Geometric characterization of Capacity

Benny Avelin (J. with Vesa Julin and Lauri Viitasaari)

CIRM: Analysis and simulations of metastable systems

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Consider the Kolmogorov process

$$dX_t = -\nabla F(X_t)dt + \sqrt{2\varepsilon}dB_t. \quad (1)$$

The generator is

$$L_\varepsilon = -\varepsilon\Delta + \nabla F \cdot \nabla.$$

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Consider now a ball of radius ε around each minima, and lets consider $h(x) = \mathbb{P}(\tau_{B_2} < \tau_{B_1})$

Then as we saw in Seo's lecture, L is self-adjoint w.r.t the Gibbs measure $e^{-F/\varepsilon}dx$ and we can arrive at the formula

$$\mathbb{E}^x[\tau_{B_1}] \approx \frac{\int_{B_1^c} he^{-F/\varepsilon}\,dx}{\text{cap}(B_2, B_1)}$$

Estimating capacity

In this case we have the identity

$$\mathrm{cap}(B_2, B_1) = \inf\left(\varepsilon \int |\nabla h|^2 e^{-\frac{F}{\varepsilon}}\, dx \;:\; h \geq 1 \text{ in } B_2, u \in H_0^1(B_1^c)\right).$$

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In the case when the saddle is non-degenerate (Hessian has a single negative eigenvalue), the capacity estimate looks like (Bovier et.al. -04)

$$\mathrm{cap}(B_\varepsilon(x_2), B_\varepsilon(x_1)) \simeq \varepsilon^{\frac{n}{2}} (2\pi)^{\frac{n-2}{2}} \frac{|\lambda_1(z)|\, e^{-\frac{F(z)}{\varepsilon}}}{\sqrt{|\det(\nabla^2 F(z))|}}$$

The capacity problem: Geometric function theory

Lets say we are interested in measuring the capacity of the pair (B_1, B_2)

In the standard case of the Laplacian, this is just

$$\mathrm{cap}(B_2, B_1) := \inf\left(\int |\nabla h|^2\, dx \ :\ h \geq 1 \text{ in } B_2, u \in H_0^1(B_1^c)\right).$$

Geometric function theory (Gehring -62, Ziemer -67)

Here, let Γ be a family of curves connecting the two sets B_1, B_2, then the modulus of Γ is the following quantity

$$\mathrm{mod}_2\Gamma := \inf_{\rho} \int_X \rho^2 dx \quad \text{(Väisälä -61)}$$

with constraint

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Think of $\rho = |\nabla h|$, and a curve being the flow line of h, then the constraint above is just the fundamental theorem of calculus and the value of the integral is just the capacity. That is,

$$\mathrm{mod}_2\Gamma = \mathrm{cap}(B_1, B_2)$$

There is a dual modulus defined for separating sets. We say that a set is separating if all paths $\gamma \in \Gamma$ must pass it. Denote the set of all separating sets as M, then the dual modulus is

$$\mathrm{mod}_{2^*}\Gamma := \inf_{\rho} \int_X \rho^2 dx \quad \text{(Sabat -60)}$$

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For a divergence free field F, the flow through each m is the same as the flow out of U_{x_1} and into U_{x_2}, and if we consider ρ on m to be $F \cdot n$, then the constraint is essentially telling us a minimal value of the flow. This is essentially Thomsons principle, i.e.

$$\mathrm{mod}_{2^*}\Gamma = \frac{1}{\mathrm{cap}(B_1, B_2)}$$

Gehring -62

Without normalization we can write all these things as

$$L(\rho) := \inf_{\gamma \in \Gamma} \int_\gamma \rho ds$$

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$$\inf_\rho \frac{\int_X \rho^2 dx}{L(\rho)^2} = \sup_\rho \frac{A(\rho)^2}{\int_X \rho^2 dx} = \mathrm{cap}(B_1, B_2)$$

Tubular case

If our domain X is tubular, i.e. we can "essentially" write it as $\gamma \times m$, where $\gamma \in \Gamma$ and $m \in M$, then

$$1 \leq \int_\gamma \rho ds \leq \left(\int_\gamma \rho^2 ds \right)^{1/2} \mathcal{H}^1(\gamma)^{1/2}$$

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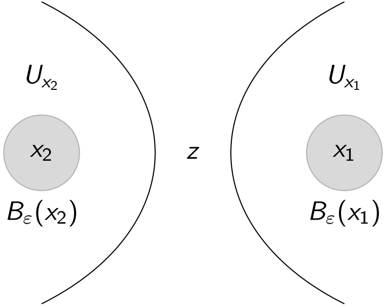
integrate both sides over a separating surface m

$$\frac{\mathcal{H}^{n-1}(m)}{\mathcal{H}^1(\gamma)} \leq \int_X \rho^2 dx$$

Geometric setup: Returning to metastability

Define the sub-levelset $U_{-\delta} = \{x : F(x) < -\delta\}$, let $U_{x_1} \cup U_{x_2} = U_{-\delta}$ be the connected components.



