

## A Network Architectures

| Layer           | CNN-3                        | CNN-9                        | CNN-18                       | CNN-45                        | CNN-60                        | CNN-69                        |
|-----------------|------------------------------|------------------------------|------------------------------|-------------------------------|-------------------------------|-------------------------------|
| Conv1.x         | $[3 \times 3, 64] \times 1$  | $[3 \times 3, 64] \times 3$  | $[3 \times 3, 64] \times 6$  | $[3 \times 3, 64] \times 15$  | $[3 \times 3, 64] \times 20$  | $[3 \times 3, 64] \times 23$  |
| Pool1           | 2x2 Max Pooling, Stride 2    |                              |                              |                               |                               |                               |
| Conv2.x         | $[3 \times 3, 96] \times 1$  | $[3 \times 3, 96] \times 3$  | $[3 \times 3, 96] \times 6$  | $[3 \times 3, 96] \times 15$  | $[3 \times 3, 96] \times 20$  | $[3 \times 3, 96] \times 23$  |
| Pool2           | 2x2 Max Pooling, Stride 2    |                              |                              |                               |                               |                               |
| Conv3.x         | $[3 \times 3, 128] \times 1$ | $[3 \times 3, 128] \times 3$ | $[3 \times 3, 128] \times 6$ | $[3 \times 3, 128] \times 15$ | $[3 \times 3, 128] \times 20$ | $[3 \times 3, 128] \times 23$ |
| Pool3           | 2x2 Max Pooling, Stride 2    |                              |                              |                               |                               |                               |
| Fully Connected | 256                          | 256                          | 256                          | 256                           | 256                           | 256                           |

Table 5: Our plain CNN architectures with different convolutional layers. Conv1.x, Conv2.x and Conv3.x denote convolution units that may contain multiple convolution layers. E.g.,  $[3 \times 3, 64] \times 3$  denotes 3 cascaded convolution layers with 64 filters of size  $3 \times 3$ .

| Layer   | ResNet-32 for Section 4.2                                  | ResNet-32 for Section 4.3                                  | ResNet-18 for Section 4.6                                    |
|---------|--|--|--|
| Conv0.x | N/A  | N/A  | $[7 \times 7, 256]$ , Stride 2<br>3x3, Max Pooling, Stride 2 |
| Conv1.x | $[3 \times 3, 64] \times 1$<br>$[3 \times 3, 64] \times 5$ | $[3 \times 3, 96] \times 1$<br>$[3 \times 3, 96] \times 5$ | $[3 \times 3, 256] \times 2$                                 |
| Conv2.x | $[3 \times 3, 96] \times 5$                                | $[3 \times 3, 192] \times 5$                               | $[3 \times 3, 512] \times 2$                                 |
| Conv3.x | $[3 \times 3, 128] \times 5$                               | $[3 \times 3, 384] \times 5$                               | $[3 \times 3, 768] \times 2$                                 |
| Conv4.x | N/A  | N/A  | $[3 \times 3, 1024] \times 2$                                |
|         | Average Pooling  |  |  |

Table 6: Our ResNet architectures with different convolutional layers. Conv0.x, Conv1.x, Conv2.x, Conv3.x and Conv4.x denote convolution units that may contain multiple convolutional layers, and residual units are shown in double-column brackets. Conv1.x, Conv2.x and Conv3.x usually operate on different size feature maps. These networks are essentially the same as [6], but some may have different number of filters in each layer. The downsampling is performed by convolutions with a stride of 2. E.g.,  $[3 \times 3, 64] \times 4$  denotes 4 cascaded convolution layers with 64 filters of size  $3 \times 3$ , and S2 denotes stride 2.

## B Experimental Details for Imagenet-2012

For the input data of the Imagenet-2012 experiment, we only use the minimum data augmentation. Specifically, we first resize the images to  $256 \times 256$  resolution and then randomly crop patches of size  $224 \times 224$  from the resized images. Besides that, we also randomly flip the image horizontally. For SphereResNet-18-v1, we use the cosine SphereConv and the cosine W-Softmax loss. For SphereResNet-18-v2, we use the cosine SphereConv and the softmax loss. Generally, we find that the standard softmax loss and all kinds of W-Softmax loss usually have similar empirical performance. Note that, we could obtain better performance by using the other SphereConvs (sigmoid SphereConv with  $k = 0.3$  is a good choice), but it requires more GPU memory. Due to the width of our architecture and the limitation of GPU memory, the mini-batch size is set to 40 for all methods in the Imagenet-2012 experiment.

