On power chi expansions of $f$-divergences

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Abstract

We consider both finite and infinite power chi expansions of $f$-divergences derived from Taylor’s expansions of smooth generators, and elaborate on cases where these expansions yield closed-form formula, bounded approximations, or analytic divergence series expressions of $f$-divergences.

Keywords: $f$-divergence, chi-squared distance, exponential family, Taylor expansions, binomial and multinomial theorems, analytic formula, bounded density ratio.

1 Introduction

1.1 Statistical $f$-divergences

Let $(\mathcal{X}, \mathcal{F})$ be a measurable space [7], where $\mathcal{X}$ denotes the sample space and $\mathcal{F}$ is a $\sigma$-algebra of measurable events on $\mathcal{X}$. For a convex function $f : (0, \infty) \to \mathbb{R}$, strictly convex at 1, the $f$-divergence [8, 13] between two probability measure $P$ and $Q$ is defined by:

$$I_f(P : Q) := \left\{ \begin{array}{ll}
\int_{\mathcal{X}} f \left( \frac{dQ}{dP} \right) dP, & Q \ll P \\
+\infty, & Q \not\ll P
\end{array} \right.,$$

where $Q \ll P$ denoting that $Q$ is absolutely continuous [7] with respect to $P$. Notice that the integral defining the $f$-divergence may potentially diverge: In that case, we have $I_f(P : Q) = +\infty$.

The strict convexity of the generator $f$ at 1 is required for satisfying the law of the indiscernibles of the $f$-divergence: $I_f(P : Q) = 0$ if and only if $P = Q$ almost everywhere (a.e.). Since it follows from Jensen’s inequality that $I_f(P : Q) \geq f(1)$, we assume in the remainder that $f(1) = 0$. Moreover, let $f_{\alpha}(u) = f(u) + \alpha(u - 1)$. We have $I_{f_{\alpha}} = I_f$ for any $\alpha \in \mathbb{R}$. Thus we fix the generator $f_{\alpha}$ that satisfies $f'_{\alpha}(1) = 0$. In information geometry, a standard $f$-divergence [2] further satisfies the scaling normalization $f''_{\alpha}(1) = 1$ (see Appendix [A] for details).
When the probability measures $P$ and $Q$ are defined on the same measure space $(\mathcal{X}, \mathcal{F}, \mu)$ where $\mu$ is a base $\sigma$-finite positive measure (with $P, Q \ll \mu$), let $p$ and $q$ denote their respective Radon-Nikodym densities $\frac{dp}{d\mu}$ and $\frac{dq}{d\mu}$. Then the $f$-divergence between $p$ and $q$ is then defined by

$$I_f^\mu(p : q) := \int_{\mathcal{X}} p(x)f \left( \frac{q(x)}{p(x)} \right) \, d\mu(x) \geq f(1) = 0.$$  

(2)

We adopt the following conventions for the mathematically undefined expressions in Eq. (2)

$$f(0) = \lim_{\omega \to 0^+} f(\omega), \quad 0f \left( \frac{0}{0} \right) = 0, \quad 0f \left( \frac{a}{0} \right) = \lim_{\omega \to 0^+} \left( \frac{a}{1} \right).$$

It can be shown that the $f$-divergence between $P$ and $Q$ is independent of the choice of the dominating measure $\mu$ (in particular, one can choose $\mu = \frac{P + Q}{2}$). Thus we write concisely $I_f(p : q)$ for $I_f^\mu(p : q)$. In the remainder, we consider all measures dominated by the base measure $\mu$ (e.g., the Lebesgue or counting measures), and function $f$ shall be called the generator of the divergence (with $f(1) = 0$ and $f'(1) = 0$).

Let us give some examples of $f$-divergences in disguise: The total variation distance $TV(p, q) = \frac{1}{2} \int |p(x) - q(x)| d\mu(x)$ is a metric $f$-divergence obtained for the generator $f_{TV}(u) = |u - 1|$ which is strictly convex at $u = 1$ (and only convex otherwise). Another example is the chi-squared distance [21] which is $f$-divergences obtained for the generator $f_{\chi^2}(u) = (u - 1)^2$:

$$\chi^2(p : q) = \int \frac{(q(x) - p(x))^2}{p(x)} \, d\mu(x).$$

In theory, the definite integral of the $f$-divergences of Eq. (2) may be computed using Risch semi-algorithm of symbolic integration [6]. However, this semi-algorithm requires to test whether some expressions are equivalent to zero or not. It is not known whether such an algorithm exists or not. Worse, when the absolute value function belongs to the set of the elementary functions, it can be proved that no such algorithm exists [3] Thus in practice, one often relies on stochastic Monte Carlo integrations for estimating $f$-divergences, or on various approximation bounds [21].

