Neural Tangent Kernel: Convergence and Generalization in Neural Networks

Arthur Jacot, Franck Gabriel, Clément Hongler

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- If time allows we can dwelve deeper into the matter

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- Stack features and targets into matrices:

$$\boldsymbol{X} \in \mathbb{R}^{n \times d_0} \text{ and } \boldsymbol{y} \in \mathbb{R}^n$$

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- **Same** notation as last time :)

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- Again **identical** to first presentation

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- Assume that the loss decomposes over the samples:

$$L(f_{\boldsymbol{\theta}}(\boldsymbol{X}), \boldsymbol{y}) = \sum_{i=1}^{n} L(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), y_i)$$

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- **Non-linear** ODE, hard to solve... If we could solve it, no need to train NNs since the solution describes the trajectory through time

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This means in particular that for $k, k' \in \{1, \dots, d_L\}$ and $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{d_0}$

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and thus $\Theta^{(L)}(\boldsymbol{x}, \boldsymbol{x}') \in \mathbb{R}^{d_L \times d_L}$ (multi-dimensional kernel)

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- **Question:** Why should we care about this object???

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- What can we say about the **function space** dynamics?

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&= -\sum_{i=1}^{n} \frac{\partial L(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i, y_i)}{\partial f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)} \boldsymbol{\Theta}_t^{(L)}(\boldsymbol{x}, \boldsymbol{x}_i)
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- ODE hence **not** analytically solvable (again if it were, no need to train NNs at all)

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We hence don't have to worry about the initialization and time-dependence anymore!

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- Gradient flow hence converges to the **global minimum** in the infinite regime.

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- Can't do it for just $d_L = 1$, otherwise induction doesn't work. Have to do it for **general** d_L...

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Remember: $\boldsymbol{\Theta}_{kk'}^{(L)}(\boldsymbol{x}, \boldsymbol{x}') = \sum_{p=1}^{P} \partial_{\theta_p} f_{\boldsymbol{\theta},k}(\boldsymbol{x}) \partial_{\theta_p} f_{\boldsymbol{\theta},k'}(\boldsymbol{x}')$

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Notice: We didn't take any limit because input dimension d_0 of course remains fixed.

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This **proves** the base case.

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We can now **split** the NTK:

$$\boldsymbol{\Theta}_{kk'}^{(l+1)}(\boldsymbol{x}, \boldsymbol{x}') = \underbrace{\sum_{l=1}^{\tilde{P}} \partial_{\tilde{\theta}_l} f_{\boldsymbol{\theta},k}(\boldsymbol{x}), \partial_{\tilde{\theta}_l} f_{\boldsymbol{\theta},k'}(\boldsymbol{x}')}_{A} + \underbrace{\sum_{i,j=1}^{d_l,d_{l+1}} \partial_{W_{ij}^{(L)}} f_{\boldsymbol{\theta},k}(\boldsymbol{x}), \partial_{W_{ij}^{(L)}} f_{\boldsymbol{\theta},k'}(\boldsymbol{x}')}_{B}$$

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Let us study the terms $A = \sum_{l=1}^{\tilde{P}} \partial_{\tilde{\theta}_l} f_{\boldsymbol{\theta},k}(\boldsymbol{x}) \partial_{\tilde{\theta}_l} f_{\boldsymbol{\theta},k'}(\boldsymbol{x}')$ due to $\tilde{\boldsymbol{\theta}}$:

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$$\frac{1}{d_l} \sum_{p=1}^{\tilde{P}} \left(\sum_{j=1}^{d_l} W_{kj}^{(L)} \dot{\sigma}\left(\tilde{\alpha}_j^{(l)}(\boldsymbol{x})\right) \partial_{\tilde{\theta}_p} \tilde{\alpha}_j^{(l)}(\boldsymbol{x}) \right) \left(\sum_{j'=1}^{d_l} W_{k'j'}^{(l)} \dot{\sigma}\left(\tilde{\alpha}_{j'}^{(l)}(\boldsymbol{x}')\right) \partial_{\tilde{\theta}_p} \alpha_{j'}^{(l)}(\boldsymbol{x}') \right)$$

