Stochastic neighbor embedding (SNE) for dimension reduction and visualization using arbitrary divergences

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Nonlinear embedding
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A B S T R A C T
We present a systematic approach to the mathematical treatment of the t-distributed stochastic neighbor embedding (t-SNE) and the stochastic neighbor embedding (SNE) method. This allows an easy adaptation of the methods or exchange of their respective modules. In particular, the divergence which measures the difference between probability distributions in the original and the embedding space can be treated independently from other components like, e.g., the similarity of data points or the data distribution. We focus on the extension for different divergences and propose a general framework based on the consideration of Fréchet-derivatives. This way the general approach can be adapted to the user specific needs.

1. Introduction

Various dimension reduction techniques have been introduced based on the aim of preserving specific properties of the original data. The spectrum ranges from linear projections of original data, such as principal component analysis (PCA) or classical multidimensional scaling (MDS) to a variety of locally linear and nonlinear approaches, such as isomap, locally linear embedding (LLE), local linear coordination (LLC), or charting.

Other methods aim at the preservation of the classification accuracy in lower dimensions and incorporate the available label information for the embedding, e.g., linear discriminant analysis (LDA) and its variants thereof [9]. Extensions of the self-organizing map (SOM) [10], incorporating class labels [11], and limited rank matrix learning vector quantization (LiRaM LVQ) [12,13]. For a comprehensive review on nonlinear dimensionality reduction methods, we refer to [14].

Recently, the stochastic neighbor embedding (SNE) [15] and extensions thereof have become popular for visualization. SNE approximates the probability distribution in the high-dimensional space, defined by neighboring points, with their probability distribution in a lower-dimensional space. In [16] the authors proposed a technique called t-SNE, which is a variation of SNE considering a particular statistical model assumption for data distributions. The similarity of the distributions is quantified in terms of the Kullback–Leibler divergence. In [17] it is argued that the preservation of shift-invariant similarities as employed by SNE and its variants is superior in comparison to distance preservation as performed by many traditional dimension reduction techniques.

Functional metrics like Sobolev distances, kernel-based dissimilarity measures and divergences have attracted attention recently for the processing of data showing a functional structure. These dissimilarity measures were for example investigated as alternatives to the most common choice, the Euclidean distance [18–22]. The application of divergences for Vector Quantization and Learning Vector Quantization schemes have been investigated in [23,24].

This work bases on [25], where the self-organized neighbor embedding (SONE), which can be seen as a hybrid between the self-organizing map (SOM) and SNE, has been extended to the use of arbitrary divergences. In this contribution, we formulate a mathematical framework based on Fréchet derivatives which allows to generalize the concept of SNE and t-SNE to arbitrary divergences. This leads to a new dimension reduction and visualization scheme, which can be adapted to the user specific requirements in an actual problem. We summarize the general classes of divergences following the scheme introduced by [26] and extended in [23].

The mathematical framework for functional derivatives of continuous divergences is given by the functional-analytic generalization of common derivatives, known as Fréchet derivatives [27,28]. It is the generalization of partial derivatives for the discrete variants of the divergences.
We introduce a general mathematical framework for the extension of SNE and t-SNE for arbitrary divergences. The different classes of divergences are characterized and for various examples the Fréchet derivatives are identified. We demonstrate the proposed framework for the example case of the Gamma divergence. The behavior of different divergences stemming from the identified divergence families are shown on several examples in the image analysis domain.

2. Review of SNE and t-SNE

Generally, dimensionality reduction methods convert a high dimensional data set \( \{ x_i \}_{i=1}^n \in \mathbb{R}^d \) into low dimensional data \( \{ \tilde{x}_i \}_{i=1}^n \in \mathbb{R}^D \). A probabilistic approach to visualize the structure of complex data sets, preserving neighbor similarities is stochastic neighbor embedding (SNE), proposed by Hinton and Roweis [15]. SNE converts high-dimensional Euclidean distances between data points into probabilities that represent similarities. The conditional probabilities \( p_{ij} \) that a data point \( x_i \) would pick \( x_j \) as its neighbor is given by

\[
p_{ij} = \frac{\exp(-||x_i-x_j||^2/2\sigma_i^2)}{\sum_{j'} \exp(-||x_i-x_{j'}||^2/2\sigma_i^2)},
\]

with \( p_{ii} = 0 \). The variance \( \sigma_i \) of the Gaussians centered around \( x_i \) is determined by a binary search procedure [16]. The density of the data is likely to vary. In dense regions a smaller value of \( \sigma \) is more appropriate than in sparse regions. Let \( P_i \) be the conditional probability distribution over all other data points given \( x_i \). This distribution has an entropy which increases as \( \sigma_i \) increases. SNE performs a binary search for the value of \( \sigma_i \), which produces a \( P_i \) with a fixed perplexity specified by the user. The perplexity is defined as

\[
\text{perpl}(P_i) = 2^{H(P_i)},
\]

where \( H(P_i) \) is the Shannon entropy of \( P_i \) measured in bits: \( H(P_i) = -\sum p_{ij} \log p_{ij} \). It can be interpreted as a smooth measure of the effective number of neighbors and typical values ranges between 5 and 50 dependent on the data set size.

The low-dimensional counterparts \( \tilde{z}_i \) and \( \tilde{z}_j \) of the high-dimensional data points \( x_i \) and \( x_j \) are modeled by similar probabilities

\[
q_{ij} = \frac{\exp(-||\tilde{z}_i-\tilde{z}_j||^2)}{\sum_{j'} \exp(-||\tilde{z}_i-\tilde{z}_{j'}||^2)},
\]

with again \( q_{ii} = 0 \). SNE tries to find a low-dimensional data representation which minimizes the mismatch between the conditional probabilities \( p_{ij} \) and \( q_{ij} \). As a measure of mismatch the Kullback–Leibler divergence \( D_{KL} \) is used such that the cost function SNE is given by

\[
C = \sum_{ij} D_{KL}(P_i||Q_{ij}) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}},
\]

where \( Q_{ij} \) is defined similar to \( P_i \) as the conditional probability distribution over all other points given \( \tilde{z}_i \). The cost function is not symmetric and focuses on retaining the local structure of the data in the mapping. Large costs appear for mapping nearby data points widely separated in the embedding, but there is only small cost for mapping widely separated data points close together. The minimization of the cost function equation (4) is performed using a gradient descent approach. For details we refer to [15].

The so-called “crowding problem” may be observed in SNE and other local techniques, like for example Sammon mapping [16]. The (even very small) attractive forces might crush together moderately dissimilar points in the center of the map. Therefore, in [16] van der Maaten and Hinton presented a technique called t-SNE, which is a variation of SNE considering another statistical model assumption for the data distribution to avoid this problem. Instead of using the conditional probabilities \( p_{ij} \) and \( q_{ij} \) the joint probability distributions \( P \) and \( Q \) are used to optimize a symmetric version of SNE with the cost function

\[
C = D_{KL}(P||Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}
\]

with \( p_{ii} = q_{ii} = 0 \). Here, the pairwise similarities in the high-dimensional space are defined by the conditional probabilities

\[
p_q = \frac{p_{ij} + p_{ji}}{2n},
\]

and the low-dimensional similarities are given by

\[
q_q = \frac{1}{\sum_k \frac{1}{1 + ||\tilde{z}_i-\tilde{z}_k||^2}},
\]

The application of the heavy-tailed Student t-distribution with one degree of freedom allows to model moderate distances in the high-dimensional space by much larger distances in the embedding. Therefore, the unwanted attractive forces between map points that represent moderately dissimilar data points is eliminated. See [16] for further details.

