# Gaussian kernel on 1D Gaussian data eigendecomposition

## 1 Problem statement and solution

Given $w, \sigma > 0$, solve for $\lambda_n, \phi_n$, such that

$$K(x,y) := e^{-\frac{(x-y)^2}{2w^2}} = \sum_n \lambda_n \phi_n(x)\phi_n(y), \quad \mathbb{E}_{X\sim N(0,\sigma^2)}[\phi_n(X)\phi_k(X)] = \delta_{nk}$$

Define $v := w/\sigma$ as a helper variable.

Begin with **Mehler's formula**. For any $r \in (-1, +1)$,

$$\sum_{n=0}^{\infty} r^n h_n(x)h_n(y) = \frac{1}{\sqrt{1-r^2}} \exp\left[-\frac{r^2(x^2+y^2) - 2rxy}{2(1-r^2)}\right] \tag{1}$$

where $h_n(x) = \mathrm{He}(x)/\sqrt{n!}$ is the normalized probabilist's Hermite polynomial.

Equivalently, for any $\beta > 0$,

$$\sum_{n=0}^{\infty} \sqrt{1-r^2}\, r^n \left[e^{-\frac{r}{2(1+r)\beta^2}x^2} h_n(x/\beta) e^{-\frac{r}{2(1+r)\beta^2}y^2} h_n(y/\beta)\right] = \exp\left[-\frac{(x-y)^2}{2\beta^2(1-r^2)/r}\right] \tag{2}$$

Define the ansatz:

$$\phi_n(x) = c e^{-\frac{x^2}{2\alpha^2}} h_n\left(\frac{x}{\beta}\right) \tag{3}$$

where $c, \alpha^2, \beta > 0$ are parameters to be determined.

**First relation: kernel**

$$\sum_n \lambda_n \phi_n(x)\phi_n(y) = \sum_n c^2 \lambda_n e^{-\frac{x^2}{2\alpha^2}} h_n\left(\frac{x}{\beta}\right) e^{-\frac{y^2}{2\alpha^2}} h_n\left(\frac{y}{\beta}\right) \tag{4}$$

We want this to equal $e^{-\frac{(x-y)^2}{2w^2}}$. This is a direct application of the slightly generalized form of Mehler's formula, as long as we have the following relationships:

$$\begin{cases} c^2\lambda_n &= \sqrt{1-r^2}\, r^n \\ \frac{(1+r)\beta^2}{r} &= \alpha^2 \\ w^2 &= \beta^2(1-r^2)/r \end{cases} \tag{5}$$

**Second relation: orthonormality**

$$\mathbb{E}_{X\sim N(0,\sigma^2)}[\phi_n(x)\phi_k(x)] = \int \frac{e^{-\frac{x^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}} \cdot c e^{-\frac{x^2}{2\alpha^2}} h_n\left(\frac{x}{\beta}\right) c e^{-\frac{x^2}{2\alpha^2}} h_k\left(\frac{x}{\beta}\right) dx \tag{6}$$

By routine manipulation, it is equal to

$$\frac{c^2}{\sqrt{2\pi}} \frac{1}{\sqrt{1+\frac{2\sigma^2}{\alpha^2}}} \int e^{-\frac{1}{2}x^2} h_n\left(\frac{\sigma}{\beta\sqrt{1+\frac{2\sigma^2}{\alpha^2}}} x\right) h_k\left(\frac{\sigma}{\beta\sqrt{1+\frac{2\sigma^2}{\alpha^2}}} x\right) dx \tag{7}$$

Since $\frac{1}{\sqrt{2\pi}}\int e^{-\frac{1}{2}x^2}h_n(x)h_k(x)dx = \delta_{nk}$, orthonormality holds if we have

$$\begin{cases} \sigma &= \beta\sqrt{1+\frac{2\sigma^2}{\alpha^2}} \\ c &= \left(1+\frac{2\sigma^2}{\alpha^2}\right)^{1/4} \end{cases} \tag{8}$$

Now we have 5 equations in 5 unknowns, which is enough. It remains to solve them, which is completely routine.

$$\begin{cases} c^2\lambda_n &= \sqrt{1-r^2}r^n \\ \frac{(1+r)\beta^2}{r} &= \alpha^2 \\ w^2 &= \beta^2(1-r^2)/r \\ \sigma &= \beta\sqrt{1+\frac{2\sigma^2}{\alpha^2}} \\ c &= \left(1+\frac{2\sigma^2}{\alpha^2}\right)^{1/4} \end{cases} \tag{9}$$

Applying the equations, we have

$$\alpha^2 = \frac{w^2}{1-r}, \beta^2 = \frac{w^2 r}{1-r^2}, \sigma^2 = \frac{w^2 r}{1-r^2} + \frac{2r}{1+r}\sigma^2 \tag{10}$$

The last equation then gives a quadratic equation for $r$

$$\frac{(1-r)^2}{r} = \frac{w^2}{\sigma^2} = v^2 \tag{11}$$

with 2 solutions

$$r = \frac{1}{2}\left[v^2+2\pm\left(\sqrt{v^2+4}\right)v\right] \tag{12}$$

Since we need $1-r^2>0$, we pick the negative root. Now plug $r$ into the other equations, we have the complete solution.

