Kernel generalization error under isotropic distribution

Week 1

1 Setting

Let us consider a kernel $K(\vec{x}, \vec{y})$ where $\vec{x} \in \mathbb{R}^d$. We will only consider inner-product kernels (or dot-product kernels):

$$K(\vec{x}, \vec{y}) = h(\langle \vec{x}, \vec{y} \rangle)$$

where $h \in \mathcal{C}^\infty$. This way, we should be able to express h as a power series $h(t) = \sum_m^\infty h_m t^m$.

When studying the generalization error of a kernel machine, we are interested in identifying the spectrum of the operator T:

$$Tf(x) = \int d^d\vec{y}\, p(\vec{y}) K(\vec{x}, \vec{y}) f(\vec{y})$$

where $p(\vec{x})$ is the probability distribution of the data. In this first report, we are going to consider a gaussian isotropic case where $p = \mathcal{N}(0, \mathbb{I}_d)$

The operator T is linear, symmetric and compact (!), $T : L_2(p) \to L_2(p)$ and can be diagonalized:

$$\int d^d\vec{y}\, p(\vec{y}) K(\vec{x}, \vec{y}) f_\beta(\vec{y}) = \lambda_\beta f_\beta(\vec{x})$$

By Mercer's theorem, this is equivalent to:

$$K(\vec{x}, \vec{y}) = \sum_i \lambda_i \varphi_i(\vec{x}) \varphi_i(\vec{y})$$

where φ_β are an orthonormal basis of the $L_2(p)$ space. In this specific case, they can be represented through Hermite polynomials.

In general, one can show (?) the eigenvalues can be indexed through a multi-index $\beta = (\beta_1, \beta_2, \ldots, \beta_d)$ yielding:

$$K(\vec{x}, \vec{y}) = \sum_\beta \lambda_\beta He_\beta(\vec{x}) He_\beta(\vec{y})$$

where

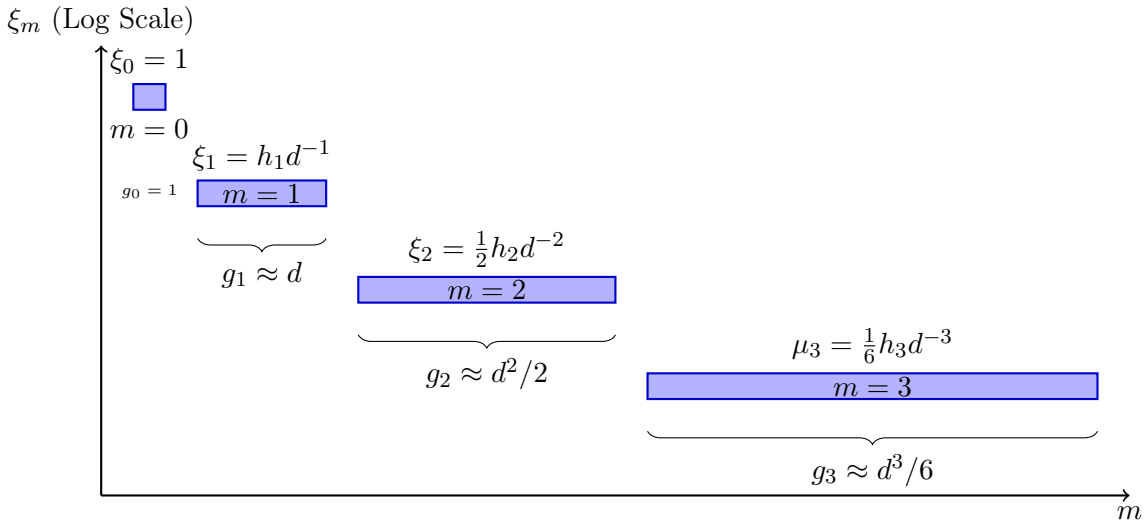
$$He_\beta(\vec{x}) = \prod_i He_{\beta_i}(x_i)$$

Using an argument of symmetry (the gaussian isotropic measure is invariant under rotation and the same goes for dot-product kernel), we should get a Mercer decomposition of the kind:

$$K(\vec{x}, \vec{y}) = h(\langle \vec{x}, \vec{y} \rangle) = \sum_m^\infty \xi_m \sum_{|\beta|=m} He_\beta(\vec{x}) He_\beta(\vec{y})$$

