GENERALIZED INTEGRALS

OF MACDONALD AND GEGENBAUER FUNCTIONS

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Plan of the talk:

1. Bilinear integrals of Macdonald and Gegenbauer functions.
2. Generalized bilinear integrals of Macdonald and Gegenbauer functions.
3. Applications to Green's functions on the Euclidean space, hyperbolic space and sphere with point-like interactions.

Consider a Sturm-Liouville operator

$$\mathcal{C} := -\rho(r)^{-1}\Big(\partial_r p(r)\partial_r + q(r)\Big)$$

acting on functions on an interval $]a, b[$. $\mathcal{C}$ is formally symmetric for the bilinear scalar product with the density ρ:

$$\langle f|g\rangle := \int_a^b f(r)g(r)\rho(r)\mathrm{d}r.$$

Let us describe a method to compute the scalar product of two eigenfunctions of $\mathcal{C}$.

Let us first consider eigenfunctions f_i corresponding to two distinct eigenvalues E_i, $i = 1, 2$. Then the following is true:

$$\int_a^b f_1(r) f_2(r) \rho(r) \mathrm{d}r = \frac{\mathcal{W}(b) - \mathcal{W}(a)}{E_1 - E_2}$$

where $\mathcal{W}(r) := f_1(r)p(r)f_2'(r) - f_1'(r)p(r)f_2(r)$ is the Wronskian.

(Sometimes, it is called Green's identity, or the integrated Lagrange identity). The right hand side can be often easily evaluated if a, b are singular points of the corresponding differential equation.

Then, using an appropriate limiting procedure we can often compute the scalar product for $f = f_1 = f_2$:

$$\langle f|f\rangle = \int_a^b f(r)^2 \rho(r) \mathrm{d}r.$$

The following two families of Sturm-Liouville operators are especially important for applications: the Bessel operator and the Gegenbauer operator:

$$\mathcal{B}_\alpha := -\frac{1}{r}\partial_r r \partial_r + \frac{\alpha^2}{r^2},$$
$$\mathcal{G}_\alpha := -(1-w^2)^{-\alpha}\partial_w (1-w^2)^{\alpha+1}\partial_w.$$

The modified Bessel equation is the eigenequation of $\mathcal{B}_\alpha$ with eigenvalue -1. The (standard) Bessel equation is its eigenequation for the eigenvalue 1. The separation of variables in the Laplacian on the Euclidean space $\mathbb{R}^d$ leads to the Bessel operator on $[0, \infty[$ with density $\rho = r$ and $\alpha = \frac{d-2}{2}$.

The Gegenbauer equation is the eigenequation of $\mathcal{G}_\alpha$ with eigenvalue $\lambda^2 - \left(\alpha + \frac{1}{2}\right)^2$. The Gegenbauer operator on $[-1, 1]$ with density $\rho(w) = (1 - w^2)^{\frac{d-2}{2}}$ arises when we separate variables in the Laplacian on the sphere $\mathbb{S}^d$. The Gegenbauer operator on $[1, \infty[$ with density $\rho(w) = (w^2 - 1)^{\frac{d-2}{2}}$ arises when we separate variables in the Laplacian on the hyperbolic space $\mathbb{H}^d$.

The scaled Macdonald functions $K_\alpha(br)$, is an exponentially decaying eigenfunction of the Bessel operator with eigenvalue $-b^2$.

Applying the above method we obtain for $a > 0$, $b > 0$

$$\int_0^\infty K_\alpha(ar)K_\alpha(br)2r\mathrm{d}r = \frac{\pi\big((a/b)^\alpha - (b/a)^\alpha\big)}{\sin(\pi\alpha)(a^2-b^2)}, \qquad |\operatorname{Re}(\alpha)| < 1, \ \alpha \neq 0;$$

$$\int_0^\infty K_0(ar)K_0(br)2r\mathrm{d}r = \frac{2\ln\frac{a}{b}}{a^2-b^2},$$

$$\int_0^\infty K_\alpha(br)^2 2r\mathrm{d}r = \frac{\pi\alpha}{b^2\sin(\pi\alpha)}, \qquad |\operatorname{Re}(\alpha)| < 1, \ \alpha \neq 0;$$

$$\int_0^\infty K_0(br)^2 2r\mathrm{d}r = \frac{1}{b^2}.$$

The first identity follows directly by Green's identity. The next three identities are obtained by applying the de l'Hôpital rule to $\alpha = 0$ and $a = b$. Unfortunately, for $|\,\mathrm{Re}(\alpha) \geq 1$ these integrals are divergent.