1.2 Power chi pseudo-distances: Closed-form formula for affine exponential families

Let us define the following $i$-th power chi pseudo-distance:

$$\chi_i^\pm(p : q) = \int \frac{(q(x) - p(x))^i}{p(x)^{i-1}} d\mu(x), \quad i \in \{2, 3, \ldots \}.$$  

(3)

We have $\chi_2^\pm(p : q) = \chi^2(p : q)$. Although $\chi_i^\pm$ is a distance for even integer $i \geq 2$, it is not a distance for odd $i$ as $\chi_i^\pm$ maybe negative (hence the notation $\chi_i^\pm$) and even fail to satisfy the law of the indiscernibles (i.e., $\chi_i^\pm(p : q) = 0$ if and only if $p = q$). To see this, consider binary categorical distributions $p = (\lambda_p, 1 - \lambda_p)$ and $q = (\lambda_q, 1 - \lambda_q)$. Then we have

$$\chi_2^+(p : q) = \frac{(\lambda_q - \lambda_p)^2}{\lambda_p^{1-i}} + \frac{(1 - \lambda_q - 1 + \lambda_p)^2}{(1 - \lambda_p)^{1-i}}.$$

[1]https://en.wikipedia.org/wiki/Risch_algorithm
When $i$ is odd, we get
\[ \chi^\pm_i(p : q) = (\lambda_q - \lambda_p)^i \left( \frac{1}{\lambda_p^{i-1}} - \frac{1}{(1 - \lambda_p)^{i-1}} \right). \]

Thus for $\lambda_p = 1 - \lambda_p = \frac{1}{2}$, we have $\chi^\pm_i(p : q) = 0$ for odd $i$, independent of the values of $\lambda_q$.

In the remainder, we term the $\chi_i^\pm$’s the $i$-order chi pseudo-distances or the power chi distances for short.

Notice that the $\chi_i^\pm$’s are $f$-divergences for even integer $i$ for the generators $f_{\chi^\pm_i}(u) = (u - 1)^i$.

Let us further extend the definition as follows (for any $\lambda \neq 0$):
\[ \chi^\pm_{i,\lambda}(p : q) := \int \frac{(q(x) - \lambda p(x))^i}{p(x)^{i-1}} d\mu(x), \quad i \in \{2, 3, \ldots \}. \tag{4} \]

We note that $\chi^\pm_{i,\lambda}(p : q) = \chi^\pm_i(p : q)$. We shall define $\lambda^j = \text{sign}(\lambda)^j |\lambda|^j$ for any integer $j \in \mathbb{N}$, where
\[ \text{sign}(\lambda) = \begin{cases} 1 & \text{if } \lambda > 0, \\ -1 & \text{if } \lambda < 0, \\ 0 & \text{if } \lambda = 0. \end{cases} \]

An full natural exponential family $\{f(x; \theta) d\mu\}$ is a set of probability distributions with densities with respect to a base measure $\mu$ written canonically \[18\] \[19\] as $f(x; \theta) = \exp(t(x)^\top \theta - F(\theta) + k(x))1_{X}(x)$, where $X$ is the support, $t(x)$ a vector of sufficient statistics, $\theta$ the natural parameter, $k(x)$ an auxiliary carrier measure term and $F(\theta)$ the log-normalizer (also called log-partition function or cumulant function). The order $D$ of the family is the dimension of $t(x)$ or $\theta$. The natural parameter space \[18\] is $\Theta = \{\theta : \int f(x; \theta) d\mu < \infty\}$ (with $\Theta \subset \mathbb{R}^D$). Following \[20\], we report a closed-form formula for exponential families \[18\] with a natural parameter space being affine. These exponential families are termed Affine Exponential Families, or AEF for short.

Affine exponential families \[18\] include the isotropic Gaussian family, the Poisson family, the multinomial family, the von Mises-Fisher distributions\[2\], etc. See Table \[11\].

Let $p = f(x; \theta_p)$ and $q = f(x; \theta_q)$ be two densities belonging to the same affine exponential family. Then we have:
\[ \chi^\pm_{i,\lambda}(p : q) = \sum_{j=0}^{i} (-\lambda)^{i-j} \binom{i}{j} \exp \left( F((1-j)\theta_p + j\theta_q) - ((1-j)F(\theta_p) + jF(\theta_q)) \right). \tag{5} \]

This can be easily seen be writing $\chi_i^\pm$ as $\chi_i^\pm(p : q) = \int p(x)^{1-i}(q(x) - p(x))^i d\mu(x)$ and plugging the canonical densities of exponential families. The binomial coefficients can be computed efficiently using Pascal’s triangle.

