

Diffusion Kernels on q -Gaussian Manifold

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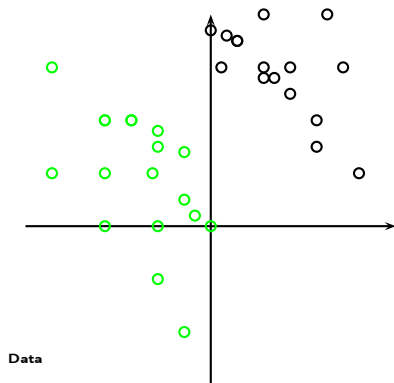
Doctoral Seminar 2
Universidad EAFIT
Department of Mathematical Sciences
PhD in Mathematical Engineering

Objetive of the presentation

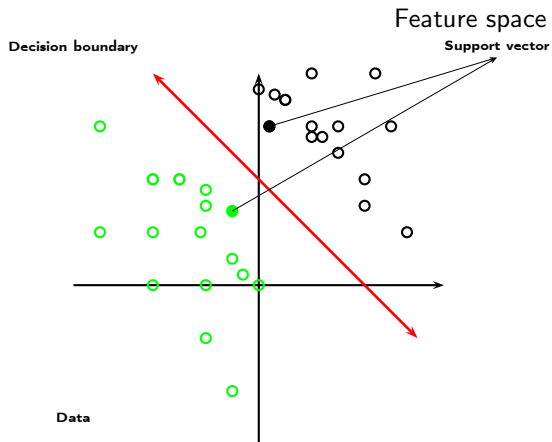
A diffusion kernel is a term coined by Laferty (2005) and it alludes to a Mercer kernel (or classifier in the context of Machine Learning), this results from solving the heat equation (diffusion equation) in the modeled manifold in the data set that have a known distribution (multinomial, gaussian, q -gaussian, etc.). In this short presentation the path that has been developed to obtain a diffusion kernel will be shown with the hypothesis that the data have a q -gaussian distribution with parameters (μ, σ) .

Example Support Vector Machine (SVM)

