NEURAL COLLAPSE WITH CROSS-ENTROPY LOSS

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Abstract. We consider the variational problem of cross-entropy loss with \( n \) feature vectors on a unit hypersphere in \( \mathbb{R}^d \). We prove that when \( d \geq n - 1 \), the global minimum is given by the simplex equiangular tight frame, which justifies the neural collapse behavior. We also show a connection with the frame potential of Benedetto & Fickus.

1. Introduction and Results

1.1. Introduction. We consider the following variational problem

\[
\min_u \mathcal{L}_\alpha(u) := \min_u \sum_{i=1}^n \log \left( 1 + \sum_{j \neq i}^n e^{\alpha \langle u_j, u_i \rangle} \right).
\]

where \( \alpha > 0 \) is a parameter and for \( i = 1, \ldots, n \), \( u_i \in \mathbb{R}^d \) such that \( \|u_i\| = 1 \). Here and in the sequel, we use \( \| \cdot \| \) to denote the Euclidean norm of a vector, and \( \langle \cdot, \cdot \rangle \) denotes the Euclidean inner product. The question we would like to address in this note is the solution structure of such variational problems. The problem has several motivations from some recent works in the literature of machine learning.

Our main motivation comes from the very nice recent paper [3]. In that paper, the authors proposed and studied the neural collapse behavior of training of deep neural networks for classification problems. Following the work [3] by choosing a cross-entropy loss, while taking unconstrained features (i.e., not parametrized by some nonlinear functions like neural networks) to be vectors on the unit sphere in \( \mathbb{R}^d \), this amounts to the study of the variational problem

\[
\min_{u,v} \mathcal{L}(u, v) := \min_{u,v} \sum_{i=1}^n \log \left( \frac{\sum_{j=1}^n e^{\langle v_j, u_i \rangle}}{e^{\langle v_i, u_i \rangle}} \right).
\]

where \( u_i, v_i \in \mathbb{R}^d \) such that \( \|u_i\| = 1 \) for each \( i \). Note that the model in [3] also contains a bias vector, so that \( \langle v_j, u_i \rangle \) in (2) is replaced by \( \langle v_j, u_i \rangle + b_j \), for \( b \in \mathbb{R}^n \). We drop the bias to remove some degeneracy of the problem for simplicity. Another, more crucial, difference is that in actual deep learning, as considered in [3], the feature vectors \( u_i \) are given by output of deep neural networks acting on the input data, this would make the variational problem much harder to analyze and thus we will only study the simplified scenario.

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1.2. Results. The connection between the two variational problems is evident, as (1) can be viewed as a symmetric version of (2). In particular, if we choose \( v_i = \alpha u_i \) for some parameter \( \alpha > 0 \), then \( \mathcal{L}(\alpha u, u) = \mathcal{L}_\alpha(u) \). In fact, we will prove that the minimum of (2) is indeed achieved by such symmetric solutions. There is a small caveat though as one can take the norm of \( v_i \) to infinity (or \( \alpha \to \infty \) for the symmetric problem) to reduce the loss. Thus, in order to characterize better the solution structure, we will consider the problem for a fixed scaling of \( v_i \), and in fact \( \|v_i\| = 1 \) (the case of \( \|v_i\| = \alpha \) will be discussed below). We show that the solution of the variational problem is given by a simplex equiangular tight frame (ETF). This proves the neural collapse behavior for (2), which provides some justification to the observation of such behavior in deep learning.

**Theorem 1.** Consider the variational problem

\[
\min_{u,v} \mathcal{L}(u, v)
\]

such that \( u_i, v_i \in \mathbb{R}^d, \|u_i\| = \|v_i\| = 1, \quad i = 1, \ldots, n. \)

If \( d \geq n - 1 \), the global minimum of the problem corresponds to the case where \( \{u_i\}_{i=1}^n \) form a simplex equiangular tight frame and \( u_i = v_i \) for all \( i = 1, \ldots, n \).