## C More Discussions for Sphere-normalized Softmax Loss

The sphere-normalized softmax (S-Softmax) loss is essentially applying the SphereConv to the fully connected layer in the softmax loss<sup>2</sup>. However, simply applying the SphereConv can not make such loss work, because this loss function is difficult to converge in practice. To address this, we rescale the logit output of the S-Softmax loss with a scaling factor  $s$ . Therefore, the output range is changed from  $[-1, 1]$  to  $[-s, s]$ . Typically, setting  $s$  from 10 to 70 works pretty well in practice. We could also use the cross-validation strategy to set the hyperparameter  $s$ .

<sup>2</sup>The softmax loss is defined as the combination of the last fully connected layer, the softmax function and the cross-entropy loss.

## D Proofs of Lemmas

### D.1 Proof of Lemma 1

The gradient is

$$\nabla \mathcal{G}(U, V) = \begin{bmatrix} \nabla_U \mathcal{G}(U, V) \\ \nabla_V \mathcal{G}(U, V) \end{bmatrix} = \begin{bmatrix} (UV^\top - F)V \\ (VU^\top - F^\top)U \end{bmatrix}$$

The Hessian matrix is

$$\begin{aligned} \nabla^2 \mathcal{G}(U, V) &= \begin{bmatrix} \nabla_U^2 \mathcal{G}(U, V) & \nabla_{U,V}^2 \mathcal{G}(U, V) \\ \nabla_{V,U}^2 \mathcal{G}(U, V) & \nabla_V^2 \mathcal{G}(U, V) \end{bmatrix} \\ &= \begin{bmatrix} V^\top V \otimes I_n & (UV^\top - F) \otimes I_k + U \boxtimes V \\ (VU^\top - F^\top) \otimes I_k + V \boxtimes U & U^\top U \otimes I_m \end{bmatrix}, \end{aligned} \quad (12)$$

where  $I_n$  is an  $n \times n$  identity matrix for any integer  $n$ , given matrices  $A \in \mathbb{R}^{n \times r}$  and  $B \in \mathbb{R}^{m \times k}$  with  $A_{:,i}$  denoting the  $i$ -th column of  $A$ ,  $A \boxtimes B \in \mathbb{R}^{nk \times mr}$  is defined as

$$A \boxtimes B = \begin{bmatrix} A_{:,1} B_{:,1}^\top & A_{:,2} B_{:,1}^\top & \cdots & A_{:,r} B_{:,1}^\top \\ A_{:,1} B_{:,2}^\top & A_{:,2} B_{:,2}^\top & \cdots & A_{:,r} B_{:,2}^\top \\ \vdots & \vdots & \ddots & \vdots \\ A_{:,1} B_{:,k}^\top & A_{:,2} B_{:,k}^\top & \cdots & A_{:,r} B_{:,k}^\top \end{bmatrix}.$$

At a global optimum, we have  $UV^\top = F$ . Then it is easy to see that for any real  $c$ , if  $\tilde{U} = cU$  and  $\tilde{V} = V/c$ , then we have

$$\nabla^2 \mathcal{G}(\tilde{U}, \tilde{V}) = \begin{bmatrix} \frac{1}{c^2} V^\top V \otimes I_n & U \boxtimes V \\ V \boxtimes U & c^2 U^\top U \otimes I_m \end{bmatrix}$$

We have that at a global optimal point,  $\nabla^2 \mathcal{G}(U, V)$  is a positive semidefinite matrix with the smallest eigenvalue equal to 0. Specifically, due to the existence of the invariance, i.e.,  $UV^\top = UR(VR)^\top$  for any orthogonal matrix  $R \in \mathbb{R}^{r \times r}$ , there are  $r(r-1)/2$  number of eigenvectors of  $\nabla^2 \mathcal{G}(U, V)$  at  $UV^\top = F$  corresponding to 0 eigenvalue [10]. Then for any  $c > 1$ , we have

$$\begin{aligned} \text{Tr}(\nabla^2 \mathcal{G}(\tilde{U}, \tilde{V})) &= \frac{1}{c^2} \text{Tr}(V^\top V \otimes I_n) + c^2 \text{Tr}(U^\top U \otimes I_m) \\ &\geq \frac{c^2}{2} (\text{Tr}(V^\top V \otimes I_n) + \text{Tr}(U^\top U \otimes I_m)) = \frac{c^2}{2} \text{Tr}(\nabla^2 \mathcal{G}(U, V)). \end{aligned}$$

