Diffusion Kernels on $q$-Gaussian Manifold

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Objective 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 $(\mu, \sigma)$. 
Example Support Vector Machine (SVM)

Feature space

Data
Example Support Vector Machine (SVM)

Feature space

Decision boundary

Support vector

Data
Example Support Vector Machine (SVM)

Feature space

Decision boundary
Support vector
Data
Margin
Example Support Vector Machine (SVM)

- Feature space
- Decision boundary
- Support vector
- Data
- Margin
Figure 1: Ideas about the operation of SVM
Concepts, notations and equations of interest

⋆ $p(x, \theta)$: Probability distribution for $x$ a random variable in $\Omega$ y $\theta$ a vector of parameters in $\mathbb{R}^n$. 
Concepts, notations and equations of interest

☆ \( p(x, \theta) \): Probability distribution for \( x \) a random variable in \( \Omega \) and \( \theta \) a vector of parameters in \( \mathbb{R}^n \).

☆ \( \psi(\theta) \): Potential function, it results from writing the distribution \( p(x, \theta) \) as \( p(x, \theta) = \exp(F(x) \cdot \theta - \psi(\theta)) \) called exponential family, where \( F(x) = (F_1(x), F_2(x), \ldots, F_n(x)) \) and \( \theta = (\theta_1, \theta_2, \ldots, \theta_n) \).
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★ \( E[f(x)] \): Expected value with respect to the distribution \( p \) for a function \( f(x) \), is written

\[
E[f(x)] = \int_{\Omega} f(x)p d\mu
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- **$\partial_i f(x)$**: Partial derivative of $f(x)$ with respect to the $i$-th component of the vector $\theta$, is written

$$\partial_i f(x) = \frac{\partial f(x)}{\partial \theta_i}.$$
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★ \( \ell = \log p \): Score function, logarithm of the probability distribution.
Concepts, notations and equations of interest

* $g^F_{ij}$: Components of Fisher’s metric, defined as

$$g^F_{ij} = \int_\Omega (\partial_i \ell) (\partial_j \ell) \, pd\mu.$$

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Diffusion Kernels on $q$-Gaussian Manifold
Concepts, notations and equations of interest

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- $\frac{\partial f}{\partial t} = \Delta_g f$: Heat equation or diffusion equation where $\Delta$ is the operator Laplace - Beltrami defined in terms of the metric as

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

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

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where \( g^{ij} \) are the components of the inverse of the metric \( g = [g_{ij}] \).

- \( \Gamma_{ij,k} \): Christoffel symbols, defined as

\[
\Gamma_{ij,k} = \sum_{h=1}^n \frac{1}{2} \left[ \partial_i g_{jh} + \partial_j g_{ih} - \partial_h g_{ij} \right] g^{hk}.
\]
Concepts, notations and equations of interest

- $R_{ijk}^l$: Components of the metric tensor, are calculated by means of the expression

$$R_{ijk}^l = \sum_{h=1}^{n} \left[ \Gamma_{ik}^h \Gamma_{jh}^l - \Gamma_{jk}^h \Gamma_{ih}^l \right] + \partial_j \Gamma_{ik}^l - \partial_i \Gamma_{jk}^l.$$
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\]

\( \text{Geodesic curve} \): It is obtained by solving the system of homogeneous second order differential equations

\[
\frac{d\theta_{k}}{dt} + \sum_{i,j=1}^{n} \Gamma_{ij,k} \frac{d\theta_{i}}{dt} \frac{d\theta_{j}}{dt}
\]

where each \( \theta_{i} \) are the components of the parameter \( \theta \).
Concepts, notations and equations of interest

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where each $\theta_i$ are the components of the parameter $\theta$.