The full derivation for the derivation of ξ_m can be found in [Paper 2]:

$$\xi_m = h_m m! d^{-m}$$



the degeneracies of a level m is given by the possible ways of arranging $(\beta_1, \beta_2, \ldots, \beta_d)$ such that $|\beta| = \beta_1 + \beta_2 + \cdots + \beta_d = m$. It turns out this is equivalent to:

$$g_m = \binom{d+m-1}{m}$$

when $d \gg 1$, $g_m = \frac{1}{m!} d^m$

NUMERICAL PLOTS CON EMPIRICAL DIAGONALIZATION

2 Kernel error, $\lambda = 0$

From Paper1, we know that the kernel generalization error is given once we compute the quantity ν defined through the self-consistency equation:

$$n - \frac{\lambda}{\nu} = Tr(\Sigma(\Sigma + \mathbb{I}\nu)^{-1}) = df(\nu) \tag{1}$$

where Σ is the diagonal matrix of the eigenvalues of $k(\vec{x}, \vec{y})$. In this work, we will use the following scaling:

$$n = \alpha d^{\kappa}$$

that is, $n \sim O(d^{\kappa})$ where κ quantifies the sample complexity and α is a constant (of order 1). We will consider a case where $d, n \to \infty$ while α remains finite.

2.1 Computation for ν

Take Eq.1 and substitute $\lambda = 0$ and $n = \alpha d^{\kappa}$:

$$\alpha = d^{-\kappa} df(\nu) = d^{-\kappa} \sum_i^{\infty} \frac{\lambda_i}{\lambda_i + \nu} \tag{2}$$

We know that in the isotropic case the eigenvalues are distributed in degenerate shells, hence:

$$\alpha = d^{-\kappa} \sum_m^{\infty} g_m \frac{\xi_m}{\xi_m + \nu} = d^{-\kappa} \sum_m^{\infty} \frac{d^m}{m!} \frac{h_m m! d^{-m}}{h_m m! d^{-m} + \nu} \tag{3}$$

Let's define $h_m m! = \delta_m$. In all usual cases, $\delta_m \sim O(1)$ w.r.t m (for polynomials, it eventually becomes zero. For regular functions like the exponential, $d_m = 1, \forall m$). The trick here is to work

under the thermodynamic limit dividing the sum in three terms:

$$\begin{aligned}\alpha &= d^{-\kappa}\sum_{m}^{\infty}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\nu} = \\ &= d^{-\kappa}\left(\sum_{m=0}^{k-1}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\nu}+\frac{d^\kappa}{\kappa!}\frac{\delta_\kappa d^{-\kappa}}{\delta_\kappa d^{-\kappa}+\nu}+\sum_{m=k+1}^{\infty}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\nu}\right)\end{aligned} \tag{4}$$

To make things work, we have to make an ansatz. We will guess:

$$\nu = \xi d^{-\kappa}$$

PLOT NUMERICI PER CONFERMARE ANSATZ Let's consider the three terms separately:

- **First term**:

$$d^{-\kappa}\sum_{m=0}^{k-1}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\xi d^{-\kappa}} \tag{5}$$

  Fix a value for $0 \leq m \leq k-1$. Then the eigenvalue term:

$$\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\xi d^{-\kappa}} = \frac{1}{1+\frac{\xi}{\delta_m}d^{m-k}} \xrightarrow{d\gg 1, m<k} 1 \tag{6}$$

  Since ξ is independent of d by construction and δ_m is of order 1 with respect to m.

  The first term then becomes:

$$\sum_{m=0}^{\kappa-1}\frac{d^m}{m!} = \sum_{m=0}^{\kappa-1}\frac{d^{m-\kappa}}{m!} \xrightarrow{d\gg 1} 0 \tag{7}$$

- **Central term**: This is easy, as it evaluates to something of order 1:

$$d^{-\kappa}\frac{d^\kappa}{\kappa!}\frac{\delta_\kappa d^{-\kappa}}{\delta_\kappa d^{-\kappa}+\xi d^{-\kappa}} = \frac{1}{\kappa!}\frac{\delta_k}{\delta_k+\xi} \tag{8}$$

- **Third term**: Again, we write

$$d^{-\kappa}\sum_{m=k+1}^{\infty}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\xi d^{-\kappa}} \tag{9}$$