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$$= \mathbb{E}_{\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \tilde{\boldsymbol{\Sigma}}^{(l)})} \left[\sigma(z_1)\, \sigma(z_2)\right] \mathbb{1}_{\{k=k'\}}$$

Terms in B

Let's calculate the gradients w.r.t. last layer weights

$$\partial_{W_{ij}^{(l)}} f_{\boldsymbol{\theta},k}(\boldsymbol{x}) = \frac{1}{\sqrt{d_l}} \alpha_j^{(l)}(\boldsymbol{x}) \mathbb{1}_{\{k=i\}}$$

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$$= \frac{1}{d_l} \sum_{j=1}^{d_{l+1}} \alpha_j^{(l)}(\boldsymbol{x}) \alpha_j^{(l)}(\boldsymbol{x}') \mathbb{1}_{\{k=k'\}} \xrightarrow{d_l \to \infty} \mathbb{E}\left[\sigma(\tilde{\alpha}_{j,\infty}^{(l)}(\boldsymbol{x})) \sigma(\tilde{\alpha}_{j,\infty}^{(l)}(\boldsymbol{x}'))\right] \mathbb{1}_{\{k=k\}}$$

$$= \mathbb{E}_{\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \tilde{\boldsymbol{\Sigma}}^{(l)})}\left[\sigma(z_1)\, \sigma(z_2)\right] \mathbb{1}_{\{k=k'\}} = \Sigma^{(l+1)}(\boldsymbol{x}, \boldsymbol{x}') \mathbb{1}_{\{k=k'\}}$$

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- This concludes the proof!

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Then: $\boldsymbol{\Theta}_t^{(L)} \xrightarrow{d_1,\ldots,d_{L-1}\to\infty} \boldsymbol{\Theta}_\infty^{(L)} \otimes \mathbb{1}_{d_L \times d_L}$ *for all* $t \in [0, T]$

