Spherical Harmonics and Neural Tangent Kernel

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- *Regularization with Dot-Product Kernels* (Williamson et al)
- The goal is to understand the eigenspectrum of the NTK if the data is supported **uniformly on the sphere**

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- **Notice**: No assumption on the target distribution made

Mercer Decomposition (I)

- **Recall** the Helmholz operator T_K associated to the kernel K:

$$(T_K\phi)(\boldsymbol{x}) = \int_{\mathcal{X}} K(\boldsymbol{x}, \boldsymbol{y})\phi(\boldsymbol{y})p(\boldsymbol{y})d\boldsymbol{y}$$

  where $\mathcal{X}$ denotes the support of the input data distribution p.

- We are interested in the **eigenfunctions** of this operator:

$$(T_K\phi)(\boldsymbol{x}) = \lambda\phi(\boldsymbol{x})\ \forall \boldsymbol{x} \in \mathcal{X}$$

- Why? Because we get the decomposition

$$K(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=0}^{\infty} \lambda_i\phi_i(\boldsymbol{x})\phi_i(\boldsymbol{y})$$

Mercer Decomposition (II)

- Usually p is of course **unknown** for real datasets
- Moreover, performing the integral is usually **hard** even for known p
- Here we choose $p(\boldsymbol{x}) \sim \mathcal{U}(\mathbb{S}^{d-1})$ to make life easy
- Moreover, NTK (and NNGP) is a **dot-product kernel**:

$$\boldsymbol{\Theta}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{\Theta}(\boldsymbol{x}^T \boldsymbol{y})$$

- Turns out that the **spherical harmonics** play a crucial role

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- Key ingredient in finding the **eigenfunctions** of the Helmholz operator associated with the NTK
- We will mostly look at the **three dimensional** case but extensions are analogous

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- Rewrite it in **polar** coordinates $x = r\cos(\theta), y = r\sin(\theta)$:

$$\Delta f = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{1}{r}\frac{\partial f}{\partial r}$$

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  - $-r^2\ddot{R}(r) - r\dot{R}(r) = \lambda$
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- The solution for the **angular part**, due to required periodicity (forcing $\lambda = -k^2$) is given by

$$\Theta_k(\theta) = C_k e^{ik\theta} \ \forall k \in \mathbb{Z}$$

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- This is exactly the **Fourier basis**!

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- **First step:** Translate Laplacian to **spherical** coordinates:

$$\Delta f = \frac{\partial^2 f}{\partial r^2} + \frac{2}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2 \sin(\theta)}\left(\cos(\theta)\frac{\partial f}{\partial \theta} + \sin(\theta)\frac{\partial^2 f}{\partial \theta^2}\right) + \frac{1}{r^2 \sin^2(\theta)}\frac{\partial^2 f}{\partial \phi^2}$$

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- Again a **separation ansatz**: $f(r, \theta, \phi) = R(r)Y(\theta, \phi)$

Radial Part of Laplacian

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- We get the following ODE for the radius:

$$\left(\ddot{R}(r) + \frac{2}{r}\dot{R}(r)\right)\frac{r^2}{R(r)} = \lambda \iff r^2\ddot{R}(r) + 2r\dot{R}(r) - \lambda R(r) = 0$$

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- The solutions are given by $R_l(r) = r^l$ where l satisfies:

$$l(l-1) + 2l - \lambda = 0 \iff \lambda = l(l+1)$$

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- We get the partial differential equation for the **angle**:

$$\cos(\theta)\,Y'(\theta,\phi)+\sin(\theta)\,Y''(\theta,\phi)+\frac{1}{r^2\sin^2(\theta)}\,Y^{**}(\theta,\phi)=-\lambda\sin(\theta)\,Y(\theta,\phi)$$

where $f^{'}(\theta,\phi)=\frac{\partial f}{\partial\theta}$ and $f^{*}(\theta,\phi)=\frac{\partial f}{\partial\phi}$

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- Again make the **separation ansatz**: $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$ splitting into the polar and azimuthal angles.

