Heat kernels of diffusion and jump processes on fractals

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Analysis on metric spaces: integration

Let (M, d) be a metric space and μ be a Radon measure on M. Assume in what follows that M is *α-regular*, that is, for any metric ball

$$B(x, r) := \{y \in M : d(x, y) < r\}$$

of any radius $r < r_0$, we have

$$\mu(B(x, r)) \simeq r^\alpha, \tag{1}$$

where $\alpha > 0$. The sign $\simeq$ means that the ratio of the two sides is bounded from above and below by positive constants.

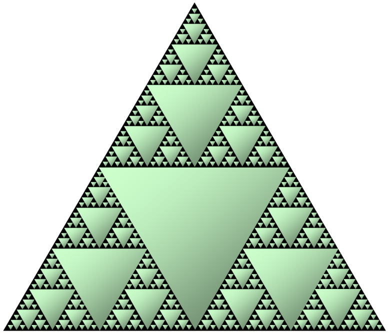
It follows from (1) that

$$\dim_H M = \alpha \quad \text{and} \quad \mathcal{H}_\alpha \simeq \mu.$$

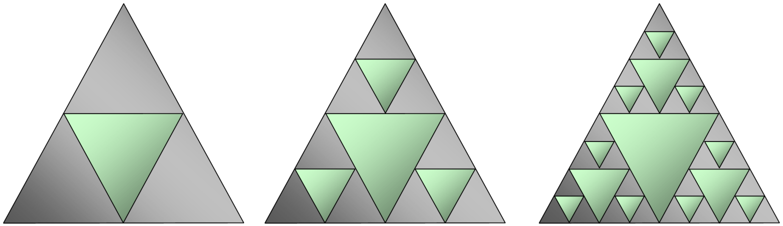
In some sense, α is a numerical characteristic of the integral calculus on M.

Spaces with fractional α are called *fractals*. They appeared in mathematics as curious examples that initially served as counterexamples to illustrate various theorems.

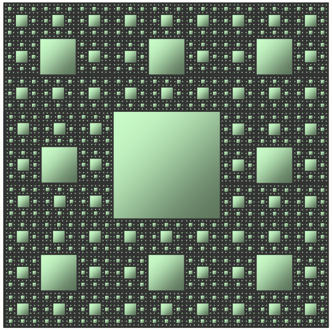
The most famous fractal is the *Cantor set*. Here are some examples of fractals relevant for this presentation:



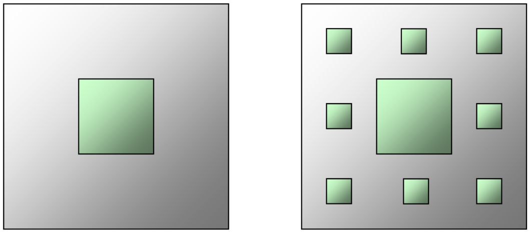
Sierpinski gasket (SG), $\alpha = \frac{\log 3}{\log 2} \approx 1.59$



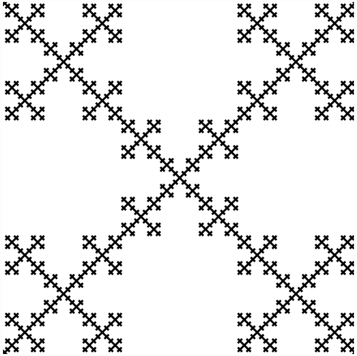
Three steps of construction of SG



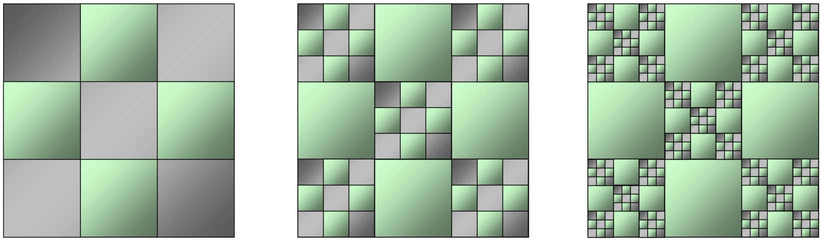
Sierpinski carpet (SC), $\alpha = \frac{\log 8}{\log 3} \approx 1.90$



Two steps of construction of SC



Vicsek snowflake (VS), $\alpha = \frac{\log 5}{\log 3} \approx 1.47$



Three steps of construction of VS

Analysis on metric spaces: differentiation

On many families of fractals, it is possible to construct a *Laplace-type* operator, by means of the theory of Dirichlet forms of Fukushima.