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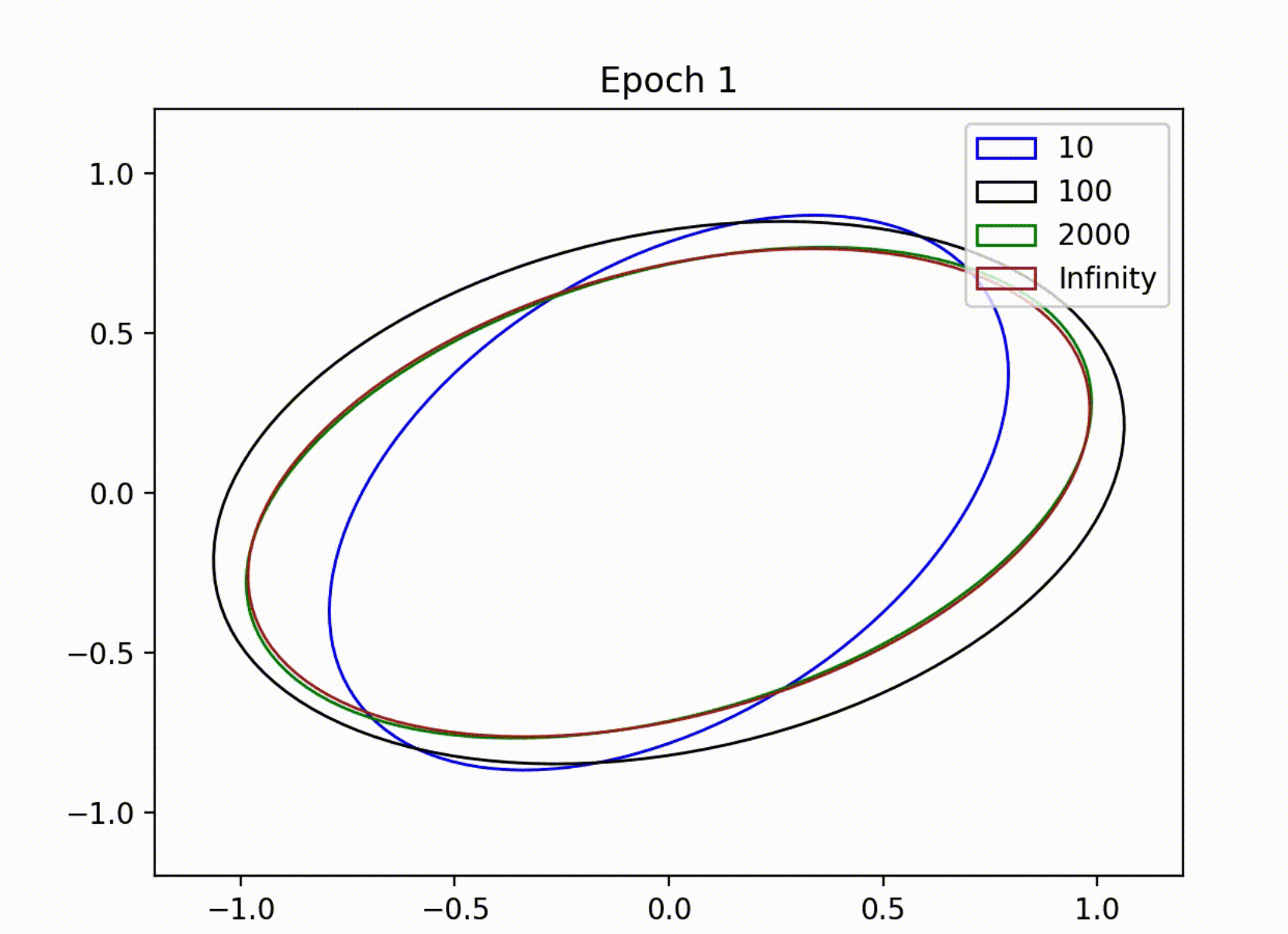
$$\sim \mathcal{O}(\partial_t W_{kj}^{(l)}) + \mathcal{O}(\partial_t \tilde{\alpha}_j^{(l)}) + \mathcal{O}(\partial_t \alpha_j^{(l)}) = \mathcal{O}\left(\frac{1}{\sqrt{d_l}}\right)$$