This indicates that the largest eigenvalue of  $\nabla^2 \mathcal{G}(\tilde{U}, \tilde{V})$  is on the order of  $\Theta(c^2)$  times the largest eigenvalue of  $\nabla^2 \mathcal{G}(U, V)$  following the perturbation bound analysis [15] and  $U$  and  $V$  are balanced. Using a similar idea, the smallest nonzero eigenvalue of  $\nabla^2 \mathcal{G}(\tilde{U}, \tilde{V})$  is no greater than the smallest nonzero eigenvalue of  $\nabla^2 \mathcal{G}(U, V)$ , which results in our claim on the restricted condition number.

### D.2 Proof of Lemma 2

The gradient of  $\mathcal{G}_S(U, V)$  is

$$\nabla \mathcal{G}_S(U, V) = \begin{bmatrix} \nabla_U \mathcal{G}_S(U, V) \\ \nabla_V \mathcal{G}_S(U, V) \end{bmatrix} \quad \text{with}$$

$$\begin{aligned} \nabla_U \mathcal{G}_S(U, V) &= D_U(D_U UV^\top D_V - F)D_V V - (D_U^3(D_U UV^\top D_V - F) \otimes_k (UV^\top D_V)) \odot U, \\ \nabla_V \mathcal{G}_S(U, V) &= D_V(D_V VU^\top D_U - F^\top)D_U U - (D_V^3(D_V VU^\top D_U - F^\top) \otimes_k (VU^\top D_U)) \odot V, \end{aligned}$$

Note that after each iteration of SGD, we perform the entry-wise normalization for both  $U$  and  $V$ , which means  $D_U = I_n$  and  $D_V = I_m$ . Then the gradient of  $\mathcal{G}_S(U, V)$  is

$$\nabla \mathcal{G}_S(U, V) = \begin{bmatrix} \nabla_U \mathcal{G}_S(U, V) \\ \nabla_V \mathcal{G}_S(U, V) \end{bmatrix} = \begin{bmatrix} (UV^\top - F)V - ((UV^\top - F) \otimes_k (UV^\top)) \odot U \\ (VU^\top - F^\top)U - ((VU^\top - F^\top) \otimes_k (VU^\top)) \odot V \end{bmatrix},$$

where given matrices  $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times m}$  with  $\mathbf{A}_{:,i}$  denoting the  $i$ -th column of  $\mathbf{A}$ ,  $\mathbf{A} \odot \mathbf{B} \in \mathbb{R}^{n \times m}$  is the Hadamard (pointwise) product, and the operation  $\mathbf{A} \otimes_k \mathbf{B} \in \mathbb{R}^{n \times k}$  is defined as

$$\mathbf{A} \otimes_k \mathbf{B} = \begin{bmatrix} \mathbf{A}_{1,:} \mathbf{B}_{1,:}^\top \\ \mathbf{A}_{2,:} \mathbf{B}_{2,:}^\top \\ \vdots \\ \mathbf{A}_{n,:} \mathbf{B}_{n,:}^\top \end{bmatrix} \mathbf{1}_{1 \times k},$$

where  $\mathbf{1}_{1 \times k}$  is a  $1 \times k$  vector with all entries equal to 1.

