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Information in Infinite Ensembles of Infinitely-Wide Neural Networks

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Abstract

In this preliminary work, we study the generalization properties of infinite ensembles of infinitely-wide neural networks. Amazingly, this model family admits tractable calculations for many information-theoretic quantities. We report analytical and empirical investigations in the search for signals that correlate with generalization.

1. Introduction

A major area of research is to understand deep neural networks' remarkable ability to generalize to unseen examples. One promising research direction is to view deep neural networks through the lens of information theory (Tishby and Zaslavsky, 2015). Abstractly, deep connections exist between the information a learning algorithm extracts and its generalization capabilities (Bassily et al., 2017; Banerjee, 2006). Inspired by these general results, recent papers have attempted to measure information-theoretic quantities in ordinary deterministic neural networks (Shwartz-Ziv and Tishby, 2017; Achille and Soatto, 2017; Achille and Soatto, 2019).

Both practical and theoretical problems arise in the deterministic case (Amjad and Geiger, 2018; Saxe et al., 2018; Kolchinsky et al., 2018). These difficulties stem from the fact that mutual information (MI) is reparameterization independent (Cover and Thomas, 2012).[1] One workaround is to make a network explicitly stochastic, either in its activations (Alemi et al., 2016) or its weights (Achille and Soatto, 2017). Here we take an alternative approach, harnessing the stochasticity in our choice of initial parameters. That is, we consider an *ensemble* of neural networks, all trained with the same training procedure and data. This will generate an ensemble of predictions. Characterizing the generalization properties of the ensemble should characterize the generalization of individual draws from this ensemble.

Infinitely-wide neural networks behave as if they are linear in their parameters (Lee et al., 2019). Their evolution is fully described by the *neural tangent kernel* (NTK). The NTK is

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1. This implies that if we send a random variable through an invertible function, its MI with respect to any other variable remains unchanged.

constant in time and can be tractably computed (Anonymous, 2020). For our purposes, it can be considered to be a function of the network's architecture, e.g. the number and the structure of layers, nonlinearity, initial parameters' distributions, etc.

All told, the output of an infinite ensemble of infinitely-wide neural networks initialized with Gaussian weights and biases and trained with gradient flow to minimize a square loss is simply a conditional Gaussian distribution:

$$p(z|x) \sim \mathcal{N}(\mu(x,\tau), \Sigma(x,\tau)), \tag{1}$$

where z is the output of the network and x is its input. The mean $\mu(x,\tau)$ and covariance $\Sigma(x,\tau)$ functions can be computed (Anonymous, 2020). For more background on the NTK and NNGP as well as full forms of μ and Σ, see appendix A.

This simple form allows us to bound several interesting information-theoretic quantities including: the MI between the representation and the targets ($I(Z;Y)$, appendix C.2), the MI between the representation and the inputs after training ($I(Z;X|D)$, appendix C.3), and the MI between the representations and the training set, conditioned on the input ($I(Z;D|X)$, appendix C.4), We are also able to compute in closed form: the Fisher information metric (appendix C.5), the distance the parameters move (appendix C.6), and the MI between the parameters and the data ($I(\Theta;D)$, appendix C.7). Because infinitely-wide neural networks are linear in their parameters, their information geometry in parameter space is very simple. The Fisher information metric is constant and flat, so the trace of the Fisher does not evolve as in Achille and Soatto (2019). While the Euclidean distance the parameters move is small (Lee et al., 2019), the distance they move according to the Fisher metric is finite. Finally, the MI between the data and the parameters tends to infinity, rendering PAC Bayes style bounds on generalization vacuous (Achille and Soatto, 2017; Banerjee, 2006; Bassily et al., 2017).