A *Dirichlet form* in $L^2(M,\mu)$ is a pair $(\mathcal{E},\mathcal{F})$ where $\mathcal{F}$ is dense subspace of $L^2(M,\mu)$ and $\mathcal{E}$ is a bilinear form on $\mathcal{F}$ with the following properties:

1. It is *positive definite*, that is, $\mathcal{E}(f,f) \geq 0$ for all $f \in \mathcal{F}$.

2. It is *closed*, that is, $\mathcal{F}$ is complete with respect to the norm

$$\|f\|_{\mathcal{F}} := \left(\int_M f^2 d\mu + \mathcal{E}(f,f) \right)^{1/2}.$$

3. It is *Markovian*, that is, if $f \in \mathcal{F}$ then $\widetilde{f} := \min(f_+, 1) \in \mathcal{F}$ and $\mathcal{E}(\widetilde{f},\widetilde{f}) \leq \mathcal{E}(f,f)$.

Any Dirichlet form has the generator: a positive definite self-adjoint operator $\mathcal{L}$ in $L^2(M,\mu)$ with a dense domain $\operatorname{dom}(\mathcal{L}) \subset \mathcal{F}$ such that

$$(\mathcal{L}f, g) = \mathcal{E}(f,g) \text{ for all } f \in \operatorname{dom}(\mathcal{L}) \text{ and } g \in \mathcal{F}.$$

For example, the bilinear form

$$\mathcal{E}(f,g)=\int_{\mathbb{R}^n}\nabla f\cdot\nabla g\,dx \tag{2}$$

in the domain $\mathcal{F}=W_2^1\left(\mathbb{R}^n\right)$ is a Dirichlet form (its quadratic part is the Dirichlet integral), and its generator is $\mathcal{L}=-\Delta$ with $\operatorname{dom}\left(\mathcal{L}\right)=W_2^2\left(\mathbb{R}^n\right)$.

Another example of a Dirichlet form in $\mathbb{R}^n$ is

$$\mathcal{E}(f,f)=\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\frac{\left(f\left(x\right)-f\left(y\right)\right)^2}{\left|x-y\right|^{n+s}}dxdy, \tag{3}$$

where $s\in(0,2)$ and $\mathcal{F}=B_{2,2}^{s/2}\left(\mathbb{R}^n\right)$. Its generator is $\mathcal{L}=\left(-\Delta\right)^{s/2}$.

A Dirichlet form $(\mathcal{E},\mathcal{F})$ is called *strongly local* if $\mathcal{E}(f,g)=0$ whenever $f=\text{const}$ in a neighborhood of $\operatorname{supp} g$. For example, the form (2) is strongly local, while (3) is nonlocal.

A Dirichlet form $(\mathcal{E},\mathcal{F})$ is called *regular* if $C_0\left(M\right)\cap\mathcal{F}$ is dense both in $\mathcal{F}$ and $C_0\left(M\right)$. The both Dirichlet forms (2) and (3) are regular.

The generator of any regular Dirichlet form determines a *heat semigroup* $\left\{e^{-t\mathcal{L}}\right\}_{t\geq0}$, as well as a Markov processes $\{X_t\}_{t\geq0}$ on M with the transition semigroup $e^{-t\mathcal{L}}$, that is,

$$\mathbb{E}_x f\left(X_t\right)=e^{-t\mathcal{L}}f\left(x\right)\quad\text{for all } f\in C_0\left(M\right).$$

If $(\mathcal{E}, \mathcal{F})$ is local then $\{X_t\}$ is a diffusion while otherwise the process $\{X_t\}$ contains jumps.

