1}^{d_0} \theta_{ji}^{(1)} x_i^{(0)}\right)\right)\right)$$

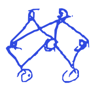
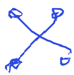
$$x_j^{(1)} = g\left(\sum \theta_{ji}^{(1)} x_i^{(0)}\right)$$

$$f : \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$$



$$x_k^{(2)} = \sum \theta_{kj}^{(2)} \underbrace{\sum \theta_{ji}^{(1)}} x_i^{(0)} =$$

last layer g is typically taken to be linear

 $\equiv$ 

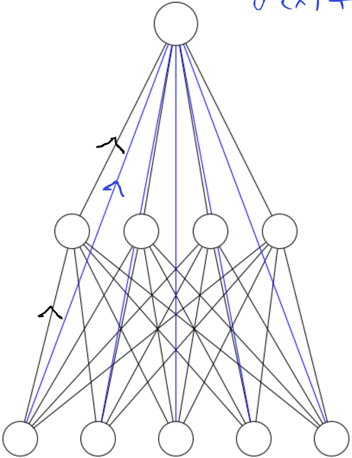
✎ complex neural network architectures:

⛔ anything goes, but “loops” are not allowed!

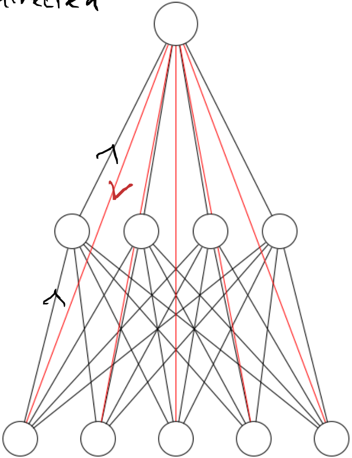
Formally, a neural net is mapped to a DAG — graph

directed acyclic

$\mathcal{F}(x) + x$



X



biological neural networks v.s. deep neural networks

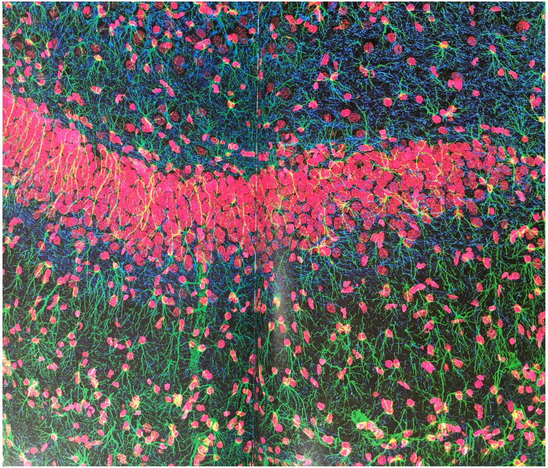


Figure: human brain: 10^{11} neurons, 10^{15} synapses
10 layers, feedback, 100 Hz, spike timing

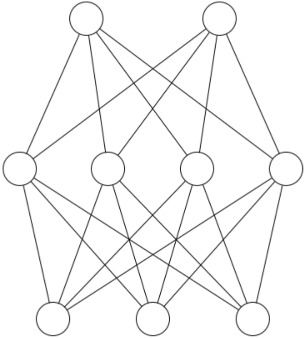
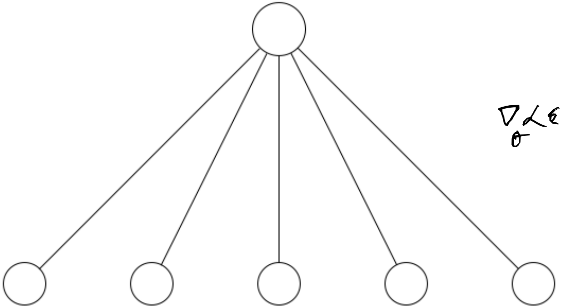


Figure: GPT-4: 10^{6} neurons, 10^{11} parameters (weights), 100 layers
DAG, GHz, backprop (rate coding)

What are we missing in this comparison?

