Convolutional Neural Tangent Kernel

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William Cappelletti

Abstract

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2.1 Tensor Programs

Our goal is to study how Artificial Neural Networks (ANN) behaves when their sizes become arbitrarily big and their parameters are initialized at random, following Glorot initialization [2].

To study such functions, Yang introduces the concept of *Tensor Program* in [7] and [8]. This framework is used to bind the sizes of parameters across different parts of the network, by explicitly binding to a line of the program introduction and usage of each parameter and non-linearity. In particular, *Tensor Programs* allow the input of vectors (**VecIn**) and matrices (**MatIn**) and their usage in linear combination of vectors (**LinComb**), matrix multiplication (**MatMul**), matrix transpose (**T**) and application of general (possibly nonlinear) functions (**Nonlin**). A more precise definition can be found in [7, Section 3], along with examples.

We can immediately see that Tensor Programs cover almost every standard Deep Learning architecture, and, in particular, they describe MLPs and CNNs. In spite of being more cumbersome of the usual algebraic formulation, this notation makes it easier to study ANN as we let their increase arbitrarily.

Intuitively, each program line binds a variable assignment and a dimension annotation, such that one can use each line result in other operations and keep track of the relations between dimensions. It follows that lines of type T, MatMul, LinComb, and Nonlin induce equality constraints on the dimensions of each line. We call *G-vars* the outputs of VecIn, MatMul and LinComb, and, similarly, *A-vars* those produced by MatIn and T and *H-vars* the results of Nonlin. Given a program π and a possible set of additional dimensional constraints Λ, we can consider the smallest equivalence relation $\sim$ on G-vars such that $g \sim g'$ if their dimensions are constrained to be equal by Λ or by some line of the program. With this relation, we can split the G-vars into classes and we call each class a *common dimension class* (CDC); we write $\mathfrak{C}$ the collection of all CDCs for a program π and additional constraints Λ. The CDCs are the main instrument to understand the ANN behaviour when we let the network's dimensions increase, as all its elements scale together.

2.2 The Infinite Width Limit

We study how ANNs behave when we let their dimensions go to infinity, in what is called the Infinite Width Limit. Before we go deeper into theoretical results, we want to clarify what it means, for different architectures, to become infinitely wide. The easiest case is the MLP, in which all layers are fully connected. In this case, without additional constraints, the only dimensions that are bound are those of the input of a layer and the output of the previous one. Therefore, each layer gives its own CDC and the dimensions that go to infinity are the number of nodes in each layer (i.e the columns in each weight matrix and bias vector). This justifies the approach used in [3], where the authors make the layers sizes increase to infinity sequentially.

A different intuition arises when considering CNNs. In this case, by the definition of convolution, one cannot have the size of the filter to grow to infinity, as that would impose all layers to grow to infinity together and it would require an infinite size input, which is absurd. Therefore, in such a situation, the filter size stays the same, and the dimension that grows to infinity is the number of channels. To visualize what that means in terms of tensor programs, we can consider an image

with different channels. We take a vector across channels for every single pixel and we can see each filter application as first multiplying each pixel-vector by a weight matrix, giving as result a pixel-vector with a different number of channels, and then obtaining the preactivations for each coordinate of the new tensor as linear combinations of the latter pixel-vectors. Finally, one can apply the nonlinearity pointwise. For a complete example, we refer the reader to [7, Appendix B.6].

In the same way, we can express through tensor programs more complex architectures, such as Residual Neural Networks and other kinds of transformer, as shown in [7, Appendix B]. After we understand what dimensions go to infinity, we see that some similar behaviour arises, in spite of the architectures being significantly different. The first consequence is that in the *Infinite Width Limit* (IWL) all ANNs behave like *Gaussian Processes*.

Neal first proved, in [5], that a single-layer neural network with random parameters can converge in distribution to a Gaussian process as its width goes to infinity. [7] extends this result to any network that can be described by a tensor program.