Consequently, the Hessian matrix is

$$\begin{aligned} \nabla^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) &= \begin{bmatrix} \nabla_{\mathbf{U}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) & \nabla_{\mathbf{U}, \mathbf{V}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) \\ \nabla_{\mathbf{V}, \mathbf{U}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) & \nabla_{\mathbf{V}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) \end{bmatrix} \text{ with} \\ \nabla_{\mathbf{U}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) &= \mathbf{V}^\top \mathbf{V} \otimes \mathbf{I}_n - \text{diag}(\text{vec}((\mathbf{U}\mathbf{V}^\top - \mathbf{F}) \otimes_k (\mathbf{U}\mathbf{V}^\top))) \\ &\quad - \begin{bmatrix} \text{diag}(\mathbf{U}_{:,1} \odot ((2\mathbf{U}\mathbf{V}^\top - \mathbf{F})\mathbf{V}_{:,1})) & \cdots & \text{diag}(\mathbf{U}_{:,1} \odot ((2\mathbf{U}\mathbf{V}^\top - \mathbf{F})\mathbf{V}_{:,k})) \\ \vdots & \ddots & \vdots \\ \text{diag}(\mathbf{U}_{:,k} \odot ((2\mathbf{U}\mathbf{V}^\top - \mathbf{F})\mathbf{V}_{:,1})) & \cdots & \text{diag}(\mathbf{U}_{:,k} \odot ((2\mathbf{U}\mathbf{V}^\top - \mathbf{F})\mathbf{V}_{:,k})) \end{bmatrix} \\ \nabla_{\mathbf{U}, \mathbf{V}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) &= \mathbf{I}_k \otimes (\mathbf{U}\mathbf{V}^\top - \mathbf{F}) + \mathbf{U} \boxtimes \mathbf{V} \\ &\quad - \begin{bmatrix} (2\mathbf{U}\mathbf{V}^\top - \mathbf{F}) \odot ((\mathbf{U}_{:,1} \odot \mathbf{U}_{:,1})\mathbf{1}_{1 \times m}) & \cdots & (2\mathbf{U}\mathbf{V}^\top - \mathbf{F}) \odot ((\mathbf{U}_{:,1} \odot \mathbf{U}_{:,k})\mathbf{1}_{1 \times m}) \\ \vdots & \ddots & \vdots \\ (2\mathbf{U}\mathbf{V}^\top - \mathbf{F}) \odot ((\mathbf{U}_{:,k} \odot \mathbf{U}_{:,1})\mathbf{1}_{1 \times m}) & \cdots & (2\mathbf{U}\mathbf{V}^\top - \mathbf{F}) \odot ((\mathbf{U}_{:,k} \odot \mathbf{U}_{:,k})\mathbf{1}_{1 \times m}) \end{bmatrix} \\ \nabla_{\mathbf{V}, \mathbf{U}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) &= (\nabla_{\mathbf{U}, \mathbf{V}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}))^\top \\ \nabla_{\mathbf{V}}^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}) &= \mathbf{U}^\top \mathbf{U} \otimes \mathbf{I}_n - \text{diag}(\text{vec}((\mathbf{V}\mathbf{U}^\top - \mathbf{F}^\top) \otimes_k (\mathbf{V}\mathbf{U}^\top))) \\ &\quad - \begin{bmatrix} \text{diag}(\mathbf{V}_{:,1} \odot ((2\mathbf{V}\mathbf{U}^\top - \mathbf{F}^\top)\mathbf{U}_{:,1})) & \cdots & \text{diag}(\mathbf{V}_{:,1} \odot ((2\mathbf{V}\mathbf{U}^\top - \mathbf{F}^\top)\mathbf{U}_{:,k})) \\ \vdots & \ddots & \vdots \\ \text{diag}(\mathbf{V}_{:,k} \odot ((2\mathbf{V}\mathbf{U}^\top - \mathbf{F}^\top)\mathbf{U}_{:,1})) & \cdots & \text{diag}(\mathbf{V}_{:,k} \odot ((2\mathbf{V}\mathbf{U}^\top - \mathbf{F}^\top)\mathbf{U}_{:,k})) \end{bmatrix} \end{aligned}$$

Then we have  $\lambda_i(\nabla^2 \mathcal{G}_S(\tilde{\mathbf{U}}, \tilde{\mathbf{V}})) = \lambda_i(\nabla^2 \mathcal{G}_S(\mathbf{U}, \mathbf{V}))$  for all  $i \in [(n+m)k] = \{1, 2, \dots, (n+m)k\}$  by noticing that we normalize the data as  $\frac{\mathbf{U}_{i,j}}{\|\mathbf{U}_{i,:}\|_2}$  for all  $i \in [n]$  and  $\frac{\mathbf{V}_{i,j}}{\|\mathbf{V}_{i,:}\|_2}$  for all  $i \in [m]$ . This finishes the proof.