Positive Definite Functions on the Unit Sphere

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Positive definite functions

Let $\mathbb{S}^{d-1}$ be the unit sphere of $\mathbb{R}^d$. Let $d(x, y)$ be the geodesic distance of $\mathbb{S}^{d-1}$,

$$d(x, y) := \arccos(\langle x, y \rangle), \qquad x, y \in \mathbb{S}^{d-1}.$$

Definition

A continuous function $g : [0, \pi] \to \mathbb{R}$ is positive definite on $\mathbb{S}^{d-1}$, written $g \in \mathrm{PD}_{d-1}$, if for all distinct point sets $\mathcal{X} = \{x_1, \ldots, x_n\}$ on $\mathbb{S}^{d-1}$ and all $n \in \mathbb{N}$, the matrices $M_{\mathcal{X}} := \left[g(d(x_i, x_j))\right]_{i,j=1}^{n}$ are positive semi-definite, that is, $c^T M_{\mathcal{X}} c \geq 0$ for all $c \in \mathbb{R}^n$.

The function g is strictly positive definite on $\mathbb{S}^{d-1}$, written $g \in \mathrm{SPD}_{d-1}$, if the matrices are all positive definite, that is, $c^T M_{\mathcal{X}} c > 0$, for all nonzero $c \in \mathbb{R}^n$.

Scatted data Interpolation

I. J. Schoenberg characterized PD functions in 1942. The study of SPD functions is motivated by Scatted data Interpolation.

Given $\mathcal{X} = \{x_1, \ldots, x_n\}$ on $\mathbb{S}^{d-1}$ and data (x_i, y_i). If $g \in \mathrm{SPD}_{d-1}$, then we can choose λ_j such that

$$s(x) = \sum_{j=1}^{n} \lambda_j g(d(x, x_j))$$

solves the interpolation problem, that is,

$$s(x_i) = \sum_{j=1}^{n} \lambda_j g(d(x_i, x_j)) = y_i \qquad 1 \leq i \leq n.$$

Indeed, the linear system of equation has a unique solution if and only if the matrix $M_{\mathcal{X}} = \left[g(d(x_i, x_j))\right]_{i,j=1}^{n}$ is nonsingular.

Zonal functions and its Fourier series

A function f is called a zonal function if $f(x) = g(\langle x, y\rangle)$ for a fixed $y \in \mathbb{S}^{d-1}$ and $g : [-1, 1] \mapsto \mathbb{R}$. The reproducing kernel of spherical harmonics of degree n on $\mathbb{S}^{d-1}$ is zonal:

$$Z_{n,d}(t) := \frac{n+\lambda}{\lambda} C_n^\lambda(t), \qquad \lambda = \frac{d-2}{2},$$

where C_n^λ is the Gegenbauer (ultraspherical) polynomial of degree n, orthogonal with respect to

$$\langle f, g\rangle_\lambda := \int_{-1}^{1} f(t)g(t)w_\lambda(t)dt, \quad w_\lambda(t) = (1-t^2)^{\lambda-1/2}.$$

If f is zonal, $f(x) = g(\langle x, y\rangle)$, we can rotate y to $(1, 0, \ldots, 0)$, so that $f(x) = g(x_1)$. The Fourier series (in spherical harmonics) of f becomes Fourier-Gegenbauer series of g.

Fourier-Gegenbauer series and PDF

For $g \in L^2(w_\lambda, [-1,1])$, its Fourier-Gegenbauer series is defined by

$$g = \sum_{n=0}^{\infty} \widehat{g}_n^\lambda \frac{C_n^\lambda}{\|C_n^\lambda\|_\lambda^2}, \qquad \widehat{g}_n^\lambda = \int_{-1}^{1} g(t) C_n^\lambda(t) w_\lambda(t) dt$$

For PD functions on $\mathbb{S}^{d-1}$, $g(d(x,y)) = g(\arccos\langle x,y\rangle)$ is zonal. For $g : [0,\pi] \mapsto \mathbb{R}$ in $\mathrm{PD_{d-1}}$, we expand $g(\theta) = f(\cos\theta)$ as a series and we always require $\sum_{n=0}^{\infty} \widehat{g}_n^\lambda C_n^\lambda(1)/\|C_n^\lambda\|^2 < \infty$.