The Gegenbauer equation is the special case of the hypergeometric equation with the symmetry $w \to -w$ and the singular points at $-1, 1, \infty$:

$$\left((1-w^2)\partial_w^2 - 2(1+\alpha)w\partial_w + \lambda^2 - \left(\alpha + \frac{1}{2}\right)^2\right) f(w) = 0.$$

It is arguably more convenient than the equivalent associated Legendre equation.

We will use two kinds of Gegenbauer functions: one is characterized by its asymptotics $\sim \frac{1}{\Gamma(\alpha+1)}$ at 1:

$$\mathbf{S}_{\alpha,\pm\lambda}(w) := \sum_{j=0}^{\infty} \frac{\left(\frac{1}{2}+\alpha+\lambda\right)_j \left(\frac{1}{2}+\alpha-\lambda)\right)_j}{\Gamma(\alpha+1+j)j!} \Big(\frac{1-w}{2}\Big)^j.$$

The other has the asymptotics $\sim \frac{1}{w^{\frac{1}{2}+\alpha+\lambda}\Gamma(\lambda+1)}$ at ∞:

$$\mathbf{Z}_{\alpha,\lambda}(w) := \frac{1}{(w\pm 1)^{\frac{1}{2}+\alpha+\lambda}} \sum_{j=0}^{\infty} \frac{\left(\frac{1}{2}+\lambda\right)_j \left(\frac{1}{2}+\lambda+\alpha\right)_j}{\Gamma(\lambda+1)(1+2\lambda)_j j!} \Big(\frac{2}{1\pm w}\Big)^j.$$

We note the identities

$$\mathbf{S}_{\alpha,\lambda}(w) = \mathbf{S}_{\alpha,-\lambda}(w), \quad \mathbf{Z}_{\alpha,\lambda}(w) = \frac{\mathbf{Z}_{-\alpha,\lambda}(w)}{(w^2-1)^{\alpha}},$$

as well as the slightly more subtle Whipple identity:

$$\mathbf{Z}_{\alpha,\lambda}(w) := (w^2-1)^{-\frac{1}{4}-\frac{\alpha}{2}-\frac{\lambda}{2}}\mathbf{S}_{\lambda,\alpha}\left(\frac{w}{(w^2-1)^{\frac{1}{2}}}\right),$$

$$\mathbf{S}_{\alpha,\lambda}(w) := (w^2-1)^{-\frac{1}{4}-\frac{\alpha}{2}-\frac{\lambda}{2}}\mathbf{Z}_{\lambda,\alpha}\left(\frac{w}{(w^2-1)^{\frac{1}{2}}}\right), \qquad \mathrm{Re}(w) > 0.$$

Here are the basic bilinear integrals of Gegenbauer functions. We assume $|\operatorname{Re}(\alpha)| < 1$, $\alpha \neq 0$ and $\operatorname{Re}(\lambda) > 0$:

$$\int_{-1}^{1} \mathbf{S}_{\alpha,\mathrm{i}\beta_1}(w)\mathbf{S}_{\alpha,\mathrm{i}\beta_2}(w)(1-w^2)^{\alpha}\mathrm{d}2w$$
$$=\frac{2^{2\alpha+2}}{(\beta_1^2-\beta_2^2)\sin\pi\alpha}\Big(\frac{\cosh(\pi\beta_1)}{\Gamma(\frac{1}{2}+\alpha-\mathrm{i}\beta_2)\Gamma(\frac{1}{2}+\alpha+\mathrm{i}\beta_2)}-(\beta_1\leftrightarrow\beta_2)\Big)$$

$$\int_{1}^{\infty} \mathbf{Z}_{\alpha,\lambda_1}(w)\mathbf{Z}_{\alpha,\lambda_2}(w)(w^2-1)^{\alpha}\mathrm{d}2w$$
$$=\frac{2^{\lambda_1+\lambda_2+1}}{(\lambda_1^2-\lambda_2^2)\sin\pi\alpha}\Big(\frac{1}{\Gamma(\frac{1}{2}-\alpha+\lambda_1)\Gamma(\frac{1}{2}+\alpha+\lambda_2)}-(\lambda_1\leftrightarrow\lambda_2)\Big),$$