We consider a sequence (in $t \in \mathbb{N}$) of dimensions $\{n^{lt}\}_{g^l \text{or} h^l} \cup \{n_1^{lt}, n_2^{lt}\}_{A^l}$ respecting the equivalence relation $\sim$ (defined in Section 2.1) in the program π, where g^l, h^l and A^l are, respectively, G, H, and A-vars appearing at line l in π. At time t, we sample independently $A_{ij}^{lt} \sim \mathcal{N}(0, (\sigma^{lt})^2/n_2^{lt})$, for each i, j, for a set $\{\sigma^{lt}\}_{A^l}$. For each common dimension class $\mathfrak{c}$, we also sample independenty $g^{\mathfrak{c}_{\text{in}}t} \sim \mathcal{N}(\mu^{\mathfrak{c}_{\text{in}}t}, K^{\mathfrak{c}_{\text{in}}t})$ for each i. Here $\mathfrak{c}_{\text{in}}$ is the set of input G-vars in $\mathfrak{c}$, $g^{\mathfrak{c}_{\text{in}}t} = (g_i^{lt})_{g^l \in \mathfrak{c}_{\text{in}}}$, and $\mu^{\mathfrak{c}_{\text{in}}t} : \mathfrak{c}_{\text{in}} \to \mathbb{R}, K^{\mathfrak{c}_{\text{in}}t} : \mathfrak{c}_{\text{in}} \times \mathfrak{c}_{\text{in}} \to \mathbb{R}$ are specified mean and covaiance at time t. Thus, given (π, Λ), the data $\{n^{\mathfrak{c}t}\}_{\mathfrak{c} \in \mathfrak{C}}$, $\{\sigma^{lt}\}_{A^l}$, $\{\mu^{\mathfrak{c}_{\text{in}}t}\}_{\mathfrak{c} \in \mathfrak{C}}$ and $\{K^{\mathfrak{c}_{\text{in}}t}\}_{\mathfrak{c} \in \mathfrak{C}}$ realize a random program $\pi(\{n^{\mathfrak{c}t}\}_{\mathfrak{c} \in \mathfrak{C}}, \{\sigma^{lt}\}_{A^l}, \{\mu^{\mathfrak{c}_{\text{in}}t}\}_{\mathfrak{c} \in \mathfrak{C}}, \{K^{\mathfrak{c}_{\text{in}}t}\}_{\mathfrak{c} \in \mathfrak{C}})$.

Furthermore, we assume that as $t \to \infty$, for all $\mathfrak{c}$, $\mathfrak{c}' \in \mathfrak{C}$:

1. $n^{\mathfrak{c}t}$ is increasing with t and $n^{\mathfrak{c}t} \to \infty$.
2. $\lim_{t \to \infty} n^{\mathfrak{c}t}/n^{\mathfrak{c}'t} = \alpha_{\mathfrak{c},\mathfrak{c}'} \in (0, \infty)$, for some constant $\alpha_{\mathfrak{c},\mathfrak{c}'}$ depending only on $\mathfrak{c}' \in \mathfrak{C}$.
3. $\sigma^{lt} \to \sigma^{l\infty}$ for some finite $\sigma^{l\infty} > 0$ for each input A-var A^l.
4. $\mu^{\mathfrak{c}_{\text{in}}t} \to \mu^{\mathfrak{c}_{\text{in}}\infty}$ and $K^{\mathfrak{c}_{\text{in}}t} \to K^{\mathfrak{c}_{\text{in}}\infty}$ for some finite $\mu^{\mathfrak{c}_{\text{in}}\infty}$ and $K^{\mathfrak{c}_{\text{in}}\infty}$, and $\operatorname{rank} K^{\mathfrak{c}_{\text{in}}t} = \operatorname{rank} K^{\mathfrak{c}_{\text{in}}\infty}$ for all large t.

For this section main theorem, we need to restrict to a general class of nonlinearities, which we can intuitively think as meaning that the function is at most exponential.

Definition 2.1. For $\alpha > 0$, a function $\phi : \mathbb{R}^k \to \mathbb{R}$ is said to be *alpha-controlled* if for some C, $c > 0$, we have

$$|\phi(x)| \leq \exp\left(C \sum_{i=1}^{k} |x_i|^\alpha + c\right) \tag{2.1}$$

for all $x \in \mathbb{R}^k$.

Theorem 2.2 ([8])**.** *Consider ro correlations, but otherwise are asympthotically independent, unless they appear togheter in a LinComb. dimension costraints Λ and a program π without T lines, i.e. no transpose allowed. Suppose the nonlinearities are α-controlled for some $\alpha < 2$. Sample all input vars as explained beforhand (Glorot initialization). Then, for any $\mathfrak{c} \in \mathfrak{C}$ and any α-controlled function $\phi : \mathbb{R}^{\mathfrak{c}} \to \mathbb{R}$, $\alpha < 2$,*