3. A generalized framework

In this paper we provide the mathematical framework for the generalization of t-SNE and SNE, with respect to the use of arbitrary divergences in the cost-function for the gradient descent. We generalize the definitions towards continuous measures of the Gaussians centered around \( x_i \) and a low-dimensional space \( \mathcal{E} = \{ \tilde{z}_i \} \in \mathbb{R}^M \). The pairwise similarities in the high-dimensional original data space are set to

\[
p = p_{xy} = \frac{p_{xy} + p_{yx}}{2 \cdot \int dy},
\]

with conditional probabilities

\[
p_{y|x} = \frac{\exp(-||x-y||^2/2\sigma_y^2)}{\int \exp(-||x-y||^2/2\sigma_y^2) dy}.
\]

3.1. The generalized t-SNE gradient

Let \( D(p||q) \) be a divergence for non-negative integrable measure functions \( p = p(r) \) and \( q = q(r) \) with a domain \( V \) and \( \tilde{z}_i, \tilde{z}_j \in \mathcal{E} \) distributed according to \( \Pi_E \) [26]. Further, let \( r(\tilde{z}_i, \tilde{z}_j) : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{R} \) with the distribution \( \Pi_r = \phi(r, \Pi_E) \). Let us use the squared Euclidean distance in the low dimensional space:

\[
r = r(\tilde{z}_i, \tilde{z}_j) = ||\tilde{z}_i-\tilde{z}_j||^2.
\]

For t-SNE, \( q \) is obtained by means of a Student t-distribution, such that

\[
q(r(\tilde{z}_i, \tilde{z}_j)) = \frac{1}{\int (1 + r(\tilde{z}_i, \tilde{z}_j))^{-1} d\tilde{z}_i d\tilde{z}_j}.
\]

which we will abbreviate below for reasons of clarity as

\[
q(r') = \frac{1}{\int (1 + r')^{-1} d\tilde{z}_i d\tilde{z}_j} = f(r') \cdot |1|.
\]

Now let us consider the derivative of \( D \) with respect to \( \tilde{z}_i \):

\[
\frac{\partial D}{\partial \tilde{z}_i} = \frac{\partial D(p,q(r(\tilde{z}_i)))}{\partial \tilde{z}_i} = \int \frac{\partial D}{\partial r} \frac{\partial r}{\partial \tilde{z}_i} \frac{d\tilde{z}_j}{d\tilde{z}_i} = \int \frac{\partial D}{\partial r} \frac{\partial r(\tilde{z}_i, \tilde{z}_j)}{\partial \tilde{z}_i} d\tilde{z}_j.
\]

\[
= \int \frac{\partial D}{\partial r} \frac{\partial r(\tilde{z}_i, \tilde{z}_j)}{\partial \tilde{z}_i} d\tilde{z}_j = 4 \int \frac{\partial D}{\partial r} \frac{\partial r(\tilde{z}_i, \tilde{z}_j)}{\partial \tilde{z}_i} d\tilde{z}_j.
\]
We now have to consider $\frac{\delta D}{\delta r(\zeta, \zeta')}$. Again, using the chain rule for functional derivatives we get

$$
\frac{\delta D}{\delta r(\zeta, \zeta')} = \int \frac{\delta D}{\delta q(r(\zeta, \zeta'))} \frac{\delta q(r(\zeta, \zeta'))}{\delta r(\zeta, \zeta')} d\zeta d\zeta',
$$

where

$$
\frac{\delta q(r(\zeta, \zeta'))}{\delta r(\zeta, \zeta')} = \frac{\delta f(r)}{\delta r} I^{-1} - f(r') I^{-1} \frac{\delta f(\zeta)}{\delta r} dr',
$$

holds with

$$
\frac{\delta f(r)}{\delta r} = -\delta_{rr}(1+r)^{-2} \quad \text{and} \quad \frac{\delta f(\zeta)}{\delta r} = -(1+r)^{-2}.
$$

So we obtain

$$
\frac{\delta q(r(\zeta, \zeta'))}{\delta r} = f(r') I^{-1} - \frac{1}{(1+r)^2} \delta_{rr}(1+r)^{-2} I
$$

$$
= q(r') q(r) \frac{1}{(1+r)^2} \delta_{rr}(1+r)^{-1} q(r)
$$

$$
= -(1+r)^{-2} q(r) \delta_{rr} - q(r'))).
$$

Substituting these results in Eq. (13), we get

$$
\frac{\delta D}{\delta r} = \int \frac{\delta D}{\delta q(r')} \frac{\delta q(r')}{\delta r} I r' dr'
$$

$$
= q(r) \frac{1}{1+r} \int \frac{\delta D}{\delta q(r')} (\delta_{rr} - q(r')) I r' dr'
$$

$$
= \frac{q(r)}{1+r} \left( \int \frac{\delta D}{\delta q(r')} q(r') I r' dr' \right).
$$

Finally collect all terms and get

$$
\frac{\delta D}{\delta r} = 4 \int \frac{\delta D}{\delta q(r')} (\xi - \xi') d\xi
$$

$$
= 4 \int \frac{q(r)}{1+r} \left[ \int \frac{\delta D}{\delta q(r')} q(r') I r' dr' \right] (\xi - \xi') d\xi.
$$

We now have the obvious advantage that we can derive $\frac{\delta D}{\delta r}$ for several divergences $D(p/q)$ directly from Eq. (14), if the Fréchet derivative $\frac{\delta D}{\delta q(r)}$ of $D$ with respect to $q(r)$ is known. The concept of Fréchet derivatives and explicit formulas for different divergences are given in Section 6.

3.2. The generalized SNE gradient

In symmetric SNE, the pairwise similarities in the low dimensional map are given by [16]

$$
q_{SNE}(r) = \frac{\exp(-r(\zeta, \zeta'))}{\int \exp(-r(\zeta, \zeta')) d\zeta d\zeta'},
$$

which we will abbreviate below for reasons of clarity as

$$
q_{SNE}(r) = \frac{\exp(-r)}{\int \exp(-r) d\zeta d\zeta'} = g(r') J^{-1},
$$

with $g(r') = \exp(-r)$ and $J$ representing the integral in the denominator. Consequently, if we consider $\frac{\delta D}{\delta \zeta}$, we can use the results from above for t-SNE. The only term that differs is the derivative of $q_{SNE}(r')$ with respect to $r$. Therefore we get

$$
\frac{\delta q_{SNE}(r')}{\delta r} = \frac{\delta g(r')}{\delta r} J^{-1} - g(r') J^{-2} \frac{\delta J}{\delta r},
$$

with

$$
\frac{\delta g(r')}{\delta r} = -\delta_{rr} \exp(-r) \quad \text{and} \quad \frac{\delta J}{\delta r} = -\exp(-r),
$$

which leads to

$$
\frac{\delta q_{SNE}(r')}{\delta r} = -\delta_{rr} \exp(-r) + g(r') J^{-2} \exp(-r)
$$

$$
= -\delta_{rr} g(r') + g(r') g(r) = -\delta_{rr} q_{SNE}(r') + q_{SNE}(r') q_{SNE}(r).
$$

Substituting these results in Eq. (13), we get

$$
\frac{\delta D}{\delta r} = \int \frac{\delta D}{\delta q_{SNE}(r')} \frac{\delta q_{SNE}(r')}{\delta r} I r' dr'
$$

$$
= -q_{SNE}(r') \int \frac{\delta D}{\delta q_{SNE}(r')} (\delta_{rr} - q_{SNE}(r')) I r' dr'
$$

$$
= -q_{SNE}(r') \left( \int \frac{\delta D}{\delta q_{SNE}(r')} q_{SNE}(r') I r' dr' \right).
$$

Finally, substituting this result in Eq. (12), we obtain

$$
\frac{\delta D}{\delta \zeta} = 4 \int \frac{\delta D}{\delta q_{SNE}(r')} (\zeta - \zeta') d\zeta'
$$

$$
= 4 \int q_{SNE}(r') (\xi - \xi') \left[ \int \frac{\delta D}{\delta q_{SNE}(r')} q_{SNE}(r') I r' dr' \right] d\zeta'.
$$

4. Specifications of divergences

Divergences are derived from simple component-wise errors, e.g., the Euclidean and Minkowski metrics [26]. These frequently used metrics are intuitive and they are optimal estimators in case of Gaussian noise or error. However, if the observations are corrupted not only by Gaussian noise but also by outliers, estimators based on these metrics can be strongly biased. They also suffer from the curse of dimensionality, which means that observations become equidistant in terms of the Euclidean distance for high-dimensional data. In many applications like pattern matching, image analysis, statistical learning, etc. the noise is not necessarily Gaussian and information divergences are used. Employing generalized divergences might provide a compromise between the efficiency and robustness and/or compromise between a mean squared error and bias.