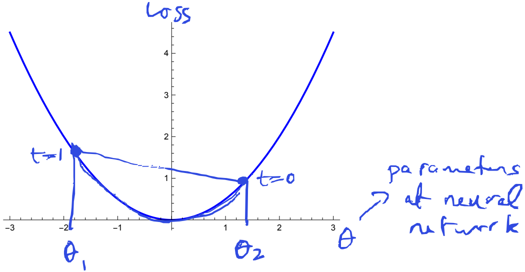
single-layer neural networks: the linear and logistic regression

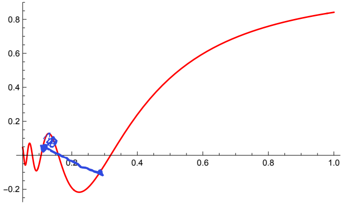


$$\mathcal{L}(\theta) = \frac{1}{2}\left(y - \underbrace{\theta^T x}_{nn(x\,;\,\theta^{(1)} \ldots \theta^{(L)})}\right)^2$$

$$\nabla_\theta \mathcal{L} = \underbrace{(y - \theta^T x)}_{\text{error}}\ \underline{x}$$

convex and non-convex functions





Recall from the multivariate calculus that the gradient of the function $f : \mathbb{R}^m \to \mathbb{R}$ is the vector

$$\nabla f(\theta_1, \dots, \theta_m) = \left(\frac{\partial f}{\partial \theta_1}, \dots, \frac{\partial f}{\partial \theta_m}\right)^\top$$

- The gradient is the direction that leads to maximal increase of f (steepest ascent). Equivalently, the negative gradient is the direction of steepest descent.
- Formally, a function f is convex if for all θ_1, θ_2 in $\mathbb{R}^m$ and $t \in [0,1]$:

$$f(t\theta_1 + (1-t)\theta_2) \leq f(\theta_1) + (1-t)f(\theta_2)$$

- convex functions have a single (global) minimum.

Given $u(z_1, z_2) = (z_1 + z_2)^2/2$, where $z_1(x_1, x_2) = x_1 \sin x_2$ and $z_2(x_1, x_2) = (\sin x_2)^2$; determine $\nabla_x u$ using the chain rule:

- brute force:

$$u(x_1, x_2) = \frac{1}{2}\left(x_1 \sin x_2 + \sin^2 x_2\right)^2 = \frac{1}{2} x_1^2 \sin^2 x_2 + x_1 \sin^3 x_2 + \frac{1}{2} \sin^4 x_2$$

$$\frac{\partial u(x_1, x_2)}{\partial x_2} = x_1^2 \sin x_2 \cos x_2 + 3x_1 \sin^2 x_2 \cos x_2 + 2 \sin^3 x_2 \cos x_2$$

- chain rule:

$$\frac{\partial u}{\partial x_2} = \underbrace{\frac{\partial u}{\partial z_1}}_{(z_1+z_2)} \frac{\partial z_1}{\partial x_2} + \underbrace{\frac{\partial u}{\partial z_2}}_{(z_1+z_2)} \frac{\partial z_2}{\partial x_2}$$

$$= (z_1 + z_2)\left(\frac{\partial z_1}{\partial x_2} + \frac{\partial z_2}{\partial x_2}\right)$$

$$= (x_1 \sin x_2 + \sin^2 x_2)(x_1 \cos x_2 + 2 \sin x_2 \cos x_2)$$

$$= x_1^2 \sin x_2 \cos x_2 + 2x_1 \sin^2 x_2 \cos x_2$$

$$+ x_1 \sin^2 x_2 \cos x_2 + 2 \sin^3 x_2 \cos x_2$$

the geometrical meaning of the gradient

Prove that $\nabla f(\theta)$, the gradient of the function $f : \Theta \to \mathbb{R}$ at any point θ, is perpendicular to the level set of f at that point.[2]