$$\begin{cases} r &= \frac{1}{2}\left(v^2+2-v\sqrt{v^2+4}\right) \\ \alpha^2 &= \frac{w^2}{1-r} = \frac{v+\sqrt{v^2+4}}{2v}w^2 \\ \beta &= w\sqrt{\frac{r}{1-r^2}} = w\sqrt{\frac{1}{v\sqrt{v^2+4}}} \\ c &= \left(\frac{\sqrt{v^2+4}}{v}\right)^{\frac{1}{4}} \\ \lambda_n &= \frac{\sqrt{1-r^2}}{c^2}r^n \end{cases} \tag{13}$$

It's easy to check that $c^4 = \frac{1+r}{1-r}$, which implies $\sum_{n=0}^{\infty}\lambda_n = 1$, so we can write the solution in a notationally cleaner form involving just $w$ and $r$:

$$\begin{cases} \alpha/w &= \sqrt{\frac{1}{1-r}} \\ \beta/w &= \sqrt{\frac{r}{1-r^2}} \\ c &= \left(\frac{1+r}{1-r}\right)^{\frac{1}{4}} \\ \lambda_n &= \frac{r^n}{1-r} \end{cases} \tag{14}$$

Let $\phi_{n,w,\sigma}$ and $\lambda_{i,w,\sigma}$ be defined as above, then our result states that

$$\sum_n \lambda_{n,w,\sigma}\phi_{n,w,\sigma}(x)\phi_{n,w,\sigma}(y) = e^{-\frac{(x-y)^2}{2w^2}}, \quad \mathbb{E}_{X\sim N(0,\sigma^2)}[\phi_{n,w,\sigma}(X)\phi_{k,w,\sigma}(X)] = \delta_{nk}$$

Let $x\sim\mu=\mathcal{N}(0,\boldsymbol{\Lambda})$ and $K(x,x') = e^{-\frac{1}{2}(x-x')^\top \boldsymbol{M}(x-x')}$ where $\boldsymbol{\Lambda}, \boldsymbol{M}$ are positive definite matrices. We would again like to find an orthonormal eigendecomposition of the kernel

$$K(x,x') = \sum_n \lambda_n\phi_n(x)\phi_n(x') \tag{15}$$

such that $\langle \phi_n, \phi_{n'} \rangle = \delta_{nn'}$.

To solve this, do a linear transform to whiten the gaussian $\mathcal{N}(0, \boldsymbol{\Lambda})$ and diagonalize the kernel $\boldsymbol{M}$, then apply the previous case.

Whiten the random variable under the measure $x \sim \mathcal{N}(0, \boldsymbol{\Lambda})$. Define

$$z = \boldsymbol{\Lambda}^{-\frac{1}{2}} x \quad \Longrightarrow \quad z \sim \mathcal{N}(0, I).$$

Diagonalize $\boldsymbol{M}$ in those whitened coordinates. First set

$$\boldsymbol{N} = \boldsymbol{\Lambda}^{\frac{1}{2}} \boldsymbol{M} \boldsymbol{\Lambda}^{\frac{1}{2}},$$

which is again positive definite. Diagonalize $\boldsymbol{N}$ as $\boldsymbol{\Omega}$

$$\boldsymbol{N} = \boldsymbol{U} \boldsymbol{\Omega} \boldsymbol{U}^\top,$$

where $\boldsymbol{\Omega}$ is diagonal with entries $1/w_1^2, \ldots, 1/w_d^2$. Then define

$$u = \boldsymbol{U}^\top z, \quad u \sim \mathcal{N}(0, I).$$

Under these transformations, the kernel becomes

$$K(x, x') = e^{-\frac{1}{2}(x-x')^\top \boldsymbol{M}(x-x')} = e^{-\frac{1}{2}(z-z')^\top \boldsymbol{N}(z-z')} = e^{-\frac{1}{2}(u-u')^\top \boldsymbol{\Omega}(u-u')}.$$

Because $\boldsymbol{\Omega}$ is diagonal, we can write

$$e^{-\frac{1}{2}(u-u')^\top \boldsymbol{\Omega}(u-u')} = \prod_{j=1}^{d} e^{-\frac{1}{2w_i^2}(u_j - u_j')^2}.$$

Take the tensor product of the 1D case. The solution:

$$\begin{cases} \phi_{n,\boldsymbol{M},\boldsymbol{\Lambda}}(x) & = \prod_j \phi_{n,w_j,1}(u_j) \\ \lambda_{n,\boldsymbol{M},\boldsymbol{\Lambda}} & = \prod_j \lambda_{n,w_j,1} \\ \boldsymbol{\Lambda}^{\frac{1}{2}} \boldsymbol{M} \boldsymbol{\Lambda}^{\frac{1}{2}} & = \boldsymbol{U} \operatorname{diag}(1/w_1^2, \ldots, 1/w_d^2) \boldsymbol{U}^\top \\ u & = \boldsymbol{U}^\top \boldsymbol{\Lambda}^{-\frac{1}{2}} x \end{cases} \tag{16}$$