  Fix a value for $m > \kappa$. Then the eigenvalue term:

$$\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\xi d^{-\kappa}} = \frac{1}{1+\frac{\xi}{\delta_m}d^{m-k}} \approx \frac{\delta_m}{\xi}d^{\kappa-m} \text{ when } d \gg 1 \tag{10}$$

  This term alone converges to 0 but it needs to be considered inside the summation:

$$d^{-\kappa}\sum_{m=k+1}^{\infty}\frac{d^m}{m!}\frac{\delta_m d^{-m}}{\delta_m d^{-m}+\xi d^{-\kappa}} \approx d^{-\kappa}\sum_{m=k+1}^{\infty}\frac{d^m}{m!}\frac{\delta_m}{\xi}d^{\kappa-m} = \sum_{m=k+1}^{\infty}\frac{\delta_m}{\xi m!} \tag{11}$$

  We will define:

$$l(\kappa) = \sum_{m=k+1}^{\infty}\frac{\delta_m}{m!}$$

  and the third term can be rewritten as $\frac{l(\kappa)}{\xi}$[1]

[1] If δ_m is of order 1, then this function should always converge, approfondisci meglio

Putting all of this together, we get:

$$\alpha = \frac{1}{\kappa!}\frac{\delta_k}{\delta_k + \xi} + \frac{l(\kappa)}{\xi} \tag{12}$$

Let's solve for ξ:

$$\xi = \xi(\alpha, \kappa) = \frac{1}{2\alpha}\left[\left(\frac{1}{\kappa!}\delta_\kappa + l(\kappa) - \alpha\delta_\kappa\right) + \sqrt{\left(\frac{1}{\kappa!}\delta_\kappa + l(\kappa) - \alpha\delta_\kappa\right)^2 + 4\alpha l(\kappa)\delta_\kappa}\right] \tag{13}$$

which is independent of d, confirming our scaling ansatz. Finally, one has:

$$\nu = \xi(\alpha, \kappa)d^{-\kappa} \tag{14}$$

NUMERICAL FIGURE DISPLAYING THE PERFECT AGREEMENT WITH A NUMERICAL SOLVER

2.2 Extreme cases

When using an exponential kernel, one has $\delta_\kappa = 1, \forall\kappa$ (note that δ_κ is just the derivative of the h function evaluated at 0.)

What happens when we use a polynomial kernel of degree κ_0? This essentialy means $\delta_m = 0\ \forall m \geq \kappa_0$. There can be two cases:

- When $\kappa < \kappa_0$, then $\delta_\kappa \neq 0$ and $l(\kappa) \neq 0$, hence we can safely use Eq.14
- When $\kappa > \kappa_0$, then $\delta_\kappa = 0$ and $l(\kappa) = 0$. This implies $\nu = 0$. [?? BIAS NULLO MA VARIANZA MAL DEFINITA]

2.3 Computation for $Var(\alpha, \kappa)$

Again, from Paper 1 (but also Cheng, Montanari) we have:

$$V(\alpha, \beta, \lambda = 0) = V = \sigma_\epsilon^2\frac{Tr(\Sigma^2(\Sigma+\nu)^{-2})}{n - Tr(\Sigma^2(\Sigma+\nu)^{-2})} = \frac{\frac{1}{n}Tr(\Sigma^2(\Sigma+\nu)^{-2})}{1 - \frac{1}{n}Tr(\Sigma^2(\Sigma+\nu)^{-2})} = \frac{\tau}{1-\tau} \tag{15}$$

Let's compute τ, the procedure is similar to the one we have seen above.

$$\tau = \frac{1}{n}Tr(\Sigma^2(\Sigma+\nu)^{-2}) = \frac{1}{n}\sum_m g_m\frac{\xi_m^2}{(\xi_m+\nu)^2} \tag{16}$$

As usual, we divide the summation in three pieces and let $n = \alpha d^\kappa$.

$$\tau = \alpha^{-1}d^{-\kappa}\sum_{m=0}^{k-1} g_m\frac{\xi_m^2}{(\xi_m+\nu)^2} + \alpha^{-1}d^\kappa g_\kappa\frac{\xi_\kappa^2}{(\xi_\kappa+\nu)^2} + \alpha^{-1}d^\kappa\sum_{m=k+1}^{\infty} g_m\frac{\xi_m^2}{(\xi_m+\nu)^2} \tag{17}$$