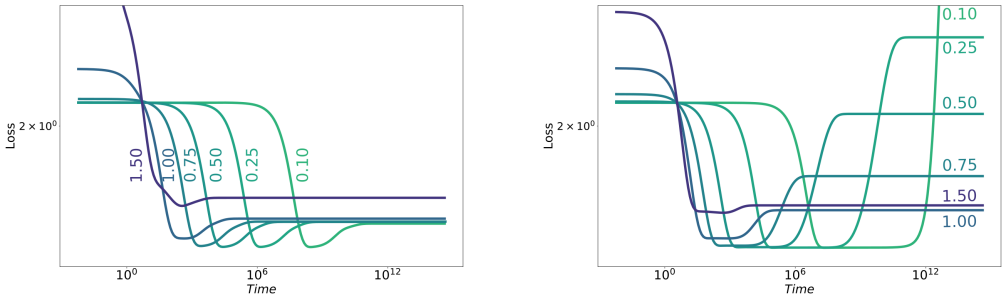
2. Experiments

For jointly Gaussian data (inputs X and targets Y), the Gaussian Information Bottleneck (Chechik et al., 2005) gives an exact characterization of the optimal tradeoff between $I(Z;X)$ and $I(Z;Y)$, where Z is a stochastic representation, $p(z|x)$, of the input. Below we fit infinite ensembles of infinitely-wide neural networks to jointly Gaussian data and measure estimates of these mutual informations. This allows us to assess how close to optimal these networks perform.

The Gaussian dataset we created (for a details, see appendix B) has $|X| = 30$ and $|Y| = 1$. We trained a three-layer FC network with both ReLU and Erf activation functions.

Figure 1 shows the test set loss as a function of time for different choices of initial weight variance (σ_w^2). For both the ReLU and Erf networks, at the highest σ_w shown (darkest purple), the networks *underfit*. For lower initial weight variances, they all show signs of *overfitting* in the sense that the networks would benefit from early stopping. This overfitting is worse for the Erf non-linearity where we see a divergence in the final test set loss as σ_w decreases. For all of these networks the training loss goes to zero.

In fig. 2 we show the performance of these networks on the information plane. The x-axis shows a variational lower bound on the complexity of the learned representation: $I(Z;X|D)$. The y-axis shows a variational lower bound on learned relevant information:

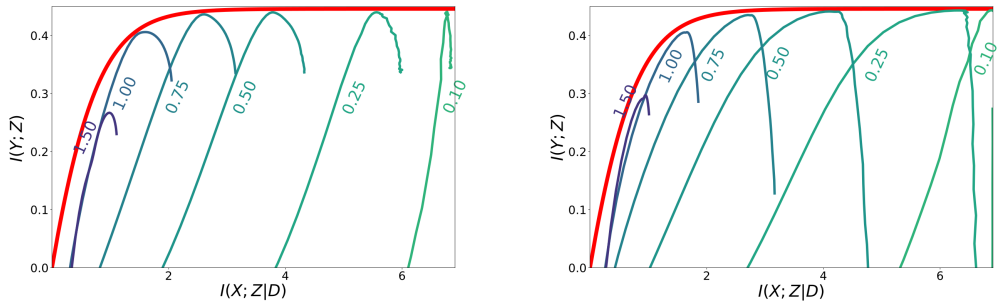


(*a*) ReLU (*b*) Erf

Figure 1: Loss as function of time for different initial weights' variances on the Gaussian dataset.

$I(Y;Z)$. For details on the calculation of the MI estimates see appendix C. The curves show trajectorites of the networks' representation as time varies from $\tau = 10^{-2}$ to $\tau = 10^{10}$ for different weight variances (the bias variance in all networks was fixed to 0.01). The red line is the optimal theoretical IB bound.

There are several features worth highlighting. First, we emphasize the somewhat surprising result that, as time goes to infinity, the MI between an infinite ensemble of infinitely-wide neural networks output and their input is finite and quite small. Even though every individual network provides a seemingly rich deterministic representation of the input, when we marginalize over the random initialization, the ensemble compresses the input quite strongly. The networks overfit at late times. For Erf networks, the more complex representations ($I(Z;X|D)$) overfit more. With optimal early stopping, over a wide range, these models achieve a near optimal trade-off in prediction versus compression. Varying the initial weight variance controls the amount of information the ensemble extracts.