Divergences are functionals $D(p/q)$ designed as dissimilarity measures between two non-negative integrable functions $p$ and $q$ [26]. In practice, usually $p$ corresponds to the observed data and $q$ denotes the estimated or expected data. We assume $p(r)$ and $q(r)$ are positive measures defined on $r$ in the domain $V$. The weight of the functional $p$ is defined as

$$
W(p) = \int_V p(r) dr.
$$

Positive measures with the additional constraint $W(p) = 1$ can be interpreted as probability density functions. Generally speaking, divergences measure a quasi-distance or directed difference, while we are mostly interested in separable measures, which satisfy the condition

$$
D(p/q) \begin{cases} > 0 & \text{for } p \neq q, \\ 0 & \text{if } p = q. \end{cases}
$$

In contrast to a metric, divergences may be non-symmetric $D(p/q) \neq D(q/p)$, and do not necessarily satisfy the triangular inequality $D(p/q) \leq D(p/z) + D(z/q)$. Following [26] one can distinguish at least three main families of divergences with the same consistent properties: Bregman-divergences, Csiszár's $f$-divergences and $\gamma$-divergences. Note that all these families contain the Kullback–Leibler (KL)
divergence as a special case, so the KL-divergence can be seen as
the non-empty intersection between the sets of divergences.

In general we assume \( p \) and \( q \) to be positive measures. In case they are normalized we refer to them as probability densities. We review some basic properties of divergences in the following sections. For detailed information we refer to [26,29].

An overview of the family of divergences, examples and their relationship to each other can be found in Fig. 1. Some important properties are summarized in Tables 1 and 2. We review the families of divergences and some examples in the following sections.

### 4.1. Bregman divergences

A Bregman divergence is defined as a pseudo-distance between two positive measures \( p \) and \( q \): \( D_{\phi}(p||q) : \mathcal{L} \times \mathcal{L} \to \mathbb{R}^+ \). Let \( \phi \) be a strictly convex real-valued function with the domain of the Lebesgue-integrable functions \( \mathcal{L} \) and twice continuously Fréchet-differentiable [28]. Then the Bregman divergence can be defined by

\[
D_{\phi}(p||q) = \int \phi(p) - \phi(q) - \delta \phi(q) \frac{p - q}{q} \, dr.
\]

\( \gamma = 1 \)

**Fig. 1.** Overview over the families of divergences and their relationship to each other. The shortcut Prob. denotes the special case of probability densities. For the sake of clarity we show the most important relations only and do not claim completeness.

### Table 1

<table>
<thead>
<tr>
<th>Divergence (generating function)</th>
<th>(most) Important properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bregman ( D_{\phi}(p</td>
<td></td>
</tr>
<tr>
<td>Gen. Kullback–Leibler ( \int (u \log u - u) , dr )</td>
<td>Shannon Entropy ( H_s(p) = - \int \Phi(p) , dr )</td>
</tr>
<tr>
<td>Itakura–Saito ( \int (\log u - u \log dr) )</td>
<td>Burg Entropy ( H_b(p) = \int p \log p )</td>
</tr>
<tr>
<td>Eta-div. ( \Phi(u) = \int \frac{u - 1}{\eta - 1} )</td>
<td>Related to scaling</td>
</tr>
<tr>
<td>Beta-divergence ( \Phi(u) = \int \frac{u^\alpha - \beta}{\beta} )</td>
<td>Reisz divergence ( D_s(p</td>
</tr>
</tbody>
</table>
| Beta-divergence \( \Phi(u) = \int \frac{u^\alpha + u + \beta}{\beta} \) | Symmetric

**Table 2**

<table>
<thead>
<tr>
<th>Divergence (generating function)</th>
<th>(most) Important properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gamma divergence ( \int u^\alpha , dr )</td>
<td>Related to Rényi Entropy</td>
</tr>
</tbody>
</table>
| Cauchy–Schwarz \( \gamma = 1 \) | Symmetric

\( \gamma = 1 \)
where $\delta\phi(q)/\delta q$ is the Fréchet derivative of $\phi$ with respect to $q$ [23]. Well known fundamental properties of the Bregman divergences are [26]:

**Convexity**: A Bregman divergence is always convex in its first argument but not necessary in its second.

**Non-negativity**: $D_B^p(p|q) \geq 0$ and $D_B^q(p|q) = 0$ iff $p=q$.

**Linearity**: Bregman divergences are linear according to the generating function $\phi$. Any positive linear combination of Bregman divergences is also a Bregman divergence:

$$D_B^{\mu_1\phi_1 + \cdots + \mu_n\phi_n}(p|q) = \sum_{i=1}^n \mu_i D_B^{\phi_i}(p|q), \quad \mu_i, \phi_i > 0.$$  

**Invariance**: A Bregman divergence is invariant under affine transformations. Thus, $D_B^p(p|q) = D_B^q(p|q)$ is valid for any affine transformation $f(q) = \phi(q) + \Psi_{\phi}(q) + c$, with linear operator

$$\Psi_{\phi}(q) = \frac{\delta f(q)}{\delta q} \cdot q - \frac{\delta \phi(q)}{\delta q} : q$$

for positive measures $g$ and $q$ and scalar $c$.

**Three-point property**: For any triple $p, q, g$ of positive measures the property holds:

$$D_B^p(p|q) = D_B^q(p|g) + D_B^g(q|g) + (p-q)\left(\frac{\delta \phi(q)}{\delta q} - \frac{\delta \phi(p)}{\delta q}\right).$$

**Generalized Pythagorean theorem**: Let $P_{\phi}(q) = \arg \min_{p \in \Omega} D_B^q(\phi(p)/q)$ be the Bregman projection onto the convex set $\Omega$ and $p \in \Omega$. The inequality

$$D_B^p(p|q) \geq D_B^q(P_{\phi}(p)|q) + D_B^q(P_{\phi}(p)|q)$$

is known as generalized Pythagorean theorem. If $\Omega$ is an affine set it holds with equality.

**Optimality**: In [30] an optimality property is stated. Given a set $S$ of positive measures $p$ with mean $\mu = E[S]$ and $\mu \in S$ the unique minimizer $E_{p,q}(\mathbb{D}^p(\mu|q))$ is minimum for $q=\mu$ if $D$ is a Bregman divergence. This property favors the Bregman divergences for optimization and clustering problems [31–35].

The Bregman divergence includes many prominent dissimilarity measures like [26,23,36]:

- The generalized Kullback–Leibler (or $\mathfrak{L}$-) divergence for positive measures $p$ and $q$:

$$D_{\mathcal{KL}}(p|q) = \int p \log \left(\frac{p}{q}\right) d\mu - \int (p-q) d\mu$$

using the generating function

$$\Phi(f) = \int (f \cdot \log f - f) d\mu.$$  

Some three-dimensional isosurfaces for the generalized Kullback–Leibler divergence with respect to different reference points can be found in the first column of Figs. 2 and 4. Dependent on the choice of the divergence and its possible parameters the scaling and shape of the isosurfaces vary. For probability densities $p$ and $q$, Eq. (25) simplifies to the Kullback–Leibler divergence [37,38]:

$$D_{KL}(p|q) = \int p \log \left(\frac{p}{q}\right) d\mu,$$

which is related to the Shannon-entropy [39]. Equidistance contours for three-dimensional probability densities using Kullback–Leibler divergence with respect to different reference points are displayed in the first row of Figs. 3 and 5.