Changing variables, we define

$$\widehat{f}_n^\lambda := \int_0^\pi f(\cos\theta) C_n^\lambda(\cos\theta)(\sin\theta)^{2\lambda} d\theta.$$

Characterization of PD and PSD functions

Theorem (Schoenberg 1942)

Let f be a continuous function on $[-1,1]$ and $g(\theta) := f(\cos\theta)$. Then $g \in \mathrm{PD}_{d-1}$ on the sphere if and only if all coefficients in

$$f(\cos\theta) = \sum_{k=0}^{\infty} a_k C_k^{(d-2)/2}(\cos\theta), \qquad \theta \in [0,\pi],$$

are nonnegative, that is, $a_k \geq 0$ for $k \in \mathbb{N}_0$.

- If all $a_k > 0$, $k \in \mathbb{N}_0$, then g is in SPD_{d-1} (Cheney-Xu [1992]).
- Chen, Menegatto and Sun [2003] proved that $g \in \mathrm{SPD}_{d-1}$, $d \geq 3$, if and only if $a_k \geq 0$ for all k and infinitely many a_k of even index, and infinitely many of odd index, are positive.

Problem: Find a simple criterion that determines if a function is PD_{d-1} or SPD_{d-1}.

Positive definite functions on $\mathbb{R}^d$

Theorem (Bochner 1933)

Let Φ be a continuous function $\Phi : \mathbb{R}^d \mapsto \mathbb{C}$. Then Φ is positive definite if and only if there is a finite nonnegative Borel measure μ on $\mathbb{R}^d$ such that

$$\Phi(x) = \int_{\mathbb{R}^d} e^{i\langle x,\xi\rangle} \, d\mu(\xi).$$

- A sufficient condition on $\mathbb{R}$ is Pólya's criterion:
  An even function f which is continuous and convex on $[0, \infty)$, and vanishes at infinity, is positive definite on $\mathbb{R}$.
- For $t > 0$, the function $(t - \|x\|)_+^\delta$ is strictly positive definite on $\mathbb{R}^d$ if and only if $\delta \geq \frac{d+1}{2}$. (Askey [1973], Gasper [1975], Fields-Ismail [1975])

The Pólya criterion on the sphere

Theorem

Let $d = 3, 4, 5, \ldots$ and $\lambda = \lceil \frac{d-2}{2} \rceil$. Let the real-valued function $g(\cdot) = f(\cos \cdot)$ on $[0, \pi]$ satisfy the following conditions:

(i) $g \in C^{\lambda}[0, \pi]$,

(ii) $supp(g) \subset [0, \pi)$,

(iii) *the derivative, from the right,* $g^{(\lambda+1)}(0)$ *exists, and is finite,*

(iv) $(-1)^{\lambda} g^{(\lambda)}$ *is convex.*

Then g is a positive definite function on $\mathbb{S}^{d-1}$.

If, in addition to the above properties, $g^{(\lambda)}$, restricted to $(0, \pi)$, does not reduce to a linear polynomial, then g is a strictly positive definite function on $\mathbb{S}^{d-1}$.

The essential part of the proof, via Peano kernel, is to show that a family of cut-off function is a PDF.

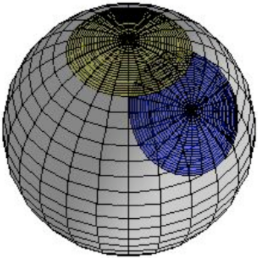
Beatson-zu Castell-X [IMA J. Numer. Math. (2014)]

A family of PDF on $\mathbb{S}^{d-1}$

For $\delta > 0$, $0 < t < \pi$, define

$$g_{t,\delta}(\theta) = (t - \theta)_+^{\delta}.$$

Fix $e \in \mathbb{S}^{d-1}$, the corresponding zonal function $(t - d(x,y))_+^{\delta}$ is supported on the spherical cap $\{x \in \mathbb{S}^{d-1} : d(x,e) \le t\}$.