We remark that similar results have been proved for different loss functions: for a large deviation type loss function in [3] and for a \( L^2 \)-loss function in [2], both for models with unconstrained feature vectors (i.e., without neural network parametrization of \( u_i \)'s). To the best of our knowledge, Theorem 1 is the first justification for the cross-entropy loss, which is considered in the large-scale experiments in [3] and also perhaps the most popular choice for classification problems.

In Theorem 1 the restriction of the scale of \( \|v_i\| = 1 \) does not in fact sacrifice generality. As we will comment towards the end of the proof, if instead \( \|v_i\| \leq \alpha \) is assumed, the solution would be given by \( v_i = \alpha u_i \). This is related to the following result for the symmetric problem (1).

**Theorem 2.** Consider the variational problem

\[
\min_u \mathcal{L}_\alpha(u)
\]

such that \( u_i \in \mathbb{R}^d, \|u_i\| = 1, \quad i = 1, \ldots, n. \)

If \( d \geq n - 1 \), then for any \( \alpha > 0 \), the global minimum of the problem corresponds to the case where \( \{u_i\}_{i=1}^n \) form a simplex equiangular tight frame.

We prove Theorem 2 first in Section 2; the idea of the proof extends to that of Theorem 1 which will be presented in Section 3.

1.3. The Frame Potential. We conclude with a simple observation: for \( \alpha \to 0^+ \), the functional \( \mathcal{L}_\alpha \) has a Taylor expansion with quite excellent properties.

**Proposition 3.** For a fixed set of point \( \{u_1, \ldots, u_n\} \subset \mathbb{S}^d \), we have, as \( \alpha \to 0 \),

\[
\sum_{i=1}^n \log \left( \sum_{j=1}^n e^{\alpha \langle u_i, u_j \rangle} \right) = n \log n + \frac{\alpha}{n} \sum_{i=1}^n \|u_i\|^2 + \frac{\alpha^2}{2n} \sum_{i,j=1}^n \langle u_i, u_j \rangle^2 - \frac{\alpha^2}{2n} \sum_{i=1}^n \left( \sum_{j=1}^n u_i \right) \left( \sum_{j=1}^n u_j \right)^2 + O(\alpha^3).
\]
This expansion has a very interesting consequence: if $\alpha$ is quite small, then the linear term dominates and minimizers of the energy functional will be forced to have $\|\sum_{i=1}^{n} u_i\|$ quite small. This has implications for the third term which will then also be small. As such we would expect that there is an emerging effective energy given by

$$E(u_1, \ldots, u_n) = \frac{\alpha}{n} \left\| \sum_{i=1}^{n} u_i \right\|^2 + \frac{\alpha^2}{2n} \sum_{i,j=1}^{n} \langle u_i, u_j \rangle^2.$$  

This object function, however, is strongly connected to the frame potential

$$F(u_1, \ldots, u_n) = \sum_{i,j=1}^{n} \langle u_i, u_j \rangle^2.$$  

The frame potential was introduced in the seminal work of Benedetto & Fickus [1] and has since played an important role in frame theory. What is utterly remarkable is that the Frame Potential has a large number of highly structured minimizers (see, for example, Fig. 1). As shown by Benedetto & Fickus, for any $\{u_1, \ldots, u_n\} \subset \mathbb{S}^{d-1}$

$$F(u_1, \ldots, u_n) = \sum_{i,j=1}^{n} \langle u_i, u_j \rangle^2 \geq \frac{n^2}{d}$$

with equality if and only if the set of points form a tight frame, i.e. if

$$\forall \ u \in \mathbb{R}^d : \sum_{i=1}^{n} \langle u, u_i \rangle^2 = \frac{n}{d} \|u\|^2.$$  

![Figure 1. The 72 vertices of the Dodecahedron-Icosahedron compound form a unit norm tight frame of $\mathbb{R}^3$. The point configuration is also a global minimizer of the frame potential.](image)