Furthermore, this formula can be extended to $\chi^\pm_i(p : \sum_{i=1}^l w_i q_i)$ where $\sum_{i=1}^l w_i q_i$ is a mixture of exponential families by using the multinomial expansion \[17\] instead of the binomial expansion:

\[ \chi^\pm_i(p : \sum_{i=1}^l w_i q_i) = \sum_{j=0}^{l} (-\lambda)^{i-j} \binom{i}{j} \exp \left( F((1-j)\theta_p + j\theta_q) - ((1-j)F(\theta_p) + jF(\theta_q)) \right). \]
Poi(\(\lambda\)) : \(f(x; \lambda) = \frac{\lambda^x e^{-\lambda}}{x!}, \lambda > 0, x \in \{0, 1, \ldots\}\)

Cat(\(p\)) : \(f(x; p) = p_0^{x_1} \cdots p_d^{x_d}, x_i \in \{0, 1\}, \sum_{i=0}^{d} x_i = 1\)

vmF(\(\theta\)) : \(f(x; \theta) = \frac{\exp(x^\top \theta)}{\,_{d}F_{1}(; \frac{\|\theta\|^2}{4})}\)

Nor(\(m, I\)) : \(f(x; \mu) = \frac{1}{(2\pi)^{\frac{d}{2}}} e^{-\frac{1}{2}(x-m)^\top (x-m)}, m \in \mathbb{R}^d, x \in \mathbb{R}^d\)

### Table 1: Examples of exponential families with affine natural parameter spaces.

| Density           | \(\theta\) | Domain | Log-normalizer \(F(\theta)\) | Base measure |
|-------------------|-------------|--------|-----------------------------|--------------|
| Categorical       | \(\theta_i = \log \frac{p_i}{p_0}, i \in \{1, \ldots, d\}\) | \(\mathbb{R}^d\) | \(\log(1 + \sum_{i=1}^{d} e^{\theta_i})\) | \(\mu_c\)   |
| Poisson           | \(\log \lambda\) | \(\mathbb{R}\) | \(e^{\theta}\) | \(\mu_c\)   |
| Isotropic Gaussian | \(m\) | \(\mathbb{R}^d\) | \(\frac{1}{2} \theta^\top \theta\) | \(\mu_L(d)\) |
| von-Mises Fisher  | \(\theta\) | \(\mathbb{R}^{d-1}\) | \(\log_{0} F_{1}(; \frac{\|\theta\|^2}{4})\) | \(\mu_S(d-1)\) |

Following [17], when \(p(x) = f(x; \theta)\) and \(q_u(x) = f(x; \theta_u)\) are densities of the same affine exponential family, we have

\[
\chi^+_{i, \lambda} \left( p : \sum_{i=1}^{l} w_i q_i \right) = \int \frac{\left( \sum_{i=1}^{l} w_i q_i(x) - \lambda p(x) \right)^i}{p(x)^{i-1}} d\mu(x),
\]

\[
= \int \left( \sum_{s=0}^{i} \binom{i}{s} (-\lambda p(x))^{1-s} \left( \sum_{u=1}^{l} w_u q_u(x) \right)^s \right) d\mu(x),
\]

\[
= \sum_{s=0}^{i} \binom{i}{s} (-\lambda)^{1-s} \sum_{\alpha_1, \ldots, \alpha_l}^{\alpha} \int p(x)^{1-s} \prod_{u=1}^{l} (w_u q_u(x))^\alpha_j d\mu(x).
\]

Following [17], when \(p(x) = f(x; \theta)\) and \(q_u(x) = f(x; \theta_u)\) are densities of the same affine exponential family, we have

\[
\int p(x)^{1-s} \prod_{u=1}^{l} (w_u q_u(x))^\alpha_j d\mu(x) = \exp \left( F \left( (1-s)\theta + \sum_{u=1}^{l} \alpha_u \theta_u \right) - \left( (1-s) F(\theta) + \sum_{u=1}^{l} \alpha_u F(\theta_u) \right) \right).
\]  

**Theorem 1.** The power chi pseudo-distances between a member and a mixture of an affine exponential family can be calculated in closed-form.
For isotropic Gaussian distributions $p \sim N(m_1, I)$ and $q \sim N(m_2, I)$ (where $I$ denotes the identity matrix), we get:

$$
\chi_i^\pm (p : q) = \chi_i^\pm (m_1 : m_2) = \sum_{j=0}^{i} (-1)^{i-j} \binom{i}{j} \exp \left( \frac{j(j-1)}{2} \|m_1 - m_2\|^2 \right).
$$