If we assume for a saddle $z = 0$, $F(z) = 0$ there is a coordinate system such that

$$|F(y) + g_z(y_1) - G_z(y')| \leq \omega(g_z(y_1)) + \omega(G_z(y'))$$

where g_z, G_z are convex functions that have their minimum at 0, ω is an increasing function satisfying

$$\lim_{s \to 0} \frac{\omega(s)}{s} = 0.$$

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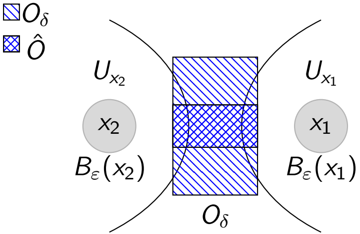
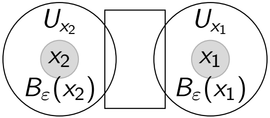
Then we can construct a bridge between U_{x_1}, U_{x_2} of the form

$$O_\delta = \{y_1 : g(y_1) < 3\delta\} \times \{y' \in \mathbb{R}^{n-1} : G(y') < 3\delta\}$$



Local domain, curve families and separating sets

We define $\Omega_\delta = U_{-\delta} \cup O_\delta$ that is, the two components + the bridge.



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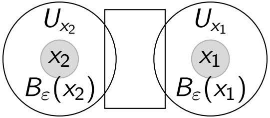

Let Γ be the set of curves going from $B_\varepsilon(x_1)$ to $B_\varepsilon(x_2)$ while staying inside Ω_δ. Consider the set of all smooth hypersurfaces M with the property that every curve must pass each set, we call these the **separating sets**.

Weighted length and area

Geodesic distance, replaces $\mathcal{H}(\gamma)$

$$d_\varepsilon(B_\varepsilon(x_1), B_\varepsilon(x_2)) = \inf_{\gamma\in\Gamma} \int_\gamma e^{F(x)/\varepsilon} d\mathcal{H}^1(x). \tag{2}$$

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Minimal cut, replaces $\mathcal{H}^{n-1}(m)$

$$V_\varepsilon(B_\varepsilon(x_1), B_\varepsilon(x_2)) = \inf_{m \in M} \int_m e^{-F(x)/\varepsilon} d\mathcal{H}^{n-1}. \tag{3}$$

Main result

Theorem (Avelin, Julin, Viitasaari -22)

In the case of two minimas x_1, x_2 and a saddle z satisfying the above condition, and Ω as before, then

$$\mathrm{cap}(B_\varepsilon(x_1), B_\varepsilon(x_2)) \simeq \epsilon \frac{V_\varepsilon(B_\varepsilon(x_1), B_\varepsilon(x_2))}{d_\varepsilon(B_\varepsilon(x_1), B_\varepsilon(x_2))} e^{F(z)/\varepsilon}$$

Where $\simeq$ means that the comparison constant approaches 1 as $\varepsilon \to 0$.

Idea of the proof (lower bound)

- Localize the energy to the bridge
- Characterize the energy of the saddle in terms of the saddle expansion
- Characterize these integrals geometrically

Localizing the energy around the saddle

Lets go back to our weighted setting, assume for simplicitly that the saddle $z = 0$ we have $F(0) = 0$ Then by simply constructing a proposal function we immediately get

$$\operatorname{cap}(B_2, B_1) \lesssim \varepsilon^{-q}$$

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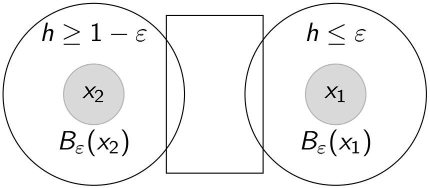
Now, regularity theory of the equation $Lh = 0$ gives that

$$\text{osc}_{U_{x_1}} h \leq \varepsilon$$

for ε small enough.