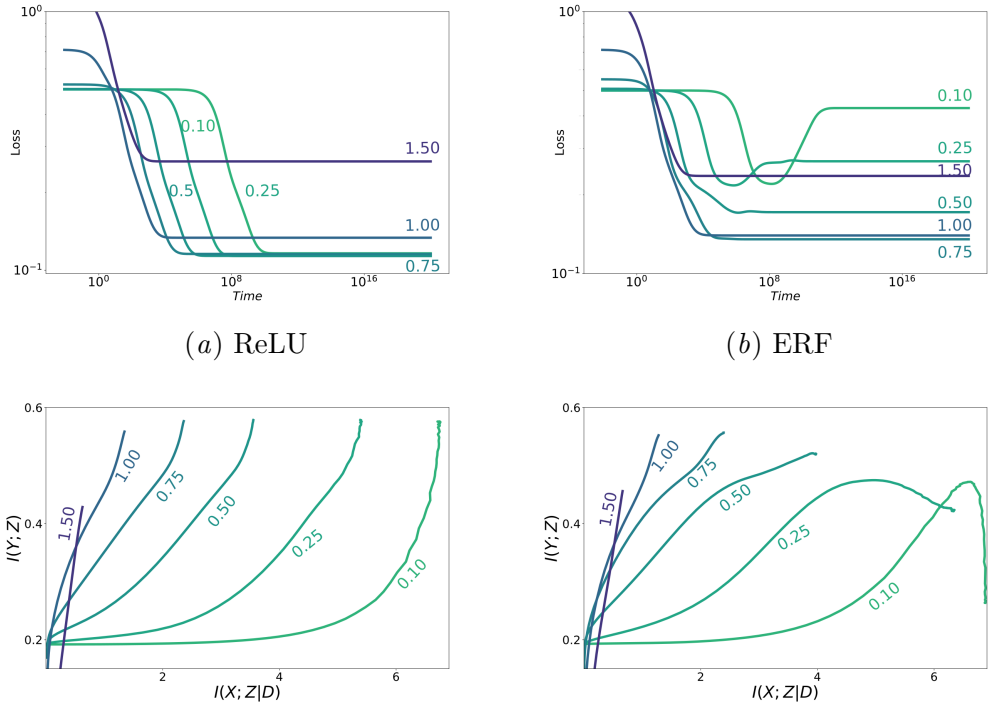


(*a*) ReLU (*b*) Erf

Figure 2: Trajectories of the (bounds on) MI between the representation Z and the input X versus time. Curves differ only in their initial weight variance. The red line is the optimal IB as predicted by theory. Our estimate for $I(Z;X)$ is upper bounded by the log of the batch size ($\log 1000 = 6.9$.)

Next, we repeat the result of the previous section on the MNIST dataset (LeCun and Cortes, 2010). Unlike the normal setup we turn MNIST into a binary regression task for the parity of the digit (even or odd). The network this time is a standard two-layer convolutional neural network with 5×5 filters and either ReLU or Erf activation functions.

Figure 3 shows the results. Unlike in the jointly Gaussian dataset case, here both networks show some region of initial weight variances that do not overfit in the sense of demonstrating any advantage from early stopping. The Erf network at higher variances does show overfitting at low initial weight variances, but the ReLU network does not. Notice that in the information plane, the Erf network shows overfitting at higher representational complexities ($I(Z;X)$ large), while the ReLU network does not.



(a) ReLU (b) ERF

(c) ReLU (d) ERF

Figure 3: Loss as function of time and information plan trajectories for different initial weights' variances on MNIST.

3. Conclusion

Infinite ensembles of infinitely-wide neural networks provide an interesting model family. Being linear in their parameters they permit a high number of tractable calculations of information-theoretic quantities and their bounds. Despite their simplicity, they still can achieve good generalization performance (Arora et al., 2019). This challenges existing claims for the purported connections between information theory and generalization in deep neural networks. In this preliminary work, we laid the ground work for a larger-scale empirical and

theoretical study of generalization in this simple model family. Given that real networks approach this family in their infinite width limit, we believe a better understanding of generalization in the NTK limit will shed light on generalization in deep neural networks.

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Appendix A. Background on the NTK

Infinitely-wide neural networks behave as though they were linear in their parameters (Lee et al., 2019):

$$z(x,\theta) = z_0(x) + \frac{\partial z_0}{\partial \theta}(\theta - \theta_0) \quad z_0(x) \equiv z(x,\theta_0). \tag{2}$$

This makes them particularly analytically tractable. An infinitely-wide neural network, trained by gradient flow to minimize squared loss admits a closed form expression for evolution of its predictions as a function of time:

$$z(x,\tau) = z_0(x) - \Theta(x,\mathcal{X})\Theta^{-1}\left(I - e^{-\tau\Theta}\right)(z_0(\mathcal{X}) - \mathcal{Y}). \tag{3}$$