Applying the de l'Hôpital rule we extend these identities to $\alpha = 0$ $\lambda_1 = \lambda_2$, and $\beta_1 = \beta_2$. However, for $|\operatorname{Re}(\alpha) \geq 1$ these integrals are divergent, which is annoying.

Fortunately one can introduce the generalized integral, with which one can cover all $\alpha \in \mathbb{C}$. This concept can be traced back to Hadamard and Riesz, see the book by Paycha for a modern exposition.

We say that a function f on $]0,\infty[$ is integrable in the generalized sense if it is integrable on $]1,\infty[$ and if there exists a finite set $\Omega \subset \mathbb{C}$ and $f_k \in \mathbb{C}$, $k \in \Omega$, such that $f - \sum_{k\in\Omega} f_k r^k$ is integrable on $]0,1[$.

We define the generalized integral as

$$\operatorname{gen}\int_0^\infty f(r)\mathrm{d}r$$

$$:= \sum_{k\in\Omega\backslash\{-1\}} \frac{f_k}{k+1} + \int_0^1 \Big(f(r) - \sum_{k\in\Omega} f_k r^k\Big)\mathrm{d}r + \int_1^\infty f(r)\mathrm{d}r.$$

For $f \in L^1[0,\infty[$ the generalized and standard integrals coincide:

$$\operatorname{gen}\int_0^\infty f(r)\mathrm{d}r = \int_0^\infty f(r)\mathrm{d}r.$$

The generalized integral is called anomalous if for some $n \in \mathbb{N}$ we have $f_{-n} \neq 0$. Non-anomalous generalized integrals have much better properties. They are often easy to compute: one just applies analytic continuation. They are invariant wrt change of variables:

$$\mathrm{gen}\int_0^\infty f(r)\mathrm{d}r = \mathrm{gen}\int_0^\infty f(g(u))g'(u)\mathrm{d}u.$$

Anomalous integrals are more interesting. They have a scaling anomaly:

$$\mathrm{gen}\int_0^\infty f(r)\mathrm{d}r = \mathrm{gen}\int_0^\infty f(\alpha u)\,\alpha\mathrm{d}u + f_{-1}\ln(\alpha),$$

but $$\mathrm{gen}\int_0^\infty f(r)\mathrm{d}r = \mathrm{gen}\int_0^\infty f(u^\alpha)\,\alpha u^{\alpha-1}\mathrm{d}u.$$

Let $a, b > 0$. For $\alpha \notin \mathbb{Z}$ the generalized integrals of Macdonald functions are analytic continuations of the standard integrals:

$$\operatorname{gen}\int_0^\infty K_\alpha(ar)K_\alpha(br)2r\mathrm{d}r = \frac{\pi}{\sin(\pi\alpha)}\frac{\left(\left(\frac{a}{b}\right)^\alpha - \left(\frac{b}{a}\right)^\alpha\right)}{(a^2-b^2)},$$

$$\operatorname{gen}\int_0^\infty K_\alpha(br)^2 2r\mathrm{d}r = \frac{\pi\alpha}{b^2\sin(\pi\alpha)}.$$

They have poles at $\alpha \in \mathbb{Z}$.

For $\alpha \in \mathbb{Z}$ the generalized integrals are anomalous and more complicated to compute. In particular, they do not coincide with the finite parts of the expressions from the previous slides:

$$\operatorname{gen}\int_0^\infty K_\alpha(ar)K_\alpha(br)2r\mathrm{d}r = (-1)^\alpha 2\frac{\Big(\big(\frac{a}{b}\big)^\alpha \ln\big(\frac{a}{2}\big) - \big(\frac{b}{a}\big)^\alpha \ln\big(\frac{b}{2}\big)\Big)}{(a^2-b^2)}$$

$$-\frac{(-1)^\alpha}{ab}\sum_{k=0}^{|\alpha|-1}\left(\frac{a}{b}\right)^{2k-|\alpha|+1}\big(\psi(1+k)+\psi(|\alpha|-k)\big);$$

$$\operatorname{gen}\int_0^\infty K_\alpha(br)^2 2r\mathrm{d}r = \frac{(-1)^\alpha}{b^2}\Big(|\alpha|\ln\big(\tfrac{b^2}{4}\big) + 1 + 2|\alpha|\big(1-\psi(1+|\alpha|)\big)\Big).$$

