ECE 046211 - Technion - Deep Learning

HW2 - Multilayer NNs and Convolutional NNs



Part 1 - Theory

- You can choose whether to answser these straight in the notebook (Markdown + Latex) or use another editor (Word, LyX, Latex, Overleaf...) and submit an additional PDF file, **but no** handwritten submissions.
- You can attach additional figures (drawings, graphs,...) in a separate PDF file, just make sure to refer to them in your answers.
- LATEX Cheat-Sheet (to write equations)
 - Another Cheat-Sheet

Question 1 - Generalization in A Teacher-Student Setup

Recall from lecture 4 the Bayes Risk $\overline{\mathcal{R}}(w)$:

$$\overline{\mathcal{R}}(w) riangleq \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma_{\epsilon}^2 I), w_{true} \sim \mathcal{N}(0, rac{\sigma_w^2}{d} I)} \left[\mathcal{R}
ight],$$

where

$$\mathcal{R}(w_{\mu}) = \left| \left| w_{\mu} - w_{true}
ight|
ight|^2 = \left| \left| (H_{\mu}^{-1} H - I) w_{true} + H_{\mu}^{-1} X^T \epsilon
ight|
ight|^2$$

Prove:

$$\overline{\mathcal{R}}(w_{\mu}) = \sum_{i=1}^d rac{(\sigma_w^2/d)\mu^2 + \sigma_\epsilon^2 \lambda_i}{(\lambda_i + \mu)^2}$$

Hints:

•
$$\mathbb{E}\left[\epsilon^T X H_{\mu}^{-1} H_{\mu}^{-1} X^T \epsilon\right] = \sum_{i,j}^N \mathbb{E}[\epsilon_i \epsilon_j] \left(X H_{\mu}^{-1}\right)_i \left(H_{\mu}^{-1} X^T\right)_j$$

•
$$\mathbb{E}[\epsilon_i \epsilon_j] = \sigma^2_{\epsilon} \delta_{ij}$$

•
$$\sum_{i=1}^{N} \left(XH_{\mu}^{-1}\right)_{i} \left(H_{\mu}^{-1}X^{T}\right)_{i} = Tr\left[XH_{\mu}^{-2}X^{T}\right]$$

Setup

Solution 1 - Generalization in A Teacher-Student

$$\begin{split} & \mathcal{R} = \mathbb{E} \left\| \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right) \mathbf{w}_{\text{true}} + \mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \boldsymbol{\epsilon} \right\|^{2} \\ & = \mathbb{E} \left\| \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right) \mathbf{w}_{\text{true}} \right\|^{2} + \mathbb{E} \left\| \mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \boldsymbol{\epsilon} \right\|^{2} \\ & = \mathbb{E} \left[\mathbf{w}_{\text{true}}^{\top} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right) \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right) \mathbf{w}_{\text{true}} \right] + \mathbb{E} \left\| \boldsymbol{\epsilon}^{\top} \mathbf{X} \mathbf{H}_{\mu}^{-1} \mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \boldsymbol{\epsilon} \right\| \\ & = \sum_{i,j=1}^{d} \mathbb{E} \left[w_{i,\text{true}} w_{j,\text{true}} \right] \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{i}^{\top} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{j} + \sum_{i,j=1}^{N} \mathcal{C}_{\epsilon}^{2} \delta_{ij} \left(\mathbf{X} \mathbf{H}_{\mu}^{-1} \right)_{i} \left(\mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \right)_{j} \\ & = \sum_{i,j=1}^{d} \sigma_{w}^{2} \delta_{ij} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{i}^{\top} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{j} + \sum_{i,j=1}^{N} \sigma_{\epsilon}^{2} \delta_{ij} \left(\mathbf{X} \mathbf{H}_{\mu}^{-1} \right)_{i} \left(\mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \right)_{j} \\ & = \sigma_{w}^{2} \sum_{i=1}^{d} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{i}^{\top} \left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)_{i} + \sum_{i,j=1}^{N} \sigma_{\epsilon}^{2} \left(\mathbf{X} \mathbf{H}_{\mu}^{-1} \right)_{i} \left(\mathbf{H}_{\mu}^{-1} \mathbf{X}^{\top} \right)_{j} \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{X} \mathbf{H}_{\mu}^{-2} \mathbf{X}^{\top} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{I} \right]^{-2} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H}_{\mu}^{-1} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{I} \right]^{-2} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H} + \mu \mathbf{I} \right)^{-1} \mathbf{H} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{I} \right]^{-2} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H} \mathbf{H} - \mathbf{I} \right)^{-1} \mathbf{H} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{H} \right]^{-2} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H} \mathbf{H} - \mathbf{H} - \mathbf{I} \right)^{-1} \mathbf{H} \mathbf{H} - \mathbf{I} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{H} \right]^{-2} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H} \mathbf{H} - \mathbf{H} - \mathbf{I} \right)^{-1} \mathbf{H} \mathbf{H} - \mathbf{H} \right)^{2} \right] + \sigma_{\epsilon}^{2} \operatorname{Tr} \left[\mathbf{H} \mathbf{H} + \mu \mathbf{H} \mathbf{H} - \mathbf{H} \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[\left(\mathbf{H} \mathbf{H} - \mathbf{H} - \mathbf{H} - \mathbf{H} \right)^{-1} \mathbf{H} \mathbf{H} - \mathbf{H} \mathbf{H} - \mathbf{H} \right) \right] \\ & = \sigma_{w}^{2} \operatorname{Tr} \left[$$