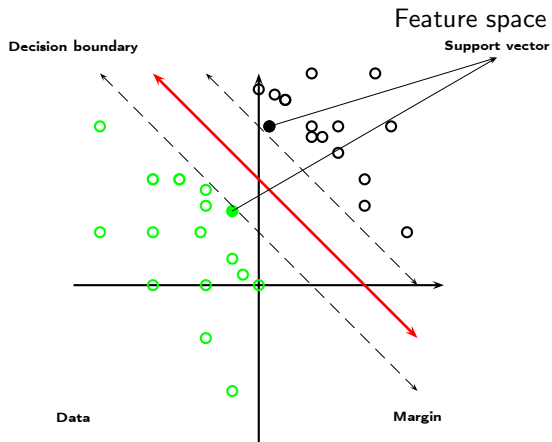
Feature space



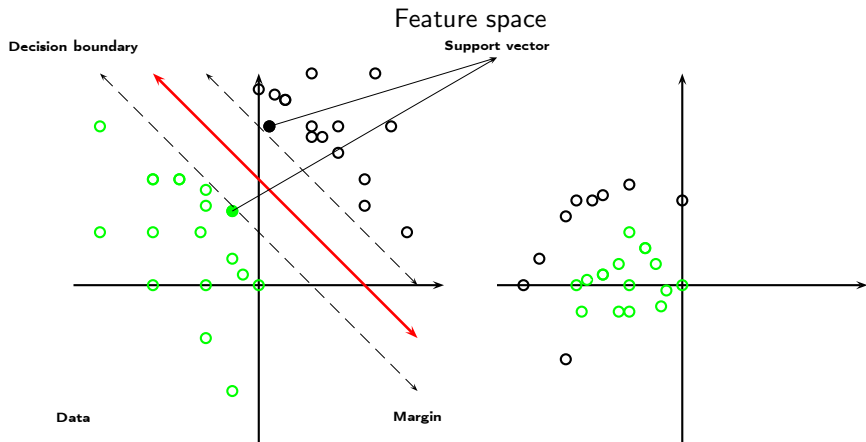
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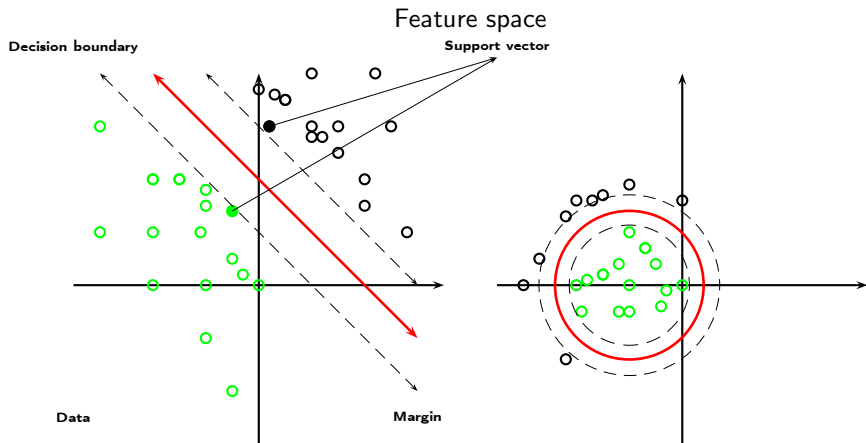


Figure 1: Ideas about the operation of SVM

Concepts, notations and equations of interest

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- ★ $\ell = \log p$: Score function, logarithm of the probability distribution.

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$$\Delta_g f = \frac{1}{\sqrt{\det g}} \sum_j \frac{\partial}{\partial x_j} \left(\sum_i g^{ij} \sqrt{\det g} \frac{\partial f}{\partial x_i} \right) ,$$

g^{ij} are the components of the inverse of the metric $g = [g_{ij}]$.

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★ $\Gamma_{ij,k}$: Christoffel symbols, defined as

$$\Gamma_{ij,k} = \sum_{h=1}^n \frac{1}{2} [\partial_i g_{jh} + \partial_j g_{ih} - \partial_h g_{ij}] g^{hk} .$$

Concepts, notations and equations of interest

- ★ R^l_{ijk} : Components of the metric tensor, are calculated by means of the expression

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- ★ **Geodesic curve**: It is obtained by solving the system of homogeneous second order differential equations

$$\frac{d\theta_k}{dt} + \sum_{i,j=1}^n \Gamma_{ij,k} \frac{d\theta_i}{dt} \frac{d\theta_j}{dt}$$

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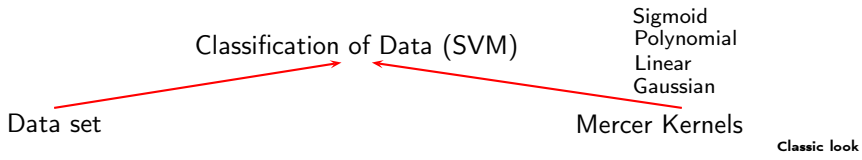
- ★ ρ : Geodesic distance, parametrizing the geodesic curve as $\gamma(t)$, this distance is

$$\rho = \int_a^b \sqrt{g_\gamma(\dot{\gamma}, \dot{\gamma})} dt$$

where $\dot{\gamma}$ is the derivate of γ with respect to t .