Here z denotes the output of our neural network acting on the input x. τ is a dimensionless representation of the time of our training process. $\mathcal{X}$ denotes the whole training set of examples, with their targets $\mathcal{Y}$. $z_0(x) \equiv z(x, \tau = 0)$ denotes the neural networks output at initialization. The evolution is governed by the *neural tangent kernel* (NTK) Θ (Jacot et al., 2018). For a finite width network, the NTK corresponds to JJ^T, the gram matrix of neural network gradients. As the width of a network increases to infinity, this kernel converges in probability to a fixed value. There exist tractable ways to calculate the exact infinite-width kernel for wide classes of neural networks (Anonymous, 2020). The shorthand Θ denotes the kernel function evaluated on the train data ($\Theta \equiv \Theta(\mathcal{X},\mathcal{X})$).

Notice that the behavior of infinitely-wide neural networks trained with gradient flow and squared loss is just a time-dependent affine transformation of their initial predictions. As such, if we now imagine forming an infinite ensemble of such networks as we vary their initial weight configurations, if those weights are sampled from a Gaussian distribution, the law of large numbers enforces that the distribution of outputs of the ensemble of networks at initialization is Gaussian, conditioned on its input. Since the evolution is an affine transformation of the initial predictions, the predictions remain Gaussian at all times. For more details see Lee et al. (2019).

$$p(z|x) \sim \mathcal{N}(\mu(x,\tau), \Sigma(x,\tau)) \tag{4}$$

$$\mu(x,\tau) = \Theta(x,\mathcal{X})\Theta^{-1}\left(I - e^{-\tau\Theta}\right)\mathcal{Y} \tag{5}$$

$$\Sigma(x,\tau) = \mathcal{K}(x,x) + \Theta(x,\mathcal{X})\Theta^{-1}\left(I - e^{-\tau\Theta}\right)\left(\mathcal{K}\Theta^{-1}\left(I - e^{-\tau\Theta}\right)\Theta(\mathcal{X},x) - 2\mathcal{K}(\mathcal{X},x)\right). \tag{6}$$

Here, $\mathcal{K}$ denotes yet another kernel, the *neural network gaussian process* kernel (NNGP). For a finite width network, the NNGP corresponds to the expected gram matrix of the outputs: $\mathbb{E}\left[zz^T\right]$. In the infinite width limit, this concentrates on a fixed value. Just as for the NTK, the NNGP can be tractably computed (Anonymous, 2020), and should be considered just a function of the neural network architecture.

Appendix B. Gaussian Dataset

For our experiments we used a jointly Gaussian dataset, for which there is an analytic solution for the optimal representation (Chechik et al., 2005).

Imagine a jointly Gaussian dataset, where we have $x_{ij} = L^x_{jk}\epsilon^x_{ik}$ with $\epsilon \sim \mathcal{N}(0,1)$. Make y just an affine projection of x with added noise.

$$y_{ij} = L^y_{jk}\epsilon_{ik} + A_{jk}x_{ik} = L^y_{jk}\epsilon^y_{ik} + A_{jk}L^x_{km}\epsilon^x_{im}. \tag{7}$$

Both x and y will be mean zero. We can compute their covariances.

$$\Sigma^x_{jk} = \langle x_{ij} x_{ik} \rangle = \langle L_{jm} \epsilon_{im} L_{kl} \epsilon_{il} \rangle = L_{jm} L_{kl} \delta_{ml} = L_{jm} L_{km} \tag{8}$$

Next look at the covariance of y.

$$\begin{aligned}
\Sigma^y_{jk} &= \langle y_{ij} y_{ik} \rangle \\
&= \left\langle \left(L^y_{jl} \epsilon^y_{il} + A_{jl} L^x_{lm} \epsilon^x_{im} \right) \left(L^y_{kn} \epsilon^y_{in} + A_{kn} L^x_{no} \epsilon^x_{io} \right) \right\rangle \\
&= L^y_{jl} L^y_{kn} \delta_{ln} + A_{jl} L^x_{lm} A_{kn} L_{no} \delta_{mo} \\
&= L^y_{jn} L^y_{kn} + A_{jl} \Sigma^x_{ln} A_{kn}
\end{aligned}$$

