Attention in machine learning: how to explain the empirical formula

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1. Attention as a way to better classification

- In many practical situations, we have several objects.
- Each object i is characterized by vector $x_i = (x_{i,1}, \ldots, x_{i,N})$ consisting of this object's numerical characteristics.
- For example, we have many picture of pets, and you want to classify them into cats and dogs.
- One of the difficulties is that objects within each class are different.
- For example, dogs can be large and small, of different breeds, etc.
- To make classification task easier, it is desirable:
  - to replace each specific vector x_i
  - with a weighted average $y_i = \sum_j w_{ij} \cdot x_j$ of all the objects x_j which are similar to x_i.
- This way, the role of individual characteristics will diminish, and the classification task will become easier.

2. Attention as a way to better classification (cont-d)

- A natural way to describe the closeness between the objects x_i and x_j is to use the usual metric $d(a,b)=\sqrt{\sum_k (a_k-b_k)^2}$.
- The smaller this distance, the larger should be the weight.
- So we must have $w_{ij}\sim f(d(x_i,x_j))$ for some decreasing function $f(v)$.
- The sum of the weights should be equal to 1, so we must have

$$w_{ij}=\frac{f(d(x_i,x_j))}{\sum_\ell f(d(x_i,x_\ell))}.$$

- This expression can be simplified if we take into account that overall, the values x_{ij} are reasonably random.
- In this case the value $x_i^2=\sum_k x_{i,k}^2$ is close to some constant C (which is N time average of $x_{i,j}^2$).
- Then, $d^2(x_i,x_j)=x_i^2+x_j^2-2x_i\cdot x_j\approx 2C-2x_i\cdot x_j$.
- So, a decreasing function of $d(x_i,x_j)$ can be described as an increasing function of the dot product $x_i\cdot x_j$.

3. Attention as a way to better classification (cont-d)

- Thus,
$$w_{ij}=\frac{F(x_i\cdot x_j)}{\sum_\ell F(x_i\cdot x_\ell)}.$$
- Empirical evidence shows that out of all increasing functions $F(v)$, functions $F(v)=\exp(\alpha\cdot v)$ work the best.
- How can we explain this empirical fact?

4. Our explanation

- It is based on the fact that measurements are noisy.
- So, a natural requirement is that the resulting values y_i should be affected by the noise as little as possible.
- What if we replace the original values $x_{i,j}$ with noisy values $\widetilde{x}_{i,k} = x_{i,k} + n_{i,k}$ for some noise $n_{i,k}$ with 0 mean.
- Then the dot product $\widetilde{x}_i \cdot \widetilde{x}_j$ becomes $x_i \cdot x_j + x_i \cdot n_i + n_i \cdot x_j + n_i \cdot n_j$.
- The expected value of terms $x_i \cdot n_j$ is 0, so the only non-zero addition to the dot product is $E[n_i \cdot n_j]$.
- For local noise, this expected value is 0; however:
  - if the noise had a global component with mean square value m,
  - then, on average, all dot products are increased by the same constant m.
- So, we want to find the function $F(v)$ for which adding a constant m to all dot product would not change the weights.

5. Our explanation (cont-d)

- In particular, for two objects, this means that
$$\frac{F(a+m)}{F(a+m)+F(b+m)}=\frac{F(a)}{F(a)+F(b)} \text{ for all } a,b, \text{ and } m.$$
- If we apply $1/z$ to both sides of this equality and subtract 1 from both sides, we get
$$\frac{F(b+m)}{F(a+m)}=\frac{F(b)}{F(a)}.$$
- Multiplying both sides by $F(a+m)/F(b)$, we get
$$\frac{F(b+m)}{F(b)}=\frac{F(a+m)}{F(a)} \text{ for all } a \text{ and } b.$$
- So, the ratio $F(a+m)/F(a)$ does not depend on a, it only depends on m: $F(a+m)/F(a)=g(m)$ for some function $g(m)$.
- Thus, $F(a+m)=g(m)\cdot F(a)$.

6. Our explanation (cont-d)

- It is known that the only increasing solution to this functional equation is $F(a) = c \cdot \exp(\alpha \cdot a)$.
- From the viewpoint of the weights $w_{i,j}$, it is equivalent to

$$F(a) = \exp(\alpha \cdot a).$$

- This is exactly what we needed to explain.

7. Comment: how to solve the functional equation

- To solve the functional equation, differentiate both sides by m and take $m = 0$.
- Then $F'(a) = g'(0) \cdot F(a)$, with $\alpha \stackrel{\text{def}}{=} g'(0)$, i.e.,

$$\frac{dF}{da} = \alpha \cdot F \text{ and } \frac{dF}{F} = \alpha \cdot da.$$

- Integrating, we get $\ln(F) = \alpha \cdot a + \text{const}$, so $F(a) = \text{const} \cdot \exp(\alpha \cdot a)$.

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