Question 2 - "Typical" Generalization in Multilayer Neural Networks

We examine a "student" neural network $f_{\mathbf{w}}\left(\mathbf{x}\right)$ with parameter vector $\mathbf{w} \in \mathbb{R}^{k}$ and input $\mathbf{x} \in \mathbb{R}^{d_{0}}$ used in a binary classification problem where the training set is $\mathcal{S} = \left\{\mathbf{x}^{(n)}\right\}_{n=1}^{N}$ sampled i.i.d. from P_{X} , where the binary (± 1) labels are generated by a "teacher" neural network $f_{\mathbf{w}_{\star}}\left(\mathbf{x}\right)$ with the same architecture. To understand the "typical" generalization of the student, we examine the following

"Guess and Check" algorithm to learn its weights: we randomly sample parameters vectors $\mathbf{w}_1, \mathbf{w}_2, \ldots$ i.i.d.from P_W , in which each parameter is sampled independently from a uniform distribution over $Q = \{-\left(q-1\right)/2, \ldots, -1, 0, 1, \ldots, \left(q-1\right)/2\}$ quantization levels, where q = |Q| is an odd positive number. We do this until a stopping time t in which we perfectly fit the dataset: $\forall n: f_{\mathbf{w}_t}\left(\mathbf{x}^{(n)}\right) = f_{\mathbf{w}_\star}\left(\mathbf{x}^{(n)}\right)$. We examine a two-layer neural network with d_1 hidden neurons

$$f_{\mathbf{w}}\left(\mathbf{x}
ight) = \mathrm{sign}\left(\mathbf{w}_{2}^{ op}[\mathbf{W}_{1}\mathbf{x}]_{+}
ight)$$

where $[\cdot]_+$ is the ReLU activation function, the teacher has at most $d_1^{\star} < d_1$ non-zero neurons (i.e., the other $d_1 - d_1^{\star}$ hidden neurons in the teacher to have all the incoming and outgoing weights equal to zero). Each of the teacher's weights are also in Q.

- 1. Calculate the probability $P_{\mathbf{w} \sim P_W}\left(\mathbf{w} = \mathbf{w}_\star
 ight)$.
- 2. Prove that

$$(1) \ p_{\star} \triangleq P_{\mathbf{w} \sim P_{W}} \left(\forall \mathbf{x} : f_{\mathbf{w}} \left(\mathbf{x} \right) = f_{\mathbf{w}_{\star}} \left(\mathbf{x} \right) \right) \ge q^{-d_{0}d_{1}^{*} - d_{1}}. \tag{1}$$

3. Show that for any constant T>0, we can bound the probability of stopping time t>T as

$$(2) \quad \lfloor T \rfloor \leq \frac{\log P\left(t > T\right)}{\log(1 - p_{\star})} \,. \tag{2}$$

4. Prove the generalization bound:

Theorem 1 *With probability* $(1 - \eta)(1 - \delta)$,

$$(3) \ \epsilon < \frac{\left(d_0 d_1^{\star} + d_1\right) \log q + \log \frac{1}{\delta} + \log \log \frac{1}{\eta}}{N}$$

Hint: Combine the results from previous sections, using the approximations $\lfloor T \rfloor \approx T$ and $\log(1-p_\star) \approx -p_\star$ (treat these approximations as exact), and the following basic generalization bound (which we learned in class):

Theorem 2 For any $f \in |\mathcal{F}|$ $f \in |\mathcal{F}|$, with probability $1 - \delta$,

$$(4) \ \epsilon \triangleq \mathbb{P}_{\mathbf{x}} \left(f_{\mathbf{w}} \left(\mathbf{x} \right) \neq f_{\mathbf{w}_{\star}} \left(\mathbf{x} \right) \right) < \frac{\log |\mathcal{F}| + \log \frac{1}{\delta}}{N} \,. \tag{4}$$

5. Is the bound in eq. (3) better than the bound in eq. (4) in which $\mathcal{F}=\left\{f_{\mathbf{w}}:\mathbf{w}\in Q^k\right\}$ is the student hypothesis class (in which each parameter can have one of q values)? Explain and ignore the (negligble) $\log\log\frac{1}{n}$ term.