NTK Animation



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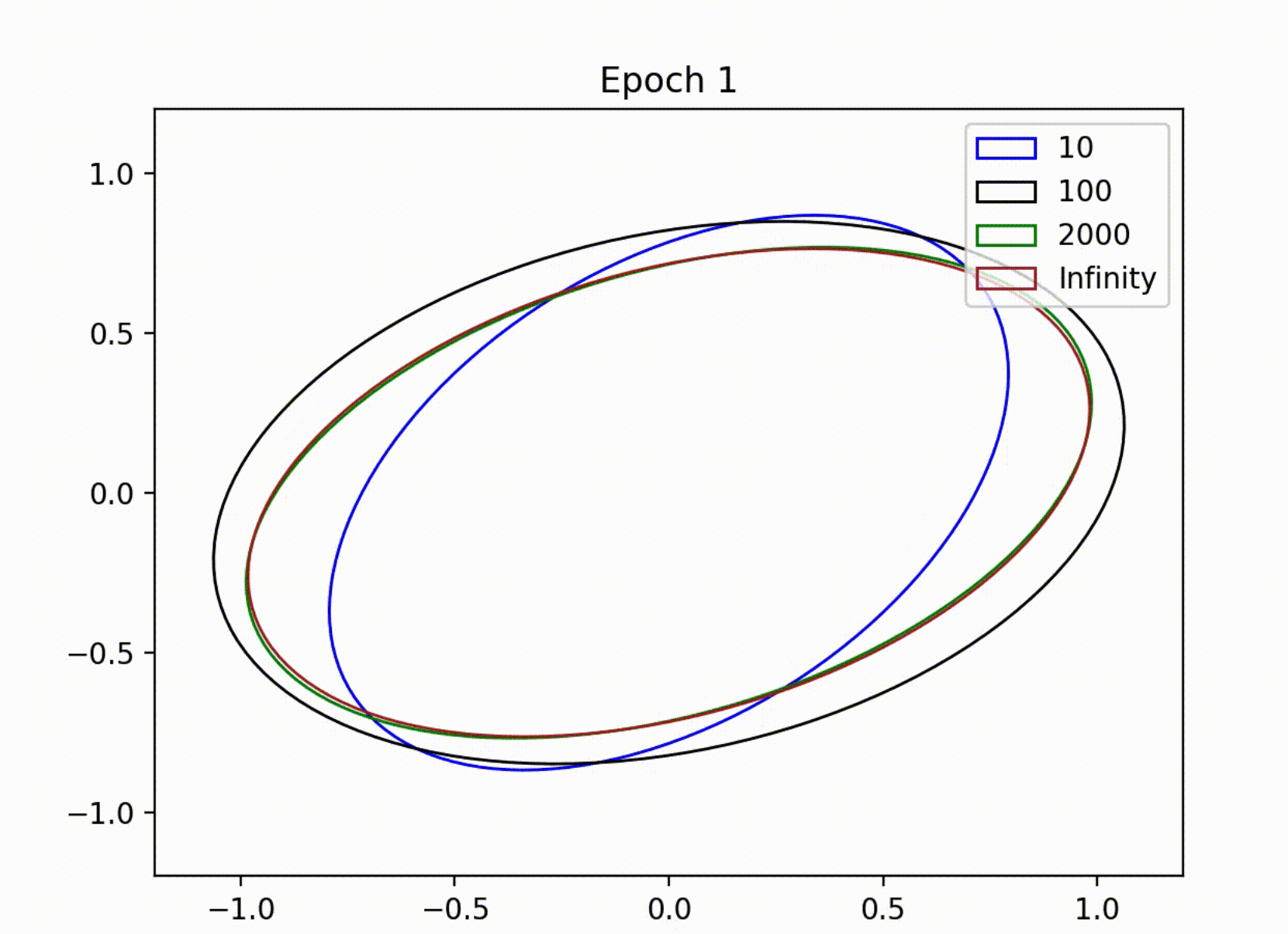

