

Il Porcodio: Deep Learning Cheatsheet

1 Matrix based notation

The activation z_j^l of the j -th neuron of the l -th layer is

$$z_j^l = \sigma \left(\sum_k w_{jk}^l z_k^{l-1} + b_j^l \right)$$

Now take \mathbf{W}^l as the matrix

$$\begin{bmatrix} w_{00}^l & w_{01}^l & w_{02}^l & \cdots \\ w_{10}^l & w_{11}^l & w_{12}^l & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

in matrix notation we write then

$$\mathbf{z}^l = \sigma(\mathbf{W}^l \mathbf{z}^{l-1} + \mathbf{b}^l)$$

and we define

$$\mathbf{a}^l := \mathbf{W}^l \mathbf{z}^{l-1} + \mathbf{b}^l$$

so that $\mathbf{z}^l = \sigma(\mathbf{a}^l)$.

Hadamard product: stupid retarded product of matrices:

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \odot \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \times 2 \\ 3 \times 4 \end{bmatrix}.$$

2 Cost function

It must be:

- Expressed as mean of the single inputs;
- It must be a function of the outputs of the network.

Example: quadratic cost function

$$C = \frac{1}{2n} \left\| \mathbf{y}(x) - \mathbf{z}^L(x) \right\|^2.$$

3 The Four Fundamental Equations

Define δ_j^l as the error at level l of neuron j :

$$\delta_j^l = \frac{\partial C}{\partial a_j^l}.$$

3.1 BP1

$$\begin{aligned} \delta_j^L &= \frac{\partial C}{\partial z_j^L} \cdot \sigma'(a_j^L) \\ &\downarrow \\ \delta^L &= \nabla_z C \odot \sigma'(\mathbf{a}^L). \end{aligned}$$

3.2 BP2

$$\begin{aligned} \delta_j^l &= \sum_k w_{kj}^{l+1} \delta_k^{l+1} \sigma'(a_j^l) \\ &\downarrow \\ \delta^l &= ((\mathbf{W}^{l+1})^\top \delta^{l+1}) \odot \sigma'(\mathbf{a}^l). \end{aligned}$$

3.3 BP3

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l.$$

3.4 BP4

$$\frac{\partial C}{\partial w_{jk}^l} = z_k^{l-1} \delta_j^l \quad \frac{\partial C}{\partial w} = z_{\text{in}} \delta_{\text{out}}.$$

Proof 3.1: BP1

Show that $\delta_j^L := \frac{\partial C}{\partial a_j^L} = \frac{\partial C}{\partial z_j^L} \sigma'(a_j^L)$. Use the chain rule:

$$\begin{aligned} \delta_j^L &= \frac{\partial C}{\partial a_j^L} \\ &= \sum_k \frac{\partial C}{\partial z_k^L} \frac{\partial z_k^L}{\partial a_j^L} \\ &= \frac{\partial C}{\partial z_j^L} \frac{\partial z_j^L}{\partial a_j^L} \\ &= \frac{\partial C}{\partial z_j^L} \sigma'(a_j^L). \end{aligned}$$

Proof 3.2: BP2

Here we must show that

$$\begin{aligned} \delta_j^l &:= \frac{\partial C}{\partial a_j^l} = \left[(\mathbf{W}^{l+1})^\top \delta^{l+1} \odot \sigma'(\mathbf{a}^l) \right]_j \\ &= \sum_k w_{kj}^{l+1} \delta_k^{l+1} \cdot \sigma'(a_j^l). \end{aligned}$$

Start from the fact that we can think of C as a function of a_k^{l+1} so we can use the chain rule:

$$\begin{aligned} \delta_j^l &:= \frac{\partial C}{\partial a_j^l} = \sum_k \frac{\partial C}{\partial a_k^{l+1}} \frac{\partial a_k^{l+1}}{\partial a_j^l} \\ &\quad \text{by def. } \delta_k^{l+1} \\ &= \sum_k \delta_k^{l+1} \frac{\partial a_k^{l+1}}{\partial a_j^l}. \end{aligned}$$