- **First term**:

$$\begin{aligned}
\alpha^{-1}d^{-\kappa}\sum_{m=0}^{k-1} g_m\frac{\xi_m^2}{(\xi_m+\nu)^2} &= \alpha^{-1}d^{-\kappa}\sum_{m=0}^{k-1}\frac{1}{m!}d^m\frac{\delta_m^2 d^{-2m}}{\xi^2 d^{-2\kappa} + \delta_m^2 d^{-2m} + \delta_m\xi d^{-m-k}} = \\
&= \alpha^{-1}\sum_{m=0}^{k-1}\frac{1}{m!}\frac{\delta_m^2 d^{-\kappa-m}}{\xi^2 d^{-2\kappa} + \delta_m^2 d^{-2m} + \delta_m\xi d^{-m-k}} = \\
&= \alpha^{-1}\sum_{m=0}^{k-1}\frac{1}{m!}\frac{\delta_m^2}{\xi^2 d^{m-\kappa} + \delta_m^2 d^{-m+\kappa} + \delta_m\xi} \underset{d\gg 1}{\approx} \\
&\underset{d\gg 1}{\approx} \sum_{m=0}^{\kappa-1}\frac{1}{\alpha m!}d^{\kappa-m} \xrightarrow{d\gg 1} 0
\end{aligned} \tag{18}$$

Since, again, the terms δ_m, ξ are assumed to be $O(1)$ with respect to d.

- **Central term**

$$\alpha^{-1}d^{-\kappa}\frac{1}{\kappa!}d^{\kappa}\frac{\delta_\kappa^2}{(\delta_\kappa+\xi)^2}=\frac{1}{\alpha\kappa!}\frac{\delta_\kappa^2}{(\delta_\kappa+\xi)^2} \tag{19}$$

- **Third term**

$$\begin{aligned}\alpha^{-1}d^{-\kappa}\sum_{m=\kappa+1}^{\infty}g_m\frac{\xi_m^2}{(\xi_m+\nu)^2}=\alpha^{-1}\sum_{m=\kappa+1}^{\infty}\frac{1}{m!}\frac{\delta_m^2}{\xi^2d^{m-\kappa}+\delta_m^2d^{-m+\kappa}+\delta_m\xi}\overset{d\gg1}{\approx}\\ \overset{d\gg1}{\approx}\alpha^{-1}\sum_{m=\kappa+1}^{\infty}\frac{1}{m!}d^{\kappa-m}\xrightarrow{d\gg1}0\end{aligned} \tag{20}$$

So for the variance, the only term that counts is the one of order $m=\kappa$. Finally, we obtain:

$$\tau\approx\frac{1}{\alpha\kappa!}\frac{\delta_\kappa^2}{(\delta_\kappa+\xi(\alpha,\kappa))^2} \tag{21}$$

where $\xi(\alpha,\kappa)$ can be computed as in Eq.14. The full variance will then become:

$$Var(\alpha,\kappa,\lambda=0)=\sigma_\epsilon^2\frac{1-\tau}{\tau}=\sigma_\epsilon^2\frac{\delta_\kappa^2}{\alpha\kappa!(\delta_\kappa+\xi)^2-\delta_\kappa^2} \tag{22}$$

[TO DO: CONDITION SUCH THAT DENOMINATOR IS POSITIVE?]

[NUMERICAL PLOT OF VARIANCE SHAPE, TENDS TO ZERO AS ALPHA GROWS]

2.4 Computation for $B(\alpha,\kappa)$

The bias term is given by:

$$B(\alpha,\kappa)=\frac{\nu^2\langle\vec{\theta},(\Sigma+\nu)^{-2}\vec{\theta}\rangle}{1-\tau} \tag{23}$$

where $\vec{\theta}$ is the orthonormal decomposition of the target function $f_\star(\vec{x})\in L_2(\mathcal{N}(0,\mathcal{I}_\lceil))$. In particular, given the generalized d-dimensional Hermite polynomials, we can write:

$$f_\star(\vec{x})=\sum_{\beta\in\mathbb{N}^d}\theta_\beta He_\beta(\vec{x})=\sum_{\beta\in\mathbb{N}^d}\theta_\beta\prod_{i=1}^{d}He_{\beta_i}(x_i) \tag{24}$$

In general, the eigendecomposition of $f_\star$ cannot be organized in degenerate levels since we are only assuming $f_\star$ is square-integrable:

$$||f_\star||_{L_2}^2=\sum_{\beta\in\mathbb{N}^d}\theta_\beta^2=1$$

but $f_\star$ may easily be not rotationally invariant (as was the case for the kernel $k(x,x')$).