In fact, our effective energy $E(u_1, \ldots, u_n)$ may be understood as the frame potential with an additional strong incentive for the point configuration to have mean value 0. It would be interesting to have a better understanding whether $\mathcal{L}_\alpha$ inherits some of the good properties of the Frame Potential for $\alpha$ small. Is it possible to say anything about minimal energy configurations of $\mathcal{L}_\alpha$ when $n \gg d$? We note that Jensen’s inequality implies

$$\sum_{i=1}^{n} \log \left( \frac{1}{n} \sum_{j=1}^{n} e^{\alpha \langle u_j, u_i \rangle} \right) \leq n \log \left( \frac{1}{n} \sum_{i,j=1}^{n} e^{\alpha \langle u_i, u_j \rangle} \right).$$
In addition, \(e^{\alpha \langle \cdot, \cdot \rangle}\) is a positive definite kernel on \(S^d\) and thus minimizers are asymptotically uniformly distributed. However, we also note that the Fourier coefficients of this kernel decay quite rapidly making the kernel rather insensitive to high frequency perturbations.

2. Proof for Theorem 2

Proof. Recall the variational problem under consideration

\[
\min_u \mathcal{L}_\alpha(u) := \min_u \sum_{i=1}^{n} \log \left( 1 + \sum_{j=1 \atop j \neq i}^{n} e^{\alpha \langle u_j, u_i \rangle - 1} \right).
\]

Using Jensen’s inequality, we have, for any fixed \(1 \leq i \leq n\),

\[
\frac{1}{n-1} \sum_{j=1 \atop j \neq i}^{n} e^{\alpha \langle u_j, u_i \rangle} \geq \exp \left( \frac{1}{n-1} \sum_{j=1 \atop j \neq i}^{n} \alpha \langle u_j, u_i \rangle \right)
\]

\[
= \exp \left( \frac{\alpha}{n-1} \left( \langle U, u_i \rangle - 1 \right) \right),
\]

where we introduce the sum

\[
U = \sum_{i=1}^{n} u_i.
\]

Thus, since the logarithm is monotone,

\[
\mathcal{L}_\alpha(u) = \sum_{i=1}^{n} \log \left( 1 + \sum_{j=1 \atop j \neq i}^{n} e^{\alpha \langle u_j, u_i \rangle} \right)
\]

\[
\geq \sum_{i=1}^{n} \log \left( 1 + (n-1)e^{-\frac{\alpha}{n-1}} e^{\alpha \langle U, u_i \rangle} \right).
\]

Note that for any \(a, b > 0\), the function \(t \mapsto \log(1 + ae^{bt})\) is convex, applying Jensen’s inequality again, we have

\[
\frac{1}{n} \mathcal{L}_\alpha(u) \geq \frac{1}{n} \sum_{i=1}^{n} \log \left[ 1 + (n-1)e^{-\frac{\alpha}{n-1}} \exp \left( \frac{\alpha}{n-1} \langle U, u_i \rangle \right) \right]
\]

\[
\geq \log \left[ 1 + (n-1)e^{-\frac{\alpha}{n-1}} \exp \left( \frac{\alpha}{n-1} \frac{1}{n} \sum_{i=1}^{n} \langle U, u_i \rangle \right) \right]
\]

\[
= \log \left[ 1 + (n-1)e^{-\frac{\alpha}{n-1}} \exp \left( \frac{\alpha}{n-1} \frac{1}{n} \|U\|^2 \right) \right]
\]

\[
\geq \log \left( 1 + (n-1)e^{-\frac{\alpha}{n-1}} \right).
\]

Therefore, we arrive at

\[
\mathcal{L}_\alpha(u) \geq n \log \left( 1 + (n-1)e^{-\frac{\alpha}{n-1}} \right).
\]