$$\frac{1}{n^{\mathfrak{c}t}} \sum_{i=1}^{n^{\mathfrak{c}t}} \phi(g_i^{\mathfrak{c}t}) \xrightarrow{a.s.} \mathbb{E}\phi(Z), \tag{2.2}$$

where $g_i^{\mathfrak{c}t} = (g_i^{lt})_{g^l \in \mathfrak{c}}$ *and* $\mathbb{R}^{\mathfrak{c}} \ni Z = (Z^g)_{g \in \mathfrak{c}} \sim \mathcal{N}(\mu^{\mathfrak{c}}, K^{\mathfrak{c}})$*, with* $\mu^{\mathfrak{c}}$ *and* $K^{\mathfrak{c}}$ *defined respectively in* (2.3) *and* (2.4)*.*

For any $\mathfrak{c} \in \mathfrak{C}$, we recursively define

$$\text{(mean)} \quad \mu^{\mathfrak{c}}(g^l) = \begin{cases} \mu^{\mathfrak{c}_{\text{in}}\infty}(g^l) & \text{if } g^l \in \mathfrak{c}_{\text{in}} \\ \sum_i a_{ji}^l \mu^{\mathfrak{c}}(g_i^j) & \text{if } g^l := \sum_i a_{ji}^l g_i^j \\ 0 & \text{if } g^l := A^k g^j \text{ or } g^l := A^k h^j \end{cases} \tag{2.3}$$

and recursively define

$$\text{(covariance)} \quad K^{\mathfrak{c}}(g^l, g^m) = \begin{cases} K^{\mathfrak{c}_{\text{in}}\infty}(g^l, g^m) & \text{if } g^l, g^m \in \mathfrak{c}_{\text{in}} \\ \sum_i a_{ji}^m K^{\mathfrak{c}}(g^l, g_i^j) & \text{if } g^m := \sum_i a_{ji}^m g_i^j \\ \sum_i a_{ji}^l K^{\mathfrak{c}}(g_i^j, g^m) & \text{if } g^l := \sum_i a_{ji}^l g_i^j \\ (\sigma^{k\infty})^2 \mathbb{E}_z[f^a(z) f^b(z)] & \text{if } g^l := A^k h^a, g^m := A^k h^b \\ 0 & \text{else} \end{cases} \tag{2.4}$$

where $h^a := f^a(g_1^j, \ldots, g_k^j), h^b := f^b(g_1^{j'}, \ldots, g_k^{j'})$ and $z \sim \mathcal{N}(\mu^{\mathfrak{c}}, K^{\mathfrak{c}})$. We also make branch 4 cover the case when $g^l := A^k g^a$ or $g^m := A^k g^b$ by "typecasting" g^a to an H-var and setting $f^a = \text{id}$ (similarly for g^b). Note that, f^a will ignore irrelevant components of a, and the expectations only depend on the entries of $\mu^{\mathfrak{c}}$ and $K^{\mathfrak{c}}$ that correspond to already-defined values, so this describes a valid recursion.

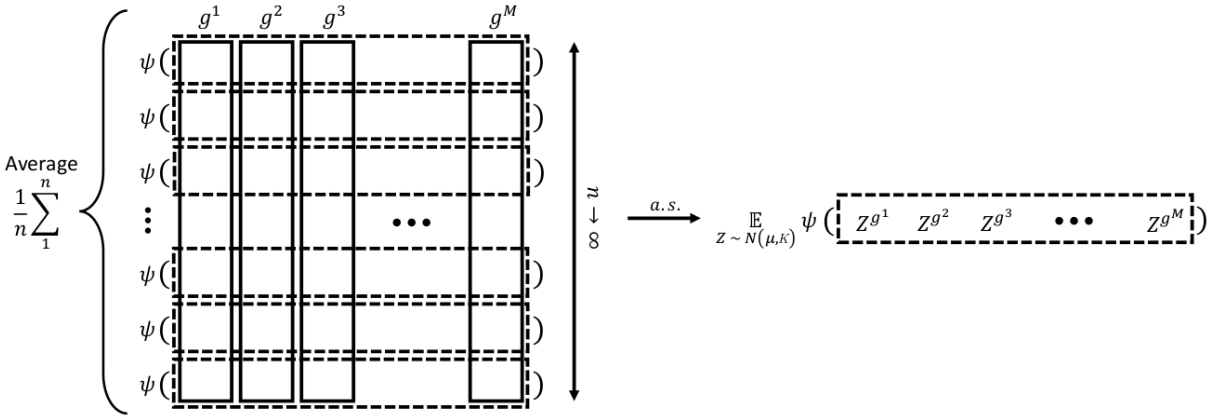

Figure 1: Illustration of Theorem 2.2, from [8]. If we suppose that $g^1, \ldots, g^M$ are all the G-vars in a CDC (i.e. $g^{\mathfrak{c}} = (g^1, \ldots, g^M)$), then, as the dimension n increase, the empirical mean along the coordinates of the G-vars of an α-controlled function ψ converges to the expected value. Or, more intuitively, for each i, $(g_i^1, \ldots, g_i^M) \approx \mathcal{N}(\mu, K)$.