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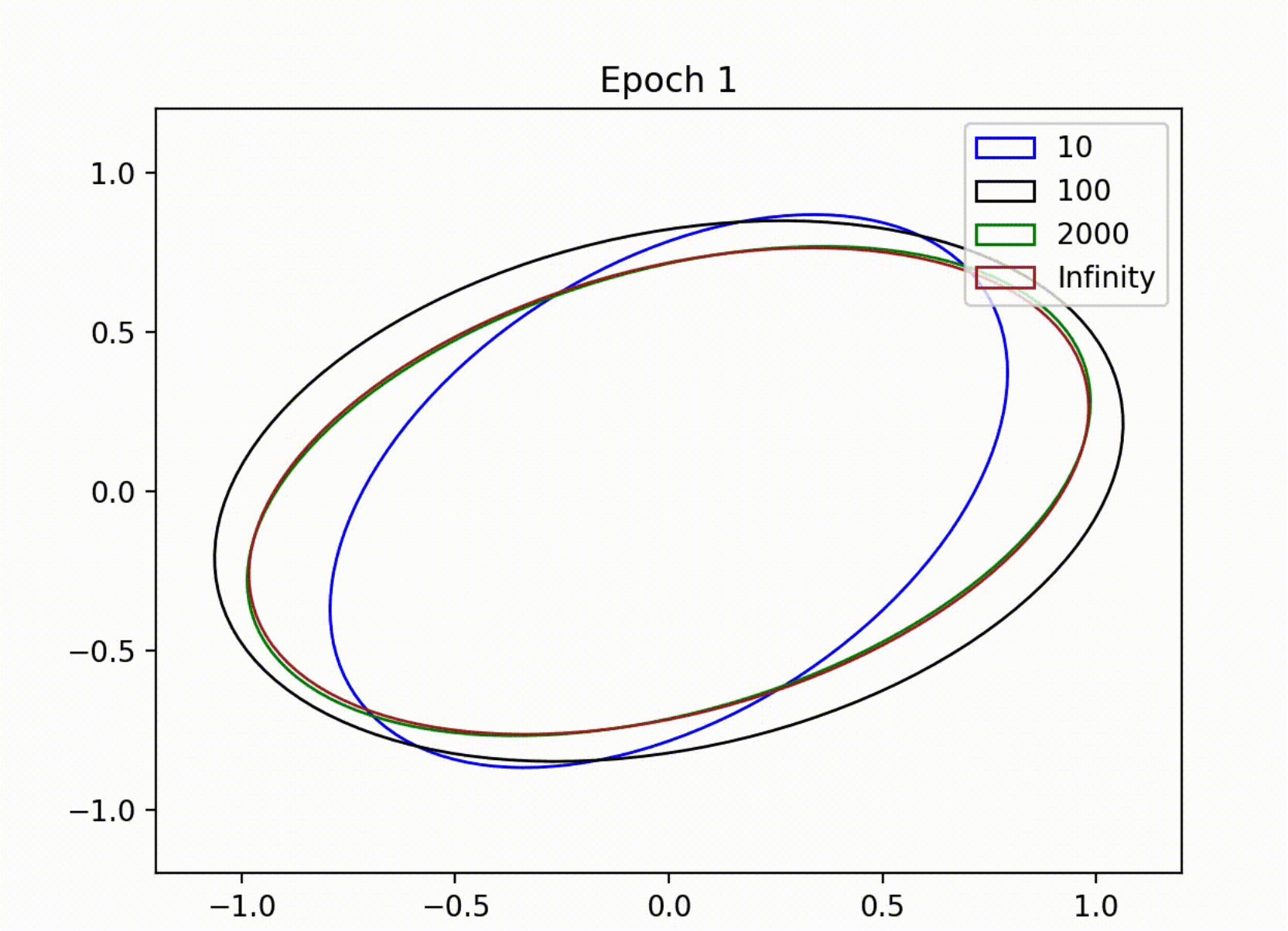