Solution 2 - "Typical" Generalization in Multilayer Neural Networks

1. To get a specific weights we set each of the k weights to recieve a specific value out of q possible values. Since the weights are i.i.d this entails

$$P_{\mathbf{w}\sim P_W}\left(\mathbf{w}=\mathbf{w}_\star
ight)=q^{-k}\,.$$

2. In this case, we need to sample correctly all the input and output weights of the d_1^\star hidden neurons in the teacher neural network. In addition we need to sample '0' in the output weights of all the $\left(d_1-d_1^\star\right)$ student neurons that are not in the teacher neurons. Therefore, we get

$$p_\star \geq q^{-d_0 d_1^\star - d_1}$$
 .

3. If t > T it means we were not able to fit the training set for T times,

$$P\left(t > T\right) = \left(1 - P_{\mathbf{w} \sim P_W}\left(\forall \mathbf{x} \in \mathcal{S} : f_{\mathbf{w}}\left(\mathbf{x}\right) = f_{\mathbf{w}_{\star}}\left(\mathbf{x}\right)\right)\right)^T \leq \left(1 - p_{\star}\right)^T,$$

where in the inequality we used the fact the probability of achieving a perfect classification on the training set can be lower bounded by the probability of achieving the same function as the teacher. Taking the log of both sides of the inequality we get

$$\log\left(1-p_{\star}\right)^{T} \geq \log P\left(t>T\right) \Rightarrow T\log(1-p_{\star}) \geq \log P\left(t>T\right) \overset{\log(1-p_{\star})<0}{\Rightarrow} T \leq \frac{\log P\left(t>T\right)}{\log(1-p_{\star})} \, .$$

4. Denoting $\eta \triangleq P(t > T)$, we have that $1 - \eta = P(t < T)$. So, with probability $1 - \eta$, we have $f_{\mathbf{w}_t} \in \mathcal{F}_T = \{f_{\mathbf{w}_1}, \dots, f_{\mathbf{w}_T}\}$, and

$$egin{aligned} \log |\mathcal{F}_T| &= \log T \leq \log \left(rac{\log P\left(t > T
ight)}{\log (1 - p_\star)}
ight) = \log \left(rac{\log \eta}{\log (1 - p_\star)}
ight) \ &pprox \log \left(rac{\log \eta}{-p_\star}
ight) = \log \log rac{1}{\eta} - \log p_\star \leq \log \log rac{1}{\eta} + \left(d_0 d_1^\star + d_1
ight) \log q. \end{aligned}$$

where in the first inequality we used eq. (2), and in the last equality we used eq. (1). Plugging this into the generalization bound (eq. (4)), we get the Theorem we aimed to prove. 5. With q quantization levels, and $k=d_0d_1+d_1$ parameters we get in eq. (4)

$$\log \lvert \mathcal{F} \rvert = k \log q = (d_0 d_1 + d_1) \log q.$$

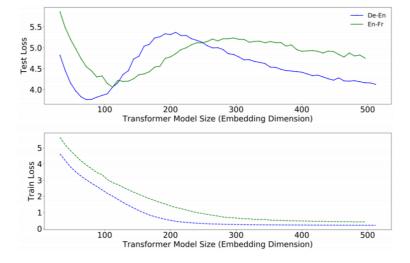
This is larger than $(d_0d_1^* + d_1) \log q$ if $d_1^* < d_1$ as we assume, and therefore leads to a worse generalization bound than in eq. (3).

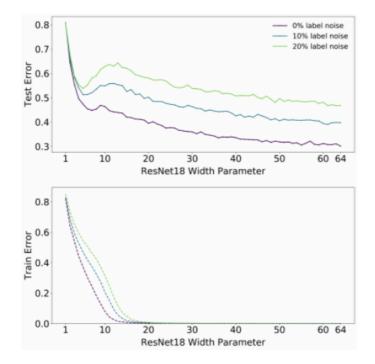


Question 3 - Deep Double Descent

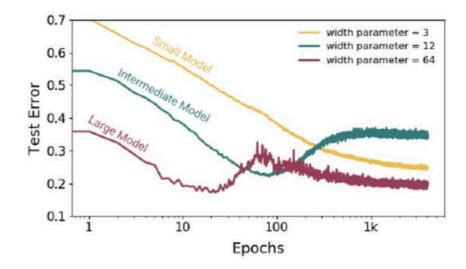
For the following plots:

- 1. Where is the critical point (the point of transition between the "Classical Regime" and "Modern Regime") of the deep double descent?
- 2. What type of double descent is shown? Explain. There can be more than one correct answer.





b.