Similarly we can be compute generalized bilinear integrals of $\mathbf{S}_{\alpha,\mathrm{i}\beta}$, $\mathbf{Z}_{\alpha,\lambda}$.

As $\beta,\lambda\to\infty$, Gegenbauer functions converge to Macdonald functions in the following sense:

$$\frac{\pi\mathrm{e}^{-\pi\beta}(\sin\theta)^{\alpha+\frac12}}{2^\alpha\theta^{\alpha+\frac12}}\mathbf{S}_{\alpha,\pm\mathrm{i}\beta}(-\cos\theta)$$
$$=(\theta\beta)^{-\alpha}K_\alpha(\beta\theta)\big(1+O(\beta^{-1})\big);$$

$$\frac{\sqrt{\pi}\Gamma(\frac12-\alpha+\lambda)(\sinh\theta)^{\alpha+\frac12}}{2^{\lambda+\frac12}\theta^{\alpha+\frac12}}\mathbf{Z}_{\alpha,\lambda}(\cosh\theta)$$
$$=(\lambda\theta)^{-\alpha}K_\alpha(\lambda\theta)\big(1+O(\lambda^{-1})\big).$$

The generalized integrals of Gegenbauer functions converge to the corresponding generalized integrals of Macdonald functions:

$$\frac{\pi^2 \mathrm{e}^{-2\pi\beta}\beta^{2\alpha}}{2^{2\alpha}} \operatorname{gen}\int_{-1}^{1} \mathbf{S}_{\alpha,\mathrm{i}\beta}(w)^2(1-w^2)^\alpha \mathrm{d}2w$$
$$=\Big(1+\mathcal{O}\big(\tfrac{1}{\beta}\big)\Big) \operatorname{gen}\int_0^\infty K_\alpha(\beta r)^2 2r\mathrm{d}r;$$

$$\frac{\pi\Gamma\big(\frac{1}{2}+\alpha+\lambda\big)^2}{2^{2\lambda+1}\lambda^{2\alpha}} \operatorname{gen}\int_1^\infty \mathbf{Z}_{\alpha,\lambda}(w)^2(w^2-1)^\alpha \mathrm{d}2w$$
$$=\Big(1+\mathcal{O}\big(\tfrac{1}{\lambda}\big)\Big) \operatorname{gen}\int_0^\infty K_\alpha(\lambda r)^2 2r\mathrm{d}r.$$

The convergence of these generalized integrals is straightforward in the non-anomalous case. In the anomalous case one has to choose the variables carefully, which we did:

$$2r\mathrm{d}r = \mathrm{d}r^2, \quad 2\cosh\theta - 1 \simeq r^2, \quad 1 - 2\cos\theta \simeq r^2.$$

Note that the generalized integral is invariant wrt the change of variables $r \to r^2$, but not wrt scaling.

Let us now describe an application of generalized integrals to operator theory.

Consider the Laplacian Δ_d on the Euclidean space $\mathbb{R}^d$. Let $G_d(z;x,x')$ be the Euclidean Green's function, that is the integral kernel of the resolvent $(-z-\Delta_d)^{-1}$.

It is well-known that for $\operatorname{Re}\beta > 0$,

$$G_d(-\beta^2;x,x') = \frac{1}{(2\pi)^{\frac{d}{2}}}\Big(\frac{\beta}{|x-x'|}\Big)^{\frac{d}{2}-1} K_{\frac{d}{2}-1}\big(\beta|x-x'|\big).$$

The hyperbolic space is

$$\mathbb{H}^d := \{x \in \mathbb{R}^{1,d} \mid [x|x] = 1\}$$

where $[x|y] = x^0y^0 - x^1y^1 - \cdots - x^dy^d$ is the Minkowskian pseudoscalar product. The hyperbolic distance between $x, x' \in \mathbb{H}^d$ is given by $\cosh(r) = [x|x']$.