Intuitively, Theorem 2.2 states that $g_i^{\mathfrak{c}t} \overset{\text{d}}{\approx} \mathcal{N}(\mu^{\mathfrak{c}}, K^{\mathfrak{c}})$ for large t, iid for each i. This, jointly with the definitions of (2.3) and (2.4), means, roughly speaking, that the G-vars (preactivations, CFR Section 2.1) created from the same matrix A^k have nonzero correlations, but otherwise are asymptotically independent unless they appear together in a LinComb.

2.3 Neural Tangent Kernel

Has we have seen in Section 2.2, each neaural network architecture is equivalent, in the IWL to a Gaussian Process. This implies that we can study the regression we perform with the ANN as a kernel method, once we understand which kernel corresponds to its training. In this section, $\{x^i\}_{i\in[N]} \subset \mathbb{R}^{\dim_{\text{in}}}$ denote the network inputs, $\theta \in \mathbb{R}^P$ contains all the parameters, distributed at initialization as in Section 2.2, and $f(\theta, x)$ is the output of the network, which, for notation simplicity, we suppose unidimensional.

As in [3] and [1], we consider a training dataset $\{(x^i, y^i)\}_{i=1}^N \subset \mathbb{R}^{d_{\text{in}}} \times \mathbb{R}$ and we train the neural network by minimizing a convex loss function

$$l(\theta) = \sum_{i=1}^{N} \mathcal{L}(f(\theta, x^i), y^i).$$

We update the parameters at step t using gradient descent with an infinitesimally small learning rate $\frac{d\theta(t)}{dt} = -\nabla l(\theta(t))$. With this setup, if we consider l to be the mean squared error, by a simple differentiation [1, Lemma 3.1] we see that the outputs of the network $u(t) = (f(\theta(t), x^i))_{i\in[N]}$ evolve according to

$$\frac{du(t)}{dt} = -\operatorname{NTK}(f_t) \cdot (u(t) - y), \tag{2.5}$$

where $\operatorname{NTK}(f_t)$ is the $n \times n$ positive semidefinite matrix given by the *Neural Tangent Kernel*.

Definition 2.3. With the notation previously introduced, we define the *Neural Tangent Kernel* $\operatorname{NTK}(\cdot, \cdot)$ as the kernel whose values on points x, x' are given by

$$\operatorname{NTK}(x, x') = \left\langle \frac{\partial f(\theta, x)}{\partial \theta}, \frac{\partial f(\theta, x')}{\partial \theta} \right\rangle. \tag{2.6}$$

As the values of θ are randomly initialized, we also define

$$\operatorname{NTK}_\infty(x, x') = \mathbb{E}_\theta[\operatorname{NTK}(x, x')]. \tag{2.7}$$

Finally, for any kernel K, we abuse the notation and, when the context make it clear, use K, or specifically NTK, to define the matrix whose entries i, j are given by $K(x^i, x^j)$.

As we can see, the NTK depends on the parameters of the network and thus it is random at initialization and varies during training. Nonetheless, in [3], the authors prove that, if the ANN is an MLP, the NTK converges in the IWL to $\operatorname{NTK}_\infty$, which is ideed deterministic. Therefore, the dynamic expressed in (2.5) is identical to that of *kernel regression* under gradient flow.

It turns out that this idea is even more general. In fact, in [3] Jacot et al. prove that the network function evolves along the kernel gradient given by the Neural Tangent Kernel for any convex loss function. We conjecture that this result holds true for any deep learning architecture.

