Neural Tangent Kernel

Convergence and Generalization of DNNs

Arthur Jacot, Franck Gabriel, Clément Hongler

Ecole Polytechnique Fédérale de Lausanne

October 28, 2019

Neural Networks

- $L+1$ layers of n_ℓ neurons with activations $\alpha^{(\ell)}(x) \in \mathbb{R}^{n_\ell}$

$$\alpha^{(0)}(x) = x$$
$$\tilde{\alpha}^{(\ell+1)}(x) = \frac{\sqrt{1-\beta^2}}{\sqrt{n_\ell}} W^{(\ell)} \alpha^{(\ell)}(x) + \beta b^{(\ell)}$$
$$\alpha^{(\ell+1)}(x) = \sigma\left(\tilde{\alpha}^{(\ell+1)}(x)\right)$$

  - Parameters: connections weights $W^{(\ell)} \in \mathbb{R}^{n_\ell \times n_{\ell+1}}$ and bias $b^{(\ell)} \in \mathbb{R}^{n_{\ell+1}}$.
  - Weights / bias balance: $\beta \in [0,1]$.
  - Non-linearity: $\sigma : \mathbb{R} \to \mathbb{R}$.
- Network function $f_\theta(x) = \tilde{\alpha}^{(L)}(x)$

Initialization: DNNs as Gaussian processes

- In the infinite width limit $n_1, ..., n_{L-1} \to \infty$
- Initialize the parameters $\theta \sim \mathcal{N}(0, Id_P)$.
- The preactivations $\tilde{\alpha}_i^{(\ell)}(\cdot; \theta) : \mathbb{R}^{n_0} \to \mathbb{R}$ converge to iid Gaussian processes of covariance $\Sigma^{(\ell)}$ (Cho and Saul, 2009; Lee et al., 2018):

$$\Sigma^{(1)}(x, y) = (1 - \beta^2) x^T y + \beta^2$$
$$\Sigma^{(\ell+1)}(x, y) = (1 - \beta^2) \mathbb{E}_{\alpha \sim \mathcal{N}(0, \Sigma^{(\ell)})} [\sigma(\alpha(x))\sigma(\alpha(y))] + \beta^2$$

- The network function $f_\theta = \tilde{\alpha}^{(L)}$ is also asymptotically Gaussian.

Training: Neural Tangent Kernel

- Training set of size N: inputs $X \in \mathbb{R}^{N \times n_0}$ and outputs $Y \in \mathbb{R}^{N \times n_L}$.
- Gradient descent on the MSE $C(\theta) = \frac{1}{N} \|f_\theta(X) - Y\|^2$

$$\partial_t \theta = -\nabla C(\theta) = \frac{2}{N} \sum_{i=1}^{N} \nabla f_\theta(x_i)(Y_i - f_\theta(x_i))$$

- Evolution of f_θ:

$$\partial_t f_\theta(x) = (\nabla f_\theta(x))^T \partial_t \theta = \frac{2}{N} \sum_{i=1}^{N} (\nabla f_\theta(x))^T \nabla f_\theta(x_i)(y_i - f_\theta(x_i))$$

- Neural Tangent Kernel (NTK):

$$\Theta^{(L)}(x, y) := (\nabla f_\theta(x))^T \nabla f_\theta(y)$$

Asymptotics of the NTK

Theorem (Arora et al., 2019; Jacot et al., 2018)

Let $n_1, \ldots, n_{L-1} \to \infty$, for any t:

$$\Theta^{(L)}(t) \to \Theta_\infty^{(L)}$$

where

$$\Theta_\infty^{(L)}(x, y) = \sum_{\ell=1}^{L} \Sigma^{(\ell)}(x, y) \dot{\Sigma}^{(\ell+1)}(x, y) \ldots \dot{\Sigma}^{(L)}(x, y)$$

with

$$\dot{\Sigma}^{(L)}(x, x') = (1 - \beta^2) \mathbb{E}_{\alpha \sim \mathcal{N}(0, \Sigma^{(L-1)})} [\dot{\sigma}(\alpha(x)) \dot{\sigma}(\alpha(x'))].$$

Convergence

The continuous-time dynamics of the outputs $Y_{\theta(t)} = f_{\theta(t)}(X)$ are described by the linear ODE

$$\partial_t Y_{\theta(t),k} = \frac{2}{N} \Theta_{\infty}^{(L)}(X, X) \left(Y - Y_{\theta(t)}\right)$$

with solution $Y_{\theta(t)} = Y - e^{\frac{2t}{N}\Theta_{\infty}^{(L)}(X,X)} \left(Y - Y_{\theta(0)}\right)$.