For example, the Dirichlet form (2) determines Brownian motion in $\mathbb{R}^n$, whose transition density is exactly the Gauss-Weierstrass function

$$p_t(x, y) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x-y|^2}{4t}\right).$$

The Dirichlet form (3) determines a jump process: a symmetric stable Levy process of the index s. In the case $s = 1$ its transition density is the Cauchy distribution

$$p_t(x, y) = \frac{c_n t}{\left(t^2 + |x-y|^2\right)^{\frac{n+1}{2}}} = \frac{c_n}{t^n}\left(1 + \frac{|x-y|^2}{t^2}\right)^{-\frac{n+1}{2}},$$

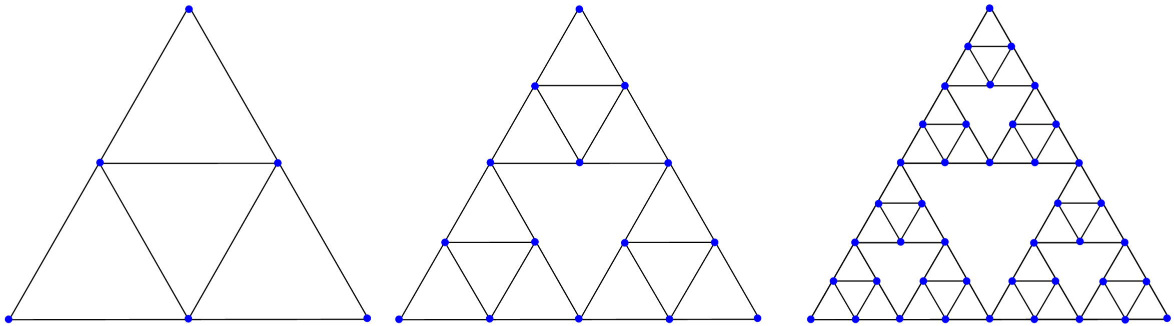
where $c_n = \Gamma\left(\frac{n+1}{2}\right)/\pi^{(n+1)/2}$. For an arbitrary $s \in (0, 2)$ we have

$$p_t(x, y) \simeq \frac{1}{t^{n/s}}\left(1 + \frac{|x-y|}{t^{1/s}}\right)^{-(n+s)}.$$

If a metric measure space M possesses a strongly local regular Dirichlet form $(\mathcal{E}, \mathcal{F})$ then its generator $\mathcal{L}$ can be regarded as an analogue of the Laplace operator. In some sense $\mathcal{L}$ determines a differential calculus on M.

Large families of fractals admit non-trivial strongly local regular Dirichlet forms respecting the self-similarity and symmetry structures. Such Dirichlet forms have been constructed on SG by Barlow–Perkins '88, Goldstein '87 and Kusuoka '87, on SC by Barlow–Bass '89 and Kusuoka–Zhou '92, on p.c.f. fractals (including VS) by Kigami '93.

In fact, each of these fractals can be regarded as a limit of a sequence of graphs Γ_n.



Approximating graphs $\Gamma_1, \Gamma_2, \Gamma_3$ for SG

Define on each Γ_n a Dirichlet form $\mathcal{E}_n$ by

$$\mathcal{E}_n(f,f) = \sum_{x,y:\, x\sim y} \left(f(x) - f(y)\right)^2$$

and then consider a scaled limit

$$\mathcal{E}(f,f) = \lim_{n\to\infty} R_n \mathcal{E}_n(f,f) \tag{4}$$

with an appropriately renormalizing sequence $\{R_n\}$. The main difficulty is to ensure the existence of $\{R_n\}$ such that this limit exists and is in $(0,\infty)$ for a dense in L^2 family of f. For p.c.f. fractals one chooses $R_n = \rho^n$ where, for example, $\rho = \frac{5}{3}$ for SG and $\rho = 3$ for VS, and the limit in (4) exists due to monotonicity.

For SC the situation is much harder. Initially a strongly local Dirichlet form on SC was constructed by Barlow and Bass '89 in a different way by using a probabilistic approach. After a work of Barlow, Bass, Kumagai and Teplyaev '10 it became possible to claim that the limit (4) exists for a certain sequence $\{R_n\}$ such that $R_n \simeq \rho^n$, where the exact value of ρ is still unknown. Numerical computation indicates that $\rho \approx 1.25$.