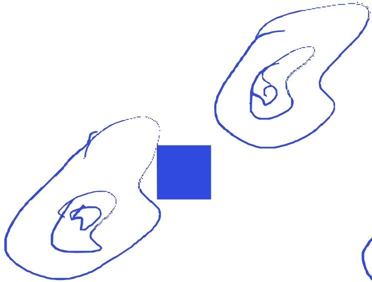
$\Theta \subseteq \mathbb{R}^m$

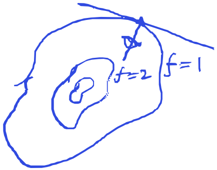
(Hint: define a path $t \to \theta$ on the level set and use the fact that by definition of the level set $\partial_t f(\theta(t)) = 0$. Use the chain rule!)

$t \to \theta \to f$

$f(\theta(t)) = \text{const}$

$\partial_t f(\theta(t)) = 0$





$f = -\frac{(\theta_1^2 + \theta_2^2)}{2}$

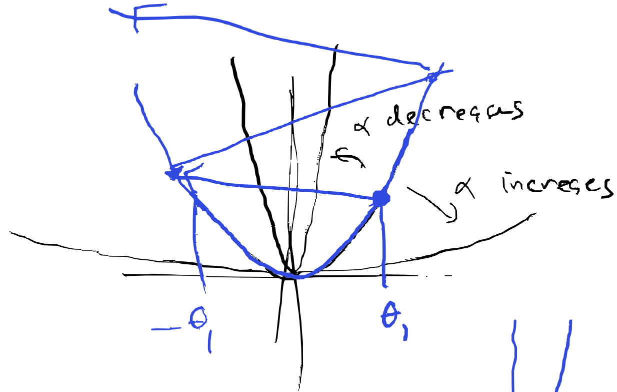
$\partial_t f(\theta(t)) = 0$

$= \frac{\partial f}{\partial \theta_1}\frac{\partial \theta_1}{\partial t} + \cdots + \frac{\partial f}{\partial \theta_m}\frac{\partial \theta_m}{\partial t}$

$= (\nabla f) \cdot \vec{v} = 0$

[2]Recall that level sets are defined by $\{\theta' : f(\theta') = f(\theta)\}$ for some constant c.

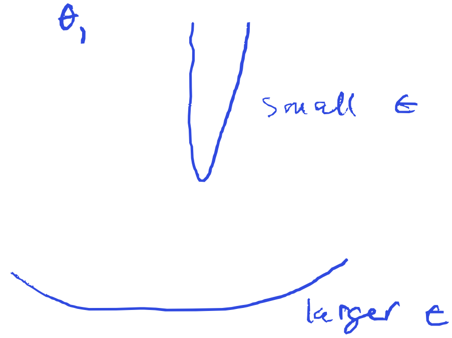
$$f(\theta) = \frac{\theta^2}{2\alpha}$$