(7)

For any prescribed integer $i$, $\chi_i^\pm (m_1 : m_2) < \infty$ and we can bound $\chi_i^\pm$ as follows:

$$
|\chi_i^\pm (m_1 : m_2)| \leq 2^i \exp \left( \frac{i(i-1)}{2} \|m_1 - m_2\|^2 \right) < \infty.
$$

Consider $\|m_1 - m_2\| = 1$ (e.g., in 1D, $m_1 = 0$ and $m_2 = 1$), then we have

\begin{align*}
\chi_2^\pm (0 : 1) & \approx 1.718281828459045, \\
\chi_3^\pm (0 : 1) & \approx 13.930691437810532, \\
\chi_4^\pm (0 : 1) & \approx 336.3963367707387, \\
\chi_5^\pm (0 : 1) & \approx 20186.99437829033, \\
\chi_6^\pm (0 : 1) & \approx 3142544.0730946246, \\
\chi_7^\pm (0 : 1) & \approx 1.2963817005597024 \times 10^9, \\
\chi_8^\pm (0 : 1) & \approx 1.4357966846042915 \times 10^{12}, \\
\chi_9^\pm (0 : 1) & \approx 4.298262439031654 \times 10^{15}, \\
\chi_{10}^\pm (0 : 1) & \approx 3.489122366600497 \times 10^{19}, \\
\text{etc.}
\end{align*}

We can notice that the $\chi$ pseudo-distances diverge very quickly with the increase of the order.

2 Power chi expansions of $f$-divergences from Taylor’s theorem

2.1 Power chi expansions

Consider the Taylor’s $k$-th order expansions [5] of the smooth generator $f$ around point $c$:

$$
f(u) = P_k(u) + R_k(u),
$$

where $P_k(u)$ is the $k$-th order Taylor polynomial:

$$
P_k(u) = \sum_{i=0}^{k} \frac{f^{(i)}(c)}{i!}(u - c)^i,
$$

and $R_k(u) = f(u) - P_k(u)$ is the Taylor remainder term. There are many ways to express (e.g., Peano, Lagrange, Cauchy, or integral forms) and bound the remainder $R_k$ in a Taylor expansion [5, 4].

In particular, when $|f^{(k+1)}(u)| \leq M$ for any $u \in (c - r, c + r)$ (with $r > 0$), then we have

$$
|R_k(u)| \leq M \frac{r^{k+1}}{(k + 1)!}.
$$
Letting \( c = 1 \) and \( u = \frac{q(x)}{p(x)} \), and using the fact that \( f(1) = f'(1) = 0 \), we get

\[
p(x)f \left( \frac{q(x)}{p(x)} \right) = \sum_{i=2}^{k} \frac{f^{(i)}(1)}{i!} \left( \frac{q(x)}{p(x)} - 1 \right)^i + R_k \left( \frac{q(x)}{p(x)} \right).
\]

Carrying the integral over the support \( \mathcal{X} \), we end up with the following power chi expansion of the \( f \)-divergence:

\[
I_f(p : q) = \sum_{i=2}^{k} \frac{f^{(i)}(1)}{i!} \chi_i^\pm(p : q) + \int_{\mathcal{X}} R_k \left( \frac{q(x)}{p(x)} \right) d\mu(x).
\]

Define the \( k \)-th order chi expansion of the \( f \)-divergence:

\[
I_{f,k}^\chi(p : q) := \sum_{i=2}^{k} \frac{f^{(i)}(1)}{i!} \chi_i^\pm(p : q).
\]

It is “chinomial” of order \( k \). Let us express the power chi remainder as:

\[
R_k^\chi(p : q) = I_f(p : q) - I_{f,k}^\chi(p : q).
\]

Then we can approximate the \( f \)-divergence by its \( k \)-th order chi expansion, and bound the error as:

\[
\left| I_f(p : q) - I_{f,k}^\chi(p : q) \right| = \left| R_k^\chi(p : q) \right| \leq \int_{\mathcal{X}} R_k \left( \frac{q(x)}{p(x)} \right) d\mu(x).
\]

### 2.2 Some illustrating examples of power chi expansions

Let us report the \( k \)-th order chi expansions for the Kullback-Leibler divergence, the Jeffreys divergence and the Jensen-Shannon divergence:

- The Kullback-Leibler (KL) divergence\(^4\) between two densities \( p \) and \( q \) is defined by

  \[
  \text{KL}(p : q) = \int p(x) \log \frac{p(x)}{q(x)} d\mu(x).
  \]