Let Δ_d^{h} denote the Laplace-Beltrami operator on $\mathbb{H}^d$. Let $G_d^{\mathrm{h}}(z; x, x')$ be the hyperbolic Green's function, that is, the integral kernel of $\Big(-z - \Delta_d^{\mathrm{h}} - \frac{(d-1)^2}{4}\Big)^{-1}$. Then

$$G_d^{\mathrm{h}}\Big(-\beta^2; x, x'\Big) = \frac{\sqrt{\pi}\Gamma(\frac{d-1}{2} + \beta)}{\sqrt{2}(2\pi)^{\frac{d}{2}}2^\beta}\mathbf{Z}_{\frac{d}{2}-1,\beta}\big([x|x']\big).$$

The unit sphere is

$$\mathbb{S}^d := \{x \in \mathbb{R}^{1+d} \mid (x|x) = 1\},$$

where $(x|y) = x^0y^0 + x^1y^1 + \cdots + x^dy^d$ is the Euclidean scalar product. The spherical distance between $x, x' \in \mathbb{S}^d$ is given by $\cos(r) = (x|x')$. Let Δ_d^{s} denote the Laplace-Beltrami operator on $\mathbb{S}^d$. Let $G_d^{\mathrm{s}}(z; x, x')$ be the spherical Green's function, that is, the integral kernel of $\Big(-z - \Delta_d^{\mathrm{s}} + \frac{(d-1)^2}{4}\Big)^{-1}$. Then

$$G_d^{\mathrm{s}}(-\beta^2; x, x') = \frac{\Gamma(\frac{d}{2} - \frac12 + \mathrm{i}\beta)\Gamma(\frac{d}{2} - \frac12 - \mathrm{i}\beta)}{2^d \pi^{\frac{d}{2}}} \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\beta}\big(-(x|x')\big).$$

Suppose that $G(-\rho) := (\rho + H)^{-1}$ is the resolvent of a self-adjoint operator H. Then $G(-\rho)$ satisfies

$$\begin{aligned}
(H + \rho)G(-\rho) &= \mathbb{1}, \\
G(-\rho)^* &= G(-\overline{\rho}), \\
\frac{\mathrm{d}}{\mathrm{d}\rho} G(-\rho) &= -G(-\rho)^2.
\end{aligned}$$

Let $-\Delta_d^\gamma$ be a self-adjoint extension of $-\Delta_d$ restricted to $C_{\mathrm{c}}^\infty(\mathbb{R}^d\backslash\{0\})$. Let

$$G_d^\gamma(-\rho) = (-\Delta_d^\gamma + \rho)^{-1}.$$

By the conditions from the previous slide its integral kernel $G_d^\gamma(-\rho, x, x')$ should satisfy

$$\begin{aligned}(-\Delta_x + \rho)G_d^\gamma(-\rho, x, x') &= \delta(x - x'), \quad x \neq 0,\\ G_d^\gamma(-\rho, x, x') &= G_d^\gamma(-\rho, x', x),\\ \partial_\rho G_d^\gamma(-\rho, x, x') &= -\int G_d^\gamma(-\rho, x, y)G_d^\gamma(-\rho, y, x')\mathrm{d}y.\end{aligned}$$

These conditions are solved by a Krein-type resolvent

$$G_d^\gamma(-\rho,x,x') = G_d(-\rho,x,x') + \frac{G_d(-\rho,x,0)G_d(-\rho,0,x')}{\gamma+\Sigma_d(\rho)},$$

where

$$\partial_\rho \Sigma_d(\rho) = \int_{\mathbb{R}^d} G_d(-\rho,0,y)^2 \mathrm{d}y,$$

and γ is an arbitrary constant. In dimensions $d=1,2,3$ the above integral is finite and we obtain

$$\Sigma_d(\beta^2) = \begin{cases} -\frac{1}{2\beta} & d=1; \\ \frac{\ln(\beta^2)}{4\pi} & d=2; \\ \frac{\beta}{4\pi} & d=3. \end{cases}$$