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- We directly get the solution (again due periodicity, $\omega = m^2$)

$$\Phi(\phi) = A_m e^{i\phi m} \; \forall m \in \mathbb{Z}$$

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- For the **polar angle** we have

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- This is the **general Legendre equation**

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- They form a **basis** of continuous functions mapping from $[-1,1]$ to $\mathbb{R}$ and are orthogonal:

$$\int_{-1}^{1} P_k^m(x)P_l^m(x)dx = \frac{2(l+m)!}{(2l+1)!(l-m)!}\delta_{k,l}$$

$$\int_{-1}^{1} P_l^m(x)P_l^n(x)\frac{1}{1-x^2}dx = \frac{(l+m)!}{m(l-m)!}\delta_{m,n}$$

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- For every $l \in \mathbb{N}$ and $-l \leq m \leq l$ the angular part is called **spherical harmonic** and is given by

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- They form an **orthonormal** basis of $\{f : \mathbb{S}^2 \to \mathbb{R}\}$:

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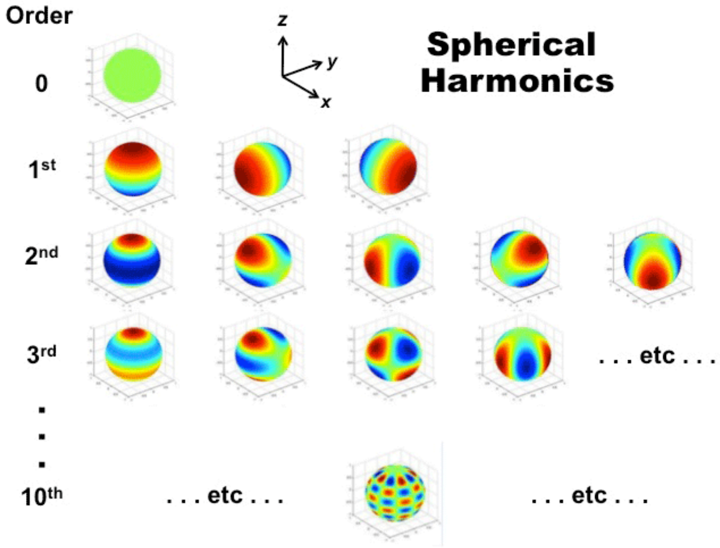
- Both stem from solving the **Laplacian equation**


Order
0
1st
2nd
3rd
10th
z
y
x
Spherical
Harmonics
. . . etc . . .
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- Now we can leverage a theorem by **Funk-Hecke**: For any continuous f defined on $[-1, 1]$ we have that

$$\int_{\mathbb{S}^2} f(\boldsymbol{x}^T \boldsymbol{y}) Y_m^l(\boldsymbol{y}) d\boldsymbol{y} = \left(\mathrm{vol}(\mathbb{S}^1) \int_{-1}^{1} f(t) G_k(t) dt\right) Y_m^l(\boldsymbol{x})$$

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- We thus have the following **Mercer decomposition**:

$$\boldsymbol{\Theta}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{l=0}^{\infty} \lambda_l \sum_{m=1}^{N(p,k)} Y_m^l(\boldsymbol{x}) Y_m^l(\boldsymbol{y})$$

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- If we only have one hidden layer with a **non-trainable** top layer and data on $\mathbb{S}^1$, then we find

$$\lambda_0 = \frac{1}{\pi^2} \text{ , } \lambda_1 = \frac{1}{4} \text{ and } \lambda_k = \frac{2(k^2+1)}{\pi^2(k^2-1)^2} \text{ for k even}$$

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- Similar but more complicated **analytical** formulas are available for $\mathbb{S}^{d-1}$

Corresponding RKHS

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- Using the decomposition we can describe the functions lying in the RKHS induced by the NTK:

$$\mathcal{H} = \left\{ f = \sum_{l:\lambda_l \neq 0} \sum_{m=1}^{N(l,m)} a_{lm} Y_m^l(\cdot) \text{ s.t. } ||f||_{\mathcal{H}}^2 = \sum_{l:\lambda_l \neq 0} \sum_{m=1}^{N(l,m)} \frac{a_{lm}}{\lambda_l} < \infty \right\}$$