$h \geq 1 - \varepsilon$
x_2
$B_\varepsilon(x_2)$
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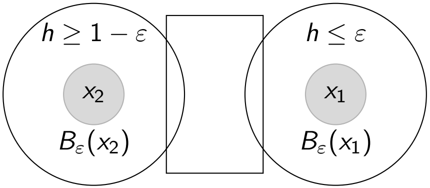

Fundamental theorem of calculus gives

$$
\begin{aligned}
1 - 2C\varepsilon &\leq \int_{\{g<\delta\}} \partial_{x_1} h(x)\, dx_1 = \int_{\{g<\delta\}} \partial_{x_1} h(x) e^{-\frac{F(x)}{2\varepsilon}} e^{\frac{F(x)}{2\varepsilon}}\, dx_1 \\
&\leq \left(\int_{\{g<\delta\}} |\nabla h(x)|^2 e^{-\frac{F(x)}{\varepsilon}}\, dx_1 \right)^{\frac{1}{2}} \left(\int_{\{g<\delta\}} e^{\frac{F(x)}{\varepsilon}}\, dx_1 \right)^{\frac{1}{2}}.
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Then integrating w.r.t x' we get

$$\int_{\hat{O}} |\nabla h_{A,B}|^2 e^{-\frac{F(x)}{\varepsilon}}\, dx \geq \frac{\int_{G<\delta/100} e^{-G(x')/\varepsilon} dx'}{d_\varepsilon(B_2, B_1)}$$

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The lower bound now follows from characterizing the integral

$$\int_{G<\delta/100} e^{-G(x')/\varepsilon} dx' \approx V_\varepsilon(B_2, B_1)$$

Characterizing the geometric quantities

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$$V_\varepsilon(B_\varepsilon(x_1), B_\varepsilon(x_2)) = \inf_{m \in M} \int_m e^{-F(x)/\varepsilon} d\mathcal{H}^{n-1}. \tag{6}$$

The hyperplane $\{y_1 = 0\}$ is separating so that gives the upper bound.

$$V_\varepsilon(B_2, B_1) \leq \int e^{-G(x')/\varepsilon} dx' \approx \int_{G<\delta/100} e^{-G(x')/\varepsilon} dx' \leq C$$

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For the lower bound, for a separating surface m that almost minimizes the area, it cuts our set into two parts, call one of the $\hat{U}_{x_1}$, then define

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for $\rho = \varepsilon^2$.

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$$v_\rho(x) = \frac{|B_\rho(x) \cap \hat{U}_{x_1}|}{|B_\rho|}$$

for $\rho = \varepsilon^2$. Since you can write v_ρ as a mollification of $\chi_{\hat{U}_{x_1}}$ we can estimate

$$\int_{\hat{O}} |\nabla v_\rho| e^{-F/\varepsilon} dx \lesssim \int |\nabla \chi_{\hat{U}_{x_1}}| e^{-F/\varepsilon} dx$$

Now by the relative isoperimetric inequality we can say that

$$\begin{aligned}\mathcal{H}^{n-1}\big(\partial\hat{U}_{x_1}\cap B_\rho(x)\big) &\geq c\min\big\{|B_\rho(x)\cap\hat{U}_{x_1}|^{\frac{n-1}{n}},|B_\rho(x)\setminus\hat{U}_{x_1}|^{\frac{n-1}{n}}\big\}\\ &\geq c\,\varepsilon^{2(n-1)}\min\big\{v_\rho(x),1-v_\rho(x)\big\}^{\frac{n-1}{n}}.\end{aligned}$$

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\end{aligned}
$$

for $x \in U_{x_1} \subset U_{-\delta}$ we have

$$
\mathcal{H}^{n-1}\big(\partial \hat{U}_{x_1} \cap B_\rho(x)\big) \leq e^{\frac{F(0)}{\varepsilon}} e^{-\frac{\delta}{4\varepsilon}} \int_{\partial \hat{U}_{x_1} \cap B_\rho(x)} e^{-\frac{F}{\varepsilon}}\, d\mathcal{H}^{n-1} \lesssim e^{-\delta/\varepsilon}
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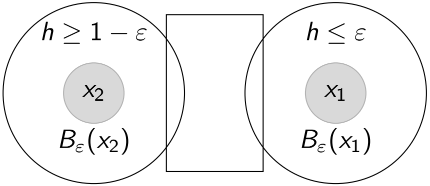

Fundamental theorem of calculus again gives

$$1 - 2C\varepsilon \leq \int_{\{g<\delta\}} \partial_{y_1} v_\rho(y_1, y')\, dy_1. \tag{7}$$

Thus simply multiplying with $e^{-G(y')/\varepsilon}$ on both sides gives

$$(1 - 2C\varepsilon) \int e^{-G(y')/\varepsilon} dy' \leq \int |\partial_{y_1} v_\rho(y_1, y')|\, e^{-G(y')/\varepsilon} dy_1 \leq \int |\nabla v_\rho(y_1, y')|\, e^{-F(y)/\varepsilon} dy$$

which is the lower bound.

Thank you for your attention