$$\theta_{t+1} = \theta_t - \epsilon \frac{\theta_t}{\alpha}$$

$$= \left(1 - \frac{\epsilon}{\alpha}\right)\theta_t$$

$$\theta_t = \left(1 - \frac{\epsilon}{\alpha}\right)^t \theta_1$$

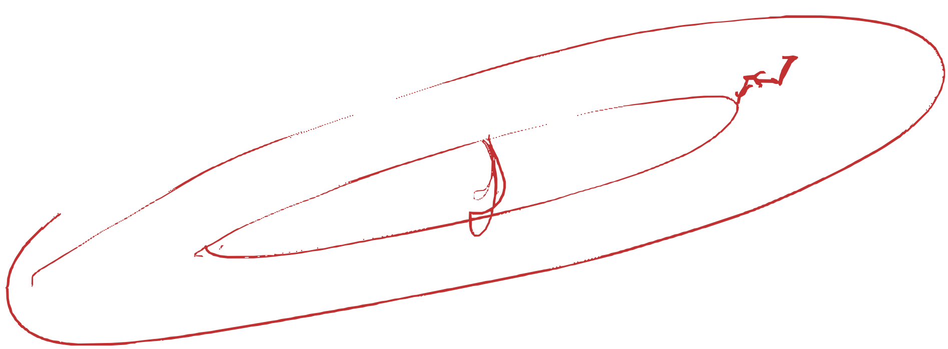


$0 < \epsilon < \alpha \Rightarrow$ $\quad 1 - \frac{\epsilon}{\alpha} < 1 \Rightarrow$ As $t \to \infty$: $\theta_t = 0$

$\epsilon = \alpha \Rightarrow$ After only a single step

$\theta_2 = \theta_{min}$

$\epsilon > 2\alpha$



α_{min} dictates the step size

stochastic gradient descent I

- at a high level the loss is always written as the sum of losses by individual points $i \in [n] := \{1, \ldots, n\}$ in the training set $\mathcal{D} = \{(x_i, y_i)\}_{i \in [n]}$:

$$\mathcal{L}(\theta) = \sum_{i=1}^{n} \mathcal{L}_i(\theta),$$

$$\nabla \mathcal{L}(\theta) = \sum_{i=1}^{n} \nabla \mathcal{L}_i(\theta)$$

where $\mathcal{L}_i(\theta)$ is short for:

$$\mathcal{L}_i(\theta) := \mathcal{L}(x_i, y_i; \theta).$$

- This is very general, but it's very easy to see where it's coming from in the maximum log-likelihood framework. We always assume the i.i.d. setting:

$$(x_i, y_i) \overset{\text{iid}}{\sim} p_\theta(x, y), \;\; i \in [n].$$

$$\nabla_\theta \mathcal{L}_i \text{ “=” } \nabla \mathcal{L} + \underline{\text{noise}}$$

Therefore,

$$\underline{p(\mathcal{D}|\theta) = \prod_{i=1}^{n} p_\theta(x_i, y_i).}$$

It follows:

$$\mathcal{L}_i(\theta) = -\log p_\theta(x_i, y_i).$$

stochastic gradient descent II

The two prominent examples so far include:

- linear regression:

$$-\log p_\theta(x_i, y_i) = \frac{1}{2\sigma^2}(y_i - \theta^\top x_i^{(0)}) + const$$

- logistic "regression":

$$-\log p_\theta(x_i, y_i) = -y_i \log g(\theta^\top x_i^{(0)}) - (1 - y_i)\log(1 - g(\theta^\top x_i^{(0)})) + const$$

- (Note that the structure of the loss is general: we are getting ready to replace $\theta^\top x_i^{(0)}$ with an L-layer neural network: $f(x_i^{(0)}; \theta^{(1)}, \ldots, \theta^{(L)})$.)

Stochastic Gradient Descent (SGD) in its pure form is defined by the following updates:

$$\theta_{t+1} = \theta_t - \epsilon_t \nabla_\theta \mathcal{L}(x_i, y_i; \theta),$$

where $i \in [n]$ is selected at random (typically without replacement) at each iteration t.

stochastic gradient descent III

- Intuitively (people have tried to study this) in high dimensions the loss landscape is "dominated" by saddle points and the noise in SGD helps to avoid them.
- SGD is convenient in the regime $n \ggg 1$.
- One pass through the data is called an epoch.
- The problem is towards the end of the training (optimization) the noise in SGD will slow down the training.
- In short: noise helps us at the beginning of training, it "hurts" us towards the end.
- Of course, one can find a compromise by dividing the dataset into (random) mini-batches of size b: in this scheme one epoch involves $\lfloor n/b \rfloor$ updates.

? Based on this picture, can you suggest a batching scheme for effective training? [3]

[3] Coming up with a mini-batch / learning rate schedule remains an art and problem dependent.