The KL divergence is a \( f \)-divergence obtained for the generator \( f_{\text{KL}}(u) = -\log u \). It is an unbounded divergence that may potentially diverge even when distributions are defined on the same support\(^5\). We have

\[
f_{\text{KL}}^{(i)}(u) = (-1)^i (i - 1)! u^{-i}, \quad i \geq 2,
\]

and it follows the \( k \)-order power chi expansion of the KL divergence:

\[
\text{KL}^\chi_k(p : q) = \sum_{i=2}^{k} \frac{(-1)^i}{i!} \chi_i^\pm(p : q).
\]

\(^4\)In the literature, a divergence is either a statistical distance or a smooth parameter distance used to define an information-geometric manifold \(^6\).

\(^5\)Let \( \mathcal{X} = (0, 1) \) and two densities (with respect to Lebesgue measure \( dx \)) \( p_1(x) = 1 \) and \( p_2(x) = ce^{-1/2} \) with \( c^{-1} = \int_0^1 e^{-1/2} dx \simeq 0.148 \) the normalizing constant. Then \( \text{KL}(p_1 : p_2) = \int_0^1 x \log \frac{p_1(x)}{p_2(x)} dx = -\log c + \int_0^1 \frac{1}{x} dx = \infty. \)
The reverse $f$-divergence $I_f^r(p : q) = I_f(q : p)$ is obtained for the conjugate generator $f^*(u) = uf \left( \frac{1}{u} \right)$. The reverse KL divergence is a $f$-divergence for the generator $f_{KL}^r(u) = u \log u$. The derivatives of the generator are:

$$f_{KL}^{(i)}(u) = (-1)^i (i - 2)!u^{-i}, \quad i \geq 2.$$

(11)

$$\text{KL}_k^\chi(p : q) = \sum_{i=2}^k (-1)^i \frac{1}{i(i-1)} \chi_i^+(p : q).$$

In general, the derivatives of the conjugate generator are

$$f^{(i)}(u) = u \left( \frac{d^i}{du^i} f \left( \frac{1}{u} \right) \right) + i \left( \frac{d^{i-1}}{du^{i-1}} f \left( \frac{1}{u} \right) \right), \quad i \geq 1.$$

We get a closed-form expression by applying the formula of Fa`a di Bruno [27]:

$$\frac{d^n}{dx^n} f(g(x)) = \sum_{1 \cdot m_1 + 2 \cdot m_2 + 3 \cdot m_3 + \cdots + n \cdot m_n = n} n! \frac{f^{(m_1 + \cdots + m_n)}(g(x)) \prod_{j=1}^n (g^{(j)}(x))^{m_j}}{m_1! \cdot m_2! \cdot m_3! \cdots \cdot m_n! \cdot n! \cdot m_n!}.$$

- The Jeffreys divergence is the following symmetrization of the KL divergence:

$$J(p : q) = \text{KL}(p : q) + \text{KL}(q : p) = \int (p(x) - q(x)) \log \frac{p(x)}{q(x)} d\mu(x).$$

It is a $f$-divergence obtained for the generator $f_J(u) = (u - 1) \log u$ (with $f_J(1) = 0$, $f_J'(u) = 1 - \frac{1}{u} + \log u$ and $f_J''(1) = 0$), and the higher-order derivatives of the generator are

$$f_J(u)^{(i)} = (-1)^i (i - 2)!u^{-i}, \quad i \geq 2.$$

Thus the $k$-order power chi expansion for the Jeffreys divergence is:

$$J_k^\chi(p : q) = \sum_{i=2}^k (-1)^i \frac{1}{i-1} \chi_i^+(p : q).$$

- The Jensen-Shannon (JS) divergence [14] is defined by:

$$\text{JS}(p, q) = \frac{1}{2} \left( \text{KL} \left( p : \frac{p + q}{2} \right) + \text{KL} \left( q : \frac{p + q}{2} \right) \right)$$

(12)

$$= \frac{1}{2} \int \left( p(x) \log \frac{2p(x)}{p(x) + q(x)} + q(x) \log \frac{2q(x)}{p(x) + q(x)} \right) d\mu(x),$$

(13)

$$= h \left( \frac{p + q}{2} \right) - h(p) + h(q),$$

(14)
where \( h(p) = -\int p(x) \log p(x) d\mu(x) \) denotes Shannon differential entropy. It is a bounded symmetrization\(^5\) of the KL divergence (i.e., \( \text{JS}(p, q) \leq \log 2 \)) obtained for the generator

\[
f_{\text{JS}}(u) = -(u + 1) \log \frac{1 + u}{2} + u \log u.
\]