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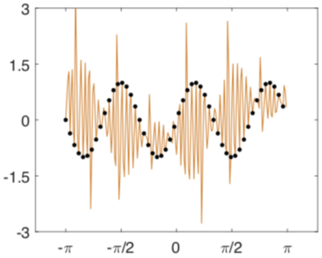
- This means that odd frequencies should be harder to learn for one hidden layer networks because $\lambda_{2k+1} = 0$.

Odd frequencies are hard to learn



Bias-free wide one hidden layer network learning $f(x) = \cos(3\theta)$ on left and $f(x) = \cos(4\theta)$ on right

One hidden layer case

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- We use a **one hidden layer** network:

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sqrt{\frac{2}{m}} \sum_{i=1}^{m} v_j \sigma \left(\boldsymbol{w}_j^T \boldsymbol{x} \right)$$

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- We can write the NTK $\boldsymbol{\Theta}(\boldsymbol{x}, \boldsymbol{x}')$ as:

$$K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\boldsymbol{x}^T \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}' \kappa_0(\boldsymbol{x}^T \boldsymbol{x}') + \kappa_1(\boldsymbol{x}^T \boldsymbol{x}')$$

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- $\kappa_0(u) = \frac{1}{\pi} (\pi - \arccos(u))$

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$$K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\boldsymbol{x}^T \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}' \kappa_0(\boldsymbol{x}^T \boldsymbol{x}') + \kappa_1(\boldsymbol{x}^T \boldsymbol{x}')$$

- $\kappa_0(u) = \frac{1}{\pi} (\pi - \arccos(u))$

- $\kappa_1(u) = \frac{1}{\pi} \left(u(\pi - \arccos(u)) + \sqrt{1 - u^2} \right)$

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We can write $\boldsymbol{\Theta}(\boldsymbol{x}, \boldsymbol{x}') = \langle \Phi_n(\boldsymbol{x}), \Phi_n(\boldsymbol{x}') \rangle$ *where*

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- This holds for **arbitrary** depth networks, proof via induction

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- We can get something similar to **Hölder-smoothness**:

$$||\Phi(\boldsymbol{x}) - \Phi(\boldsymbol{y})||_{\mathcal{H}} \leq \sqrt{||\boldsymbol{x} - \boldsymbol{y}||} + 2||\boldsymbol{x} - \boldsymbol{y}||$$

Why train all layers?

- Take any $f : \mathbb{S}^{p-1} \to \mathbb{R}$ even function such that $f(\boldsymbol{x}) \leq \eta$ and $|f(\boldsymbol{x}) - f(\boldsymbol{y})| \leq \eta ||\boldsymbol{x} - \boldsymbol{y}||_2 \; \forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^{d-1}$. Then there is $g \in \mathcal{H}$ with $||g||_{\mathcal{H}} \leq \delta$ such that

$$\sup_{\boldsymbol{x} \in \mathbb{S}^{p-1}} |f(\boldsymbol{x}) - g(\boldsymbol{x})| \leq C(p)\eta \left(\frac{\delta}{\eta}\right)^{-\frac{1}{0.5p-1}} \log\left(\frac{\delta}{\eta}\right)$$

- We can basically approximate any even Lipschitz function over $\mathbb{S}^{d-1}$ well.

- For training only top layer, we can weaker rate $\frac{\delta}{\eta}^{-\frac{1}{0.5p}}$

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- For $d = 1$, easy formulas for eigenvalues (as said before) with odd harmonics vanishing:

$$\lambda_0 = \frac{1}{\pi^2} \ , \ \lambda_1 = \frac{1}{4} \text{ and } \lambda_l = \frac{2(l^2+1)}{\pi^2 (k^2-1)^2} \text{ for l even}$$

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- Hence bound increases **linearly** with frequency

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