A SURPRISING POWER LAW RELATIONSHIP PREDICTS TRENDS IN THE TEST ACCURACY FOR VERY DEEP NEURAL NETWORKS

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Paper under double-blind review

ABSTRACT

Given two or more Deep Neural Networks (DNNs) with similar architectures, and trained on the same dataset, but trained with different solvers, hyper-parameters, regularization, etc., can we predict which DNN will have the best test accuracy, without peeking at the test data ? Solving this question of generalization would have both theoretical impact and great practical importance. In this paper, we show how to use our new theory of Implicit (Heavy Tailed) Self-Regularization for modern Deep Neural Networks to answer this. We examine over 50 different, pre-trained DNNs ranging over 15 different architectures, trained on ImagetNet, with differing test accuracies. We show that, across each architecture (VGG16, VGG19, InceptionV3/V4, ...), the reported test accuracies for each DNN are well correlated with the weighted average of the layer power law exponents. Moreover, we prove that this average complexity can be expressed simply as the average log of the Frobenius norm of the layer weight matrices. Our approach requires no changes to the underlying DNN, and does not even require access to the ImageNet data. We present and review these empirical results, and compare and contrast with recent approaches to estimate test performance of DNNs using product norms.

1 INTRODUCTION

2 THEORY OF HEAVY TAILED SELF REGULARIZATION

Let us write the Energy Landscape (or optimization function) for a typical DNN with L layers, with activation functions $h_l(\cdot)$, and with weight matrices and b iases $\mathbf{W}_l$ and $\mathbf{b}_l$, as follows:

$$E_{DNN} = h_L(\mathbf{W}_L \times h_{L-1}(\mathbf{W}_{L-1} \times h_{L-2}(\cdots) + \mathbf{b}_{L-1}) + \mathbf{b}_L). \tag{1}$$

We imagine training this model on some labeled data $\{d_i, y_i\} \in \mathcal{D}$, using Backprop, by minimizing the loss $\mathcal{L}$ For simplicity, we do not indicate the structural details of the layers (e.g., Dense or not, Convolutions or not, Residual/Skip Connections, etc.). Each layer is defined by one or more weight matrices $\mathbf{W}_L$, or tensors.

In this study, we only need to consider Linear and 2D Convolutional (Conv2D) layers. For the Linear layers, each $\mathbf{W}_L$ is a single $(N \times M)$ (real valued) 2D matrix, where $N \geq M$. These include Dense or Fully Connected (FC) layers, as well as 1D Convolutional (Conv1D) layers, Attention matrices, etc. For the Conv2D layers, with a $c\times d$ kernel, $\mathbf{W}_L$ is a 4-index Tensor, of the form $(N\times M\times c\times d)$, consisting of $c \times d$ 2D feature maps of shape $(N \times M)$. So each Linear layer l gives $n = 1$ 2D matrix $\mathbf{W}_l$, and each Conv2D layer l gives $n = c \times d$ 2D matrices $\mathbf{W}_{l,i}$. A typical modern DNN may have anywhere between 5 and 500 2D $\mathbf{W}_{l,i}$ layer matrices.

Heavy Tailed Universality For any layer weight matrix $\mathbf{W}$, we construct the associated $M \times M$ (uncentered) correlation matrix

$$\mathbf{X} = \frac{1}{N}\mathbf{W}^T\mathbf{W}, \tag{2}$$

and form the eigenvalue spectrum of $\mathbf{X}$,

$$\mathbf{X}\mathbf{v}_i = \lambda_i\mathbf{v}_i$$

(where we have dropped the l, i indices).

We call the density of eigenvalues $\rho(\lambda)$ the Empirical Spectral Density (ESD).

Small Neural Networks [charlesG: complete]

The layer matrices in all large, modern DNNs, do not have a scale cut-off, and, instead display scale-invariance. For any modern DNN, the ESD of nearly every $\mathbf{W}$ layer matrix can be fit to a power law,

$$\rho(\lambda) \sim \lambda^{-\alpha}$$

The power law exponent α lies, $80 - 90\%$ of the time, in a Universal range between 2 and 4, $\alpha \in [2, 4]$. We have verified this empirical Universality on empirical result on over 10,000 layer matrices $\mathbf{W}$ spanning over 50 pre-trained DNNs. Of course, there are exceptions, and in any real DNN, α may range anywhere from ~ 1.5 to 10 or higher.