Other methods of constructing a strongly local Dirichlet form on SC was proposed by Kusuoka and Zhou '92 and AG and M.Yang '19.

Walk dimension

In all the above examples the heat semigroup $\{e^{-t\mathcal{L}}\}$ of the Dirichlet form $(\mathcal{E},\mathcal{F})$ is a family of integral operators: for any $t>0$ and $f\in L^2(M,\mu)$

$$e^{-t\mathcal{L}}f(x)=\int_M p_t(x,y)f(y)\,d\mu(y),$$

where the integral kernel $p_t(x,y)$ is called the *heat kernel* of $(\mathcal{E},\mathcal{F})$ (or of $\mathcal{L}$). Moreover, in all the above examples the heat kernel satisfies the following *sub-Gaussian* estimate

$$p_t(x,y)\asymp\frac{C}{t^{\alpha/\beta}}\exp\left(-c\left(\frac{d^\beta(x,y)}{t}\right)^{\frac{1}{\beta-1}}\right) \tag{5}$$

for all $x,y\in M$ and $t\in(0,t_0)$ (Barlow–Perkins '88, Barlow–Bass '92).

Here α is the Hausdorff dimension while β is a new parameter that is called the *walk dimension.* It can be regarded as a numerical characteristic of differential calculus on M. It is known that always $\beta\geq 2$ and that any pair (α,β) of reals such that

$$\alpha\geq 1\quad\text{and}\quad 2\leq\beta\leq\alpha+1$$

can be realized on some fractal as parameters in the heat kernel bounds (5) (Barlow '04).

Hence, we obtain a large family of metric measure spaces that are characterized by a pair (α, β) where α is responsible for integration while β is responsible for differentiation.

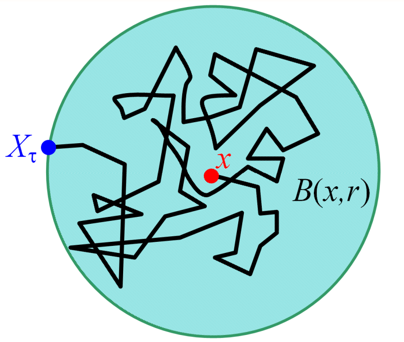
The Euclidean space $\mathbb{R}^n$ belongs to this family with $\alpha = n$ and $\beta = 2$ (in the case $\beta = 2$ the estimate (5) is called Gaussian).

On fractals the values of β is determined by the scaling parameter ρ. It is known that:

- on SG: $\beta = \frac{\log 5}{\log 2} \approx 2.32$
- on VS: $\beta = \frac{\log 15}{\log 3} \approx 2.46$
- on SC: $\beta = \frac{\log(8\rho)}{\log 3}$ (the approximation $\rho \approx 1.25$ indicates that $\beta \approx 2.10$).

The walk dimension β has the following probabilistic meaning. For any open set $\Omega \subset M$, denote by τ_Ω the first exit time of diffusion X_t from Ω:

$$\tau_\Omega = \inf \{t > 0 : X_t \notin \Omega\}.$$



If (5) holds, then, for any ball $B(x, r)$ with $r < r_0$,

$$\mathbb{E}_x \tau_{B(x,r)} \simeq r^\beta.$$

Besov spaces and characterization of β

Given an α-regular metric measure space (M, d, μ), it is possible to define a family $B^{\sigma}_{p,q}$ of Besov spaces. Here we need only the following special cases: for any $\sigma > 0$ the space $B^{\sigma}_{2,2}$ consists of functions $f \in L^2(M, \mu)$ such that

$$\|f\|^2_{\dot{B}^{\sigma}_{2,2}} := \iint\limits_{M \times M} \frac{|f(x) - f(y)|^2}{d(x,y)^{\alpha+2\sigma}} d\mu(x) d\mu(y) < \infty$$

and $B^{\sigma}_{2,\infty}$ consists of functions such that

$$\|f\|^2_{\dot{B}^{\sigma}_{2,\infty}} := \sup_{0<r<r_0} \frac{1}{r^{\alpha+2\sigma}} \iint\limits_{\{d(x,y)<r\}} |f(x) - f(y)|^2 d\mu(x) d\mu(y) < \infty.$$