C.



Solution 3 - Deep Double Descent

a. 200-300

b. 10

Both Model-wise Double Descent

c. Epoch + model-wise double descent. Sufficiently large models can undergo a "double descent" behavior where test error first decreases then increases near the interpolation threshold, and then decreases again. In contrast, for "medium sized" models, for which training to completion will only barely reach a level of error close to 0, the test error as a function of training time will follow a classical U-like curve where it is better to stop early. Models that are too small to reach the approximation threshold will remain in the "under parameterized" regime where increasing train time monotonically decreases test error.

Question 4 - Initialization

Recall that in lecture 5 we were discussing how to calculate the initialization variance, and reached the conclusion that

$$\sigma_l = rac{1}{\sqrt{\sum_j \mathbb{E}\left[arphi^2(u_{l-1}[j])
ight]}}$$

Show that for ReLU activation ($\varphi(z)=max(0,z)$), the optimal variance satisfies:

$$\sigma_l = \sqrt{rac{2}{d_{l-1}}}$$

- 1. Under the assumption that the distribution of W is symmetric (\rightarrow the distribution of u is symmetric).
- 2. Using the central limit theorem for large width.

Answer each section **separately** and assume the sections are independent.

All the notations are the same as in the lecture slides.



Solution 4 -Initialization

1. For ReLU:

$$\sigma_l = rac{1}{\sqrt{\sum_j \mathbb{E}\left[arphi^2(u_{l-1}[j])
ight]}} = rac{1}{\sqrt{d_{l-1}\mathbb{E}\left[arphi^2(u_{l-1}[j])
ight]}} = rac{1}{\sqrt{d_{l-1}\cdotrac{1}{2}}} = \sqrt{rac{2}{d_{l-1}}},$$

where the first transition is from symmetry and see below for the calculation of the expectancy.

2. For ReLU:
$$\varphi^2(z)=max(0,z^2)$$
, and $\mathbb{E}_{z\sim\mathcal{N}(0,1)}[max(0,z^2)]=rac{1}{2}\mathbb{E}_{z\sim\mathcal{N}(0,1)}[z^2]$.

We know that

$$egin{aligned} Var(z) &= \mathbb{E}[z^2] - (\mathbb{E}[z])^2 \ & o \mathbb{E}[z^2] = 1 + 0 = 1 \ \ & o \sigma_l = rac{1}{\sqrt{d_{l-1}(rac{1}{2} \cdot \mathbb{E}[z^2])}} = \sqrt{rac{2}{d_{l-1}}} \end{aligned}$$



Question 5 - Equivariance

Let $f_w(x)=\phi(Wx)$ where ϕ is a component-wise non-linearity and $W\in\mathbb{R}^{d\times d}$. Prove that $f_w:\mathbb{R}^d\to\mathbb{R}^d$ is equivariant to transformation family H if and only if:

$$orall au \in H, W[i,j] = W[au(i), au(j)]$$

- As in class, τ is an operator which re-arranges the terms in the vector it is operating on. $\tau(i)=j$ implies that component i is mapped to component j. In addition, $\tau \cdot x$ means we use τ on x.
- Assume one-by-one activations (Injective functions/one-by-one)



Solution 5 - Equivariance

Recall that ϕ operates **component-wise**, as such ϕ can be switched with τ .

1.
$$\rightarrow$$
: if $W[i,j] = W[\tau(i),\tau(j)]$ then:

$$egin{aligned} f_w(au x) &= \phi(W au x) = \phi\left(\left[egin{array}{c} | \sum_j W[i,j]x[au(j)] \ | \end{array}
ight]
ight) = \phi\left(\left[egin{array}{c} | \sum_j W[au(i), au(j)]x[au(j)] \ | \end{array}
ight]
ight) \ &= au\phi(Wx) = au f_w(x) \end{aligned}$$

2. \leftarrow : if $f_w(\tau x) = \tau f_w(x)$ then:

$$egin{aligned} \phi(W au x) &= \phi\left(\left[egin{array}{c} | \ \sum_j W[i,j]x[au(j)] \ | \ \end{array}
ight) = \phi\left(\left[egin{array}{c} | \ \sum_j W[au(i), au(j)]x[au(j)] \ | \ \end{array}
ight) \\ & o W[i,j] = W[au(i), au(j)], \end{aligned}$$

where in the second equivalence we switched from summing by j to summing by $\tau(j)$, because the order of the sum does not matter (e.g., 1+2+3=2+3+1).