For the cross covariance:

$$\begin{aligned}
\Sigma^{xy}_{jk} &= \langle x_{ij} y_{ik} \rangle \\
&= \left\langle L^x_{jm} \epsilon^x_{im} \left(L^y_{kn} \epsilon^y_{in} + A_{kn} L^x_{no} \epsilon^x_{io} \right) \right\rangle \\
&= L^x_{jm} A_{kn} L^x_{no} \delta_{mo} \\
&= L^x_{jm} A_{kn} L^x_{nm} = \Sigma^x_{jn} A_{kn}
\end{aligned}$$

So we have for our entropy of x:

$$H(X) = \frac{n_x}{2} \log(2\pi e) + n_x \log \sigma_x$$

$$H(Y|X) = \frac{n_y}{2} \log(2\pi e) + n_y \log \sigma_y$$

as for the marginal entropy, we will assume the SVD decomposition $A = U \Sigma V^T$

$$H(Y) = \frac{n_y}{2} \log(2\pi e) + \frac{n_y}{2} \log \left| \sigma_y^2 I + \sigma_x^2 A A^T \right| = \frac{n_y}{2} \log(2\pi e) + \frac{1}{2} \sum_i \log \left(\sigma_y^2 + \sigma_x^2 \Sigma_i^2 \right)$$

So, solving for the mutual information between x and y we obtain:

$$I(X;Y) = H(Y) - H(Y|X) = \frac{1}{2} \sum_i \log \left(1 + \frac{\sigma_x^2 \Sigma_i^2}{\sigma_y^2} \right)$$

Appendix C. Information Metrics

Having a tractable form for the representation of the ensemble of infinitely-wide networks enables us to compute several information-theoretic quantities of interest. This already sheds some light on previous attempts to explain generalization in neural networks, and gives us candidates for an empirical investigation into quantities that can predict generalization.

C.1. Loss

In order to compute the expected loss of our ensemble, we need to marginalize out the stochasticity in the output of the network. Training with squared loss is equivalent to assuming a Gaussian observation model $p(y|z) \sim \mathcal{N}(0, 1)$. We can marginalize out our representation to obtain

$$q(y|x) = \int dz\, q(y|z)p(z|x) \sim \mathcal{N}(\mu(x,\tau), I + \Sigma(x,\tau)). \tag{9}$$

The expected log loss has contributions both from the square loss of the mean prediction, as well as a term which couples to the trace of the covariance:

$$\mathbb{E}\left[\log q(y|z)\right] = \frac{1}{2}\mathbb{E}\left[(y - z(x,\tau))^2\right] = \frac{1}{2}(y - \mu(x,\tau))^2 + \frac{1}{2}\operatorname{Tr}\Sigma(x,\tau) - \frac{k}{2}\log 2\pi \tag{10}$$

here k is the dimensionality of y.

C.2. $I(Z;Y)$

While the MI between the network's output and the targets is intractable in general, we can obtain a tractable variational lower bound: (Poole et al., 2019)

$$I(Z;Y) = \mathbb{E}\left[\log \frac{p(y|z)}{p(y)}\right] \leq \mathbb{E}\left[\log \frac{q(y|z)}{p(y)}\right] = H(Y) + \mathbb{E}\left[\log q(y|z)\right] \tag{11}$$

C.3. $I(Z;X|D)$

The MI between the input (X) and output (Z) of our network, conditioned on the dataset (D) is:

$$I(Z;X|D) = \mathbb{E}\left[\log \frac{p(z|x,D)}{p(z|D)}\right]. \tag{12}$$

This requires knowledge of the marginal distribution $p(z|D)$. Without knowledge of $p(x)$, this is in general intractable, but there exist simple tractable multi sample upper and lower bounds (Poole et al., 2019):

$$\frac{1}{N}\sum_i \log \frac{p(z_i|x_i,D)}{\frac{1}{N}\sum_j p(z_i|x_j,D)} \leq I(Z;X|D) \leq \frac{1}{N}\sum_i \log \frac{p(z_i|x_i,D)}{\frac{1}{N-1}\sum_{j\neq i} p(z_i|x_j,D)}. \tag{13}$$

In this work, we show the minibatch lower bound estimates, which are upper bounded themselves by the log of the batch size.

C.4. $I(Z;D|X)$

We can also estimate a variational upper bound on the MI between the representation of our networks and the training dataset.

$$I(Z;D|X) = \mathbb{E}\left[\log \frac{p(z|x,D)}{p(z|x)}\right] \leq \mathbb{E}\left[\log \frac{p(z|x,D)}{p_0(z|x)}\right]. \tag{14}$$

Here, the MI we extract from the dataset involves the expected log ratio of our posterior distribution of outputs to the marginal over all possible datasets. Not knowing the data distribution, this is intractable in general, but we can variationally upper bound it with an approximate marginal. A natural candidate is the prior distribution of outputs, for which we have a tractable estimate.