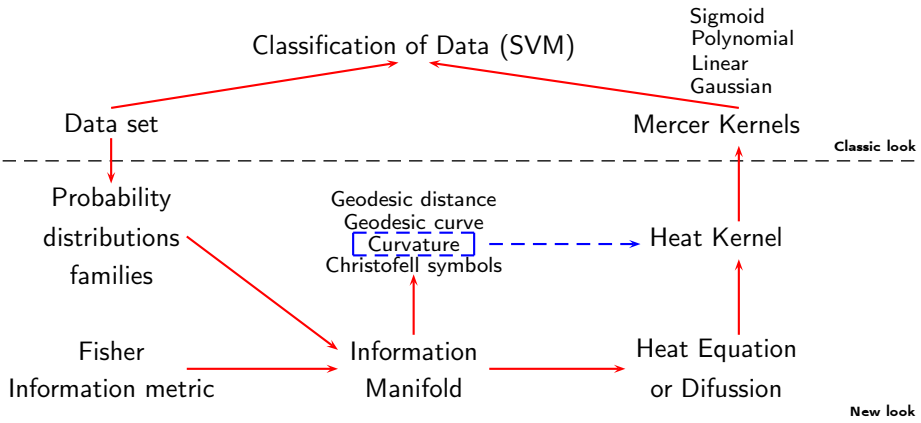
Way to obtain a diffusion kernel

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- 1 In the case of the Euclidean space \mathbb{R}^n , the Heat Kernel is given by

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

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- 2 On the hyperbolic space \mathbb{H}^n , the heat kernel is given by

$$K_t(x, x') = \begin{cases} \frac{(-1)^m}{(2\pi)^m} \frac{1}{\sqrt{4\pi t}} \left(\frac{1}{\sinh \rho} \frac{\partial}{\partial \rho}\right)^m \exp\left(-m^2 t - \frac{\rho^2}{4t}\right) & \text{If } n = 2m + 1 \\ \frac{(-1)^m}{(2\pi)^m} \frac{\sqrt{2}}{\sqrt{(4\pi t)^3}} \left(\frac{1}{\sinh \rho} \frac{\partial}{\partial \rho}\right)^m \int_{\rho}^{\infty} \frac{s \exp\left(-\frac{(2m+1)^2 t}{4} - \frac{s^2}{4t}\right)}{\sqrt{\cosh s - \cosh \rho}} ds & \text{If } n = 2m + 2 \end{cases}$$

where $\rho = d(x, x')$ is the geodesic distance between the two points in the plane \mathbb{H}^n . If $n = 2$ ($m = 0$ in the second case) then

$$K_t(x, x') = \frac{\sqrt{2}}{(4\pi t)^{\frac{3}{2}}} \exp\left(-\frac{t}{4}\right) \int_{\rho}^{\infty} \frac{s \exp\left(-\frac{s^2}{4t}\right)}{\sqrt{\cosh s - \cosh \rho}} ds.$$

Tsallis entropy

In the context of non-extensive statistical mechanics, Constantino Tsallis (in 1988) defines entropy relative to q as

$$S_q = \frac{1}{1-q} \left(\sum_i p_i^q - 1 \right) = \frac{1}{1-q} (h_q - 1)$$

where $\sum_i p(x_i) = \sum_i p_i = 1$, q is a fixed value less than 3 called **entropy index** and h_q is the functional $h_q = E[p^q]$ ($E[\cdot]$ it can be summation or integral) that allows defining an expected value relative to q . So, if $q \rightarrow 1$ the Shannon entropy

$$S = - \sum_i p(x_i) \log p(x_i)$$

used in classical statistical mechanics is obtained.

The description makes sense when defining a pair of inverse functions one of the other, called q -exponential and q -logarithm that generalize the exponential and the logarithm, recovering these when q tends to 1.

The q -exponential function

The q -exponential function is defined as

$$\exp_q(x) = [1 + (1 - q)x]_+^{\frac{1}{1-q}}$$

for $-\infty < q < 3$. The derivative for a fixed q value is

$$\frac{d}{dx} \exp_q(x) = [\exp_q(x)]^q .$$

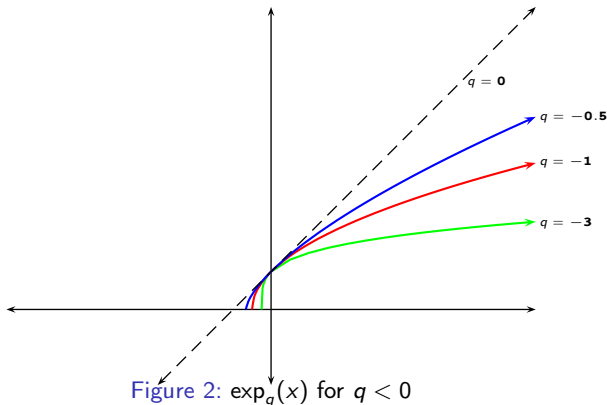
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Graphs for the function q -exponential