- The Itakura–Saito divergence [40]:

$$D_{IS}(p|q) = \int p \log \left(\frac{p}{q}\right) d\mu$$

bases on the Burg entropy, which also serves as the generating function:

$$\Phi(f) = -\int \log(f) d\mu.$$  

The Itakura–Saito divergence was originally presented as a measure of the quality of fits between two spectra and became a standard measure in the speech and image processing community due to the good perceptual properties of the reconstructed signals. It is known as negative cross-Burg entropy and fulfills the scale-invariance property $D_{IS}(c \cdot p|c \cdot q) = D_{IS}(p|q)$, which implies the same relative weight is given to low and high components of $p$, see [41] for details.

- The Eta-divergence is also known as norm-like divergence [42]:

$$D_{\eta}(p|q) = \int p^{\eta} (\eta - 1) \cdot q - \eta \cdot p \cdot q^{-\eta-1} d\mu,$$

with generating function

$$\Phi(f) = \int f^\eta d\mu \quad \text{for } \eta > 1.$$  

In the case $\eta = 2$ the Eta-divergence becomes the Euclidean distance with generating function $\Phi(f) = \int f^2 d\mu$.

- The Beta-divergence [26]:

$$D_B(p|q) = \int \log \left(\frac{p^{-\beta} - q^{-\beta}}{\beta - 1}\right) d\mu - \int \frac{p^{-\beta} - q^{-\beta}}{\beta - 1} d\mu$$

Table 2

<table>
<thead>
<tr>
<th>Divergence</th>
<th>[most]</th>
<th>Important properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen. Csiszár–f</td>
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<tr>
<td>$D_f^p(p</td>
<td>q) = \int f(p</td>
<td>q) d\mu + q f\left(\frac{p}{q}\right)$</td>
</tr>
<tr>
<td>Gen. Entropy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_p(g) = -\int f(p</td>
<td>g) d\mu$</td>
<td></td>
</tr>
<tr>
<td>Convexity to both p, q</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$cD_f = D_{f,c} &gt; 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Invariance</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f_{sym}(u) = f(u) + f^*(u)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symmetry</td>
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<tr>
<td>Bounded</td>
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<tr>
<td>Continuity</td>
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</tbody>
</table>

**Table of divergences and their properties (continued).**
Fig. 2. Isosurfaces of some Example divergences including the plane of probability densities with respect to the reference point (0.3,0.3,0.3). The first column shows Bregman divergences, the second Csiszár-f divergences and the last column shows the Gamma divergence for different values of $\gamma$. 
Fig. 3. Equidistance lines of some Example divergences for probability densities with respect to reference point (0.3,0.3,0.3). The columns show Bregman divergences, Csiszar-f divergences and Gamma divergences.
with \( \beta \neq 0 \) and \( \beta \neq 1 \) and the generating function
\[
\phi(f) = f^\beta - \beta \cdot f + \beta - 1 \quad \frac{1}{\beta(\beta - 1)} .
\]
(33)

For specific values of \( \beta \) the divergence becomes:
\( \beta \to 1 \): generalized Kullback–Leibler equation (25).
\( \beta \to 0 \): Itakura–Saito divergence equation (28).
\( \beta = 2 \): Euclidean distance (apart from a factor \( \frac{1}{2} \)).

Furthermore the Beta-divergence is equivalent to the density power divergence \([43,36,44]\) and a rescaled version of the Eta-divergence.

4.2. Csiszár-f divergences

Csiszár-f divergences are connected with the “ratio test” in the Pearson–Neyman style hypothesis testing and are in many ways “natural” concerning distributions and statistics. We denote by \( \mathcal{F} \) the class of convex, real-valued, continuous functions \( f \) satisfying \( f(1) = 0 \), with
\[
\mathcal{F} = \{ g | g : [0, \infty) \to \mathbb{R}, g - \text{convex} \} .
\]
(34)

For a function \( f \in \mathcal{F} \) the Csiszár-f divergence is given by
\[
D_{f}(p||q) = \int f(u) \left( \frac{p}{q} \right) du .
\]
(35)

with the definitions \( 0 \cdot f(0^+) = 0 \) and \( 0 \cdot f(a/0) = \lim_{\alpha \to 0} . \alpha \cdot f(a/\alpha) = \lim_{\alpha \to 0} . \alpha \cdot f(u/\alpha) [45-48] \). The f-divergence can be interpreted as an average of the likelihood ratio \( p/q \) describing the change rate of \( p \) with respect to \( q \) weighted by the determining function \( f \). For a general \( f \), which does not have to be convex, with \( f(1) = c_f \neq 0 \), this form is not invariant and we have to use the generalized \( f \)-divergence
\[
D_{f}^{g}(p||q) = c_f \left( \int (p-q) \, du + \int q f\left( \frac{P}{q} \right) du \right) .
\]
(36)

For the special case of probability densities \( p \) and \( q \) the first term vanishes and the original form of the \( f \)-divergences is obtained.

Some basic properties of the Csiszár-f divergences are \([49,26]\): Non-negativity: \( D_{f}(p||q) \geq 0 \) where the equal sign holds iff \( p = q \), which follows from Jensen’s inequality.

Generalized entropy: It corresponds to a generalized \( f \)-entropy if the form
\[
H_{f}(p) = - \int f(p(r)) \, dr .
\]
(37)

Strict convexity: The \( f \)-divergence is convex in both arguments \( p \) and \( q \):
\[
D_{f}(tp_{1}+(1-t)p_{2}||tq_{1}+(1-t)q_{2}) \leq tD_{f}(p_{1}||q_{1})+(1-t)D_{f}(p_{2}||q_{2}) \quad \forall t \in [0, 1] .
\]
(38)

Scalability: \( C_{f}D_{f}(p||q) = D_{f}(c \cdot p||c \cdot q) \) for any positive constant \( c > 0 \).

Invariance: \( D_{f}(p||q) \) is invariant with respect to a linear shift regarding the function \( f \): e.g. \( D_{f}(p||q) = D_{f}(p||q) \) iff \( f(u) = f(u) + c \cdot (u-1) \) for any constant \( c \in \mathbb{R} \).

Symmetry: For \( f \neq f^{*} \in \mathcal{F} \), where \( f^{*}(u) = u \cdot f(1/u) \) denotes the conjugate function of \( f \), the relation \( D_{f}(p||q) = D_{f}(q||p) \) is valid. It is possible to construct a symmetric Csiszár-f divergence with \( f_{sym}(u) = f(u) + f^{*}(u) \) as determining function.

Upper bound: The \( f \)-divergence is bounded by
\[
0 \leq D_{f}(p||q) \leq \lim_{u \to 0} \left( f(u) + f^{*}(u) \right) \quad \text{with} \quad u = \frac{p}{q} .
\]
(39)

The existence of this limit for probability densities \( p \) and \( q \) was shown by Liese and Vajdai in \([50]\). Villmann and Haase showed that these bounds still hold for positive measures \( p \) and \( q \) \([23]\).
which is based on the quadratic Rényi-entropy. The Cauchy–Schwarz divergence is symmetric and was introduced considering the Cauchy–Schwarz inequality for norms. It is frequently applied for Parzen window estimation, especially suitable for spectral clustering as well as related graph cut problems [55–57,23].

Some isosurfaces of the Gamma divergence for different values of $\gamma$ are shown in the last column of Figs. 2 and 4. The equidistance
Fig. 5. Equidistance lines of some example divergences for probability densities with respect to reference point (0.5,0.2,0.3). The columns show Bregman divergences, Csiszár-f divergences and Gamma divergences.
lines for the special case of probability densities can be found in the last column of Figs. 3 and 5. The Gamma divergence displays some nice properties [26,23]:

**Invariance:** $D_g(p|q)$ is invariant under scalar multiplication with positive constants

$$D_g(p|q) = D_g(c \cdot p|c \cdot q) \quad \forall c > 0, c_1, c_2 > 0.$$  

(48)

In case of positive measures the equation $D_g(p|q) = 0$ holds only if $p = c \cdot q$ with $c > 0$. For probability densities $c=1$ is required.