C.5. Fisher

Infinitely-wide networks behave as though they were linear in their parameters with a fixed Jacobian. This leads to a trivially flat information geometry. For squared loss the true Fisher can be computed simply as $F = J^T J$ (Kunstner et al., 2019). While the trace of the Fisher information has recently been proposed as an important quantity for controlling generalization in neural networks (Achille and Soatto, 2019), for infinitely wide networks we can see that the trace of the fisher is the same as the trace of the NTK, which is a constant and does not evolve with time ($\operatorname{Tr} F = \operatorname{Tr} J^T J = \operatorname{Tr} J J^T = \operatorname{Tr} \Theta$). In so much as infinite ensembles of infinitely-wide neural networks generalize, the degree to which they do or do not cannot be explained by the time evolution of the trace of the Fisher given that the trace of the Fisher does not evolve.

C.6. Parameter Distance

How much do the parameters of an infinitely-wide network change? Other work (Lee et al., 2019) emphasizes that the relative Frobenius norm change of the parameters over the course of training vanishes in the limit of infinite width. This is in fact a justification for the linearization becoming more accurate as the network becomes wider. But is it thus fair to say the parameters are not changing? Instead of looking at the Frobenius norm we can investigate the *length* of the parameters path over the course of training. This reparameterization independent notion of distance utilizes the information geometric metric provided by the Fisher information:

$$L(\tau) = \int_0^\tau ds = \int_0^\tau d\tau \sqrt{\dot{\theta}_\alpha(\tau) g_{\alpha\beta} \dot{\theta}_\beta(\tau)} = \int_0^\tau d\tau \left\| \Theta e^{-\tau\Theta} (z_0(\mathcal{X}) - \mathcal{Y}) \right\| \tag{15}$$

The length of the trajectory in parameter space is the integral of a norm of our residual at initialization projected along $\Theta e^{-\tau\Theta}$. This integral is both positive and finite even as $t \to \infty$. To get additional understanding into the structure of this term, we can consider its expectation over the ensemble, where we can use Jensen's inequality to bound the expectation of trajectory lengths. Since we know that at initialization $z_0(\mathcal{X}) \sim \mathcal{N}(0, \mathcal{K})$ we obtain further simplifications:

$$\mathbb{E}[L(\tau)]^2 \leq \mathbb{E}[L^2(\tau)] = \int_0^\tau d\tau \, \mathbb{E}\left[(z_0(\mathcal{X}) - \mathcal{Y})^T \Theta^2 e^{-2\tau\Theta} (z_0(\mathcal{X}) - \mathcal{Y}) \right] \tag{16}$$

$$= \frac{1}{2} \mathbb{E}\left[(z_0(\mathcal{X}) - \mathcal{Y})^T \Theta \left(1 - e^{-2\tau\Theta}\right) (z_0(\mathcal{X}) - \mathcal{Y}) \right] \tag{17}$$

$$= \frac{1}{2} \left[\operatorname{Tr}\left(\mathcal{K} \Theta \left(1 - e^{-2\tau\Theta}\right) \right) + \mathcal{Y}^T \Theta \left(1 - e^{-2\tau\Theta}\right) \mathcal{Y} \right]. \tag{18}$$

C.7. $I(\theta; D)$

The MI between the parameters and the dataset $I(\theta; D)$ has been shown to control for overfitting (Bassily et al., 2017). We can generate a variational upperbound on this quantity by consider the KL divergence between the posterior distribution of our parameters and the prior distribution $D_{\mathrm{KL}}\left[p(\theta|D)\|p_0(\theta)\right]$ a quantity that itself has been shown to provide generalization bounds in PAC Bayes frameworks (Achille and Soatto, 2017). For our networks, the prior distribution is known and simple, but the posterior distribution can be quite rich. However, we can use the *instantaneous change of variables* formula (Chen et al., 2018)

$$\log p(\theta_\tau) = \log p(\theta_0) - \int_0^\tau d\tau \ \mathrm{Tr}\left(\frac{\partial \dot{\theta}}{\partial \theta}\right), \tag{19}$$