It is easy to see that the space $B^{\sigma}_{2,2}$ shrinks as σ increases. Define

$$\sigma^* = \sup\left\{\sigma > 0 : B^{\sigma}_{2,2} \text{ is dense in } L^2\right\}. \tag{6}$$

If $\sigma < 1$ then $B^{\sigma}_{2,2}$ contains all Lipschitz functions with compact support, which implies $\sigma^* \geq 1$. In $\mathbb{R}^n$, if $\sigma > 1$ then $B^{\sigma}_{2,2} = \{0\}$ so that $\sigma^* = 1$. On most fractal spaces $\sigma^* > 1$.

Theorem 1 (AG, Jiaxin Hu, K.-S. Lau '03) *If $(\mathcal{E},\mathcal{F})$ is a strongly local Dirichlet form on M such that its heat kernel exists and satisfies the sub-Gaussian estimate*

$$p_t(x,y) \asymp \frac{C}{t^{\alpha/\beta}} \exp\left(-c\left(\frac{d^\beta(x,y)}{t}\right)^{\frac{1}{\beta-1}}\right) \tag{7}$$

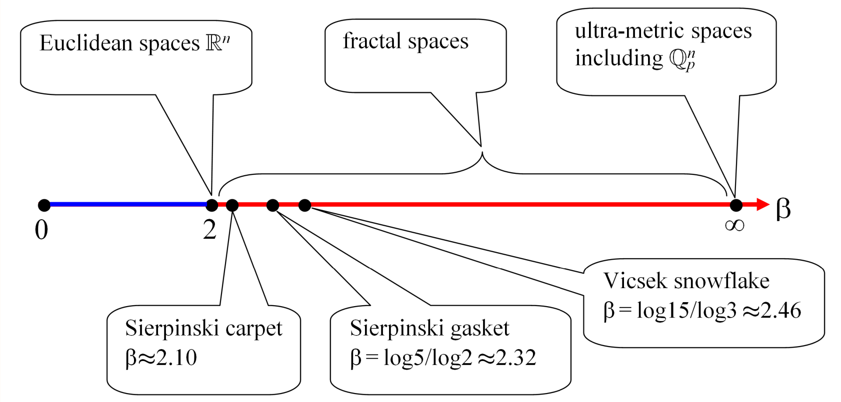
with some α and β then the following is true:

1. *the space M is α-regular, $\alpha = \dim_H M$ and $\mu \simeq \mathcal{H}_a$;*
2. *$\beta = 2\sigma^*$ (consequently, $\beta \geq 2$);*
3. *$\mathcal{F} = B^{\sigma^*}_{2,\infty}$ and $\mathcal{E}(f,f) \simeq \|f\|^2_{\dot{B}^{\sigma^*}_{2,\infty}}$.*

Corollary 2 *Both α and β in (7) are invariants of the metric structure (M,d) alone.*

Indeed, σ^* is defined by using metric d and measure μ, while in this case μ is also determined by d. Therefore, σ^* and β are also invariants of the metric space (M,d).
Note that σ^* is defined by (6) for any α-regular metric space. In the view of Theorem 1 it makes sense to redefine the notion of the walk dimension by $\beta := 2\sigma^*$. Then β becomes a second invariant of any regular metric space, after the Hausdorff dimension α.

Here is classification of α-regular spaces according to their walk dimension $\beta = 2\sigma^*$.



A metric space (M, d) is called *ultra-metric* if it satisfies a stronger triangle inequality

$$d(x,y) \le \max\left(d\left(x,z\right), d\left(y,z\right)\right) \quad \text{for all } x,y,z \in M.$$

For example, the field $\mathbb{Q}_p$ of p-adic numbers with the p-adic distance $|x-y|_p$ is an ultra-metric space. All ultra-metric spaces are totally disconnected and, hence, cannot carry a non-trivial diffusion. On the other hand, on such spaces, for any $\sigma > 0$, the space $B^{\sigma}_{2,2}$ contains indicator functions $\mathbf{1}_B$ of all balls and, hence, is dense in L^2. Consequently, $\sigma^* = \infty$.