**Pythagorean relation:** As for Bregman divergences a modified Pythagorean relation between positive measures can be stated for special choices of $p,q,r$. Let $p$ be a distortion of $q$ defined as convex combination with a positive distortion measure $\phi(r)$

$$p_t(r) = (1-e) \cdot q(r) + e \cdot \phi(r).$$  

(49)

A positive measure $g$ is denoted as $\phi$-consistent if $v_g = \int \phi(r)g(r^2 \, dr)^{1/2}$ is sufficiently small for large $\alpha > 0$. If two positive measures $q$ and $\rho$ are $\phi$-consistent with respect to a distortion measure $\phi$, then the Pythagorean relation approximately holds for $q,\rho$ and the distortion $p_\phi$ of $q$:

$$D(p_\phi(q,\rho)) = D(p_\phi(p_t(q),p_t(\rho)) - D(p_t(q)/p_t(\rho)) = O(e^{\alpha/2})$$

with $v = \max(v_g,v_\rho)$.  

(50)

This property implies the robustness of $D_\phi$ according to distortions.

5. Discussion of divergences

In this section we examine and compare some introduced divergences by means of controlled experiments. We investigate the behavior of different divergences for the comparison of images containing an increasing level of (nonlinear) noise. Therefore, we compute the histograms of gray-value images taken from the Berkeley segmentation data set and noisy versions of them.

5.1. Linearly monotonically increasing noise

In the first experiment the noisy image $I^\nu$ is obtained by adding a linear monotonically increasing transformation of gray values to the image $I$:

$$I^\nu(x,y) = l(x,y) \cdot |l \cdot (l(x,y)-I_0)| + 1,$$  

(51)

where $l$ denotes the level of noise and $I_0$ corresponds to the minimal intensity in the original image. Fig. 6 shows a picture (in the following referred to as “moon”) adding different levels of noise following Eq. (51) together with the gray-value histograms. The noise-level is ranged from $l=1$ to $l=9$. Some dissimilarity matrices comparing the 10 histograms with different divergence measures are shown in Fig. 7. The intuitively ideal dissimilarity matrix in this case is a symmetric band matrix shown in the middle of the top row. Some divergences like the generalized Rényi divergence show numerical instabilities. Others show quite similar behavior, e.g. Itakura–Saito, Alpha divergences and the Beta-divergence with $\beta = 0.5$, but they do not exhibit the desired band structure. For the original image and low noise-levels (images 1–5) the Beta-divergence with $\beta = 1.5$, Alpha divergence with $\alpha = 0.5$ and also the generalized KL divergence show a bit of the desired band structure. Ignoring the last column and last row (the extreme case) in the dissimilarity matrix of theEta-divergence shows a good approximation of a band matrix. The Gamma divergence is observed to be quite robust in this case and also exhibits a visible band structure for $\gamma \geq 1$. In the special case of $\gamma = 1$ the Gamma divergence equals the Cauchy–Schwarz divergence and is symmetric. Another symmetric example is the Alpha divergence with $\alpha = 0.5$.

As a second example we take a picture of a group of dolphins and add some noise (following Eq. (52)) using the levels $l = \{0.1, 0.2, \ldots, 0.9\}$. The resulting histograms of gray values for the different noise levels are shown in Fig. 8. As above we compute the matrices of pairwise similarities between the histograms using different divergences. The results can be found in Fig. 9. In this example the ETA-divergence especially with $\eta = 2.5$ is a good approximation of the ideal dissimilarity matrix shown in the middle of the top row. The best symmetric choice is the Gamma divergence with $\gamma = 1$ (Cauchy–Schwarz). Furthermore, dependent on the value for $\gamma$ one can chose between a better “resolution” (local) and a better preservation of the hierarchy of the histograms (global). Some other divergences, e.g. the generalized KL and Itakura–Saito, show very poor approximations of the desired dissimilarity for this example.

5.2. Additive uniform noise

In the second experiment the noisy image $I^\nu$ is obtained by adding uniform noise to the image $I$:

$$I^\nu(x,y) = l(x,y) + U(0,1),$$  

(52)

where $U(0,1)$ denotes a scalar value drawn from the uniform distribution in the interval $[0,1]$. Fig. 10 shows the picture of dolphins adding different levels of uniform noise following Eq. (52) together with the noise and more flattened gray-value histograms. The noise-level is ranged from $l = \frac{1}{255}$ to $l = \frac{128}{255}$. Some dissimilarity matrices pairwise comparing the 10 images with different divergence measures are shown in Fig. 11. Some divergences like the generalized Rényi, Itakura–Saito and some Alpha- and Beta-divergences fail to approximate the desired band structure in the pairwise dissimilarity matrix.
ignoring the extreme cases and the Gamma divergence with a small constant shown in the middle of the top row. Some divergences (marked with an asterisk * in the title) show numerical instabilities in case of zeros in the signals. In that cases a small constant $c=1$ was added to all histograms to prevent the degeneration. Other divergences, like e.g. the Gamma divergence are more robust. The Eta-divergence ignoring the extreme cases and the Gamma divergence with $\gamma \geq 1$ exhibit more of the desired band structure for this example compared to other choices.

Fig. 7. Matrix of pairwise dissimilarity of the 10 histograms shown in Fig. 6 using different divergences. The ideal dissimilarity matrix for this example is a band matrix shown in the middle of the top row. Some divergences (marked with an asterisk * in the title) show numerical instabilities in case of zeros in the signals. In that cases a small constant $c=1$ was added to all histograms to prevent the degeneration. Other divergences, like e.g. the Gamma divergence are more robust. The Eta-divergence ignoring the extreme cases and the Gamma divergence with $\gamma \geq 1$ exhibit more of the desired band structure for this example compared to other choices.

Fig. 8. Histograms of intensity values in an example picture. The original image “dolphins” (top row) together with its histogram is shown on the left side. The following pictures contain noise in the form of a linear monotonically increasing transformation of gray values following Eq. (51) using $l=\{0,1,\ldots,9\}$ corresponding to the Noise-Levels 1–9.
Fig. 9. Matrix of pairwise dissimilarity of the 10 histograms shown in Fig. 8 using different divergences. The ideal dissimilarity matrix for this example is a band matrix shown in the middle of the top row. Some divergences (marked with an asterisk * in the title) show numerical instabilities in case of zeros in the signals. In that cases a small constant c = 1 was added to all histograms to prevent the degeneration. The Eta-divergence especially with η = 2.5 shows a good approximation of the desired band structure for this example. The Gamma divergence with γ = 0.75 (Cauchy–Schwarz) is the best symmetric choice in this case.

Fig. 10. Histograms of intensity values in an example picture. The original image “dolphins” (top row) together with its histogram is shown on the left side. The following pictures contain additive uniform noise following Eq. (52) using \( I = \frac{1}{50}, \frac{1}{100}, \ldots, \frac{1}{450} \) corresponding to the Noise-Levels 1–9.
Others, like the Gamma-, Eta- and some Alpha- and Beta-divergences are nearly ideal for this example. The Kullback-Leibler divergence is nearly perfect if the original image is ignored.

