Multi-head self-attention is the core modeling component of Transformers. In this question, we'll get some practice working with the self-attention equations, and motivate why multi-headed self-attention can be preferable to single-headed self-attention.

Recall that attention can be viewed as an operation on a *query* vector $q \in \mathbb{R}^d$, a set of *value* vectors $\{v_1, \ldots, v_n\}, v_i \in \mathbb{R}^d$, and a set of *key* vectors $\{k_1, \ldots, k_n\}, k_i \in \mathbb{R}^d$, specified as follows:

$$c = \sum_{i=1}^{n} v_i \alpha_i \tag{1}$$

$$\alpha_i = \frac{\exp(k_i^\top q)}{\sum_{j=1}^{n} \exp(k_j^\top q)} \tag{2}$$

with $alpha = \{\alpha_1, \ldots, \alpha_n\}$ termed the "attention weights". Observe that the output $c \in \mathbb{R}^d$ is an average over the value vectors weighted with respect to α.

(a) (3 points) **Copying in attention.** One advantage of attention is that it's particularly easy to "copy" a value vector to the output c. In this problem, we'll motivate why this is the case.

i. (2 points) The distribution α is typically relatively "diffuse"; the probability mass is spread out between many different α_i. However, this is not always the case. **Describe** (in one sentence) under what conditions the categorical distribution α puts almost all of its weight on some α_j, where $j \in \{1, \ldots, n\}$ (i.e. $\alpha_j \gg \sum_{i \neq j} \alpha_i$). What must be true about the query q and/or the keys $\{k_1, \ldots, k_n\}$?

ii. (1 point) Under the conditions you gave in (i), **describe** the output c.

(b) (2 points) **An average of two.** Instead of focusing on just one vector v_j, a Transformer model might want to incorporate information from *multiple* source vectors.

Consider the case where we instead want to incorporate information from **two** vectors v_a and v_b, with corresponding key vectors k_a and k_b. Assume that (1) all key vectors are orthogonal, so $k_i^\top k_j = 0$ for all $i \neq j$; and (2) all key vectors have norm 1. **Find an expression** for a query vector q such that $c \approx \frac{1}{2}(v_a + v_b)$, and **justify your answer.*** (Recall what you learned in part (a).)

(c) (5 points) **Drawbacks of single-headed attention:** In the previous part, we saw how it was *possible* for a single-headed attention to focus equally on two values. The same concept could easily be extended to any subset of values. In this question we'll see why it's not a *practical* solution.

Consider a set of key vectors $\{k_1, \ldots, k_n\}$ that are now randomly sampled, $k_i \sim \mathcal{N}(\mu_i, \Sigma_i)$, where the means $\mu_i \in \mathbb{R}^d$ are known to you, but the covariances Σ_i are unknown (unless specified otherwise in the question). Further, assume that the means μ_i are all perpendicular; $\mu_i^\top \mu_j = 0$ if $i \neq j$, and unit norm, $\|\mu_i\| = 1$.

i. (2 points) Assume that the covariance matrices are $\Sigma_i = \alpha I, \forall i \in \{1, 2, \ldots, n\}$, for vanishingly small α. Design a query q in terms of the μ_i such that as before, $c \approx \frac{1}{2}(v_a + v_b)$, and provide a brief argument as to why it works.

ii. (3 points) Though single-headed attention is resistant to small perturbations in the keys, some types of larger perturbations may pose a bigger issue. In some cases, one key vector k_a may be larger or smaller in norm than the others, while still pointing in the same direction as μ_a.†
As an example, let us consider a covariance for item a as $\Sigma_a = \alpha I + \frac{1}{2}(\mu_a \mu_a^\top)$ for vanishingly small α (as shown in figure 1). This causes k_a to point in roughly the same direction as μ_a, but with large variances in magnitude. Further, let $\Sigma_i = \alpha I$ for all $i \neq a$.

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*Hint: while the softmax function will never *exactly* average the two vectors, you can get close by using a large scalar multiple in the expression.

†Unlike the original Transformer, newer Transformer models apply layer normalization before attention. In these pre-layernorm models, norms of keys cannot be too different which makes the situation in this question less likely to occur.

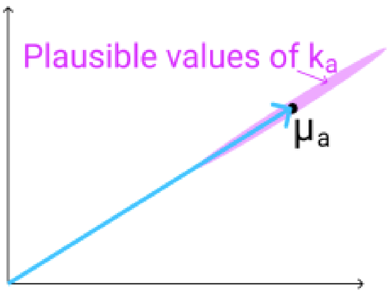

Figure 1: The vector μ_a (shown here in 2D as an example), with the range of possible values of k_a shown in red. As mentioned previously, k_a points in roughly the same direction as μ_a, but may have larger or smaller magnitude.

When you sample $\{k_1, \ldots, k_n\}$ multiple times, and use the q vector that you defined in part i., what do you expect the vector c will look like qualitatively for different samples? Think about how it differs from part (i) and how c's variance would be affected.

(d) (3 points) **Benefits of multi-headed attention:** Now we'll see some of the power of multi-headed attention. We'll consider a simple version of multi-headed attention which is identical to single-headed self-attention as we've presented it, except two query vectors (q_1 and q_2) are defined, which leads to a pair of vectors (c_1 and c_2), each the output of single-headed attention given its respective query vector. The final output of the multi-headed attention is their average, $\frac{1}{2}(c_1 + c_2)$.

As in question 1(c), consider a set of key vectors $\{k_1, \ldots, k_n\}$ that are randomly sampled, $k_i \sim \mathcal{N}(\mu_i, \Sigma_i)$, where the means μ_i are known to you, but the covariances Σ_i are unknown. Also as before, assume that the means μ_i are mutually orthogonal; $\mu_i^\top \mu_j = 0$ if $i \neq j$, and unit norm, $\|\mu_i\| = 1$.

i. (1 point) Assume that the covariance matrices are $\Sigma_i = \alpha I$, for vanishingly small α. Design q_1 and q_2 in terms of μ_i such that c is approximately equal to $\frac{1}{2}(v_a + v_b)$. Note that q_1 and q_2 should have different expressions.

ii. (2 points) Assume that the covariance matrices are $\Sigma_a = \alpha I + \frac{1}{2}(\mu_a \mu_a^\top)$ for vanishingly small α, and $\Sigma_i = \alpha I$ for all $i \neq a$. Take the query vectors q_1 and q_2 that you designed in part i. What, qualitatively, do you expect the output c to look like across different samples of the key vectors? Explain briefly in terms of variance in c_1 and c_2. You can ignore cases in which $k_a^\top q_i < 0$.

(e) (1 point) Based on part (d), briefly summarize how multi-headed attention overcomes the drawbacks of single-headed attention that you identified in part (c).