The power law exponent α is a complexity metric for a weight matrix; it describes how well that matrix encodes the complex correlations in the training data. So a natural complexity metric for a DNN is to take a weighted average of the power law exponents $\alpha_{l,i}$ for each layer weight matrix $\mathbf{W}_{l,i}$.

$$\hat{\alpha} := \frac{1}{n}\sum_{l,i} b_{l,i}\alpha_{l,i}$$

The smaller $\hat{\alpha}$, the better we expect the DNN to represent the training data. And, presumably, the better the DNN will generalize. The only question is, what are good weights $b_{l,i}$?

It turns out, we can derive the weighted average $\hat{\alpha}$ directly from the more familiar Product Norm.

[charlesG: THE REST OF THIS SECTION is to justify this complexity metric, using the product norm for DNNs. I have sketeched out some of the math,. It just needs to be presented clearly AND TO JUSTIFY computing the average log Norm (which is much faster, much simpler)]

[charles: Maybe should can state a theorem and prove it.]

THEOREM: *The data dependent VC-like complexity of a Deep Neural Network can be expressed a weighted average the of power law exponents describing the empirical spectral density of the layer weight matrices*

[charles:

PROOF:...]

Product Norm Measures of Complexity Recently it has been suggested that the complexity of a DNN, $\mathcal{C}$, can be defined by something akin to a data dependent VC complexity, the product of norms of the layer weight matrices

$$\mathcal{C} \sim \|\mathbf{W}_1\| \times \|\mathbf{W}_2\| \cdots \|\mathbf{W}_L\|$$

where $\|\mathbf{W}\|$ may be the Frobenius norm or even the L1-norm. (Here we can use either $\|\mathbf{W}\|$ or $\|\mathbf{W}\|^2$ for our complexity metric, which will make more sense below.

To that end, we consider a log complexity

$$\log \mathcal{C} \sim \log \Big[\|\mathbf{W}_1\| \times \|\mathbf{W}_2\| \cdots \|\mathbf{W}_L\| \Big]$$

$$\sim \Big[\log \|\mathbf{W}_1\| + \log \|\mathbf{W}_2\| \cdots \log \|\mathbf{W}_L\| \Big]$$

We define the average log norm of the weight matrices as

$$\langle \log \|\mathbf{W}\| \rangle = \frac{1}{L}\sum_{i=1}^{L} \log_{10} \|\mathbf{W}_i\|$$

which we explicitly define in terms of the base-10 log.

Relation to Heavy Tailed Universality We note the log matrix norm squared (and dropping the l, i subscripts) is just twice the log norm

$$\log \|\mathbf{W}\|^2 = 2 \log \|\mathbf{W}\|$$

which makes the following analysis much simpler.

We now note that the Frobenius norm is related to the integral of the ESD, over the range the power law is a good fit.

$$\|\mathbf{W}_{l,i}\|^2 \sim \int_{x_{min}}^{x_{max}} \lambda \rho_{l,i}(\lambda) d\lambda$$

Technically, the power only describes the tail of the ESD, for the range $\lambda \in [\lambda_{min}, \lambda_{max}]$. But for most DNN layer matrices, this range covers most the ESD. So this should be a pretty good approximation.

So far we have

$$\begin{aligned} \log \|\mathbf{W}\|^2 &\approx \log \int_{\lambda_{min}}^{\lambda_{max}} \lambda \rho(\lambda) d\lambda \\ &= \log \int_{\lambda_{min}}^{\lambda_{max}} \lambda^{1-\alpha} d\lambda \end{aligned}$$

But this integral is difficult to evaluate. To get an expression we can work with, we will use a trick from statistical mechanics.