6. The Fréchet derivative

In this section we introduce the concept of Fréchet derivatives used for the generalization to arbitrary divergences. Suppose $V$ and $W$ are Banach spaces and $U \subset V$ is an open subset of $V$. The function $f : U \to W$ is called Fréchet differentiable at $r \in U$, if there exists a bounded linear operator $A_r : V \to W$, such that for $h \in U$

$$\lim_{h \to 0} \frac{|f(r+h)-f(r)-A_r(h)|_W}{\|h\|_V} = 0. \quad (53)$$

This general definition can be used for functions $L : B \to \mathbb{R}$, defined as mappings from a functional Banach space $B$ to $\mathbb{R}$. Further let $B$ be equipped with a norm $\| \cdot \|$ and $f, h \in B$ are two functionals. The Fréchet derivative $\delta L[f]/\delta f$ of $L$ at point $f$ (i.e. in a function $f$) in the direction $h$ is formally defined as

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} (L[f+\epsilon h]-L[f]) = \frac{\delta L[f]}{\delta f}[h]. \quad (54)$$

The Fréchet derivative in finite-dimensional spaces reduces to the usual partial derivative. Thus, it is a generalization of the directional derivatives.

Following [23] we introduce the functional derivatives of divergences in the next paragraphs. An overview is given in Table 3.
<table>
<thead>
<tr>
<th>Divergence family</th>
<th>Formula</th>
<th>Fréchet derivative</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bregman divergence</td>
<td>( D_b^\phi(p</td>
<td>q) = \phi(p) - \phi(q) - \frac{\delta \phi(q)}{\delta q} (p - q) )</td>
</tr>
<tr>
<td>Gen. Kullback-Leibler</td>
<td>( D_{KL}(p</td>
<td>q) = \int p \log \left( \frac{p}{q} \right) dr - (p - q) \frac{d}{dq} )</td>
</tr>
<tr>
<td>Kullback-Leibler</td>
<td>( D_{KL}(p</td>
<td>q) = \int p \log \left( \frac{p}{q} \right) dr )</td>
</tr>
<tr>
<td>Itakura-Saito</td>
<td>( D_{IS}(p</td>
<td>q) = \int \frac{p^q - q^p}{q - p} \frac{d}{dq} (q - p) )</td>
</tr>
<tr>
<td>Eta-divergence</td>
<td>( D_{\eta}(p</td>
<td>q) = \int p^\eta (q - 1) - q^\eta \frac{d}{dq} )</td>
</tr>
<tr>
<td>Beta-divergence</td>
<td>( D_{B}(p</td>
<td>q) = \int \frac{(p^\beta - q^\beta)}{(p - q)} \frac{d}{dq} (p - q) )</td>
</tr>
<tr>
<td>Gen. Csiszár-f</td>
<td>( D_{C}(p</td>
<td>q) = \int q \left( \frac{p^q}{\int p^q dr} \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Csiszár-f divergence</td>
<td>( D_{C}(p</td>
<td>q) = \int q \left( \frac{p^q}{\int p^q dr} \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Alpha divergence</td>
<td>( D_{A}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Gen. Rényi</td>
<td>( D_{R}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Rényi</td>
<td>( D_{R}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Tsallis</td>
<td>( D_{T}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Hellinger</td>
<td>( D_{H}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Gamma</td>
<td>( D_{G}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
<tr>
<td>Cauchy–Schwarz</td>
<td>( D_{C}(p</td>
<td>q) = \int q \log \left( \int q^q ddr \right)^\frac{1}{\eta} )</td>
</tr>
</tbody>
</table>

### 6.1. Fréchet derivatives: Bregman divergences

The Fréchet-derivative of \( D_b^\phi \), Eq. (19) with respect to \( q \) is formally given by

\[
\frac{\delta D_b^\phi(p|q)}{\delta q} = \frac{\delta \phi(p)}{\delta q} - \frac{\delta \phi(q)}{\delta q} - \frac{\delta \phi(q)}{\delta q} (p - q),
\]

with

\[
\frac{\delta \phi(q)}{\delta q} = \frac{\delta^2 \phi(q)}{\delta q^2} (p - q) - \frac{\delta \phi(q)}{\delta q}.
\]

For the generalized Kullback–Leibler divergence equation (25) this simplifies to

\[
\frac{\delta D_{KL}(p|q)}{\delta q} = -\frac{p}{q} + 1,
\]

whereas for the Kullback–Leibler divergence equation (27) in the special case of probability densities it reads

\[
\frac{\delta D_{KL}(p|q)}{\delta q} = -\frac{p}{q}.
\]

For the Itakura–Saito divergence equation (28) we get

\[
\frac{\delta D_{IS}(p|q)}{\delta q} = \frac{1}{q^2} (q - p)
\]

and for the Eta-divergence equation (30) the Fréchet-derivative is

\[
\frac{\delta D_{\eta}(p|q)}{\delta q} = q^{\eta - 1} (1 - \eta \cdot \eta \cdot (p - q)).
\]

In the case of \( \eta = 2 \) it reduces to the derivative of the Euclidean distance \(-2(p - q)\). The Fréchet-derivative for the subset of Beta-divergences equation (32) is given by

\[
\frac{\delta D_{B}(p|q)}{\delta q} = -p \cdot q^{\beta - 1} + q^{\beta - 1}.
\]

### 6.2. Fréchet derivatives: Csiszár-f divergences

For the Csiszár-f divergences equation (35) the Fréchet derivative is

\[
\frac{\delta D_{C}(p|q)}{\delta q} = f \left( \frac{p}{q} \right) + q \frac{\partial f(u)}{\partial u} \frac{1}{\eta}.
\]

with \( u = p/q \). For the set of Alpha divergences equation (40) we get

\[
\frac{\delta D_{A}(p|q)}{\delta q} = \frac{1}{q} \left( q^{\frac{1}{\eta}} - 1 \right).
\]

The related generalized Rényi divergence equation (42) yields

\[
\frac{\delta D_{R}(p|q)}{\delta q} = \frac{1}{q} \left( q^{\frac{1}{\eta}} - 1 \right).
\]
which reduces in the case of the Rényi divergence for probability densities to
\[
\frac{\partial D_\alpha(p||q)}{\partial q} = -p^\alpha q^{\alpha-1} \frac{\partial}{\partial q} \int p^\alpha q^{\alpha-1} dr.
\] (65)

For the Tsallis divergence equation (44) the Fréchet derivative reads
\[
\frac{\partial D_\gamma(p||q)}{\partial q} = -p^\gamma q^{\gamma-1} \frac{\partial}{\partial q} \int p^\gamma q^{\gamma-1} dr,
\] (66)

and for the well-known Hellinger divergence equation (45) the derivative is
\[
\frac{\partial D_{\text{H}}(p||q)}{\partial q} = 1 - \frac{p}{q}
\] (67)

6.3. Fréchet derivatives: Gamma divergences

The Fréchet derivative of the Gamma divergence equation (46) can be written as
\[
\frac{\partial D_\gamma(p||q)}{\partial q} = \frac{q^\gamma}{\int q^{\gamma} dr} - \frac{p}{\int p \cdot q dr}.
\] (68)

Considering the important special case \(\gamma = 1\), i.e. Cauchy–Schwarz divergence equation (47),
\[
\frac{\partial D_{\text{C}}(p||q)}{\partial q} = \frac{q}{\int q^2 dr} - \frac{p}{\int p \cdot q dr},
\] (69)

7. t-SNE gradients for various divergences

In this section we explain the t-SNE gradients for various divergences. There exists a large variety of divergences which can be collected into several classes according to their mathematical properties and structural behavior. Here we follow the classification proposed in [26]. For this purpose, we plug the corresponding Fréchet-derivatives into the general gradient equation (14) for t-SNE. Clearly, one can convert these results easily to the general SNE gradient equation (16) in complete analogy, because of its structural similarity to the t-SNE formula equation (14).

A technical remark should be made here: In the following we will abbreviate \(p(r)\) by \(p\) and \(p(r')\) by \(p\). Further, because the integration variable \(r\) is a function \(r = r(z)\) an integration requires the weighting according to the distribution \(\Pi_r\). Thus, the integration has formally to be carried out according to the differential \(d\Pi_r(r)\) (Stieltjes-integral). We abbreviate this by \(dr\) but keeping this fact in mind, i.e. by this convention, we will drop the distribution \(\Pi_r\), if it is clear from the context.