The JS divergence gained interest in Deep Learning (DL), notably with the Generative Adversarial Network (GAN) architecture \(^{10, 23}\). We have

\[
f^{(i)}_{\text{JS}}(u) = (-1)^{i-2}(i-2)! \left( \frac{1}{u^{i-1}} - \frac{1}{(u+1)^{i-1}} \right), \quad i \geq 2,
\]

and it follows the \( k \)-order power chi expansion of the JS divergence:

\[
\text{JS}_{k}^\chi(p : q) = \sum_{i=2}^{k} (-1)^{i-2} \frac{1}{i^{i-1}} \left( 1 - \frac{1}{2i-1} \right) \chi_{i}^\pm(p : q). \tag{15}
\]

Note that the power chi expansions (e.g., \( \text{JS}_{k}^\chi \)) are not distances since they do not satisfy the law of the indiscernibles.

There are many other \( f \)-divergences, some of them are not standard\(^6\). For example, the harmonic divergence \( H(p : q) = \int \frac{2p(x)q(x)}{p(x)+q(x)} d\mu(x) \) is an uncalibrated \( f \)-divergence obtained for the generator \( f_{H}(u) = \frac{2u}{u+1} \). Indeed, in that case, we have \( f_{H}(1) = 1 \) and \( f'_{H}(1) = \frac{1}{2} \). The harmonic divergence is lower bounded by \( f_{H}(1) = 1 \) and upper bounded by 2. The higher-order derivatives are \( f^{(i)}_{H}(u) = 2(-1)^{i+1} i! \left( \frac{1}{(i+1)^{i-1}} \right) \). The power chi expansion yields

\[
H_{k}^\chi(p : q) = 1 + \sum_{i=2}^{k} (-1)^{i+1} \frac{1}{2i^{i-1}} \chi_{i}^\pm(p : q). \tag{16}
\]

Finally, the \( f \)-divergence defined for the generator \( f_{\exp}(u) = e^u - eu \) (with \( f_{\exp}(1) = 0 \) and \( f'_{\exp}(1) = 0 \)) has very simple higher-order derivatives: \( f^{(i)}_{\exp}(u) = \exp(u) \) for \( i \geq 2 \). Therefore the \( k \)-th power chi expansion is

\[
I_{f_{\exp}}^{k}(p : q) = E_{k}^\chi(p : q) = \sum_{i=2}^{k} e \frac{1}{i!} \chi_{i}^\pm(p : q).
\]

We call this \( f \)-divergence the exponential divergence for short.

### 2.3 Finite chi expansions for \( f \)-divergences with polynomial generators

**Theorem 2** (Polynomial generator). The \( f \)-divergence for any polynomial generator \( f(u) = \sum_{j=0}^{d} a_{j}u^{j} \) has a finite chi expansion. When the distributions are members of an affine exponential family, the \( f \)-divergence is calculated in closed-form.

\(^5\)Indeed, we have \( p(x) \log \frac{2p(x)}{p(x)+q(x)} \leq p(x) \log 2 \), and hence \( \text{KL}(p : \frac{1+x}{2}) \leq \log 2 \).

\(^6\)A standard \( f \)-divergence \(^{2}\) satisfies \( f(1) = f'(1) = 0 \) with \( f''(1) = 1 \).
Proof. Let \( f(u) = \sum_{j=0}^{d} a_j u^j \) be a convex polynomial generator for the \( f \)-divergence of order \( d \) (with coefficients satisfying \( f(1) = f'(1) = 0 \)). We have \( f^{(i)}(u) = 0 \) when \( i > d \), and \( f^{(i)}(u) = \sum_{j=1}^{d} a_j \frac{d}{(j-1)!} u^{j-1} \) for \( 0 \leq i \leq d \). It follows that \( I_f \) has a finite chi expansion:

\[
I_f(p : q) = \sum_{i=2}^{d} \left( \sum_{j=1}^{d} a_j \binom{j}{i} \right) \chi_i^\pm(p : q).
\]

The reverse \( f \)-divergence \( I_f^r(p : q) = I_f(q : p) \) is obtained for the conjugate generator \( f^r(u) = uf\left(\frac{1}{u}\right) \). The conjugate polynomial generator is \( f(u) = \sum_{j=0}^{d} a_j u^{1-j} = \sum_{j=0}^{d} a_j \frac{1}{u^{1-j}} \) (called a Laurent polynomial).

A necessary condition for a polynomial to be convex on \( \mathbb{R}_+ \) is to have the leading coefficient positive.