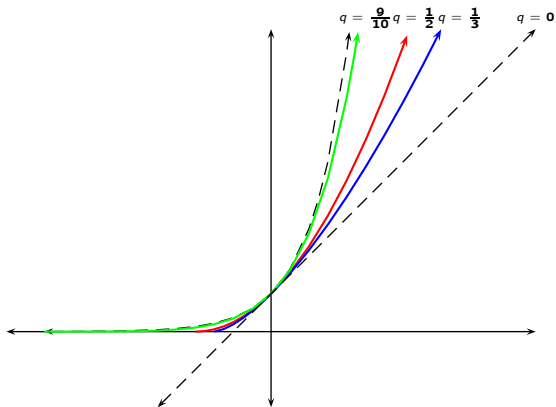


Figure 3: $\exp_q(x)$ for $0 < q < 1$

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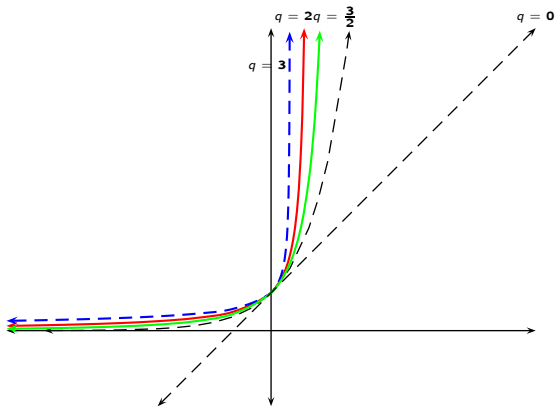


Figure 4: $\exp_q(x)$ for $1 < q < 3$

The q -logarithm function

The inverse of the q -exponential function, the q -logarithm, is given by

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q}$$

provided that $x > 0$. The graph for some values of q is presented below, as well as its derivative for q fixed.

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$$\frac{d}{dx} [\log_q(x)] = \frac{1}{x^q}$$

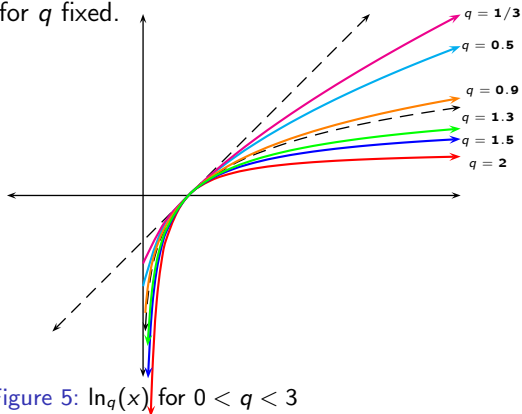


Figure 5: $\ln_q(x)$ for $0 < q < 3$

q -Gaussian Distribution

The q -gaussian distribution has density function

$$p_q(x, \theta) = \frac{1}{Z_{q,\sigma}} \exp_q \left(-\frac{(x - \mu)^2}{(3 - q)\sigma^2} \right) = \frac{1}{Z_{q,\sigma}} \left[1 - \frac{(1 - q)(x - \mu)^2}{(3 - q)\sigma^2} \right]^{\frac{1}{1 - q}}$$

where $\theta = (\mu, \sigma)$ are the parameters on which the manifold of information is defined, $Z_{q,\sigma}$ is the normalization constant that depends on q , is written as $Z_{q,\sigma} = A_q \sigma$.