Question 6 -VGG Architecture

- 1. The VGG-11 CNN architecture consists of 11 convolution (CONV)/fully-connected (FC) layers (every CONV layer has the same padding and stride, every MAXPOOL layer is 2×2 and has padding of 0 and stride 2). Fill in the table. You need to **consider the bias**.
- CONVM-N: a convolutional layer of size $M \times M \times N$, where M is the kernel size and N is the number of filters. stride = 1, padding = 1.
- ullet POOL2: 2 imes 2 Max Pooling with stride=2
 - In case the input of the layer is odd, you should round down. For example, if the output of the layer should be $3.5 \times 3.5 \times 3$, you should round to $3 \times 3 \times 3$ (i.e., ignore the last column of the input image when performing MaxPooling).
- ullet FC-N: a fully connected layer with N neurons.

| Layer | Output Dimension | Number of Parameters (Weights) |
|----------|-------------------------|--------------------------------|
| INPUT | 224x224x3 | 0 |
| CONV3-64 | - | - |

| Layer | Output Dimension | Number of Parameters (Weights) |
|-----------|------------------|--------------------------------|
| ReLU | - | - |
| POOL2 | - | - |
| CONV3-128 | - | - |
| ReLU | - | - |
| POOL2 | - | - |
| CONV3-256 | - | - |
| ReLU | - | - |
| CONV3-256 | - | - |
| ReLU | - | - |
| POOL2 | - | - |
| CONV3-512 | - | - |
| ReLU | - | - |
| CONV3-512 | - | - |
| ReLU | - | - |
| POOL2 | - | - |
| CONV3-512 | - | - |
| ReLU | - | - |
| CONV3-512 | - | - |
| ReLU | - | - |
| POOL2 | - | - |
| FC-4096 | - | - |
| FC-4096 | - | - |
| FC-1000 | - | - |
| SOFTMAX | - | - |

- 2. What is the total number of parameters? (use a calculator for this one)
- 3. What percentage of the weights are found in the fully-connected layers?



Solution 6 - VGG Architecture

1. Solution:

| Layer | Output Dimension | Number of Parameters (Weights) |
|--------------|---------------------|-----------------------------------|
| INPUT | 224x224x3 | 0 |
| CONV3- 64 | 224×224×64 | (3 	imes 3 	imes 3 + 1)64 = 1,792 |
| ReLU | 224×224×64 | 0 |

| Layer | Output Dimension | Number of Parameters (Weights) |
|---------------|---------------------|---|
| POOL2 | 112×112×64 | 0 |
| CONV3- 128 | 112×112×128 | (3	imes3	imes64+1)128=73,856 |
| ReLU | 112×112×128 | 0 |
| POOL2 | 56×56×128 | 0 |
| CONV3- 256 | 56×56×256 | $(3	imes3	imes128+1)256=295, \ 168$ |
| ReLU | 56×56×256 | 0 |
| CONV3- 256 | 56×56×256 | $(3 	imes 3 	imes 256 + 1)256 = 590, \ 080$ |
| ReLU | 56×56×256 | 0 |
| POOL2 | 28×28×256 | 0 |
| CONV3- 512 | 28×28×512 | $(3	imes3	imes256+1)512=1,180, \ 160$ |
| ReLU | 28×28×512 | 0 |
| CONV3- 512 | 28×28×512 | $(3	imes3	imes512+1)512=2,359, \ 808$ |
| ReLU | 28×28×512 | 0 |
| POOL2 | 14×14×512, | 0 |
| CONV3- 512 | 14×14×512 | $(3	imes3	imes512+1)512=2,359, \ 808$ |
| ReLU | 14×14×512 | 0 |
| CONV3- 512 | 14×14×512 | $(3	imes3	imes512+1)512=2,359, \ 808$ |
| ReLU | 14×14×512 | 0 |
| POOL2 | 7×7×512 | 0 |
| FC-4096 | 4096 | $(7	imes 7	imes 512+1)4096=102, \ 764,544$ |
| FC-4096 | 4096 | $(4096+1)	imes 4096=16,781, \ 312$ |
| FC-1000 | 1000 | (4096+1) 	imes 1000 = 4,097,000 |
| SOFTMAX | 1000 | 0 |

- 2. 132,863,336
- 3. 93%



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