But we know that

$$\begin{aligned} a_k^{l+1} &= \sum_j w_{kj}^{l+1} z_j^l + b_k^{l+1} \\ &= \sum_j w_{kj}^{l+1} \sigma(a_j^l) + b_k^{l+1} \end{aligned}$$

so we have that

$$\frac{\partial a_k^{l+1}}{\partial a_j^l} = w_{kj}^{l+1} \sigma'(a_j^l).$$

So putting all together we get

$$\delta_j^l = \sum_k w_{kj}^{l+1} \delta_k^{l+1} \sigma'(a_j^l).$$

Proof 3.3: BP3

We must show that $\frac{\partial C}{\partial b_j^l} = \delta_j^l$. Think of C as a function of a_j^l and use chain rule:

$$\begin{aligned}\frac{\partial C}{\partial b_j^l} &= \sum_k \frac{\partial C}{\partial a_k^l} \frac{\partial a_k^l}{\partial b_j^l} \\ &= \underbrace{\frac{\partial C}{\partial a_j^l}}_{=\delta_j^l} \underbrace{\frac{\partial a_j^l}{\partial b_j^l}}_{=1}.\end{aligned}$$

Proof 3.4: BP4

We must show that $\frac{\partial C}{\partial w_{jk}^l} = z_k^{l-1} \delta_j^l$. Use the chain rule:

$$\begin{aligned}\frac{\partial C}{\partial w_{jk}^l} &= \sum_i \frac{\partial C}{\partial a_i^l} \frac{\partial a_i^l}{\partial w_{jk}^l} \\ &= \frac{\partial C}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \\ &= \delta_j^l \frac{\partial a_j^l}{\partial w_{jk}^l}\end{aligned}$$

but we know that

$$\begin{aligned}\frac{\partial a_j^l}{\partial w_{jk}^l} &= \frac{\partial}{\partial w_{jk}^l} \left(\sum_k w_{jk}^l z_k^{l-1} + b_j^l \right) \\ &= z_k^{l-1}.\end{aligned}$$

So

$$\frac{\partial C}{\partial w_{jk}^l} = z_k^{l-1} \delta_j^l.$$

but since $\nabla E = 0$ we get

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H}(\mathbf{w} - \mathbf{w}^*).$$

Since $\{\mathbf{u}_i\}_i$ is an orthonormal basis we can write any vector as a linear combination of \mathbf{u}_i vectors, which allows us to write:

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2.$$

Proof 5.1: Taylor's shit

We need to show that $E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2$. We know that:

$$\begin{aligned}E(\mathbf{w}) &= E(\mathbf{w}^*) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H}(\mathbf{w} - \mathbf{w}^*) \\ &= E(\mathbf{w}^*) + \frac{1}{2} \left(\sum_i \alpha_i \mathbf{u}_i \right)^\top \mathbf{H} \left(\sum_i \alpha_i \mathbf{u}_i \right) \\ &= E(\mathbf{w}^*) + \frac{1}{2} \left(\sum_i \alpha_i \mathbf{u}_i \right)^\top \left(\sum_i \alpha_i \mathbf{H} \mathbf{u}_i \right) \\ &= E(\mathbf{w}^*) + \frac{1}{2} \left(\sum_i \alpha_i \mathbf{u}_i \right)^\top \left(\sum_i \alpha_i \lambda_i \mathbf{u}_i \right) \\ &= E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2.\end{aligned}$$

And this implies:

Proof 5.2: Gradient's shit

Show that $\nabla E = \sum_i \alpha_i \lambda_i \mathbf{u}_i$.

$$\begin{aligned}\nabla E(\mathbf{w}) &= \nabla \left(E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2 \right) \\ &= \frac{1}{2} \sum_i \lambda_i 2 \alpha_i \nabla \alpha_i.\end{aligned}$$