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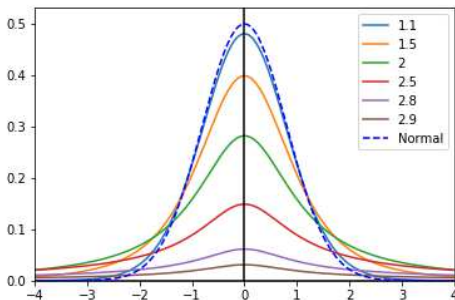


Figure 6: q -gaussian distribution

Normalization constant

The normalization constant is obtained by satisfying the expression

$$\int_{-\infty}^{\infty} f(x)dx = 1 \text{ or } Z_{q,\sigma} = \int_{-\infty}^{\infty} \left[1 - \frac{(1-q)(x-\mu)^2}{(3-q)\sigma^2} \right]^{\frac{1}{1-q}} dx .$$

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By means of a variable change, the constant A_q is defined in terms of the Beta function (or the Gamma function) for some values of q

- 1 $A_q = \sqrt{\frac{3-q}{1-q}} B\left(\frac{2-q}{1-q}, \frac{1}{2}\right)$ if $-\infty < q < 1$. In this situation the admissible domain for x is $\left[-\frac{\sigma}{\sqrt{1-q}}, \frac{\sigma}{\sqrt{1-q}}\right]$.
- 2 $A_q = \sqrt{2\pi}$ if $q = 1$.
- 3 $A_q = \sqrt{\frac{3-q}{q-1}} B\left(\frac{3-q}{2(q-1)}, \frac{1}{2}\right)$ if $1 < q < 3$. The domain for x are all real numbers.

Particular cases

- 1 Gaussian distribution ($q = 1$).
- 2 Cauchy distribution ($q = 2$).
- 3 t -Students distribution ($q = 1 + \frac{2}{n+1}$ with $n \in \mathbb{N}$).
- 4 Uniform distribution ($q \rightarrow -\infty$).
- 5 Wigner semicircle distribution ($q = -1$).

The q -gaussian distribution belong an exponential family

According to the definition of the function q -logarithm applied to the q -gaussian distribution it is possible to write

$$\log_q p_q = \frac{1}{1-q} \left(\left(\frac{1}{Z_{q,\sigma}} \exp_q \left(-\frac{(x-\mu)^2}{(3-q)\sigma^2} \right) \right)^{1-q} - 1 \right),$$

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 &= \underbrace{\frac{Z_{q,\sigma}^{q-1}}{3-q} \frac{2\mu}{\sigma^2}}_{\theta_1} \underbrace{x}_{F_1(x)} + \underbrace{\frac{Z_{q,\sigma}^{q-1}}{3-q} \frac{1}{\sigma^2}}_{\theta_2} \underbrace{(-x^2)}_{F_2(x)} - \underbrace{\left[\frac{Z_{q,\sigma}^{q-1}}{3-q} \frac{\mu^2}{\sigma^2} - \log_q \left(\frac{1}{Z_{q,\sigma}} \right) \right]}_{\psi_q(\mu,\sigma)}, \\
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Then the q -gaussian distribution is an element in the family q -exponential with parameters and function q -potential

$$\begin{aligned} \theta_1 &= \frac{Z_{q,\sigma}^{q-1}}{3-q} \frac{2\mu}{\sigma^2}, & \theta_2 &= -\frac{Z_{q,\sigma}^{q-1}}{3-q} \frac{1}{\sigma^2}, \\ \psi_q(\theta_1, \theta_2) &= -\frac{\theta_1^2}{4\theta_2} - \log_q \left[(-d_q \theta_2)^{\frac{1}{3-q}} \right], & \text{with } d_q &= \frac{3-q}{A_q^2}. \end{aligned}$$

Fisher's metrics and its representations

On the manifold defined by the q -gaussian distribution, it is possible to define two metrics. To do this, Amari (2009) defines the functional Ω_q for a probability distribution p as

$$\Omega_{q,p} = \int_{\Omega} p^q d\mu ,$$

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along with the q -expectation

$$E[f(x)] = \int_{\Omega} f(x) \hat{p}_q d\mu = \frac{1}{\Omega_{q,p}} \int_{\Omega} f(x) p^q d\mu .$$

For the q -gaussian distribution the relation is fulfilled (Tanaya, 2011)

$$\Omega_{q,p} = \frac{3-q}{2} Z_{q,p}^{1-q} = \frac{3-q}{2} A_q^{1-q} \sigma^{1-q} .$$

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One of the metrics defined in the manifold is the usual Fisher g_{ij}^F induced by the Score function $\ell = \log p_q$ and the other is the q -Fisher's metric defined by Amari (2009) and what can be written about the distribution \hat{p} as

$$g_{ij}^{(q)} = E_{\hat{p}} [(\partial_i \ell_q) (\partial_j \ell_q) q p^{q-1}] = \frac{q}{\Omega_{q,p}} \int_{\Omega} (\partial_i \ell_q) (\partial_j \ell_q) p^{2q-1} d\mu .$$

where $\ell_q = \log_q p_q$.