★ $\rho$: Geodesic distance, parametrizing the geodetic 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 $\gamma$ with respect to $t$. 
Way to obtain a diffusion kernel

Lafferty and Lebanon propose in their article *Diffusion Kernels on Statistical Manifold* (Laferty and Lebanon, 2005) the following way of work:

- **Data set**
- **Classification of Data (SVM)**
- **Mercer Kernels**
  - Sigmoid
  - Polynomial
  - Linear
  - Gaussian

*Classic look*
Way to obtain a diffusion kernel

Lafferty and Lebanon propose in their article *Diffusion Kernels on Statistical Manifold* (Lafferty and Lebanon, 2005) the following way of work.
In the case of the Euclidean space $\mathbb{R}^n$, the Heat Kernel is given by

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

where $\|x - y\|^2$ is the square of the Euclidean distance (geodesic distance) between points $x$ and $y$. 
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On the hyperbolic space $\mathbb{H}^n$, the heat kernel is given by

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

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

$$K_t(x, x') = \frac{\sqrt{2}}{(4\pi t)^{3/2}} \exp \left(-\frac{t}{4}\right) \int_\rho^\infty s \exp \left(-\frac{s^2}{4t}\right) \frac{ds}{\sqrt{\cosh s - \cosh \rho}}$$
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 $q \to 1$ 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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Figure 2: $\exp_q(x)$ for $q < 0$
Graphs for the function $q$-exponential

Figure 3: $\exp_q(x)$ for $0 < q < 1$
Graphs for the function $q$-exponential

$\exp_q(x)$ 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 $Z_{q,\sigma} = A_q \sigma$. 
**q-Gaussian Distribution**

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**Figure 6: $q$-gaussian distribution**
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 \( q \):

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

- Gaussian distribution \((q = 1)\).
- Cauchy distribution \((q = 2)\).
- \(t\)-Students distribution \((q = 1 + \frac{2}{n+1} \text{ with } n \in \mathbb{N})\).
- Uniform distribution \((q \to -\infty)\).
- 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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$$= \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \left\{ \theta_1 \exp_{q} \left( \frac{2\mu x}{3-q \sigma^2} \right) + \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \left( -\frac{x^2}{3-q \sigma^2} \right) \right\} - \left[ \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \frac{\mu^2}{\psi_q(\mu,\sigma)} - \log_q \left( \frac{1}{Z_{q,\sigma}} \right) \right] ,$$

$$= \theta_1 F_1(x) + \theta_2 F_2(x) - \psi_q(\mu,\sigma) .$$
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

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$$= \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \underbrace{2\mu}_\theta_1 \underbrace{F_1(x)}_{\theta_1} + \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \underbrace{1}_{\theta_2} \underbrace{(-x^2)}_{\theta_2} - \left[ \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} \underbrace{\mu^2}_{\psi_q(\mu, \sigma)} - \log_q \left( \frac{1}{Z_{q,\sigma}} \right) \right],$$

$$= \theta_1 F_1(x) + \theta_2 F_2(x) - \psi_q(\mu, \sigma).$$

Then the $q$-gaussian distribution is an element in the family $q$-exponential with parameters and function $q$-potential

$$\theta_1 = \frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} 2\mu , \quad \theta_2 = -\frac{Z_{q,\sigma}^{-1}}{3-q \sigma^2} 1 ,$$

$$\psi_q(\theta_1, \theta_2) = -\frac{\theta_1^2}{4\theta_2} - \log_q \left[ \left( -d_q \theta_2 \right)^{\frac{1}{3-q}} \right], \quad \text{with} \quad d_q = \frac{3-q}{A_q^2}.$$
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 $\Omega_q$ for a probability distribution $p$ as

$$\Omega_{q,p} = \int_{\Omega} p^q d\mu ,$$
Fisher’s metrics and its representations

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it allows to define a probability distribution $q$-relative

$$\hat{p}_q = \frac{1}{\Omega_{p,q}} p^q \quad \text{where} \quad \int_{\Omega} \hat{p} d\mu = 1.$$
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it allows to define a probability distribution $q$-relative

$$\hat{p}_q = \frac{1}{\Omega_{p,q}} p^q$$

where

$$\int_{\Omega} \hat{p} d\mu = 1.$$

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)

$$\Omega_{q,p} = \frac{3-q}{2} Z_{q,p}^{1-q} = \frac{3-q}{2} A_q^{1-q} \sigma^{1-q}.$$
Fisher’s metrics and its representations

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

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

where $\ell_q = \log_q p_q$. 
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where $\ell_q = \log_q p_q$. The two metrics are related by means of equality (Amari 2009)