To compute $\nabla \alpha_i$ we use the fact that $\mathbf{w} - \mathbf{w}^* = \sum_j \alpha_j \mathbf{u}_j$:

$$\begin{aligned}\mathbf{u}_i^\top (\mathbf{w} - \mathbf{w}^*) &= \mathbf{u}_i^\top \left(\sum_j \alpha_j \mathbf{u}_j \right) \\ \mathbf{u}_i^\top (\mathbf{w} - \mathbf{w}^*) &= \alpha_i \\ \sum_j w_j u_{ij} - \sum_j w_j^* u_{ij} &= \alpha_i\end{aligned}$$

so

$$\begin{aligned}\frac{\partial}{\partial w_k} \left(\sum_j w_j u_{ij} - \sum_j w_j^* u_{ij} \right) &= u_{ik} \\ &= \frac{\partial \alpha_i}{\partial w_k} \implies \nabla \alpha_i = \mathbf{u}_i.\end{aligned}$$

We have that

- $\delta \mathbf{w} = \sum_i \delta \alpha_i \mathbf{u}_i$
- $\nabla E = \sum_i \alpha_i \lambda_i \mathbf{u}_i$

4 Improving learning

Cross-entropy cost function:

$$C = -\frac{1}{n} \sum_x [y \ln z + (1-y) \ln(1-z)].$$

This yields:

$$\begin{aligned}\frac{\partial C}{\partial w_j} &= \frac{1}{n} \sum_x x_j (\sigma(a) - y) \\ \frac{\partial C}{\partial b} &= \frac{1}{n} \sum_x (\sigma(a) - y).\end{aligned}$$

We can generalize for multi-layer networks:

$$C = -\frac{1}{n} \sum_x \sum_j \left[y_j \ln z_j^L + (1-y_j) \ln(1-z_j^L) \right].$$

Soft max activation with log-likelihood cost function:

$$\begin{aligned}z_j^L &= \frac{e^{a_j^L}}{\sum_k e^{a_k^L}} \\ C &= -\ln z_y^L\end{aligned}$$

5 Convergence

Consider the quadratic approximation of the error function around the minimum point \mathbf{w}^* :

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \nabla E(\mathbf{w}^*)^\top (\mathbf{w} - \mathbf{w}^*) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H}(\mathbf{w} - \mathbf{w}^*)$$

- $\Delta \mathbf{u} = -\eta \nabla E$
- $\Delta \alpha = -\eta \lambda_i \alpha_i \implies \alpha_i^{\text{new}} = (1 - \eta \lambda_i) \alpha_i^{\text{old}}$.

This means that if $|1 - \eta \lambda_i| < 1$ then α_i decreases for each of the T steps.

- Fastest convergence: $\eta = \frac{1}{\lambda_{\max}}$ (convergence rate 0, minimum reached in one step).
- Direction of slowest convergence: λ_{\min} where the rate is $1 - \frac{\lambda_{\min}}{\lambda_{\max}}$.
- Condition number of hessian matrix: $\frac{\lambda_{\max}}{\lambda_{\min}}$. The bigger it is, the slower the convergence.

6 Momentum

Normally we have

$$\mathbf{w}^{(\tau)} = \mathbf{w}^{(\tau-1)} + \Delta \mathbf{w}^{(\tau-1)}$$

but adding the momentum we get

$$\Delta \mathbf{w}^{(\tau-1)} = -\eta \nabla E(\mathbf{w}^{(\tau-1)}) + \mu \Delta \mathbf{w}^{(\tau-2)}$$

so

$$\Delta \mathbf{w} = -\frac{\eta}{1 - \mu} \nabla E.$$

7 Learning rate scheduling

- Linear: $\eta^{(\tau)} = (1 - \frac{\tau}{K})\eta_0 + (\frac{\tau}{K})\eta_K$.
- Power law: $\eta^{(\tau)} = \eta_0(1 + \frac{\tau}{s})^c$.
- Exponential decay: $\eta^{(\tau)} = \eta_0 c^{\frac{\tau}{s}}$

8 Normalization

8.1 Data normalization

$$\tilde{x}_{ni} = \frac{x_{ni} - \mu_i}{\sigma_i}$$

for each dimension i .