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It is also shown that Fisher's q -metric is of the form

$$g_{ij}^{(q)} = \partial_i \partial_j \psi_q$$

which induces a Hessian manifold. Deriving the function q -potential in terms of parameters θ_1 and θ_2 we get the matrix $g^{(q)}$ and by a change of coordinates it is possible to obtain a matrix diagonal $g_*^{(q)}$.

q -Fisher's metrics and its matrix representations

$\psi_q(\theta_1, \theta_2) = -\frac{\theta_1^2}{4\theta_2} - \log_q \left (-d_q \theta_2)^{\frac{1}{3-q}} \right $	
Coordinates (θ_1, θ_2)	Coordinates (μ, σ)
$g^{(q)} = \begin{bmatrix} \frac{-1}{2\theta_2} & \frac{\theta_1}{2\theta_2^2} \\ \frac{\theta_1}{2\theta_2^2} & -\frac{\theta_1^2}{2\theta_2^3} + \frac{1}{3-q} \frac{\Omega_{q,\theta_2}^{-1}}{\theta_2^2} \end{bmatrix}$	$g_*^{(q)} = \begin{bmatrix} \frac{\Omega_{q,\sigma}^{-1}}{\sigma^2} & 0 \\ 0 & \frac{(3-q)\Omega_{q,\sigma}^{-1}}{\sigma^2} \end{bmatrix}$
$\det(g^{(q)}) = \frac{1}{2(3-q)} \frac{\Omega_{q,\theta_2}^{-1}}{(-\theta_2)^3}$	$\det(g_*^{(q)}) = \frac{(3-q)\Omega_{q,\sigma}}{\sigma^4}$
$[g^{(q)}]^{-1} = \begin{bmatrix} (3-q)\Omega\theta_1^2 - 2\theta_2 & (3-q)\Omega\theta_1\theta_2 \\ (3-q)\Omega\theta_1\theta_2 & (3-q)\Omega\theta_2^2 \end{bmatrix}$	$[g_*^{(q)}]^{-1} = \begin{bmatrix} \Omega\sigma^2 & 0 \\ 0 & \frac{\Omega\sigma^2}{3-q} \end{bmatrix}$

Fisher's metrics and its matrix representations

$$\psi_q(\theta_1, \theta_2) = -\frac{\theta_1^2}{4\theta_2} - \log_q \left[(-d_q \theta_2)^{\frac{1}{3-q}} \right]$$

$$g_{ij}^F = \frac{\Omega_{q,p}}{q} g_{ij}^{(q)}$$

Coordinates (θ_1, θ_2)	Coordinates (μ, σ)
$g^F = \begin{bmatrix} \frac{-\Omega}{2q\theta_2} & \frac{\Omega\theta_1}{2q\theta_2^2} \\ \frac{\Omega\theta_1}{2q\theta_2^2} & -\frac{\Omega\theta_1^2}{2q\theta_2^3} + \frac{1}{q(3-q)} \frac{1}{\theta_2^2} \end{bmatrix}$	$g_*^F = \begin{bmatrix} \frac{1}{q\sigma^2} & 0 \\ 0 & \frac{3-q}{q\sigma^2} \end{bmatrix}$
$\det(g^{(q)}) = \frac{1}{2q^2(3-q)} \frac{\Omega}{(-\theta_2)^3}$	$\det(g_*^F) = \frac{3-q}{q^2\sigma^4}$
$[g^F]^{-1} = \begin{bmatrix} (3-q)q\theta_1^2 - \frac{2q\theta_2}{\Omega} & (3-q)q\theta_1\theta_2 \\ (3-q)q\theta_1\theta_2 & (3-q)q\theta_2^2 \end{bmatrix}$	$[g_*^F]^{-1} = \begin{bmatrix} q\sigma^2 & 0 \\ 0 & \frac{q}{3-q}\sigma^2 \end{bmatrix}$