2.4 Kernel Regression

Before moving to the experimental part, we remind the rider some concepts about *kernel regression*. Suppose we have a kernel function $K(\cdot, \cdot)$ and a training dataset $\{(x^i, y^i)\}_{i=1}^N \subset \mathbb{R}^{d_{\text{in}}} \times \mathbb{R}$, kernel regression aims to approximate the underlying function with the linear combination

$$f_K(\cdot) = \sum_{i=1}^{N} \alpha^i K(\cdot, x^i). \tag{2.8}$$

The coefficients are estimated to minimize the loss function over prediction points

$$l(\alpha) = \mathcal{L}(f(x_*), y_*),$$

and in practice this minimization is carried over the training dataset

$$\widehat{\alpha} = \arg\inf \left\{ \sum_{i=1}^{N} \mathcal{L} \left(\sum_{j=1}^{N} \alpha_j K(x^i, x^j), y^i \right) : \alpha_1, \ldots, \alpha_N \in \mathbb{R} \right\}. \tag{2.9}$$

There is a nontrivial result linking a fully trained wide MLP f_{nn} to the kernel regression predictor f_{NTK}, using the NTK_∞. If we consider a fresh observation x^* and let $f_{nn} := \lim_{t\to\infty} f(\theta(t), x^*)$, where $f(\theta(t), \cdot)$ is the MLP output function as in Section 2.3, we can prove the following theorem.

Theorem 2.4 ([1])**.** *Suppose an MLP with ReLU activation function and L hidden layers with m nodes, whwre $m \geq \text{poly}(1/\kappa, L, 1/\lambda_0, N, \log(1/\delta))$, N being the size of the training dataset, $1/\kappa = \text{poly}(1/\epsilon, \log(n/\delta))$ and λ_0 being the smallest eigenvalue of the matrix NTK_∞ over the training data. Then, for any $x^* \in \mathbb{R}^{d_{in}}$ with $||x^*|| = 1$, with probability at least $1-\delta$ over the random initialization, we have*

$$|f_{nn}(x^*) - f_{\text{NTK}}(x^*)| \leq \epsilon.$$

The main consequence of this theorem is that, if a network is big enough, then we can expect its performace to be similar to that of the NTK regressor, with a non-asymptotic bound.

2.5 Multidimensional output

All we stated before about neural networks and kernels generalize immediately to the multi-dimensional case upon noting that a function $f : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}^{d_{\text{out}}}$ is equivalent to a function $\tilde{f} : \mathbb{R}^{d_{\text{in}}} \times [d_{\text{out}}] \to \mathbb{R}$ with $\tilde{f}(x, k) = f_k(x)$. This said, we can generalize kernel regression, with each entry of the kernel $K(x, x')$ now being a matrix instead of a scalar and α being a vector, such that the vector-matrix product in (2.8) produces indeed a vector output. In this case, the kernel matrix K is a block matrix, where each block is given by the matrix $K(x^i, x^j)$.

For the Neural Tangent Kernel, this means that

$$[NTK(x^i, x^j)]_{k,k'} = \left\langle \frac{\partial f_k(\theta, x^i)}{\partial \theta}, \frac{\partial f_{k'}(\theta, x^j)}{\partial \theta} \right\rangle, \tag{2.10}$$

with $k, k' \in [d_{\text{out}}]$. An interesting point of the multidimensional approach is that, as we can see in (2.10), the kernel also encodes information between different output coordinates, i.e. $k \neq k'$.

3 NTK implementation

In order to practically test the theoretical results on different deep learning architectures, we choose to work using the efficient and popular library `Pytorch` [6], which is highly optimized for tensorial calculus. We gave in (2.6) an explicit formula to compute the NTK of a given neural network. This formulation is very suitable for the `Autograd` functionality of `Pytorch`. In fact, this module creates a computational graph when an input is passed trough the ANN and it is then possible to quickly compute derivatives with respect to the network parameters.

3.1 NTK for finite networks

To get the exact NTK corresponding to a finite network, we choose therefore to compute the full Jacobian `Jac` of the function $f(\theta, (x^1, \dots, x^N))$, where we pass all the input variables in a batch. In this way, we get a tensor of size $N \times d_{\text{out}} \times P$, where N is the number of datapoints, d_{out} is the length of the response vector and P is the number of parameters in the network, i.e. the length of θ. At this point, we can compute the kernel by multiplying the Jacobian by its transpose (as it is a tensor we intend the transpose along the two fist axes, corresponding to the input number and the coordinate of the output layer) and then by adding up the entries over the third ax, namely the one corresponding to parameters. This last step cab be written in one line using Einstein summation convention, and computed efficiently in `Pytorch` with the function `einsum` and then reshaping the matrix:

```
einsum('abp, cdp -> abcd', Jac, Jac).reshape(N * dim_out, N * dim_out)
```