8.2 Batch normalization

$$\begin{aligned}\mu_i &= \frac{1}{K} \sum_{n=1}^K a_{ni} \\ \sigma_i^2 &= \frac{1}{K} \sum_{n=1}^K (a_{ni} - \mu_i)^2 \\ \hat{a}_{ni} &= \frac{a_{ni} - \mu_i}{\sqrt{\sigma_i^2 + \delta}}\end{aligned}$$

After training we use a moving average of the mean and variance.

$$\begin{aligned}\bar{\mu}_i^{(\tau)} &= \alpha \bar{\mu}_i^{(\tau-1)} + (1 - \alpha) \mu_i \\ \bar{\sigma}_i^{(\tau)} &= \alpha \bar{\sigma}_i^{(\tau-1)} + (1 - \alpha) \sigma_i\end{aligned} \quad 0 \leq \alpha \leq 1$$

9 CNNs

The cross-entropy between two discrete distributions p and q measures how much q differs from p .

$$H(p, q) = - \sum_v p(v) \cdot \log(q(v)).$$

CNNs employ the cross-entropy loss:

$$- \sum_{i=1}^S y_i \cdot \log(p_i).$$

10 Autoencoders

Remember how PCA works:

$$f(\mathbf{x}) = \arg \min_{\mathbf{h}} \|\mathbf{x} - g(\mathbf{h})\|_2$$

Where $g(\mathbf{h}) = \mathbf{D}\mathbf{h}$. So we are interested in measuring the loss of the reconstruction

$$\mathcal{L}(\mathbf{x}, g(f(\mathbf{x}))).$$

10.1 Sparse autoencoders

Here the loss function has a penalty on \mathbf{h} :

$$\mathcal{L}(\mathbf{x}, g(f(\mathbf{x}))) + \Omega(\mathbf{h}).$$

Consider the distribution

$$p_{\text{model}}(\mathbf{h}, \mathbf{x}) = p_{\text{model}}(\mathbf{h}) p_{\text{model}}(\mathbf{x}|\mathbf{h})$$

and marginalizing

$$\begin{aligned}p_{\text{model}}(\mathbf{x}) &= \sum_{\mathbf{h}} p_{\text{model}}(\mathbf{h}, \mathbf{x}) \\ &\Downarrow \\ \log p_{\text{model}}(\mathbf{x}) &= \log \sum_{\mathbf{h}} p_{\text{model}}(\mathbf{h}, \mathbf{x})\end{aligned}$$

So, given a $\tilde{\mathbf{h}}$ generated by the encoder we have

$$\begin{aligned}\log p_{\text{model}}(\mathbf{x}) &= \log \sum_{\mathbf{h}} p_{\text{model}}(\mathbf{h}, \mathbf{x}) \\ &\approx \log p(\tilde{\mathbf{h}}, \mathbf{x}) = \log p_{\text{model}}(\tilde{\mathbf{h}}) + \log p_{\text{model}}(\mathbf{x}|\tilde{\mathbf{h}}).\end{aligned}$$

If we set $\Omega(\mathbf{h}) = \lambda \sum_i |h_i|$ (L^1 norm of \mathbf{h}) then minimizing the sparsity terms is equal to maximizing the log likelihood of $p(\mathbf{h})$ assuming a Laplace prior over each component independently.

$$\begin{aligned}p_{\text{model}}(h_i) &= \frac{\lambda}{2} e^{-\lambda |h_i|} \\ &\Downarrow \\ -\log p_{\text{model}}(\mathbf{h}) &= \sum_i \left(\lambda |h_i| - \log \frac{\lambda}{2} \right) = \Omega(\mathbf{h}) + \text{const}\end{aligned}$$