They lead to well-known formulas for Green's functions with a point potential in dimensions $d = 1, 2, 3$:

$$G_d^\gamma(-\beta^2; x, x') = \begin{cases} \frac{\mathrm{e}^{-\beta|x-x'|}}{2\beta} + \frac{\mathrm{e}^{-\beta|x|}\mathrm{e}^{-\beta|x'|}}{(2\beta)^2\left(\gamma - \frac{1}{2\beta}\right)}, & d = 1; \\ \frac{K_0(\beta|x-y|)}{2\pi} + \frac{K_0(\beta|x|)K_0(\beta|y|)}{(2\pi)^2(\gamma + \frac{\ln\beta^2}{4\pi})}, & d = 2; \\ \frac{\mathrm{e}^{-\beta|x-y|}}{4\pi|x-y|} + \frac{\mathrm{e}^{-\beta|x|}\mathrm{e}^{-\beta|y|}}{(4\pi)^2|x||y|(\gamma + \frac{\beta}{4\pi})}, & d = 3. \end{cases}$$

We used the fact that for half-integer parameters the Macdonald function reduces to elementary functions.

$G_d^\gamma(-\rho; x, x')$ are integral kernels of the resolvents of well-defined self-adjoint operators $-\Delta_d^\gamma$ for $d = 1, 2, 3$. In higher dimensions, strictly speaking, these operators have no analogs. However, the functions $G_d^\gamma(-\rho; x, x')$ can be generalized to higher dimensions using the generalized integral

$$\partial_\rho \Sigma_d(\rho) = \frac{(\beta^2)^{\frac{d}{2}-1} 2\pi^{\frac{d}{2}}}{(2\pi)^d \Gamma(\frac{d}{2})} \mathrm{gen} \int_0^\infty K_{\frac{d}{2}-1}(\sqrt{\rho} r)^2 r \mathrm{d}r.$$

Thus we obtain

$$\Sigma_d(\beta^2) = \begin{cases} \dfrac{(-1)^{\frac{d+1}{2}}\beta^{d-2}}{(4\pi)^{\frac{d-1}{2}}2(\frac{1}{2})_{\frac{d-1}{2}}} & d \text{ odd;} \\ \dfrac{(-1)^{\frac{d}{2}+1}\beta^{d-2}}{(4\pi)^{\frac{d}{2}}\left(\frac{d}{2}-1\right)!}\left(2 - 2\psi\left(\frac{d}{2}\right) + \ln\dfrac{\beta^2}{4}\right) & d \text{ even.} \end{cases}$$

Similar analysis can be performed for the hyperbolic and spherical Green's functions in all dimensions.

Thus for each dimension d we obtain a family of Green's functions

$$G_d^\gamma(-\beta^2; x, x') = \frac{1}{(2\pi)^{\frac{d}{2}}}\Big(\frac{\beta}{|x - x'|}\Big)^{\frac{d}{2}-1} K_{\frac{d}{2}-1}\big(\beta|x - x'|\big)$$
$$+\frac{1}{(2\pi)^d}\Big(\frac{\beta^2}{|x||x'|}\Big)^{\frac{d}{2}-1}\frac{K_{\frac{d}{2}-1}(\beta|x|)K_{\frac{d}{2}-1}(\beta|x'|)}{\gamma + \Sigma_d(\beta^2)}.$$

describing point interaction of strength controlled by parameter γ.

One can argue that the meaning of $G_d^\gamma(-\beta^2; x, x')$ is as follows. Suppose that V is a potential, possibly strong but with a small support. Consider the the Schrödinger operator $\Delta_d + V$. Let

$$G^V(-\beta^2) = (\beta^2 - \Delta_d + V)^{-1}$$

be its resolvent with the integral kernel $G^V(-\beta^2; x, x')$. Then for a distinguished choice of V and far from its support we can approximate $G^V(-\beta^2; x, x')$ by $G^\gamma(-\beta^2; x, x')$.

This is related to the idea often expressed in the context of quantum field theory and of the theory of critical phenomena, attributed to Keneth Wilson: for large distances correlation functions have a universal behavior independent of the details of the interaction, described by few parameters.

THAN YOU FOR YOUR ATTENTION