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\[
g_{ij}^{(q)} = E_{\hat{p}} \left[ (\partial_i \ell_q) (\partial_j \ell_q) q p^{q-1} \right] = \frac{q}{\Omega_{q,p}} \int_{\Omega} (\partial_i \ell_q) (\partial_j \ell_q) p^{2q-1} d\mu.
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where \( \ell_q = \log_q p_q \). The two metrics are related by means of equality (Amari 2009)

\[
g_{ij}^{(q)} = \frac{q}{\Omega_{q,p}} g_{ij}^F.
\]

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 \( \theta_1 \) and \( \theta_2 \) 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

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

<table>
<thead>
<tr>
<th>Coordinates $(\theta_1, \theta_2)$</th>
<th>Coordinates $(\mu, \sigma)$</th>
</tr>
</thead>
</table>
| $g(q) = \begin{bmatrix}
\frac{-1}{2\theta_2} & \frac{\theta_1}{2\theta_2} \\
\frac{\theta_1}{2\theta_2} & -\frac{\theta_1^2}{2\theta_2} + \frac{1}{3-q} \Omega^{-1}_{q, \theta_2}
\end{bmatrix}$ | $g_{\ast}(q) = \begin{bmatrix}
\frac{\Omega^{-1}_{q, \sigma}}{\sigma^2} & 0 \\
0 & \frac{(3-q)\Omega^{-1}_{q, \sigma}}{\sigma^2}
\end{bmatrix}$ |
| $\det(g(q)) = \frac{1}{2(3-q)} \Omega^{-1}_{q, \theta_2}$ | $\det(g_{\ast}(q)) = \frac{(3-q)\Omega_{q, \sigma}}{\sigma^4}$ |
| $\left[ g(q) \right]^{-1} = \begin{bmatrix}
(3-q)\Omega\theta_1^2 - 2\theta_2 & (3-q)\Omega\theta_1\theta_2 \\
(3-q)\Omega\theta_1\theta_2 & (3-q)\Omega\theta_2^2
\end{bmatrix}$ | $\left[ g_{\ast}(q) \right]^{-1} = \begin{bmatrix}
\Omega\sigma^2 & 0 \\
0 & \frac{\Omega\sigma^2}{3-q}
\end{bmatrix}$ |
Fisher’s metrics and its matrix representations

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

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

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\[
g^F = \begin{bmatrix}
-\frac{\Omega}{2q\theta_2} & \frac{\Omega\theta_1}{2q\theta_2^2} \\
\frac{\Omega\theta_1}{2q\theta_2^2} & -\frac{\Omega}{2q\theta_2^2} + \frac{1}{q(3-q)} \frac{1}{\theta_2^2}
\end{bmatrix}
\]

\[
g^*_F = \begin{bmatrix}
\frac{1}{q\sigma^2} & 0 \\
0 & \frac{3-q}{q\sigma^2}
\end{bmatrix}
\]

\[
\det(g^{(q)}) = \frac{1}{2q^2(3-q)} \frac{\Omega}{(-\theta_2)^3}
\]

\[
\det(g^F) = \frac{3-q}{q^2\sigma^4}
\]

\[
[g^F]^{-1} = \begin{bmatrix}
(3-q)q\theta_1^2 - \frac{2q\theta_2}{\Omega} & (3-q)q\theta_1\theta_2 \\
(3-q)q\theta_1\theta_2 & (3-q)q\theta_2^2
\end{bmatrix}
\]

\[
[g^*_F]^{-1} = \begin{bmatrix}
q\sigma^2 & 0 \\
0 & \frac{q}{3-q}\sigma^2
\end{bmatrix}
\]
Christoffel symbols and curvature

Deriving the components of the matrix $g^F_*$ regarding the parameters $(\mu, \sigma)$, it is possible to obtain the Christoffel symbols as summarized in continuation

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Geodesic curves

Assuming that the coordinates \((\mu, \sigma)\) 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

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

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 \(\mu\). If \(q = 2\) (Cauchy distribution) the curves are circumferences of radio \(\frac{1}{k}\).
Further works

★ Find the geodesic distance for a $q$-gaussiana 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 $(\mu, \sigma)$ 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).
Bibliographic references


Thank you!!