Convergence and loss surface(Jacot et al., 2019a):

1. Eigenvalues: speed of convergence along the eigenvector
2. Narrow valley structure:
   - 2.1 Large eig. are the 'cliffs'
   - 2.2 Small eig. are the 'bottom'
3. Condition number $\kappa = \lambda_{max}/\lambda_{min}$

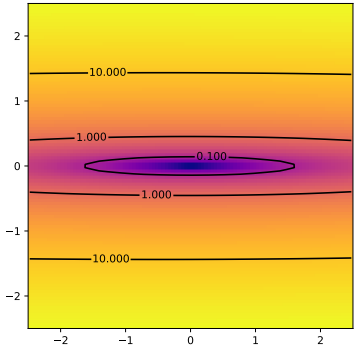


Figure: Narrow valley in the loss surface.

Freeze and Chaos

Two regimes appear (as in Poole et al. (2016); Schoenholz et al. (2017))

Theorem (Jacot et al., 2019b)

Consider a twice differentiable σ satisfying $\mathbb{E}_{z\sim\mathcal{N}(0,1)}[\sigma(z)] = 1$ and two inputs x, y with $\|x\| = \|y\| = \sqrt{n_0}$. The characteristic value

$$r_{\sigma,\beta} = (1-\beta^2)\mathbb{E}_{z\sim\mathcal{N}(0,1)}\left[\dot{\sigma}(z)^2\right]$$

determines two regimes:

FREEZE (r<1): *For $x, y \in \mathbb{S}_{n_0}$*

$$1 \geq \frac{\Theta_\infty^{(L)}(x,y)}{\Theta_\infty^{(L)}(x,x)} \geq 1 - CLr^L$$

CHAOS (r>1): *If $x \neq \pm y$:*

$$\frac{\Theta_\infty^{(L)}(x,y)}{\Theta_\infty^{(L)}(x,x)} \to 0$$

Freeze and Chaos: Properties

- **FREEZE (r<1):**
  - Almost constant NTK Gram Matrix
  - Bad conditioning $\lambda_{max}/\lambda_{min}$
  - Slow convergence
- **CHAOS (r>1):**
  - Almost identity NTK Gram Matrix
  - Fast convergence
  - Generalization?
- **EDGE:** For the RELU: $r = 1 - \beta^2 \approx 1$
  - Converges to $\mathrm{Id} + c$
  - Strong constant mode for large N
  - Slow convergence

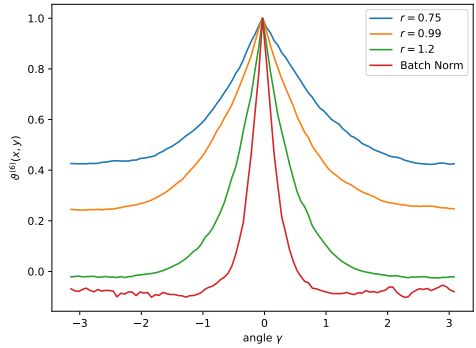


Figure: The NTK in the different regimes for $L = 6$.

Chaos: normalization

- Normalize the non-linearity (over $z \sim \mathcal{N}(0,1)$):

$$\bar{\sigma}(x) = \frac{\sigma(x) - \mathbb{E}\left[\sigma(z)\right]}{\sqrt{Var\left[\sigma(z)\right]}}.$$

- If $\sigma \neq id$ we have $\mathbb{E}\left[\dot{\bar{\sigma}}(z)^2\right] > 1$, and for small enough $\beta > 0$

$$r = (1 - \beta^2)\mathbb{E}\left[\dot{\bar{\sigma}}(z)^2\right] > 1.$$

- Asymptotically equivalent to Layer Normalization.