To see when the minimum is achieved, note that in (5), due to strict convexity of the exponential function, equality only holds when, for \(j \neq i\),

\[
\langle u_j, u_i \rangle = c_i \quad \text{is independent of } j.
\]
Equality in (7) only holds if
\[ \langle U, u_i \rangle = c \]
independent of \( i \).
Finally, inequality in the last part of (7) only holds when \( U = 0 \). If \( U = 0 \), then
\[ c = \langle U, u_i \rangle = \left( \sum_{j=1}^{n} u_j, u_i \right) = 1 + \left( \sum_{j \neq i}^{n} u_j, u_i \right) = 1 + (n-1)c_i. \]
This shows that \( c_i \) does not actually depend on \( i \) and thus \( \langle u_i, u_j \rangle \equiv c \) for some constant \( c \) whenever \( i \) is different from \( j \). Thus, we conclude
\[
0 = \left\| \sum_{i=1}^{n} u_i \right\|^2 = n + \sum_{i \neq j} \langle u_i, u_j \rangle = n + n(n-1)c.
\]
This implies that
\[ \langle u_i, u_j \rangle = -\frac{1}{n-1}. \]
Therefore, the global minimum is achieved if and only if when \( \{u_i\}_{i=1}^{n} \) form a simplex equiangular tight frame (recall \( d \geq n-1 \) so it is achievable). \( \square \)

3. PROOF OF THEOREM \( \blacksquare \)

Proof. The proof follows along similar lines as the proof of Theorem \( \blacksquare \) Recall
\[ \mathcal{L}(u, v) = \sum_{i=1}^{n} \log \left( \sum_{j=1}^{n} e^{\langle v_j, u_i \rangle} \right) = \sum_{i=1}^{n} \log \left( 1 + \sum_{j \neq i}^{n} e^{\langle v_j-u_i, u_i \rangle} \right) \]
Applying Jensen’s inequality, we have, for fixed \( 1 \leq i \leq n \),
\[
\sum_{j \neq i}^{n} e^{\langle v_j-u_i, u_i \rangle} = e^{-\langle v_i, u_i \rangle} \sum_{j \neq i}^{n} e^{\langle v_j, u_i \rangle} \geq (n-1)e^{-\langle v_i, u_i \rangle} \exp \left( \frac{1}{n-1} \sum_{j \neq i}^{n} \langle v_j, u_i \rangle \right) \]
\[ = (n-1)e^{-\langle v_i, u_i \rangle} \exp \left( \frac{\langle V, u_i \rangle - \langle v_i, u_i \rangle}{n-1} \right) \]
\[ = (n-1) \exp \left( \frac{\langle V, u_i \rangle - n\langle v_i, u_i \rangle}{n-1} \right), \]
where we denote the sum of \( v_i \) as
\[ V = \sum_{i=1}^{n} v_i. \]
Thus, using the monotonicity of logarithm,
\[
\mathcal{L}(u, v) = \sum_{i=1}^{n} \log \left( 1 + \sum_{j \neq i}^{n} e^{\langle v_j-v_i, u_i \rangle} \right) \geq \sum_{i=1}^{n} \log \left[ 1 + (n-1) \exp \left( \frac{\langle V, u_i \rangle - n\langle v_i, u_i \rangle}{n-1} \right) \right]
\]
Applying Jensen’s inequality to the convex function \( t \mapsto \log(1 + ae^{bt}) \) for \( a, b > 0 \), we have

\[
\mathcal{L}(u, v) \geq n \log \left[ 1 + (n-1) \exp \left( \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\langle V, u_i \rangle}{n-1} - \frac{n}{n-1} \langle v_i, u_i \rangle \right) \right) \right]
\]

\[
= n \log \left[ 1 + (n-1) \exp \left( \frac{1}{n} \left( \langle V, U \rangle \sum_{i=1}^{n} (\langle v_i, u_i \rangle) \right) - \frac{n}{n-1} \sum_{i=1}^{n} \langle v_i, u_i \rangle \right) \right],
\]

where \( U = \sum_{i} u_i \). For the equalities to hold in the above inequalities (10) and (12), we require for some constants \( c_i \) and \( c \) such that

\[
\langle v_j, u_i \rangle = c_i, \quad \forall \ j \neq i
\]

and

\[
\frac{\langle V, u_i \rangle}{n-1} - \frac{n}{n-1} \langle v_i, u_i \rangle = c, \quad \forall \ i.
\]

