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Radial Kernels via Scale Derivatives and Wavelets

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- New radial kernels
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Radial kernels are suited for sparse multivariate interpolation problems

$$\mathcal{K}(x,y) = \Phi(x-y) = \phi(\|x-y\|_2) =: f(\|x-y\|_2^2/2) \quad x,y \in \mathbb{R}^d$$

with a scalar function $\phi:[0,+\infty)\to\mathbb{R}$.

Properties:

- Radial symmetry,
- Dimension free,
- Invariant under affine transformations.

Examples of well-known kernels in literature:

- Gaussian,
- Multiquadrics,
- Whittle-Matérn functions,
- Wendland functions,
- Polyharmonics,
- ...



The *d*-variate Fourier transform $\hat{\Phi}$ is radial again and coincides with the Hankel transform using the *f*-form of the kernel

$$\hat{\Phi}(\omega) = \hat{f}\left(\frac{\|\omega\|_2^2}{2}\right),$$

with

$$\hat{f}(t) := \int_0^\infty f(s) s^{\nu} h_{\nu}(st) ds, \quad f(s) = \int_0^\infty \hat{f}(t) t^{\nu} h_{\nu}(ts) dt,$$

and $h_{\nu}(z^2/4):=(z/2)^{-\nu}J_{\nu}(z)$, J_{ν} Bessel function of the first kind and $\nu=(d-2)/2$.

Theorem

Let Φ be a continuous function in $L^1(\mathbb{R}^d)$. Φ is strictly positive definite if and only if Φ is bounded and its Fourier transform is non-negative and not identically equal to zero.



The main ideas in [Bozzini, Rossini, Schaback, V. '15] are:

• to introduce a scaling $z \in \mathbb{R}^+$ in the transform

$$\widehat{f(\cdot z)}(u) = z^{-\nu-1}\widehat{f(\cdot)}(u/z)$$

ullet to consider a functional λ^z that act linearly respect to z and commute with integrals

$$(\lambda^z f(\cdot z))^{\wedge}(u) = \lambda^z (z^{-\nu-1} \hat{f}(u/z))$$

As a linear functional λ we take the k-th derivative respect to z

$$\lambda^z f(z) = \frac{\mathrm{d}^k}{\mathrm{d}z^k} f(z),$$

so the previous relation becomes

$$\left(\frac{d^k}{dz^k}f(\cdot z)\right)^{\wedge}(u) = \left(f^{(k)}(\cdot z)(\cdot)^k\right)^{\wedge}(u) = \frac{d^k}{dz^k}\left(z^{-\nu-1}\widehat{f(\cdot)}(u/z)\right)$$



We specialise to the first derivative k = 1

$$(tf'(tz))^{\wedge}(u) = \frac{d}{dz}(z^{-\nu-1}\widehat{f(\cdot)}(u/z))$$

Moreover if we consider z = 1 we have

$$(t f'(t))^{\wedge}(u) = \frac{d}{dz} \int_{\mathbb{R}^{n}} \left(z^{-\nu - 1} \widehat{f(\cdot)}(u/z) \right)$$

In the following we define the new kernels ψ as the right term and its Fourier transform $\hat{\psi}$ the function in the left term.

With this choice and using the previous cited Theorem we will see that new kernels are positive definite.



We consider classes of kernels Φ that are closed under taking derivatives in f-form

$$f_p'(s) = c(p)f_{D(p)}(s)$$

where $s = ||x - y||^2/2$ and the parameter p in the definition of the kernel Φ goes to a new parameter D(p), moreover there is a factor c(p).

Theorem

The transition $\Phi\to -\Delta\Phi$ on radial kernels generates a radial kernel consisting of a weighted sum

$$-\Delta^{x}\Phi(x-y) = -\|x-y\|^{2}f''\left(\frac{\|x-y\|^{2}}{2}\right) - df'\left(\frac{\|x-y\|^{2}}{2}\right)$$

of two radial kernels, if f is the f-form of Φ , and if the action of $-\Delta$ is valid on the kernel. If, furthermore, the class of kernels is invariant under taking derivatives of f-forms, then the resulting kernel is a weighted linear combination of two radial kernels of the same family.



Theorem

For all classes of radial kernels that are closed under taking derivatives in f-form, the procedure with derivatives generates kernels that are images of the negative Laplacian applied to Fourier transforms of kernels of the same class.