Now let's compute the numeratore of Eq.23:

$$\nu^2\langle\vec{\theta},(\Sigma+\nu)^{-2}\vec{\theta}\rangle=\sum_{\beta\in\mathbb{N}^d}\theta_\beta^2\frac{\nu^2}{(\lambda_\beta+\nu)^2}=\sum_{m=0}^{\infty}\frac{\nu^2}{(\xi_m+\nu)^2}\sum_{|\beta|=m}\theta_\beta^2 \tag{25}$$

Let's define:

$$\Theta(m)=\sum_{|\beta|=m}\theta_\beta^2$$

So that finally:

$$\nu^2\langle\vec{\theta},(\Sigma+\nu)^{-2}\vec{\theta}\rangle=\sum_{m=0}^{\infty}\Theta(m)\frac{\xi^2 d^{-2k}}{(\delta_m d^{-m}+\xi d^{-k})^2}=\sum_{m=0}^{\infty}\Theta(m)\frac{\xi^2 d^{-2k}}{\delta_m^2 d^{-2m}+\xi^2 d^{-2\kappa}+2\delta_m\xi d^{-m-\kappa}}=$$
$$=\sum_{m=0}^{\infty}\Theta(m)\frac{\xi^2}{\delta_m^2 d^{2(-m+\kappa)}+\xi^2+2\delta_m\xi d^{-m+\kappa}}$$

To solve asymptotically this equation, we will perform the usual trick.

- When $0\leq m\leq\kappa$, then the terms $d^{-m+\kappa}$ and $d^{2(-m+\kappa)}$ will both diverge to infinity. Consequently, the whole fraction will converge to 0 as $d\to\infty$. The prefactor $\Theta(m)$ is independent of d^2, so the whole term goes to 0 when $m<\kappa$
- When $m=\kappa$, we obtain:
$$\Theta(\kappa)\frac{\xi^2}{(\xi+\delta_\kappa)^2} \tag{26}$$
- When $m>\kappa$, then the terms $d^{-m+\kappa}$ and $d^{2(-m+\kappa)}$ will both converge to 0. We are left with:
$$\sum_{m>k}\Theta(m)\frac{\xi^2}{\delta_m^2 d^{2(-m+\kappa)}+\xi^2+2\delta_m\xi d^{-m+\kappa}}\approx\sum_{m>k}\Theta(m) \tag{27}$$
This summation here is convergent, since $||f||=\sum_m\Theta(m)<\infty$

Finally, we have:

$$\nu^2\langle\vec{\theta},(\Sigma+\nu)^{-2}\vec{\theta}\rangle=\frac{\xi^2}{(\xi+\delta_\kappa)^2}\Theta(\kappa)+\sum_{m>k}\Theta(m) \tag{28}$$

This is a nice formula! Combining all together, I get:

$$B(\alpha,\kappa,\vec{\theta})=\frac{\frac{\xi^2}{(\xi+\delta_\kappa)^2}\Theta(\kappa)+\sum_{m>k}\Theta(m)}{1-\tau}=\frac{\frac{\xi^2}{(\xi+\delta_\kappa)^2}\Theta(\kappa)+\sum_{m>k}\Theta(m)}{1-\frac{1}{\alpha\kappa!}\frac{\delta_\kappa^2}{(\delta_\kappa+\xi)^2}} \tag{29}$$

When $\alpha\to\infty$ (a lot of data, but still scaling with d^κ), then:

$$Var(\alpha,\kappa)\to 0$$

$$B(\alpha,\kappa,\vec{\theta})\approx\sum_{m>k}\Theta(m)$$

The last quantity is extremely interesting. It represents the projection of the target function $f_\star$ on the space spanned by Hermite polynomials whose degree is higher than the sample complexity κ. This is the irreducible bias, the error we cannot avoid since we do not have enough data.

ASYMPTOTIC BEHAVIOR OF ξ,τ as $\alpha\to\infty$. (both goes to 0).

[2] Is it really? Or just O(1)?