Therefore, in order to find a lower bound on \( \mathcal{L} \), we have to solve

\[
\frac{\langle V, U \rangle}{n-1} - \frac{n}{n-1} \sum_{i=1}^{n} \langle v_i, u_i \rangle \rightarrow \min.
\]

If there is a minimizing configuration of this simpler problem that also satisfies (13) and (14), then all inequalities are actually equalities. The above variational problem is equivalent to maximizing

\[
n \sum_{i=1}^{n} \langle v_i, u_i \rangle - \left( \sum_{i=1}^{n} v_i \right) \sum_{i=1}^{n} u_i = \tilde{v}^\top (nI_n - 1_n 1_n^\top) \otimes I_d \tilde{u},
\]

where \( \otimes \) denotes the Kronecker product, \( I_d (1_n) \) denotes a \( d \times d \) \((n \times n)\) identity matrix, \( 1_n \) denotes an all-1 \( n \)-vector, \( \tilde{u} \) denotes a long \( \mathbb{R}^{nd} \) column vector formed by concatenating \( u_i \in \mathbb{R}^d \) for \( i = 1, \ldots, n \), and similarly for \( \tilde{v} \). We note that, being the concatenation of unit vectors, \( \|\tilde{u}\| = \sqrt{n} = \|\tilde{v}\| \).

The eigenvalues of a Kronecker product \( A \otimes B \) are given by \( \lambda_i \mu_j \), where \( \lambda_i \) are the eigenvalues of \( A \) and \( \mu_j \) are the eigenvalues of \( B \). The matrix \( nI_n - 1_n 1_n^\top \) is acting like \( nI_n \) on vectors having mean value 0 while sending the constant vector to 0. Its spectrum is thus given by \( n \) (with multiplicity \( n-1 \)) and 0. It follows that \((nI_n - 1_n 1_n^\top) \otimes I_d \) is symmetric, its largest eigenvalue is \( n \) and its smallest eigenvalue is 0. Recalling that \( \|\tilde{u}\| = \sqrt{n} = \|\tilde{v}\| \), we have that (without constraints (13) and (14))

\[
n \sum_{i=1}^{n} \langle v_i, u_i \rangle - \left( \sum_{i=1}^{n} v_i \right) \sum_{i=1}^{n} u_i \leq n^2.
\]

However, setting \( \tilde{u} \) to be the simplex and \( \tilde{v} = \tilde{u} \), we see that \( U = 0 = V \) and we have equality in (16) while simultaneously satisfying the constraints (13) and (14) with

\[
c_i = -\frac{1}{n-1} \quad \text{and} \quad c = -\frac{n}{n-1}.
\]

We will now argue that this is the only extremal example. Using the Spectral Theorem, we see that equality in (16) can only occur if \( \tilde{u} \) is an eigenvector of the matrix corresponding to the eigenvalue \( n \). In that case, we have

\[
\langle \tilde{v}, ((nI_n - 1_n 1_n^\top) \otimes I_d) \tilde{u} \rangle = n \langle \tilde{v}, \tilde{u} \rangle \leq n \|\tilde{v}\| \|\tilde{u}\| \leq n^2.
\]
We have equality in Cauchy-Schwarz if and only if \( \vec{v} = \lambda \vec{u} \) for some \( \lambda > 0 \). For \( \alpha = 1 \), this implies that \( \vec{v} = \vec{u} \) and we are back in the symmetric case and can argue as in the proof of Theorem 2. Conditions (13) and (14) simplify to

\[
\langle u_j, u_i \rangle = c_i, \quad \forall j \neq i \quad \text{and} \quad \frac{\langle U, u_i \rangle}{n-1} - \frac{n}{n-1} \langle u_i, u_i \rangle = c, \quad \forall i.
\]