Chaos: normalization

- Normalize the non-linearity (over $z \sim \mathcal{N}(0,1)$):

$$\bar{\sigma}(x) = \frac{\sigma(x) - \mathbb{E}\left[\sigma(z)\right]}{\sqrt{Var\left[\sigma(z)\right]}}.$$

- If $\sigma \neq id$ we have $\mathbb{E}\left[\dot{\bar{\sigma}}(z)^2\right] > 1$, and for small enough $\beta > 0$

$$r = (1-\beta^2)\mathbb{E}\left[\dot{\bar{\sigma}}(z)^2\right] > 1.$$

- Asymptotically equivalent to Layer Normalization.
- For Batch Normalization we only have:
  - Applying BN after the last non-linearity controls the constant mode:

$$\frac{1}{N^2}\sum_{ij}\Theta^{(L)}(x_i, x_j) = \beta^2$$

Generative Adversarial Networks

- Two networks(Goodfellow et al., 2014)
  - Generator G: generates data $G(z)$ from a random code z.
  - Discriminator D: classifies real/generated data to guide the generator.
- If the generator lies in the **FREEZE**
  - Mode collapse: The generator G becomes constant.
- Solutions:
  - Batch Normalization
  - Chaotic generator

Deconvolutional Generator

For G a deconvolutional network with stride s

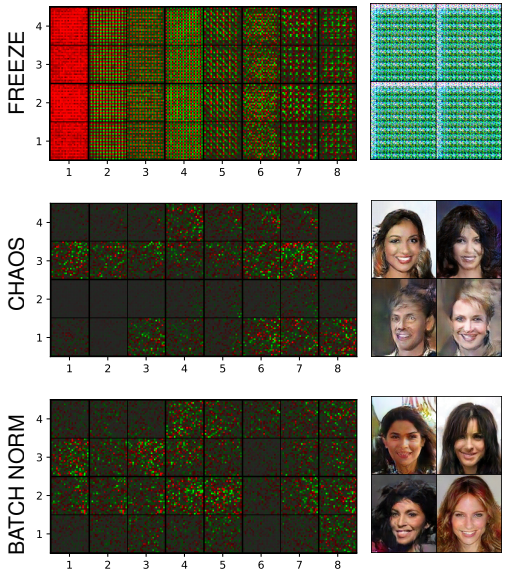
Theorem
*In the **FREEZE (r>1):***

$$\frac{1-r^{v+1}}{1-r^{L}} - C_1(v+1)r^{v} \leq \frac{\Theta^{(L)}_{p,p'}(x,y)}{\Theta^{(L)}_{p,p}(x,x)} \leq \frac{1-r^{v+1}}{1-r^{L}}$$

for v the max. in $\{0, L-1\}$ s.t. s^v divides $p-p'$

- Checkerboard patterns: images which repeat every s^v pixels
- Solution: Batch Norm / Chaos

NTK PCA



Conclusion

1. Certain architectures lead to dominating eigenvalues:
   - 1.1 Constant mode
   - 1.2 Checkerboard patterns
2. Slows down training
3. Mode collapse in GANS
4. Use the NTK to identify and fix them

Bibliography I

Arora, S., Du, S. S., Hu, W., Li, Z., Salakhutdinov, R., and Wang, R. (2019). On exact computation with an infinitely wide neural net. *arXiv preprint arXiv:1904.11955*.

Cho, Y. and Saul, L. K. (2009). Kernel Methods for Deep Learning. In *Advances in Neural Information Processing Systems 22*, pages 342–350. Curran Associates, Inc.

Goodfellow, I. J., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., Courville, A., and Bengio, Y. (2014). Generative Adversarial Networks. *NIPS'14 Proceedings of the 27th International Conference on Neural Information Processing Systems - Volume 2*, pages 2672–2680.

Jacot, A., Gabriel, F., and Hongler, C. (2018). Neural Tangent Kernel: Convergence and Generalization in Neural Networks. In *Advances in Neural Information Processing Systems 31*, pages 8580–8589. Curran Associates, Inc.

Bibliography II

Jacot, A., Gabriel, F., and Hongler, C. (2019a). The asymptotic spectrum of the hessian of dnn throughout training.

Jacot, A., Gabriel, F., and Hongler, C. (2019b). Freeze and chaos for dnns: an NTK view of batch normalization, checkerboard and boundary effects. *CoRR*, abs/1907.05715.

Lee, J. H., Bahri, Y., Novak, R., Schoenholz, S. S., Pennington, J., and Sohl-Dickstein, J. (2018). Deep Neural Networks as Gaussian Processes. *ICLR*.

Poole, B., Lahiri, S., Raghu, M., Sohl-Dickstein, J., and Ganguli, S. (2016). Exponential expressivity in deep neural networks through transient chaos. In Lee, D. D., Sugiyama, M., Luxburg, U. V., Guyon, I., and Garnett, R., editors, *Advances in Neural Information Processing Systems 29*, pages 3360–3368. Curran Associates, Inc.

Schoenholz, S. S., Gilmer, J., Ganguli, S., and Sohl-Dickstein, J. (2017). Deep information propagation.