Proof.

Using that the radial kernels is closed under taking derivatives and

$$t f(t) = \frac{\|x\|_2^2}{2} \Phi(\|x\|_2) = \frac{1}{2} (-\Delta \hat{\Phi})^{\vee} (\|x\|_2),$$

we have

$$\left(t\,f_p'(t)\right)^{\wedge}\left(\|\omega\|_2^2/2\right) = c(p)\left(t\,f_{D(p)}(t)\right)^{\wedge}\left(\|\omega\|_2^2/2\right) = -\frac{c(p)}{2}\Delta\hat{\Phi}_{D(p)}(\|\omega\|_2).$$





We have

$$c(p) (t f_{D(p)}(t))^{\wedge} (\|\omega\|_{2}^{2}/2) = -\frac{c(p)}{2} \Delta \hat{\Phi}_{D(p)}(\|\omega\|_{2})$$

$$= -\frac{c(p)}{2} (\|\omega\|^{2} \hat{f}''_{D(p)} (\frac{\|\omega\|^{2}}{2}) + d \hat{f}'_{D(p)} (\frac{\|\omega\|^{2}}{2}))$$

We define the new kernel and its Fourier transform

$$\psi(x) = -\frac{\|x\|^2}{2} \hat{f}''_{D(p)} \left(\frac{\|x\|^2}{2}\right) - \frac{d}{2} \hat{f}'_{D(p)} \left(\frac{\|x\|^2}{2}\right)$$
$$\hat{\psi}(\omega) = \frac{\|\omega\|^2}{2} f_{D(p)} \left(\frac{\|\omega\|^2}{2}\right)$$

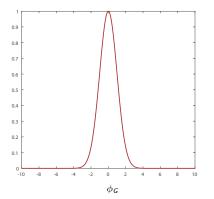
The Fourier transform $\hat{\psi}$ is non negative and not identically zero because $f_{D(p)}$ is positive definite, then the function ψ is positive definite.





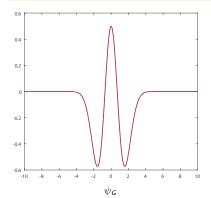
$$\phi_G(x) = \exp(-\|x\|^2/2)$$

$$\hat{\phi}_G(\omega) = \exp(-\|\omega\|^2/2)$$



$$\psi_G(x) = (d/2 - ||x||^2) \exp(-||x||^2/2)$$

$$\hat{\psi}_G(\omega) = \frac{||\omega||^2}{2} \exp(-||\omega||^2/2)$$



It's not new because, for d = 2, it is the Mexican hat.

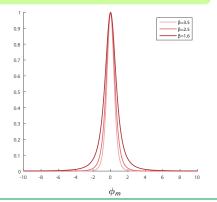


New inverse multiquadrics kernels

For $\beta > d/2 + 1$

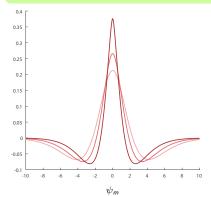
$$\phi_m(x) = (1 + \|x\|^2)^{-\beta}$$

$$\hat{\phi}_m(\omega) = \frac{2^{1-\beta}}{\Gamma(\beta)} \|\omega\|^{\beta-d/2} K_{\beta-d/2}(\|\omega\|)$$



$$\psi_{m}(x) = \frac{2^{-\beta}}{\Gamma(\beta)} \left[d\|x\|^{\beta - \frac{d}{2}} K_{\beta - \frac{d}{2}}(\|x\|) - \|x\|^{\beta - \frac{d}{2} + 1} K_{\beta - \frac{d}{2} - 1}(\|x\|) \right]$$

$$\widehat{\psi}_{m}(\omega) = \beta \|\omega\|^{2} (1 + \|\omega\|^{2})^{-\beta - 1}$$