10.2 Denoising autoencoders

They minimize

$$\mathcal{L}(\mathbf{x}, g(f(\tilde{\mathbf{x}})))$$

10.3 Contractive autoencoders

They minimize

$$\mathcal{L}(\mathbf{x}, g(f(\mathbf{x}))) + \Omega(\mathbf{h})$$

with

$$\Omega(\mathbf{h}, \mathbf{x}) = \lambda \sum_i \|\nabla_{\mathbf{x}} h_i\|^2.$$

11 Transformers

Consider the attention to embedding \mathbf{y}_n as

$$a_{nm} = \frac{\exp(\mathbf{x}_n^\top \mathbf{x}_m)}{\sum_{m'=1}^N \exp(\mathbf{x}_n^\top \mathbf{x}_{m'})}.$$

Therefore we can express our new embeddings \mathbf{Y} as

$$\begin{aligned}\mathbf{Y} &= \text{SoftMax} \left[\mathbf{X} \mathbf{X}^\top \right] \mathbf{X} \\ &= \text{SoftMax} \left[\mathbf{Q} \mathbf{K}^\top \right] \mathbf{V}.\end{aligned}$$

Where queries, keys and values are trainable.

$$\begin{aligned}\mathbf{Q} &= \mathbf{X} \mathbf{W}^{(q)} \\ \mathbf{K} &= \mathbf{X} \mathbf{W}^{(k)} \\ \mathbf{V} &= \mathbf{X} \mathbf{W}^{(v)}.\end{aligned}$$

Then the embeddings get scaled by the dimensionality of key vectors

$$\mathbf{Y} = \text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{SoftMax} \left[\frac{\mathbf{Q} \mathbf{K}^\top}{\sqrt{D_k}} \right] \mathbf{V}.$$

In a multi-head scenario where $\mathbf{H}_h = \text{Attention}(\mathbf{Q}_h, \mathbf{K}_h, \mathbf{V}_h)$ we have

$$\overbrace{\mathbf{Y}(\mathbf{X})}^{N \times D} = \overbrace{\text{Concat}[\mathbf{H}_1, \dots, \mathbf{H}_H]}^{N \times H D_v} \overbrace{\mathbf{W}^{(o)}}^{H D_v \times D}.$$

To improve learning it is possible to add a residual connection

$$\mathbf{Z} = \text{LayerNorm}[\mathbf{Y}(\mathbf{X}) + \mathbf{X}] \quad \mathbf{Z} = [\mathbf{Y}(\text{LayerNorm}(\mathbf{X})) + \mathbf{X}]$$

and then passing through a MLP with ReLU activation

$$\tilde{\mathbf{X}} = \text{LayerNorm}[\text{MLP}(\mathbf{Z}) + \mathbf{Z}] \quad \tilde{\mathbf{X}} = \text{MLP}[\text{LayerNorm}(\mathbf{Z})] + \mathbf{Z}.$$

11.1 Positional encoding

We concatenate input \mathbf{x} to positional encoding \mathbf{r} obtaining the representation $\mathbf{x} \parallel \mathbf{r}$. We can apply a linear transformation $\mathbf{w}_x \parallel \mathbf{w}_r$:

$$\begin{bmatrix} \mathbf{w}_x & \mathbf{w}_r \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{r} \end{bmatrix} = \mathbf{w}_x \mathbf{x} + \mathbf{w}_r \mathbf{r} = \mathbf{w}(\mathbf{x} + \mathbf{r}).$$

Encoding must be:

- unique for each position;
- bounded;
- generalizable to sequences of arbitrary length;
- capable of expressing relative positions.