The Annealed Approximation lets us interchange the log and the integrand when computing the expected value

$$\log \mathbb{E}[x] \leftrightarrow \mathbb{E}[\log(x)]$$

So when evaluating our power law integral, we have

$$\begin{aligned} \log \int \lambda^{1-\alpha} d\lambda &\approx \int \log \lambda^{1-\alpha} d\lambda \\ &= \int \log \frac{1}{\lambda^{\alpha-1}} d\lambda \\ &= -\int \log \lambda^{\alpha-1} d\lambda \\ &\approx -\log \int \lambda^{\alpha-1} d\lambda \end{aligned}$$

This lets us now write

$$\log \|\mathbf{W}\|^2 \approx \log \left[\frac{\lambda^{\alpha}}{\alpha} \right]_{\lambda_{min}}^{\lambda_{max}}$$

Since $\lambda_{min} \sim 0$, we have [charles: check this]

$$\log \|\mathbf{W}\|^2 = 2 \log \|\mathbf{W}\| \approx \alpha \log \lambda_{max}$$

Notice that since the power law exponents mostly display Universality empirically, the range $[\lambda_{min}, \lambda_{max}]$ is also roughly the same for all matrices, with the minimum eigenvalue is near zero, $\lambda_{min} \sim 0$, and the maximum eigenvalue is empirically bounded, roughly $\lambda_{max} \sim \mathcal{O}(10^1 - 10^2)$.

This gives

$$2 \log_{10} \|\mathbf{W}\| \approx (1 - 2) \times \alpha$$

[charles: FINISH WRITEUP AND and numerical results. In particular, we may be off by some scaling factor in $\rho(\lambda)$] [charlesG: This could all be presented as a theorem–building on work by Hidary and Poggio]

$$\text{Linear Layer:} \quad \log \|\mathbf{W}_l\|^2 \rightarrow b_l \alpha_l$$

For the Conv2D layers, we relate the 'Norm' of the 4-index Tensor $\mathbf{W}_l$ to the sum of the integrals of the $n = c \times d$ ESDs for each feature map, giving

$$\text{Conv2D Layer:} \quad \log \|\mathbf{W}_l\|^2 \rightarrow \sum_i b_{i,l} \alpha_{i,l}$$

So in the expression for the product norm for $\log \mathcal{C}$, let us replace each $\log \|\mathbf{W}_l\|$ for layer l with the sum of the power law exponents $\alpha_{l,i}$ for the n_l $\mathbf{W}_{l,i}$ layer matrices, and take the average over all N_α matrices. This lets us relate the product norm complexity metric to the weighted average of power law exponents

where

$$\hat{\alpha} := \frac{1}{N_\alpha} \sum_{i,l} b_{i,j} \alpha_{i,l}$$

We can now use $\hat{\alpha}$, or, equivalently, $2\langle \log \|\mathbf{W}\| \rangle$ to analyze numerous pre-trained DNNs...and the results are indeed surprising.

Numerical Example of Power Law / Norm Relation But first, some numerical examples of the relation between $\langle \log \|\mathbf{W}\| \rangle$ and α

BLAH

BLAH

BLAH

this is in the PowerLawExample notebook in the repo

3 Empirical Results on PreTrained DNNs

VGG and VGG BN Models We start by looking at the VGG class of models, including VGG11, VGG13, VGG16, and VGG19, and their counterparts with Batch Normalization, VGG11_BN, VGG13_BN, VGG16_BN and VGG19_BN. Figure 1

ResNet PyTorch Models

More PreTrained Models More Pretrained Models

Architecture	Model	Top1	Top5	L	N_α	$\hat{\alpha}$	$\hat{\alpha}*$
VGG11	VGG11						
	VGG11 BN						
VGG13	VGG13						
	VGG13 BN						
VGG16	VGG16						
	VGG16 BN						
VGG19	VGG19						
	VGG19 BN						