An approach to construction of local Dirichlet forms

An open question. *Let M be an α-regular metric measure space (or even self-similar). Assume $\sigma^* < \infty$ and set $\beta = 2\sigma^*$. How to construct a strongly local Dirichlet form with the heat kernel satisfying the estimate (7)? Does such a Dirichlet form exist?*

A natural approach is as follows. For any $\sigma < \sigma^*$ try first to define a quadratic form $\mathcal{E}_\sigma(f, f)$ in the domain $B^\sigma_{2,2}$ such that

$$\mathcal{E}_\sigma(f, f) \simeq \|f\|^2_{\dot{B}^\sigma_{2,2}} = \int\int_{M\times M} \frac{|f(x) - f(y)|^2}{d(x, y)^{\alpha+2\sigma}} d\mu(x)d\mu(y),$$

and then try to prove that there exists a limit

$$\lim_{\sigma\to\sigma^*} (\sigma^* - \sigma)\, \mathcal{E}_\sigma$$

and that this limit determines a local Dirichlet form on M.

This approach was realized on SG and SC by AG and M.Yang '18 and '19, but in the general case there are two many difficulties.

Heat kernel estimates of self-similar type

Let (M,d) be metric space and μ be an α-regular measure on M.

Theorem 3 (AG, T.Kumagai '08) *Let $(\mathcal{E},\mathcal{F})$ be a regular Dirichlet form on M. Assume that*

$$p_t(x,y) \asymp \frac{C}{t^{\alpha/\beta}}\Phi\left(c\frac{d(x,y)}{t^{1/\beta}}\right),$$

where $\alpha,\beta>0$ and Φ is a positive function on $[0,\infty)$. Then the following dichotomy holds:

(i) either the Dirichlet form $\mathcal{E}$ is strongly local,

$$\mathcal{F}=B^{\beta/2}_{2,\infty},\qquad \mathcal{E}(f,f)\simeq\|f\|^2_{\dot{B}^{\beta/2}_{2,\infty}}$$

and

$$\Phi(s)\asymp C\exp\left(-cs^{\frac{\beta}{\beta-1}}\right);$$

(ii) or the Dirichlet form $\mathcal{E}$ is non-local,

$$\mathcal{F}=B^{\beta/2}_{2,2},\qquad \mathcal{E}(f,f)\simeq\|f\|^2_{\dot{B}^{\beta/2}_{2,2}}$$

and

$$\Phi(s)\simeq(1+s)^{-(\alpha+\beta)}.$$

That is, in the first case $p_t(x,y)$ satisfies the sub-Gaussian estimate

$$p_t(x,y) \asymp \frac{C}{t^{\alpha/\beta}} \exp\left(-c\left(\frac{d^\beta(x,y)}{t}\right)^{\frac{1}{\beta-1}}\right) \tag{sub}$$

while in the second case we obtain a *stable-like estimate*

$$p_t(x,y) \simeq \frac{1}{t^{\alpha/\beta}}\left(1+\frac{d(x,y)}{t^{1/\beta}}\right)^{-(\alpha+\beta)} \simeq \min\left(\frac{1}{t^{\alpha/\beta}}, \frac{t}{d(x,y)^{\alpha+\beta}}\right). \tag{$stable$}$$

Next, we discuss the condition on (M,d,μ) and $(\mathcal{E},\mathcal{F})$ that ensure the estimates (sub) or $(stable)$. For that we need the notion of *generalized capacity*.

Capacity and generalized capacity

Let us fix a Dirichlet form $(\mathcal{E},\mathcal{F})$ and a parameter $\beta > 0$. Let $A \Subset B$ be two open subsets of M. Define the capacity of A in B as follows:

$$\operatorname{cap}(A,B) := \inf\left\{\mathcal{E}(\varphi,\varphi) : \varphi \in \mathcal{F},\ \varphi|_{\overline{A}} = 1,\ \operatorname{supp}\varphi \Subset B\ \right\}. \tag{8}$$