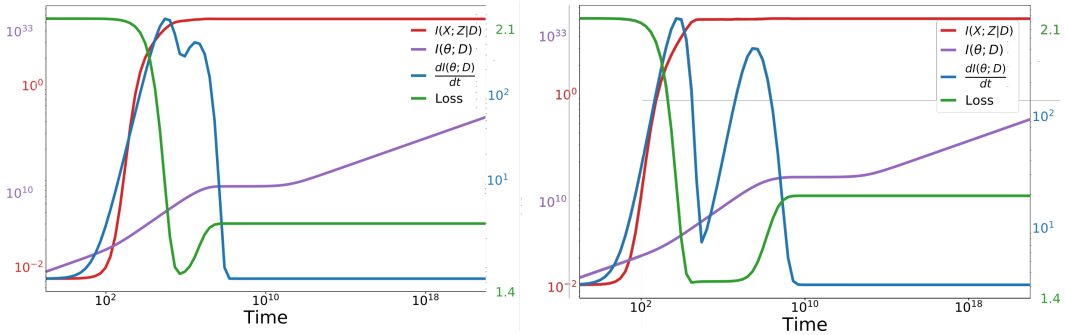
which gives us a value for the log likelihood the parameters of a trained model at any point in time in terms of its initial log likelihood and the integral of the trace of the kernel governing its time evolution. For our infinitely-wide neural networks this is tractable:

$$\begin{aligned}
I(\theta; D) &\geq \mathbb{E}_{p(\theta_\tau)}\left[\log p(\theta_\tau) - \log p_0(\theta_\tau)\right] && (20)\\
&= \mathbb{E}_{p(\theta_0)}\left[\log p(\theta_0) - \log p_0(\theta_\tau) - \int_0^\tau d\tau \ \mathrm{Tr}\left(\frac{\partial \dot{\theta}}{\partial \theta}\right)\right] && (21)\\
&= \mathbb{E}_{p(\theta_0)}\left[\log p(\theta_0) - \log p_0(\theta_0 + \Delta\theta_\tau) + \tau \,\mathrm{Tr}\,\Theta\right] && (22)\\
&= \mathbb{E}_{p(\theta_0)}\left[-\frac{1}{2}\theta_0^2 + \frac{1}{2}\left(\theta_0 + \Delta\theta_\tau\right)^2\right] + \tau \,\mathrm{Tr}\,\Theta && (23)\\
&= \mathbb{E}_{p(\theta_0)}\left[\theta_0^T \Delta\theta_\tau + \left(\Delta\theta_\tau\right)^2\right] + \tau \,\mathrm{Tr}\,\Theta && (24)\\
&= \mathbb{E}_{p(\theta_0)}\left[\theta_\tau^T \Delta\theta_\tau\right] + \tau \,\mathrm{Tr}\,\Theta && (25)\\
&= \mathbb{E}_{p(\theta_0)}\left[(z_0(\mathcal{X}) - \mathcal{Y})^T (I - e^{-\tau\Theta})^2 \Theta^{-1} (z_0(\mathcal{X}) - \mathcal{Y})\right] + \tau \,\mathrm{Tr}\,\Theta && (26)\\
&= \mathrm{Tr}\left(\mathcal{K}\Theta^{-1}(I - e^{-\tau\Theta})^2\right) + \mathcal{Y}^T \Theta^{-1} (I - e^{-\tau\Theta})^2 \mathcal{Y} + \tau \,\mathrm{Tr}\,\Theta. && (27)
\end{aligned}$$

This tends to infinity as the time goes to infinity. This renders the usual PAC-Bayes style generalization bounds trivially vacuous for the generalization of infinitely wide neural networks at late times. Yet, infinite networks can generalize well (Arora et al., 2019).

Appendix D. Additional Empirical Results

Figure 4 shows $I(X; Z|D)$, $I(\theta; D)$, $\frac{dI(\theta;D)}{dt}$ and the loss as function of time for a fixed initial weight's variance ($\sigma_w = 0.25$). (in log-log scale, notice that y-axes are different for each measure). For both the ReLU and Erf networks, we see clear features in each plot near the optimal test loss.



(*a*) ReLU (*b*) Erf

Figure 4: $I(X;Z|D)$, $I(\theta;D)$, $\frac{dI(\theta;D)}{dt}$ and the loss as function of time on our Gaussian dataset.