Christoffel symbols and curvature

Deriving the components of the matrix g_*^F regarding the parameters (μ, σ) , it is possible to obtain the Christoffel symbols as summarized in continuation

Derivadas de las componentes de la métrica

$\partial_1 g_{11}^F = 0$	$\partial_1 g_{12}^F = 0$	$\partial_1 g_{21}^F = 0$	$\partial_1 g_{22}^F = 0$
$\partial_2 g_{11}^F = -\frac{2}{q\sigma^3}$	$\partial_2 g_{12}^F = 0$	$\partial_2 g_{21}^F = 0$	$\partial_2 g_{22}^F = -\frac{2(3-q)}{q\sigma^3}$

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Christoffel symbols

$\Gamma_{11,1}^F = 0$	$\Gamma_{11,2}^F = \frac{1}{(3-q)\sigma}$	$\Gamma_{12,1}^F = -\frac{1}{\sigma}$	$\Gamma_{12,2}^F = 0$
$\Gamma_{21,1}^F = -\frac{1}{\sigma}$	$\Gamma_{21,2}^F = 0$	$\Gamma_{22,1}^F = 0$	$\Gamma_{22,2}^F = -\frac{1}{\sigma}$

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Metric Tensor

$R_{212}^1 = \frac{1}{\sigma^2}$	$R_{212}^2 = 0$	$R_{1212} = g_{11} R_{212}^1 = -\frac{1}{q\sigma^4}$
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Curvature and Geometry

$k = \frac{R_{1212}}{\det(g_*^F)} = -\frac{q}{3-q} < 0$	Negative constant curvature (hyperbolic space)
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Geodesic curves

Assuming that the coordinates (μ, σ) can be parametric depending on t and with the Christoffel symbols previously found, it is possible to define a system of homogeneous second order differential equations that describes the geodesic curves for the hyperbolic manifold generated by the q -gaussian distribution

$$\frac{d^2\mu}{dt^2} - \frac{2}{\sigma} \frac{d\mu}{dt} \frac{d\sigma}{dt} = 0$$
$$\frac{d^2\sigma}{dt^2} + \frac{1}{(3-q)\sigma} \left(\frac{d\mu}{dt}\right)^2 - \frac{1}{\sigma} \left(\frac{d\sigma}{dt}\right)^2 = 0.$$

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With the substitution $w = \frac{d\mu}{d\sigma}$ it is possible to show that the curve that solves this system is

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Assuming that the coordinates (μ, σ) can be parametric depending on t and with the Christoffel symbols previously found, it is possible to define a system of homogeneous second order differential equations that describes the geodesic curves for the hyperbolic manifold generated by the q -gaussian distribution

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With the substitution $w = \frac{d\mu}{d\sigma}$ it is possible to show that the curve that solves this system is

$$(\mu - h)^2 + (3 - q)\sigma^2 = \frac{3 - q}{k^2}$$

where h and k are constants that possibly depend on q . This curve is an ellipse with center in $(h, 0)$, that is, on the axis μ . If $q = 2$ (Cauchy distribution) the curves are circumferences of radio $\frac{1}{k}$.

Further works

- ★ Find the geodesic distance for a q -gaussian distribution for any $1 < q < 3$.
- ★ The Box-Muller method is applicable for q -gaussian distribution (Thistleton, 2007) generating random data with this distribution.
- ★ Program in Python these diffusion kernels for the manifold generated by the q -gaussian distribution.
- ★ Define appropriate Christoffel symbols for the q -metric that allow me to find the curvature for the system (μ, σ) and that is in accordance with the result $k = \frac{5-3q}{(q-3)^2(2q-3)}$ (Matsuzoe, 2014).
- ★ Study another way to find distances by means of the heat equation (Keenan, 2013).

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Thank you!!