### 2.4 The case of \( \alpha \)-divergences

The \( \alpha \)-divergences for \( \alpha \in \mathbb{R} \setminus \{\pm 1\} \) are defined by:

\[
I_\alpha(p : q) = \frac{4}{1 - \alpha^2} \left( 1 - \int p^{\frac{1-\alpha}{2}}(x)q^{\frac{1+\alpha}{2}}(x)d\mu(x) \right) = I_{-\alpha}(q : p).
\]

We have \( \lim_{\alpha \to -1} I_\alpha(p : q) = KL(p : q) \) and \( \lim_{\alpha \to 1} I_\alpha(p : q) = KL^r(p : q) = KL(q : p) \) (reverse KL divergence).

The \( \alpha \)-divergences are \( f \)-divergences for the generator \( f_\alpha(u) = \frac{4 - \alpha^2}{1 - \alpha^2}(1 - u^{\frac{1+\alpha}{2}}) \):

\[
I_\alpha(p : q) = I_{f_\alpha}(p : q) = \int p(x) \frac{4}{1 - \alpha^2} \left( 1 - \left( \frac{q}{p} \right)^{\frac{1+\alpha}{2}} \right)^2 d\mu(x),
\]

\[
= \frac{4}{1 - \alpha^2} \left( 1 - \int p^{\frac{1-\alpha}{2}}(x)q^{\frac{1+\alpha}{2}}(x)d\mu(x) \right).
\]

The derivatives for the \( \alpha \)-generators are

\[
f_\alpha^{(i)}(u) = -\frac{2}{1 - \alpha} \left( \frac{1+\alpha}{2} \right) u^{\frac{1+\alpha}{2} - i}, \quad i \geq 2,
\]

where

\[
\binom{\gamma}{i} := \begin{cases} 
\gamma(\gamma-1) \cdots (\gamma-i+1) & \text{if } i \leq \gamma, \\
0 & \text{otherwise.}
\end{cases}
\]

are the generalized binomial coefficients for any \( \gamma \in \mathbb{R} \). Symmetric divergence \( I_0 \) is known as the squared Hellinger distance:

\[
I_0(p : q) = 4 \left( 1 - \int \sqrt{p(x)} \sqrt{q(x)} d\mu(x) \right) = 2 \int (\sqrt{p(x)} - \sqrt{q(x)})^2 d\mu(x) = I_0(q : p).
\]

9
Therefore it follows that the power chi expansions for the $\alpha$-divergences is:

$$I_{\alpha,k}^\chi(p:q) = \sum_{i=2}^{k} \frac{2}{1-\alpha} \frac{1}{i!} \left(\frac{1+\alpha}{i}\right) \chi_i^\pm(p:q).$$

Consider $\frac{1+\alpha}{2}$ an integer (say, $\alpha = 2k-1$ for $k \in \{2, 3, \ldots\}$). We can directly apply Theorem [2] for the polynomial generator $f_{2k-1}(u) = \frac{1}{4k(1-k)}(1-u^k)$.

In that case, the iterated derivatives $f_{2k-1}^{(i)}$ are zero when $i > 2k-1$. Indeed, we have

$$f_{2k-1}(u) = \frac{1}{4k(1-k)}(1-u^k)$$

In that case, the iterated derivatives $f_{2k-1}^{(i)}$ are zero when $i > 2k-1$. Indeed, we have

$$f_{2k-1}^{(1)}(u) = \frac{u^{k-1}}{4(k-1)}$$

$$f_{2k-1}^{(2)}(u) = \frac{u^{k-2}}{4}$$

$$\vdots = \vdots$$

$$f_{2k-1}^{(i)}(u) = \frac{(k-2)!}{(k-i)!} \frac{u^{k-i}}{4}$$

$$\vdots = \vdots$$

$$f_{2k-1}^{(k+1)}(u) = 0.$$

Hence, we have $f_{2k-1}^{(i)}(u) = 0$ for $i > k > 0$. Notice that $f_{2k-1}^{(2)}(u)$ is positive on $u > 0$, hence $f_{2k-1}$ is strictly convex.