Table 1: VGG Architectures and DNN Models

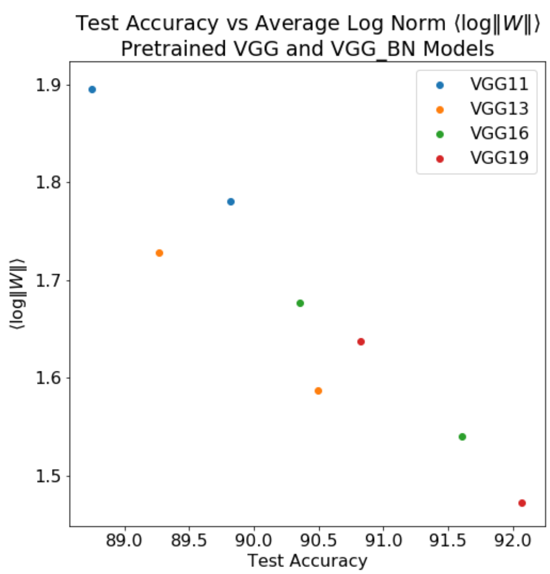


Figure 1: Pretrained VGG and VGG BN Architectures and DNNs. Test Accuracy and average log norm $\hat{\alpha}*$ for VGG11 vs VGG11_BN (blue), VGG13 vs VGG13_BN (orange), VGG16 vs VGG16_BN (green), and VGG19 vs VGG19_BN (red). Note that $\hat{\alpha}*$ does not include the last layer, connecting the model to the labels.

Architecture	Model	Test Accuracy
ResNet (larger)		
ResNet (extended)		
ResNet (b)		

Table 2: ResNet Architectures and DNN Models

Architecture	Model	Test Accuracy
GoogLeNet		
ResNeXt		
SqueezeNet		

Table 3: Other Models

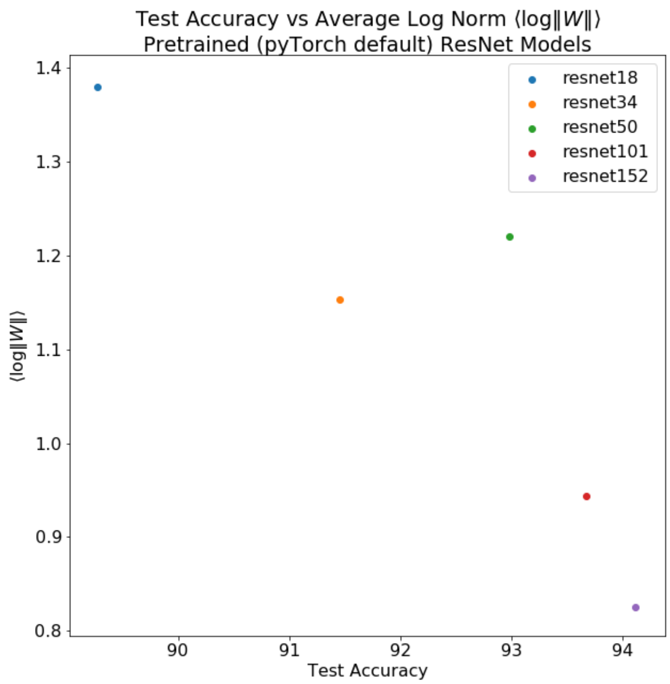
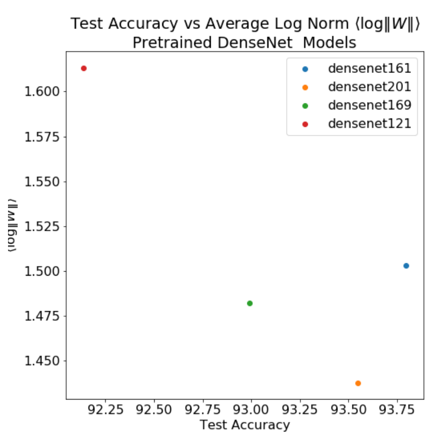
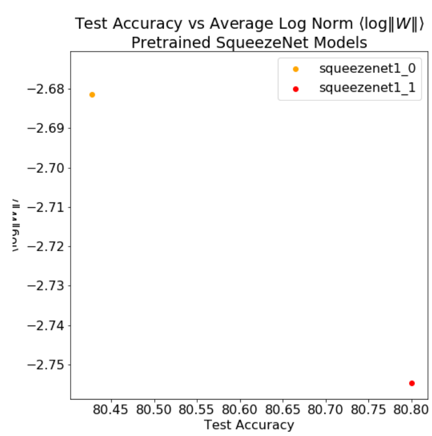


Figure 2: Pretrained ResNet models available in PyTorch



(a) DenseNet



(b) SqueezeNet

Figure 3: Densenet and SqueezeNet PyTorch Models

4 DISCUSSION

We have presented a *Unsupervised* metric which predicts the trends in the test accuracies of a trained deep neural network–without peeking at the test data. This complexity metic $\hat{\alpha}$ is a weighted average of the power law exponents α for each layer weight matrix, where α is defined in our Theory of Heavy Tailed Implicit Regularization. We prove that this new complexity metric $\hat{\alpha}$ is equivalent to the the average log of the Frobenius norm of the layer weight matrices, $\langle \log \|\mathbf{W}\| \rangle$, which is much easier to compute.