There are two main limitations to this approach. First of all, the Jacobian requires a lot of memory to be stored. For instance, if we consider an MLP with 3 hidden layers, 100 nodes in each layer and output size of 10, with biases at each layer; and we want to use it for an handwritten digit classification, for which the standard input images have 28×28 greyscale pixels, our network would have $99710 \approx 10^5$ parameters. This, jointly with a 1000 regression images, whould require a tensor of size $10^3 \times 10 \times 10^5$, thus with a billion entries. Supposing we store each digit at 32 bit precision, the Jacobian would require approximately 3GB of memory. Then, another Jacobian would be necessary for predictio, thus doubling the memory required, if we suppose the test set to have equas size as the training one.

Secondly, as a consequence of `Pythorch` differentiation implementation, in order to retrieve the full Jacobian we need to iterate both on input images and on output dimensions. This is due to the fact that differentiation always return a tensor of the same shape as the variable by which we differentiate and, thus, in case the derivative is a tensor of higher dimension, requires a direction over which aggregate the derivatives, which in this case would be a matrix with rows correspond to images and columns to output coordinates. This double loop seriously affects computation time, as the very fast `Pythorch` backend is accessed without any optimization through the `python` loops, which are very slow as it is an interpreted language.

3.2 NTK at infinite width

To estimate NTK_∞, i.e. the kernel corresponding to the ANN in the infinite width limit, we have different options. The first one would be to find an explicit formula and exactly compute the kernel function, as Arora et al. did in [1]. Altough explicit formulas are already known for MLPs and elementary CNNs, to compute them still requires to go through all layers, all input images and all output dimensions, which implies more and more computations the deeper the network is. Furthermore, every different architecture would explicitly require an explicit formula, which should be obtained beforehand.

We can avoid the latter problem leveraging on the fact that in the IWL, if our conjecture is right, each layer of the network has a kernel, which converges to the theoretical limiting one. We could thus use the already cited results, and iteratively compute an estimator of the kernel by passing through layers. By using the fact that, asympthotically, the kernel for each node is independent from the others, at least for MLPs [3], we can average of them to get an estimate of the actual

value. Nonetheless, when considering more elaborate architectures, such as CNN or transformers, obtaining the NTK is not as straightforward.

For this reason, we choose to follow the same approach as for the finite case. More precisely, we initialize many big networks, compute the NTK for each of them and then estimate the limiting kernel as their average.

4 Experimental results

In this section we focus on testing experimentally our conjecture, namely that all the results presented in Section 2 generalize to general Deep Learning architectures as well. In particular, it has already been tested that for MLPs with a single output, regression based on NTK obtains results equivalent, or even better, than those of the original network. On the other hand, the same does not holds for CNNs, where experimental results show that the actual network greatly outperform the kernel methods [1]. Our objective is to understand what the network is actually learning, to confront it with what the NTK_∞ regression function, furthermore we study networks with multidimensional output.

More precisely, given an ANN with random initialization, we can compute its actual NTK, as exaplaned in Section 3.1, and its theoretical-infinite-wide counterpart NTK_∞. Then, we train the ANN to get f_{nn}, which produces another tangent kernel NTK_{tr}. By [3], we know that NTK_∞ does not change during training, so we can study the kernel regression functions f_{NTK_∞} and $f_{\text{NTK}_{tr}}$ given respectively by the infinte-width Tangent Kernel and the NTK obtained by the finite and trained Network.

4.1 The dataset

We perform an handwritten-digit classification task, using the MNIST dataset [4]. It consist in grayscale images of handwritten digits, whose size is 28x28 pixels, and their labels, which correspond to the 10 digits from 0 to 9. We use 1000 samples for train and we study the Kernel on a test of 1000 samples The two sets are disjoint and randomly drawn from the full dataset, using `Pytorch` functionalities.

Figure 2: Sample of 8 images from the MNIST dataset. The grayscale pictures represent, in the order, the digits 5, 0, 7, 1, 6, 9, 0, 7.

We normalize the images beforehand, as the mean and standard deviation are well known, so that the observation space is supported in the unit sphere, which is one of the hypothesis used by Jacot et al. in [3].

4.2 Multilayer Perceptron

We start with the artificial neural network on which all theoretical results have been proved. In particular, we test an architecture with three hidden layers and a readout layer. The input

dimension is of $784 = 28 \cdot 28$ nodes and all hidden layers have 100 nodes. Combined with the readout layer, this gives a total of 99710 parameters.

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