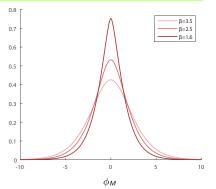


New Whittle-Matérn kernels

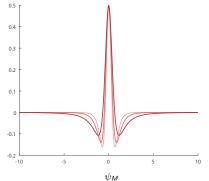
For
$$\beta > d/2 + 1$$

$$\phi_{M}(x) = \frac{2^{1-\beta}}{\Gamma(\beta)} \|x\|^{\beta-d/2} K_{\beta-d/2}(\|x\|)$$

$$\hat{\phi}_{M}(\omega) = (1 + \|\omega\|^{2})^{-\beta}$$



$$\psi_{M}(x) = \frac{d}{2}(1 + ||x||^{2})^{-\beta}$$
$$-\beta ||x||^{2} (1 + ||x||^{2})^{-\beta - 1}$$
$$\hat{\psi}_{M}(\omega) = \frac{2^{-\beta}}{\Gamma(\beta)} ||\omega||^{\beta - \frac{d}{2} + 1} K_{\beta - \frac{d}{2} - 1}(||\omega||)$$





We analyse the properties of the new kernels. They have a good decay

$$\begin{split} \left| \hat{\psi}(\omega) \right| &= O(\|\omega\|^{\alpha}) \quad \|\omega\| \to 0, \text{ for } \alpha \ge 2 \\ \left| \hat{\psi}(\omega) \right| &= O(\|\omega\|^{-\gamma}) \quad \|\omega\| \to +\infty, \text{ for } \gamma > d+2 \end{split}$$

From the construction with derivatives we have

$$\hat{\psi}(\omega) = \|\omega\|^2 \phi(\omega).$$

 $\phi(\omega)$ is bounded, since it is positive definite, so

$$\hat{\psi}(0) = 0 = \int_{\mathbb{R}^d} \psi(x) \, \mathrm{d}x.$$

The new kernels $\psi \in N_K := \{\psi_G, \psi_m, \psi_M\}$ are wavelets.





All $\psi \in N_{\mathcal{K}}$ are such that $\psi \in L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^d)$.

Moreover they satisfy

Admissibility condition

$$\int_0^{+\infty} \frac{\left|\hat{\psi}(a\omega)\right|^2}{a} \, \mathrm{d}a = C_{\psi}, \quad \forall \omega \neq 0 \text{ and } 0 < C_{\psi} < +\infty$$

We compute the constant for each $\psi \in N_K$

$$C_{\psi_G} = rac{1}{8}$$
 $C_{\psi_m} = rac{eta}{8eta + 4}$ $C_{\psi_M} = rac{4^{-1-eta}\sqrt{\pi}\Gamma(2eta - d)\Gamma(1 + eta - d/2)}{\Gamma^2(eta)\Gamma(3/2 + eta - d/2)}$

The admissibility condition allows us to recover a function $f \in L^2(\mathbb{R}^d)$ by the set of its wavelets coefficients.





Let

$$\psi_{a,b}(x) = a^{-d}\psi\left(\frac{x-b}{a}\right), \ a \in \mathbb{R}^+, \ b \in \mathbb{R}^d$$

The wavelet coefficients of f are the inner product

$$c(a,b) = (f,\psi_{a,b})_{L^2(\mathbb{R}^d)} = (f,a^{-d}\psi((\cdot-b)/a))_{L^2(\mathbb{R}^d)}$$

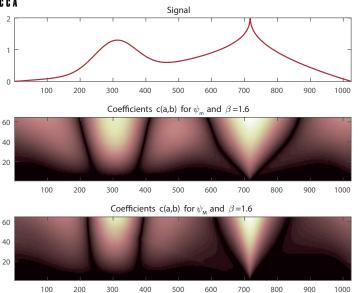
and they give all the important information about the signal.

Due to the admissibility condition we can reconstruct a function f with the wavelet continuous transform

$$f(x) = \frac{1}{C_{\psi}} \int_{0}^{+\infty} \int_{\mathbb{R}^{d}} c(a, b) \psi_{a, b}(x) db \frac{da}{a}$$



Numerical examples





It is interesting to consider discrete case with shift $k \in \mathbb{Z}^d$ and refinement matrix M, usually M = 2I.

Remark ([Ron, Shen '97])

The function ψ whose Fourier transform is positive a.e. cannot generate tight frames of the form $\psi(2^j \cdot -k)$.

For our $\psi \in N_{\mathcal{K}}$ we can not consider the classical construction of tight frames in the stationary case, we refer to a non-stationary setting.