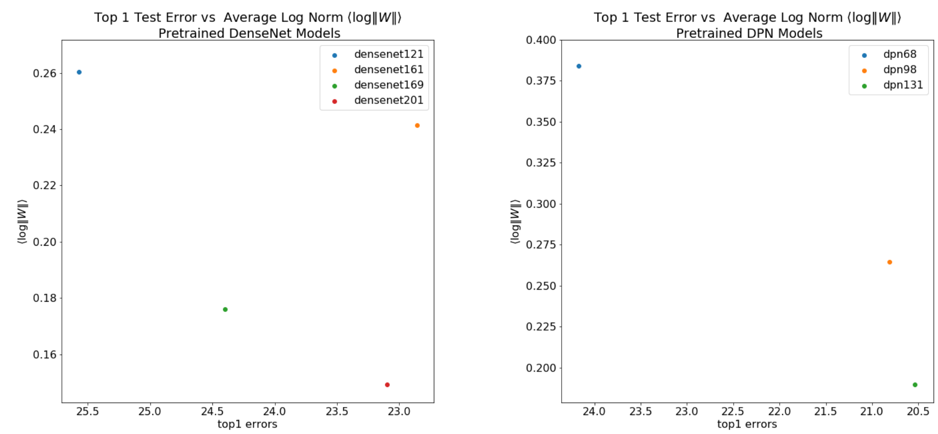
We examine several commonly available, production quality, pretrained DNNs by plotting the average complexity metric $\langle \log \|\mathbf{W}\| \rangle$ vs the reported (Top1) test accuracies. This covers classes of DNN architectures including the VGG models, ResNet, DenseNet, etc. In nearly every class, the smaller average complexity, the better the test accuracy.

The method is consistent with both recent theoretical results by Hidary and Poggio, but the approach and the intent is a bit different. Unlike their result, our approach does not require modifying the loss function. Moreover, they seek a *worst case* complexity bound. We seek *average case* metrics that can be used in production to guide the development of better DNNs.

We believe this result will have large applications in hyperparameter fine tuning DNNs. Because we do not need to peek at the test data, it may prevent information from leaking from the test set into the model, thereby helping to prevent overtraining and making fined tuned DNNs more robust.

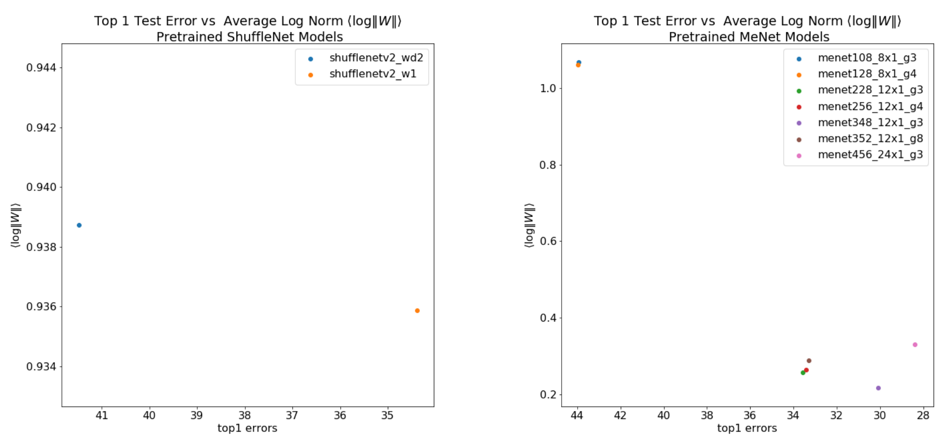
This work also leads to a much harder theoretical question; is it possible to determine if a DNN is overtrained without peeking at the test data ?