7.1. Bregman divergences

In the following we will provide the Gradients for some examples of Bregman divergences introduced in Section 4.1. As a first example we show that we obtain the same result as van der Maaten and Hinton in [16] for the Kullback–Leibler divergence equation (27). The Fréchet-derivative of \(D_{\text{KL}}\) with respect to \(q\) is given in Eq. (56). From Eq. (14) we see that
\[
\frac{\partial D_{\text{KL}}}{\partial q} = 4 \int \frac{q^{z-1} - 1}{1 + r} \left( \int p \Pi_r dr \right) d\zeta.
\] (70)

Since the integral \(I = \int p \Pi_r dr\) in Eq. (70) can be written as an double integral over all pairs of data points \(I = \int p \, d\zeta\), we see from Eq. (8) that the integral \(I\) equals 1. So, Eq. (70) simplifies to
\[
\frac{\partial D_{\text{KL}}}{\partial q} = 4 \int (1 + r)^{-1} (p - q(z - 1)) d\zeta.
\]

This is exactly the differential form of the discrete version as proposed for t-SNE in [16].

The Kullback–Leibler divergence used in original SNE and t-SNE belongs to the more general class of Bregman divergences [32]. Another representative of this class of divergences is the Itakura–Saito divergence \(D_{\text{IS}}\) equation (28) with the Fréchet-derivative equation (57). For the calculation of the gradient \(\partial D_{\text{IS}}/\partial \zeta\) we substitute the Fréchet-derivative in Eq. (14) and obtain
\[
\frac{\partial D_{\text{IS}}}{\partial \zeta} = -4 \int \frac{q}{1 + r} \left( \int q - \frac{1}{1 + r} \int \left( q - \frac{1}{1 + r} \right) \Pi_r dr \right) (\zeta - \zeta) d\zeta.
\] (71)

One more Bregman-divergence is the norm-like or Eta-divergence equation (30). The Fréchet-derivative of \(D_{\text{E}}\) with respect to \(q\) is given in Eq. (58). Again, we are interested in the gradient \(\partial D_{\text{E}}/\partial \zeta\), which is
\[
\frac{\partial D_{\text{E}}}{\partial \zeta} = 4 \eta (\eta - 1) \int \frac{\zeta - \zeta}{1 + r} (p - q) q^{\eta-1} - q \left( \int (p - q) q^{\eta-1} \Pi_r dr \right) d\zeta.
\] (72)

The last example of Bregman-divergences we handle in this paper is the class of Beta-divergences defined in Eq. (32). We use Eq. (14) and insert the Fréchet-derivative of the Beta-divergences, given by Eq. (59). Thereby the gradient \(\partial D_{\text{B}}/\partial \zeta\) reads as
\[
\frac{\partial D_{\text{B}}}{\partial \zeta} = 4 \int \frac{\zeta - \zeta}{1 + r} (p - q) q^{\alpha-1} - q \left( \int q^{\alpha-1} (p - q) \Pi_r dr \right) d\zeta.
\] (73)

7.2. Csiszar’s \(f\)-divergences

Now we will consider some divergences belonging to the class of Csiszar’s \(f\)-divergences (see Section 4.2). A well-known example is the Hellinger divergence defined in Eq. (45), with the Fréchet-derivative equation (67). The gradient of \(D_{\text{H}}\) with respect to \(\zeta\) is
\[
\frac{\partial D_{\text{H}}}{\partial \zeta} = 4 \int \frac{1}{1 + r} \left( \sqrt{pq} q - q \left( \sqrt{pq} q \Pi_r dr \right) (\zeta - \zeta) d\zeta.
\] (74)

For the Alpha divergence, see Eqs. (40) and (63), we get
\[
\frac{\partial D_{\text{A}}}{\partial \zeta} = 4 \int \frac{\zeta - \zeta}{1 + r} \left( p q^{\alpha-1} - 1 \left( \int q^{\alpha} \Pi_r dr \right) d\zeta.
\] (75)

For the Tsallis divergence, Eqs. (44) and (66), we get
\[
\frac{\partial D_{\text{T}}}{\partial \zeta} = 4 \int \frac{\zeta - \zeta}{1 + r} \left( p q^{\alpha-1} - 1 \left( \int p q^{\alpha} \Pi_r dr \right) d\zeta.
\] (76)

which is also clear from Eq. (75), since the Tsallis-divergence is a rescaled version of the Alpha divergence for probability densities.

For the Rényi-divergences, Eqs. (43) and (65), the derivative reads
\[
\frac{\partial D_{\text{R}}}{\partial \zeta} = 4 \int p q^{\alpha-1} dr \left( \int p q^{\alpha} \Pi_r dr \right) d\zeta.
\] (77)
7.3. Gamma divergences

The Fréchet-derivative of $D_\gamma(p||q)$ with respect to $q$ is given in Eq. (46) can be rewritten as

$$
\frac{\partial D_\gamma(p||q)}{\partial q} = \frac{q^{(\gamma-1)} \left[ q \int q^{(\gamma+1)} \, dr - \frac{p}{\int p q^{\gamma} \, dr} \right]}{\int q^{\gamma} \, dr} = \frac{q^{\gamma} V_\gamma - p q^{(\gamma-1)} Q_\gamma}{Q_\gamma V_\gamma}.
$$

Once again, we use Eq. (14) to calculate the gradient of $D_\gamma$ with respect to $\zeta$:

$$
\frac{\partial D_\gamma}{\partial \zeta} = \frac{4}{Q_\gamma V_\gamma} \int \frac{q(\zeta - \zeta)}{1 + \gamma} \left[ q^{\gamma} V_\gamma - p q^{(\gamma-1)} Q_\gamma \right] d\zeta
- \int \left( q^{\gamma} V_\gamma - p q^{(\gamma-1)} Q_\gamma Q_\gamma \right) d\zeta
= -\frac{4}{Q_\gamma V_\gamma} \int \frac{q(\zeta - \zeta)}{1 + \gamma} \left[ q^{\gamma} V_\gamma - p q^{(\gamma-1)} Q_\gamma \right] d\zeta
\times \int q^{(\gamma+1)} \Pi_\gamma \, dr + Q_\gamma \int p q^{\gamma} \Pi_\gamma \, dr \, d\zeta.
$$

Fig. 12. Nearest neighbor errors of the two-dimensional embeddings using the Gamma-, Renyi- and Beta-divergence on the Olivetti faces data in comparison with the original formulation using Kullback-Leibler (KL) for different perplexities.

Fig. 13. Quality of the two-dimensional embeddings using the Gamma-, Renyi- and Beta-divergence on the Olivetti faces data in comparison with the original formulation using Kullback-Leibler (KL).
For the special choice $\gamma = 1$ the Gamma divergence becomes the Cauchy–Schwarz divergence equation (47) and the gradient $\partial D_{CS}/\partial z$ for t-SNE can be directly derived from Eq. (78):

$$\frac{\partial D_{CS}}{\partial z} = 4 \int \left( \frac{r}{1 + r} \right) \left( \frac{p q i}{1 + r} - \frac{q^{i+1}}{1 + r} \right) d\zeta.$$  \hspace{1cm} (78)

$$\frac{\partial D_{CS}}{\partial z} = 4 \int \left( \frac{r}{1 + r} \right) \left( \frac{p q i}{1 + r} - \frac{q^{i+1}}{1 + r} \right) d\zeta.$$  \hspace{1cm} (79)

Fig. 14. Embeddings of the Olivetti faces based on the same initialization for different divergences and perplexity 20.
Moreover, similar derivations can be made for any other divergence, since one only needs to calculate the Fréchet-derivative of the divergence and apply it to Eq. (14).