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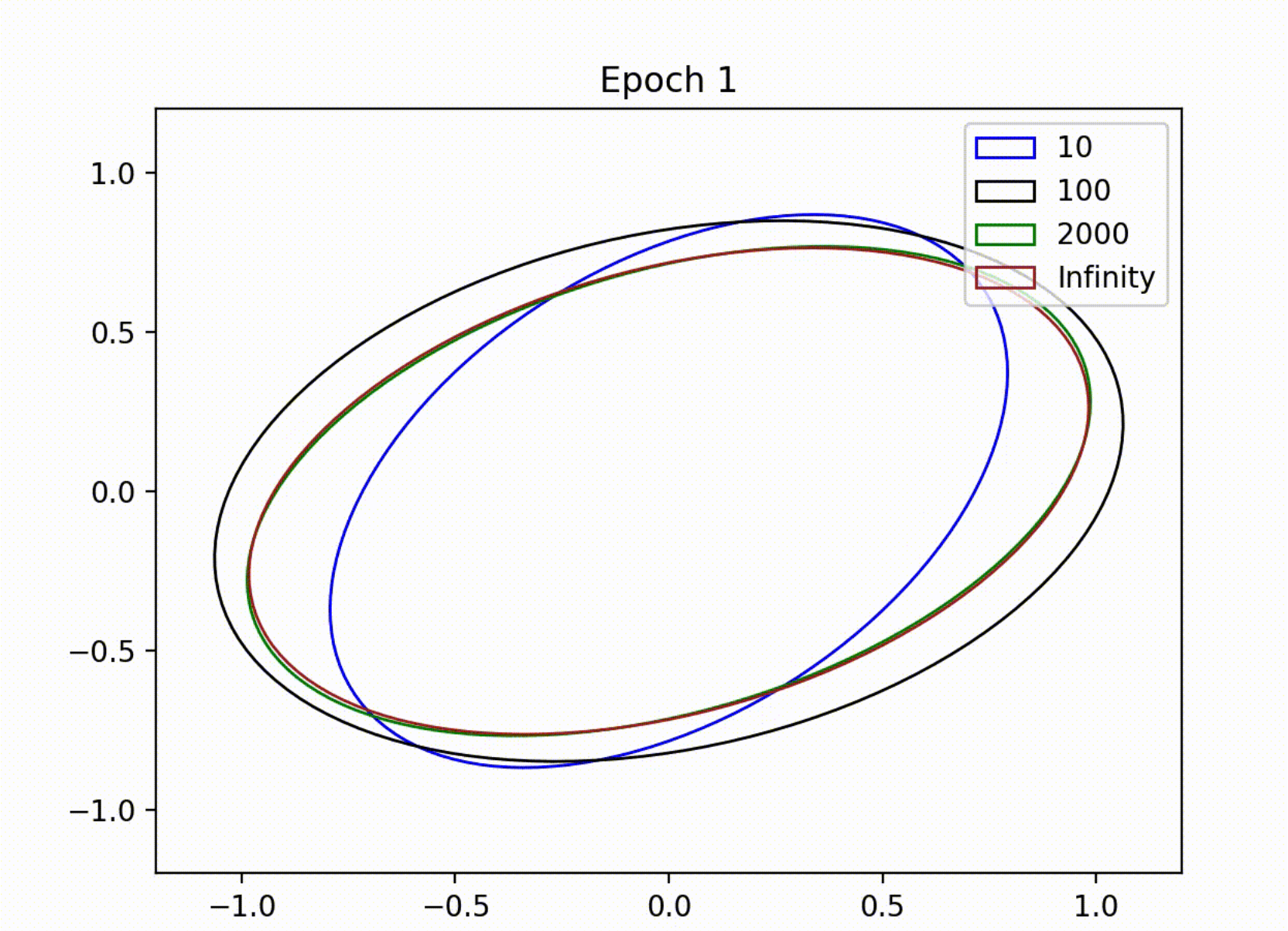

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- Can hence probably not explain why neural networks work **so** well if we take the kernel route but it may be a good start
- We observe that NNs work better with increasing width. This is a bit conflicting with infinite width as there performance decreases (Aurelien will present a paper that shows this empirically)

Backup Slides

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- We first need to solve it on the training set $\boldsymbol{X}$:

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  2) $\int e^{\boldsymbol{A}t} dt = A^{-1}\left(e^{\boldsymbol{A}t} - \mathbb{1}\right) + C$

Closed Form Solution (III)

Performing this integral gives

$$
\begin{aligned}
f_t^\infty(\boldsymbol{x}) &= \int - \left(\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{x}, \boldsymbol{X})\right)^T \left(f_t^\infty(\boldsymbol{X}) - \boldsymbol{y}\right)\, dt \\
&= \int - \left(\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{x}, \boldsymbol{X})\right)^T e^{-\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{X}, \boldsymbol{X})t} \left(f_0^\infty(\boldsymbol{X}) - \boldsymbol{y}\right)\, dt \\
&\overset{1)}{=} - \left(\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{x}, \boldsymbol{X})\right)^T \left(\int e^{-\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{X}, \boldsymbol{X})t}\, dt\right) \left(f_0^\infty(\boldsymbol{X}) - \boldsymbol{y}\right) \\
&\overset{2)}{=} \left(\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{x}, \boldsymbol{X})\right)^T \left(\left(\boldsymbol{\Theta}_\infty^{(L)}\right)^{-1} \left(e^{-\boldsymbol{\Theta}_\infty^{(L)}(\boldsymbol{X}, \boldsymbol{X})t} - \mathbb{1}\right)\right) \left(f_0^\infty(\boldsymbol{X}) - \boldsymbol{y}\right) \\
&\quad + f_0^\infty(\boldsymbol{x})
\end{aligned}
$$