Sinusoidal positional encoding:

$$\mathbf{r}_n = \begin{bmatrix} \sin(w_1 \cdot n) \\ \cos(w_1 \cdot n) \\ \sin(w_2 \cdot n) \\ \cos(w_2 \cdot n) \\ \vdots \\ \sin(w_{\frac{D}{2}} \cdot n) \\ \cos(w_{\frac{D}{2}} \cdot n) \end{bmatrix}, \quad w_i = \frac{1}{10000^{\frac{2i}{D}}}.$$

This is good because

$$\mathbf{r}_n^\top \mathbf{r}_m = \sum_{i=1}^{\frac{D}{2}} \cos(w_i \cdot (n - m)).$$

The encoding of $n + m$ can always be expressed as a linear combination of the encodings of n and m and it is always possible to find a matrix \mathbf{M} that depends only on k such that $\mathbf{r}_{n+k} = \mathbf{M} \mathbf{r}_n$.

$$\begin{bmatrix} v_1 & v_2 \\ v_3 & v_4 \end{bmatrix} \cdot \begin{bmatrix} \sin(w_i \cdot n) \\ \cos(w_i \cdot n) \end{bmatrix} = \begin{bmatrix} \sin(w_i \cdot (n + k)) \\ \cos(w_i \cdot (n + k)) \end{bmatrix}$$

Proof 11.1: Matrix shit

We have

$$\begin{bmatrix} v_1 & v_2 \\ v_3 & v_4 \end{bmatrix} \cdot \begin{bmatrix} \sin(w_i \cdot n) \\ \cos(w_i \cdot n) \end{bmatrix} = \begin{bmatrix} v_1 \sin(w_i \cdot n) & v_2 \cos(w_i \cdot n) \\ v_3 \sin(w_i \cdot n) & v_4 \cos(w_i \cdot n) \end{bmatrix}$$

but

$$\begin{bmatrix} \sin(w_i \cdot (n + k)) \\ \cos(w_i \cdot (n + k)) \end{bmatrix} = \begin{bmatrix} \sin(w_i \cdot n) \cos(w_i \cdot k) + \cos(w_i \cdot n) \sin(w_i \cdot k) \\ \cos(w_i \cdot n) \cos(w_i \cdot k) - \sin(w_i \cdot n) \sin(w_i \cdot k) \end{bmatrix}$$

so

$$\begin{aligned} & \begin{bmatrix} v_1 \sin(w_i \cdot n) + v_2 \cos(w_i \cdot n) \\ v_3 \sin(w_i \cdot n) + v_4 \cos(w_i \cdot n) \end{bmatrix} \\ &= \begin{bmatrix} \sin(w_i \cdot n) \cos(w_i \cdot k) + \cos(w_i \cdot n) \sin(w_i \cdot k) \\ \cos(w_i \cdot n) \cos(w_i \cdot k) - \sin(w_i \cdot n) \sin(w_i \cdot k) \end{bmatrix} \end{aligned}$$

and this means

$$\begin{bmatrix} v_1 & v_2 \\ v_3 & v_4 \end{bmatrix} = \begin{bmatrix} \cos(w_i \cdot k) & \sin(w_i \cdot k) \\ -\sin(w_i \cdot k) & \cos(w_i \cdot k) \end{bmatrix}$$

11.2 GPTs

The goal is to use transformers to build an autoregressive model of the form

$$p(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \prod_{n=1}^N p(\mathbf{x}_n | \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}).$$

Here the attention weights are computed using $\mathbf{Q} \mathbf{K}^\top$ as before, but we can set the attention weights to zero for all future tokens and computing $(\mathbf{Q} \mathbf{K}^\top)_{nm}^\top$ as the attention weights between tokens n and m multiplied by a mask matrix \mathbf{M} that has $-\infty$ in the upper triangular part.

$$\mathbf{Y} = \text{SoftMax} \left[\frac{\mathbf{Q} \mathbf{K}^\top}{\sqrt{D_k}} \circ \mathbf{M} \right] \mathbf{V}.$$

Temperature scaling:

$$y_i = \frac{\exp\left(\frac{a_i}{T}\right)}{\sum_j \exp\left(\frac{a_j}{T}\right)}$$