8. Demonstration of different divergences

In this section we demonstrate the use of different divergences in the t-SNE method on the bases of the Olivetti faces data set\(^1\) and the COIL-20 data set $[58]$. In the experiments we compare one divergence from all three main families: Kullback–Leibler, Beta, Rényi and Gamma as example for Bregman-, Csiszár-f- and Gamma divergences. For the Gamma divergence we include the special case of Cauchy–Schwarz in the choice of the parameter $g$ and the Rényi divergence is closely related to the Alpha divergence as shown in $[26]$.

The Olivetti data set consists of intensity-value pictures of 40 individuals with small variations in viewpoint, large variation in expression and occasional addition of glasses. The data set contains 400 images (10 per person) of size 64 $\times$ 64. The COIL-20 data set contains images of 20 different objects viewed from 72 equally spaced orientations. In total we have 1440 images of $32 \times 32 = 1024$.

---

\(^1\) The Olivetti faces data set is publicly available from http://cs.nyu.edu/~roweis/data.html.
pixels. Like suggested in [16] we preprocessed the data by extracting the mean and reducing the dimension to 30 using PCA and successive transformation to unit variance features.

For the experiments we constructed 10 independent random initializations, which we reused in the algorithm with different divergences and values of the divergence parameter. To compare the different embeddings we use the one nearest neighbor classification error using the persons as labels. A quantitative evaluation based on the quality measure as proposed by [59, 60] is included. Basically, this measure relies on $k$-intrusions and $k$-extrusions, which means it compares $k$-ary neighborhoods given in the original high-dimensional space with those occurring in the low dimensional space. Intrusions refer to samples intruding a neighborhood in the embedding space, while extrusions correspond to the number of samples.

Fig. 17. Embeddings of the COIL-20 data set based on the same initialization for different divergences and perplexity 5.
which are missing in the projected k-ary neighborhoods. The overall quality $Q$ measures the percentage of data which is neither k-intrusive nor k-extrusive. In the optimal case all neighborhoods are exactly preserved, which results in a value of $Q = 1$. The quantity $B$ measures the percentage of k-intrusions minus the percentage of k-extrusions in the projection and therefore shows the tendency of the mapping method: techniques with negative values for $B$ are characterized by extrusive behavior, while positive values display more intrusive behavior.

### 8.1. Olivetti faces

Fig. 12 shows the nearest neighbor errors of the embeddings of the Olivetti data as mean and standard deviation over the 10 random initializations for different perplexities. The parameter $\gamma$ of the Gamma divergences varies in the interval $[0.2, 2]$. For Beta and Rényi the parameter ranges in the same interval excluding 1 and 2. Depending on the perplexity the influence of the divergence varies. For small perplexities, greater values of $\gamma$ show better classification accuracy, while for large perplexities lower $\gamma$ yield better performance. The Gamma and Kullback–Leibler divergence show a quite robust behavior on this data set with respect to the parameter $\gamma$ and the perplexity. The quality and behavior of the Beta and Rényi divergence on the other hand vary a lot depending on the parameter and the actual perplexity. Also the variance with respect to the random initialization is much bigger for this data set using the Beta and Rényi divergence. The mean nearest neighbor error of the embedding is comparable to the other divergences if $\gamma = 1$ and $\beta > 1$ for all perplexities. For this data set the use of a different divergence leads to a slight improvement of the nearest neighbor classification compared to the Kullback–Leibler divergence and can be considered as an alternative measures.

### 8.2. COIL-20

Fig. 13 shows the quantitative evaluation on Olivetti using the intrusion- and extrusion measure mentioned above as mean over the 10 random initializations in the example case of perplexity 50. Again we observe small deviations in the behavior depending on the choice of the divergence. The Gamma divergence shows a little better quality for very small neighborhoods, while the Rényi divergence with $\gamma > 1$ leads to a better quality for bigger neighborhoods. Some example visualizations are shown in Fig. 14. For comparison all visualizations are based on the same initialization.

### 8.3. Table of divergences and their t-SNE gradient.

<table>
<thead>
<tr>
<th>Divergence family</th>
<th>Functional gradient for t-SNE</th>
<th>Gradients for discrete data $[x^{(n)}<em>i]</em>{i=1}^n \in \mathbb{R}^d$ and $[c^{(n)}<em>i]</em>{i=1}^n \in \mathbb{R}^d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kullback–Leibler equation (27)</td>
<td>$\frac{\partial d_{KL}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{KL}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Itakura–Saito equation (28)</td>
<td>$\frac{\partial d_{IS}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} \left[ \int \frac{e^{x}}{q} \right] P_{x_i \mid x_j} , dc_i$</td>
<td>$\frac{\partial d_{IS}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Eta-divergence equation (30)</td>
<td>$\frac{\partial d_{\eta}}{\partial c_i} = 4 \left( 1 + \frac{e^{-x}}{1 + e^{-x}} \right) (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\eta}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Beta-divergence equation (32)</td>
<td>$\frac{\partial d_{\beta}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\beta}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Alpha divergence equation (40)</td>
<td>$\frac{\partial d_{\alpha}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\alpha}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Rényi divergence equation (43)</td>
<td>$\frac{\partial d_{\gamma}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\gamma}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Tsallis divergence equation (44)</td>
<td>$\frac{\partial d_{\tau}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\tau}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Hellinger divergence equation (45)</td>
<td>$\frac{\partial d_{H}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{H}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Gamma divergence equation (46)</td>
<td>$\frac{\partial d_{\Gamma}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{\Gamma}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
<tr>
<td>Cauchy–Schwarz equation (47)</td>
<td>$\frac{\partial d_{CS}}{\partial c_i} = 4 \int \frac{e^{-x}}{1 + e^{-x}} (p - q) , dc_i$</td>
<td>$\frac{\partial d_{CS}}{\partial c_i} = 4 \sum_{k=1}^n \frac{e^{-x_k}}{1 + e^{-x_k}} (p_{x_k} - q_{x_k})$</td>
</tr>
</tbody>
</table>
an improvement for this particular data set and although error free visualizations are possible it is not satisfying, because it resembles only very close neighborhoods but scatters the trajectories. Some error free example visualizations are shown in Fig. 17. For comparison all visualizations are based on the same initialization. Note that, for example, the data points representing object 1 are chained on a bended line using the Kullback–Leibler divergence, while it is visualized in a closed loop using the Gamma divergence. Interestingly the use of the Rényi divergence with $\alpha = 1.6$ resembles the desired loop structure for nearly all objects. The cars (objects 3, 6 and 19) are visualized as rings not as long bands as seen using Kullback–Leibler and the Gamma divergence. Also objects 2 and 9 are no longer divided into pieces but a connected structure. Besides some topologic defects and the non-closed loop of object 9 the visualization using Rényi is a quite good estimate of the optimal visualization one would expect for this particular data set.

9. Conclusion and outlook

The original SNE and t-SNE formulation employ the Kullback–Leibler divergence. In this contribution we provide a mathematical foundation for the use of arbitrary divergences and their derivatives such that they can immediately be plugged into the existing algorithms. We provide the reader with alternative measures, which can be used if the results using Kullback–Leibler are not satisfying.

For this purpose we characterized main subclasses of divergences following [26]: Bregman-, $f$- and Gamma divergences. We used the mathematical framework of Fréchet derivatives to derive the gradients for a wide range of important divergences as summarized in Table 4.

We studied the behavior of the divergences in some experiments inspired by image processing. From the experiments it is clearly visible that the divergences show different behavior for different problems. Although we are not yet able to deliver an overall recipe for choosing a particular divergence in a given task, we can still argue that it might be advantageous to try alternative measures if the results are not satisfying. We demonstrate the use of divergences taken from all three main families on two example data sets, namely the Olivetti faces and COIL-20 data set. Performances are compared in terms of the nearest neighbor classification error of the embeddings, the quality as measured by intrusion- and extrusion recognition, See Table 5 and Table 6.

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