5 APPENDIX



(a) DenseNet (b) DPN

Figure 4: DenseNet, DPN



(a) ShuffleNet (b) MeNet

Figure 5: ShuffleNet, MeNet

Architecture	Model	Top 1 Error	
DenseNet	densenet121	25.57	
	densenet161	22.86	
	densenet169	24.4	
	densenet201	23.1	
DPN	dpn68	24.17	
	dpn98	20.81	
	dpn131	20.54	
MeNet	menet108_8x1_g3	43.92	
	menet128_8x1_g4	43.95	
	menet228_12x1_g3	33.57	
	menet256_12x1_g4	33.41	
	menet348_12x1_g3	30.1	
	menet352_12x1_g8	33.31	
	menet456_24x1_g3	28.4	
MobileNet	mobilenet_wd4	46.26	
	mobilenet_wd2	36.3	
	mobilenet_w3d4	33.54	
	mobilenet_w1	29.86	
MobileNetV2	mobilenetv2_wd4	49.72	
	mobilenetv2_wd2	36.54	
	mobilenetv2_w3d4	31.89	
	mobilenetv2_w1	29.31	
FDMobileNet	fdmobilenet_wd4	55.77	
	fdmobilenet_wd2	43.85	
	fdmobilenet_w1	34.7	
SE-ResNet	seresnet50	22.47	
	seresnet101	21.88	
	seresnet152	21.48	
SE-ResNeXt	seresnext50_32x4d	21.0	
	seresnext101_32x4d	19.96	
ShuffleNet	shufflenetv2_wd2	41.48	
	shufflenetv2_w1	34.39	

Table 4: Even more pretrained DNN models.

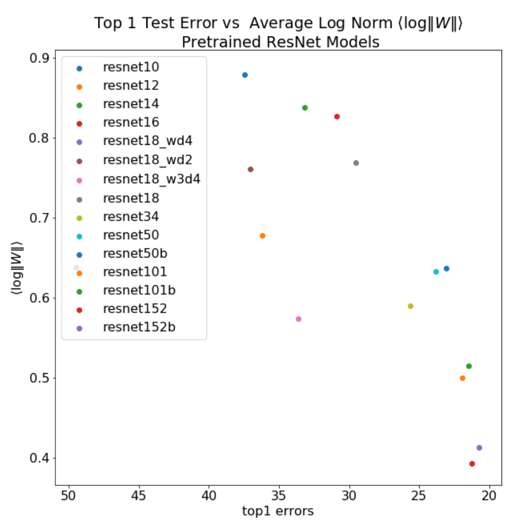
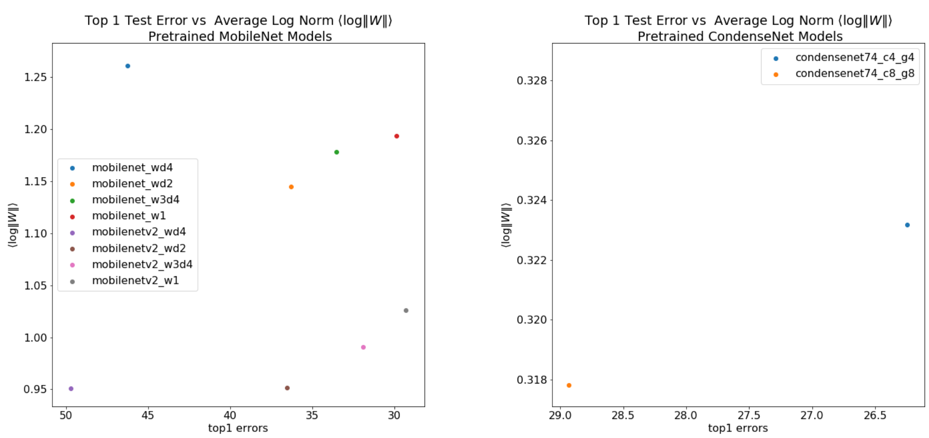


Figure 6: Pretrained ResNet models available in OSMR package

Architecture	Model	Top 1 Error	$\hat{\alpha}$
ResNet (small)	resnet10	37.46	
	resnet12	36.18	
	resnet14	33.17	
	resnet16	30.9	
	resnet18	29.52	
	resnet34	25.66	
	resnet50	23.79	
CondenseNet	condensenet74_c4_g4	26.25	
	condensenet74_c8_g8	28.93	

Table 5: Counter Examples



(a) MobileNet (b) CondenseNet

Figure 7: CounterExamples