The function $g_{t,\delta}$ is an analogue of $(t - \|x\|)_+^{\delta}$ on $\mathbb{R}^d$. The proof of the Pólya criterion reduces to show $g_{t,\delta}$ is PDF for $\delta \ge d/2$. In [BCX], the latter was established only for $d \le 8$.

Positive integrals of Gegenbauer polynomials

The function $g_{t,\delta}$ is PDF or SPDF if, for $\lambda = \frac{d-2}{2}$,

$$F_n^{\lambda,\delta}(t) := \int_0^t (t-\theta)^\delta C_n^\lambda(\theta)(\sin\theta)^{2\lambda} dt$$

are nonnegative or positive for all $n = 0, 1, 2, \ldots$ and $\delta \geq \lambda + 1$.
Here are the case of $\delta = \lambda + 1$ for $d = 2$ and 3.

$$\frac{4}{3} F_n^{2,3}(t) = \sum_{k=0}^{2} \frac{e_{k,n}}{(n+2k)^4} \left\{ \cos((n+2k)t) - \left[1 - \frac{(n+2k)^2 t^2}{2} \right] \right\}$$

with $e_{0,n} = (n+3), \quad e_{1,n} = -2(n+2), \quad e_{2,n} = (n+1).$

$$\frac{8}{3} F_n^{3,4}(t) = \sum_{k=0}^{3} \frac{f_{k,n}}{(n+2k)^5} \left\{ \sin((n+2k)t) - \left[(n+2k)t - \frac{(n+2k)^3 \, t^3}{6} \right] \right\},$$

with

$$f_{0,n} = (n+5)(n+4), \; f_{1,n} = -3(n+5)(n+2),$$
$$f_{2,n} = 3(n+4)(n+1), \; f_{3,n} = -(n+2)(n+1).$$

It is a problem of two variables, with $t \in (0, \pi)$ and $n \in \mathbb{N}_0$.

Positive integrals of Jacobi polynomials

The mixture of polynomial and trigonometric functions causes difficulty. How to solve it? Consider a more general problem!

The Jacobi polynomials $P_n^{(\alpha,\beta)}$ are orthogonal with respect to $(1-x)^\alpha(1+x)^\beta$. In particular,

$$C_n^\alpha(x) = c_n P_n^{(\alpha-\frac{1}{2},\alpha-\frac{1}{2})}(x).$$

Definition

Let $\delta > 0$, $\alpha, \beta > -\frac{1}{2}$ and $n \in \mathbb{N}_0$. For every $0 < t < \pi$, define

$$F_n^{(\alpha,\beta),\delta}(t) := \int_0^t (t-\theta)^\delta P_n^{(\alpha-\frac{1}{2},\beta-\frac{1}{2})}(\cos\theta)\left(\sin\frac{\theta}{2}\right)^{2\alpha}\left(\cos\frac{\theta}{2}\right)^{2\beta} d\theta.$$

Theorem

If $\alpha, \beta \in \mathbb{N}_0$ are not both zero, then $F_n^{(\alpha,\beta),\delta}(t) > 0$ for $n \in \mathbb{N}_0$ if $\delta \geq \alpha + 1$. Moreover, $F_n^{(0,0),\delta}(t) \geq 0$ for $n \in \mathbb{N}_0$ if $\delta \geq 1$.

[X, Proc. AMS, 2018]

Why Jacobi works?

The proof involves several reductions. First, recursive relations,

$$F_n^{(\alpha,0),\delta} \geq 0 \quad \Longrightarrow F_n^{(\alpha,\beta),\delta} \geq 0,$$

reducing the problem to $\beta = 0$. Second, quadratic transform,

$$F_n^{(\alpha,0),\delta}(t) = A_n F_n^{(\alpha,\alpha),\delta}(t/2), \qquad A_n > 0,$$

which gets back to $\beta = \alpha$ but with $t \mapsto t/2$. Eventually we use

$$\lim_{m\to\infty} m^{-\alpha} P_m^{\alpha,\beta}\left(\cos\frac{z}{m}\right) = \left(\frac{z}{2}\right)^{-\alpha} J_\alpha(z)$$

where J_α is the Bessel function and use

Theorem (Gasper, 1977)

If $0 \leq \mu \leq 1$ *and* $\alpha + \mu \geq 1/2$, *then*

$$\int_0^x (x-t)^{\alpha+2\mu-1/2} t^{\alpha+\mu} J_\alpha(t)dt \geq 0, \qquad x > 0;$$

equality holds only when $\mu = 0$, $\alpha = -1/2$ *or* $\mu = 1$, $\alpha = -1/2$.