Moreover, by summing over the second condition, we see that we want to minimize

\[
c \cdot n = \frac{\langle U, U \rangle}{n-1} - \frac{n}{n-1} \sum_{i=1}^{n} \langle u_i, u_i \rangle \to \min.
\]

We are thus interested in minimizing \( c \) which is given by

\[
c = \frac{\langle U, u_i \rangle}{n-1} - \frac{n}{n-1} \langle u_i, u_i \rangle = c_i - \langle u_i, u_i \rangle \geq c_i - 1.
\]

However, for any set of \( n \) unit vectors, the largest inner product between any pair of distinct vectors satisfies

\[
0 \leq \left\| \sum_{i=1}^{n} u_i \right\|^2 = n + n(n-1) \max_{i \neq j} \langle u_i, u_j \rangle.
\]

Thus

\[
c \geq \max_{1 \leq i \leq n} c_i - 1 \geq -\frac{1}{n-1} - 1 = -\frac{n}{n-1}.
\]

We see that equality is achieved for the simplex. Moreover, in the case of equality, we have to require that \( \langle u_i, u_j \rangle = -1/(n-1) \) for any pair of distinct vectors and this characterizes the simplex. Moreover, if \( \|u_i\| \leq \alpha \), then it is easy to see that the maximum is achieved when \( \vec{v} = \alpha \vec{u} \), we can again conclude using Theorem 2. \( \square \)

4. PROOF OF PROPOSITION 3

Proof. We are interested in asymptotics for

\[
\sum_{i=1}^{n} \log \left( \sum_{j=1}^{n} e^{\alpha \langle u_i, u_j \rangle} \right) \quad \text{as } \alpha \to 0.
\]

We have the Taylor expansion

\[
\log (1 + x) = x - \frac{x^2}{2} + O(x^3)
\]

and thus, as \( \alpha \to 0 \),

\[
\sum_{i=1}^{n} \log \left( \sum_{j=1}^{n} e^{\alpha \langle u_i, u_j \rangle} \right) = \sum_{i=1}^{n} \log \left( \sum_{j=1}^{n} 1 + \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 + \ldots \right)
\]

\[
= \sum_{i=1}^{n} \log \left( \left( 1 + \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 + \ldots \right) \right)
\]

\[
= n \log n + \sum_{i=1}^{n} \log \left( 1 + \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 + \ldots \right).
\]
Using the Taylor expansion of the logarithm and collecting all the terms that are constant, linear or quadratic in $\alpha$, we arrive at
\[
\sum_{i=1}^{n} \log \left( \sum_{j=1}^{n} e^{\alpha \langle u_i, u_j \rangle} \right) = n \log n + \sum_{i=1}^{n} \left( \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 \right) - \frac{1}{2} \sum_{i=1}^{n} \left( \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 \right)^2 + O(\alpha^3).
\]

The first term simplifies to
\[
\sum_{i=1}^{n} \left( \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 \right) = \frac{\alpha}{n} \left\| \sum_{i=1}^{n} u_i \right\|^2 + \frac{\alpha^2}{2n} \sum_{i,j=1}^{n} \langle u_i, u_j \rangle^2.
\]

The summand in the second term simplifies to, up to first and second order in $\alpha$
\[
- \frac{1}{2} \left( \frac{1}{n} \sum_{j=1}^{n} \alpha \langle u_i, u_j \rangle + \frac{\alpha^2}{2} \langle u_i, u_j \rangle^2 \right)^2 = - \frac{\alpha^2}{2n^2} \left( \sum_{j} \langle u_i, u_j \rangle \right)^2 + O(\alpha^3).
\]

\[\square\]

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