Definition. We say that $(\mathcal{E},\mathcal{F})$ satisfies the *capacity condition* if there exists a constant $C>0$ such that, for any two concentric balls $B_0 := B(x,R)$ and $B := B(x,R+r)$,

$$\operatorname{cap}(B_0,B) \le C\frac{\mu(B)}{r^\beta}. \tag{cap}$$

The condition (cap) is equivalent to the existence of a test function φ as in (8) such that

$$\mathcal{E}(\varphi,\varphi) \le C\frac{\mu(B)}{r^\beta}.$$

For any function $u \in L^\infty \cap \mathcal{F}$ and a real $\kappa \ge 1$ define the *generalized capacity* of A in B by

$$\operatorname{cap}_u^{(\kappa)}(A,B) = \inf\left\{\mathcal{E}\left(u^2\varphi,\varphi\right) : \varphi \in \mathcal{F},\ 0 \le \varphi \le \kappa,\ \ \varphi|_{\overline{A}} \ge 1,\ \varphi = 0 \text{ in } B^c\right\}.$$

For example, if $u \equiv 1$ then $\operatorname{cap}_u^{(\kappa)}(A,B) = \operatorname{cap}(A,B)$.

Definition. $(\mathcal{E},\mathcal{F})$ satisfies the *generalized capacity condition* (Gcap) if $\exists \kappa \ge 1$, $C>0$ such that, for any $u \in \mathcal{F} \cap L^\infty$ and for any two balls $B_0 := B(x,R)$ and $B := B(x,R+r)$,

$$\operatorname{cap}_u^{(\kappa)}(B_0,B) \le \frac{C}{r^\beta}\int_B u^2 d\mu. \tag{Gcap}$$

Clearly, (Gcap)$\Rightarrow$(cap).

Estimating heat kernels: strongly local case

Assume that all metric balls in (M,d) a precompact. In this section, we assume in addition that (M,d) satisfies the *chain condition*: if $\exists C$ such that for all $x,y\in M$ and for $n\in\mathbb{N}$ there exists a sequence $\{x_k\}_{k=0}^{n}$ of points in M such that $x_0=x$, $x_n=y$, and

$$d(x_{k-1},x_k)\le C\frac{d(x,y)}{n},\quad \text{for all } k=1,...,n.$$

Let μ be an α-regular measure on M and $(\mathcal{E},\mathcal{F})$ be a strongly local regular Dirichlet form.

Definition. We say that $(\mathcal{E},\mathcal{F})$ satisfies the *Poincaré inequality* with exponent β if, for any ball $B=B(x,r)$ on M and for any function $f\in\mathcal{F}$,

$$\mathcal{E}_B(f,f):=\int_B d\Gamma(f,f)\ge\frac{c}{r^\beta}\int_{\varepsilon B}\left(f-\overline{f}\right)^2 d\mu, \tag{PI}$$

where $\overline{f}=⨍_{\varepsilon B} f\,d\mu$, and c,ε are small positive constants independent of B and f.

For example, in $\mathbb{R}^n$ (PI) holds with $\beta=2$ and $\varepsilon=1$.

Theorem 4 (AG, Jiaxin Hu, K.S.Lau '15)

$$(PI)+(\text{Gcap})\Leftrightarrow(sub).$$

Conjecture. $(PI)+(\text{cap})\Leftrightarrow(sub)$

Estimating heat kernels: jump case

Let now $(\mathcal{E}, \mathcal{F})$ be a jump type Dirichlet form given by

$$\mathcal{E}(f, f) = \iint\limits_{M\times M} (f(x) - f(y))^2 J(x, y) d\mu(x) d\mu(y),$$

where J is a symmetric jump kernel. We use the following condition instead of (PI):

$$J(x, y) \simeq d(x, y)^{-(\alpha+\beta)}. \tag{J}$$

Theorem 5 (AG, Eryan Hu, Jiaxin Hu '18 and Z.Q.Chen, T.Kumagai, J.Wang '20)

$$(J) + (\text{Gcap}) \Leftrightarrow (stable).$$

In the case $\beta < 2$ it is easy to show that $(J) \Rightarrow (\text{Gcap})$ so that in this case we obtain

$$(J) \Leftrightarrow (stable).$$

This equivalence was also proved by Chen and Kumagai '03, although under some additional assumptions about the metric structure of (M, d).

Conjecture. $(J) + (\text{cap}) \Leftrightarrow (stable)$.