Let M = 2I we can define

$$\hat{\psi}_j(\omega) = rac{\hat{\psi}(\omega)}{\sqrt{\sigma_j(\omega)}}, \quad ext{where} \quad \sigma_j(\omega) := \sum_{k \in \mathbb{Z}^d} \left|\hat{\psi}(\omega + 2^{j+1}\pi k)
ight|^2$$

is a $2^{j+1}\pi$ periodic function.





With M = 2I we have to consider $2^d - 1$ cosets and the set

$$\{\psi_j^{(\ell)}(\cdot-2^{-j}k), j\in\mathbb{Z}, k\in\mathbb{Z}^d, \ell=1,\ldots,2^d-1\}.$$

We call

$$W_i := \overline{\operatorname{\mathsf{span}}\{\psi_i^{(\ell)}(\cdot - 2^{-j}k), \ k \in \mathbb{Z}^d, \ \ell = 1, \dots, 2^d - 1\}}$$

we want that $\bigcup_i W_i$ is dense in $L^2(\mathbb{R}^d)$ so $\psi_i^{(\ell)}$ are generators of $L^2(\mathbb{R}^d)$.

For this set of functions we have to show that they satisfy

Frequency localization property

Given a compact set $K \subset \mathbb{R}^d \setminus \{0\}$ and $\varepsilon > 0$, there exists $N \in \mathbb{N}$ s.t.

$$\sum_{j>N} \sup_{\omega \in K} |\hat{\psi}_j^{(\ell)}(\omega)|^2 < \varepsilon \quad \text{and} \quad \sum_{j<-N} \sup_{\omega \in K} |\hat{\psi}_j^{(\ell)}(\omega)|^2 < \varepsilon,$$

for all $\ell = 1, ..., 2^d - 1$.



In particular we want to construct an orthonormal basis. In this sense, let $\mathcal{E}:=M[0,1)^d\cap\mathbb{Z}^d$ and $\mathcal{E}_0:=\mathcal{E}\setminus\{0\}$ we observe

$$\sigma_j(\omega) = \sigma_{j+1}(\omega) + \sum_{\ell=1}^{2^d-1} \sigma_{j+1}(\omega + 2^{j+1}\pi heta_\ell), \quad heta_\ell \in \mathcal{E}_0.$$

In order to have orthogonality

• respect to $\ell = 1, \ldots, 2^d - 1$ with j fixed

$$\sum_{\gamma \in \mathcal{E}} \frac{e^{-i < \pi \gamma, \eta(\ell) - \eta(m) >}}{\sigma_j(\omega)} \sqrt{\sigma_{j+1}(\omega + 2^{j+1}\pi(\theta_\ell + \gamma))\sigma_{j+1}(\omega + 2^{j+1}\pi(\theta_m + \gamma))} = \delta_{\ell,m},$$

• between W_{i-1} and W_i

$$\sum_{\gamma \in \mathcal{E}} e^{i < \pi \gamma, \eta(\ell) >} \sqrt{\sigma_{j+1}(\omega + 2^{j+1}\pi(\theta_{\ell} + \gamma))\sigma_{j+1}(\omega + 2^{j+1}\pi\gamma)} = 0.$$

should be satisfied for $\eta:\{1,\ldots,2^d-1\}\to\mathcal{E}_0$, an opportune permutation of the representative of cosets in \mathcal{E}_0 .



In two dimensions we consider the functions

$$\hat{\psi}_{j}^{(\ell)}(\omega) = 2^{-j-1} e^{-i < 2^{-j-1}\omega, \eta(\ell) > \sqrt{\frac{\sigma_{j+1}(\omega + 2^{j+1}\pi\theta_{\ell})}{\sigma_{j}(\omega)}} \frac{\hat{\psi}(\omega)}{\sigma_{j+1}(\omega)}$$

where

$$egin{aligned} 1 &\mapsto heta_1 = (1,0)^t \ \eta: \ 2 &\mapsto heta_3 = (1,1)^t \ 3 &\mapsto heta_2 = (0,1)^t \end{aligned}$$

We proved that

$$\{\psi_i^{(\ell)}(\cdot - 2^{-j}k), k \in \mathbb{Z}^2, j \in \mathbb{Z}, \ell = 1, 2, 3\}$$

are an orthonormal basis for $\bigoplus_{i \in \mathbb{Z}} W_j$.



Thank you for the attention



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