More on positive integral ...

What if α, β are not integers?

Theorem

Let $\alpha \in \mathbb{R} \setminus \mathbb{N}_0$, $\beta \in \mathbb{R}$ and $\beta \geq 0$. If $\delta \geq \lceil \alpha \rceil + 1$, then $F_n^{(\alpha,\beta),\delta}(t) > 0$ for all $t > 0$ and $n \in \mathbb{N}_0$ when

1. $\alpha > 0$ *and* $\beta \in \mathbb{N}_0$;
2. $\alpha = \beta > 0$;
3. $0 \leq \lfloor \beta \rfloor < \alpha \leq \beta$.

The condition $\delta \geq \lceil \alpha \rceil + 1$, however, is likely not sharp.

Conjecture

For $\alpha, \beta \in \mathbb{R}_+ = (0, \infty) \setminus \mathbb{N}$, $F_n^{(\alpha,\beta),\delta}(t) > 0$ for all $t \in (0, \pi]$ and $n \in \mathbb{N}_0$ if $\delta \geq \alpha + 1$.

Back to PDF and SPDF functions

Theorem

For $d = 3, 4, 5, \ldots$ and $0 < t \leq \pi$, the function $\theta \mapsto (t - \theta)_+^\delta$ is strictly positive definite on the sphere $\mathbb{S}^{d-1}$ provided $\delta \geq \lceil \frac{d}{2} \rceil$.

The condition $\delta \geq \lceil \frac{d}{2} \rceil$ is enough for proving the Pólya criterion. The conjecture implies that it may be improved to $\delta \geq \frac{d}{2}$.

We can also consider the two-point homogeneous spaces. There are 5 such spaces,

1. $\mathbb{S}^{d-1}$ – Sphere;
2. $\mathbb{P}^d(\mathbb{R})$ – Real projective space;
3. $\mathbb{P}^d(\mathbb{C})$ – Complex projective space, $d = 4, 6, \ldots$;
4. $\mathbb{P}^d(\mathbb{H})$ – Quaternionic project space, $d = 8, 10, \ldots$;
5. $\mathbb{P}^{16}(\mathrm{Cay})$ –Cayley projective space.

The PDF and SPDF on them are given by expansions of Jacobi polynomials $P_n^{(\alpha,\beta)}$ with nonnegative/positive coefficients.

PDF on two-point homogeneous spaces

The parameters of the Jacobi polynomials are given by

1. $\mathbb{S}^{d-1}$: $\alpha = \beta = \frac{d-2}{2}$
2. $\mathbb{P}^d(\mathbb{R})$: $\alpha = \beta = \frac{d-2}{2}$ (even $P_n^{(\alpha,\beta)}$);
3. $\mathbb{P}^d(\mathbb{C})$: $\alpha = \frac{d-2}{2}$ and $\beta = 0$;
4. $\mathbb{P}^d(\mathbb{H})$: $\alpha = \frac{d-2}{2}$ and $\beta = 1$;
5. $\mathbb{P}^{16}(\mathrm{Cay})$: $\alpha = 7$, $\beta = 3$.

Theorem

For $0 < t \leq \pi$, the function $\theta \mapsto (t - \theta)_+^\delta$ is strictly positive definite on $\mathbb{P}^d(\mathbb{R})$ for $d = 3, 4, \ldots$, $\mathbb{P}^d(\mathbb{C})$ for $d = 4, 6, \ldots$, and $\mathbb{P}^d(\mathbb{H})$ for $d = 8, 10, \ldots$ if $\delta \geq \lceil \frac{d+1}{2} \rceil$ and on $\mathbb{P}^{16}(\mathrm{Cay})$ if $\delta \geq 9$.

Thank you