Thus the $(2k-1)$-divergences have finite chi expansions:

$$I_{2k-1}(p:q) = \sum_{i=2}^{k+1} \frac{(k-2)!}{i!(k-i)!} \frac{1}{4} \chi_i^\pm(p:q), \quad (18)$$

$$= \frac{1}{k(1-k)} \left(1 - \int p^{1-k}(x)q^k(x)d\mu(x)\right). \quad (19)$$

The $\alpha$-divergences between members $p = f(x; \theta_p)$ and $q = f(x; \theta_q)$ of the same affine exponential family admit the following closed-form formula for any $\alpha \in \mathbb{R}\setminus\{\pm 1\}$:

$$I_{\alpha}(p:q) = \frac{4}{1-\alpha^2} \left(1 - \exp F\left(\frac{1-\alpha}{2} \theta_p + \frac{1+\alpha}{2} \theta_q\right) - \left(\frac{1-\alpha}{2} F(\theta_p) + \frac{1+\alpha}{2} F(\theta_q)\right)\right). \quad (20)$$

This formula matches the formula obtained by the chi expansion when $\alpha = 2k-1$:

$$I_{2k-1}(p:q) = \sum_{i=2}^{k+1} \frac{(k-2)!}{i!(k-i)!} \frac{1}{4} \sum_{j=0}^{i} (-1)^{i-j} \binom{i}{j} \exp \left( (1-j)\theta_p + j\theta_q - ((1-j)F(\theta_p) + jF(\theta_q)) \right),$$

$$= \frac{1}{4k(k-1)} \sum_{i=2}^{k+1} \binom{k}{i} \sum_{j=0}^{i} (-1)^{i-j} \binom{i}{j} \exp \left( (1-j)\theta_p + j\theta_q - ((1-j)F(\theta_p) + jF(\theta_q)) \right),$$

since $\frac{(k-2)!}{i!(k-i)!} = \binom{k}{i}$. 
3 Analytic formula and power chi series

A function (or formula) is said analytic if it is locally defined by a convergent power series. For example, the exponential function \( \exp(x) = \sum_{i=0}^{\infty} \frac{x^i}{i!} \) or the function \( \sin(x) = \sum_{i=0}^{\infty} \frac{(-1)^i x^{2i+1}}{(2i+1)!} \) are (globally) analytic on \( \mathbb{R} \). We have \( \log(1 + x) = \sum_{i=1}^{\infty} \frac{(-1)^{i+1} x^i}{i} \) for \( |x| < 1 \) (locally analytic at center \( x = 0 \) with radius 1). That is, when \( |x| \geq 1 \), the power series \( \sum_{i=1}^{\infty} (-1)^{i+1} \frac{x^i}{i} \) diverge. The series \( \sum_{i=1}^{\infty} (-1)^{i+1} \frac{x^i}{i} \) is a power series for the function \( \log(1+x) \). A Taylor expansion yields in the limit a Taylor series when the Taylor polynomials converge and the Taylor remainder tends to zero.

Log-normalizers of exponential families are analytic functions. Similarly, a chi expansion tends to converge when the remainder tends to zero and the weighted sum of power chi pseudo-distances converges. Let us mention that there are cases where \( I_f(p : q) \) may admit a power chi series but not \( I_f(q : p) \) (or the reverse divergence \( I_f^p(p : q) = I_f(q : p) \)).

The JS divergence between two Gaussian distributions cannot be approximated by a finite chi expansion because the sum of weighted \( i \)-th power chi divergences diverges:

\[
\text{JS}(m_1, m_2) \neq \sum_{i=2}^{\infty} \frac{(-1)^{i-2}}{i(i-1)} \left( 1 - \frac{1}{2i-1} \right) \sum_{j=0}^{i} \frac{(-1)^{i-j} i!}{j!} \exp \left( \frac{j(j-1)}{2} \|m_1 - m_2\|^2 \right).
\]

This fact is in accordance with [28] which proved that the KL divergence between Gaussian Mixture Models (GMMs) is not analytic. See Appendix A of [21] for an English translation of the non-analytic KL GMM Japanese proof of [28].

Let us state a selected part of the Theorem 1 of [5]:

**Theorem 3** ([5]). Let \( f : (0, \infty) \rightarrow \mathbb{R} \) be \( k \) times differentiable and such that \( f^{(k)} \) is absolutely continuous on \([m, M]\), where \( 0 < m \leq 1 \leq M < \infty \), and assume that \( m \leq \frac{q(x)}{p(x)} \leq M \) almost surely on \( \mathcal{X} \), then we have

\[
|I_f(p : q) - \sum_{i=2}^{k} \frac{f^{(i)}(1)}{i!} \chi_i^\pm(p : q)| \leq \frac{1}{(k+1)!} \|f^{(k+1)}\|_\infty \chi_{k+1}(p : q),
\]

where

\[
\chi_s(p : q) = \int \frac{|q(x) - p(x)|^{s-1}}{p^s(x)} \, d\mu(x), \quad s \geq 2
\]

and \( \|f^{(k+1)}\|_\infty = \text{ess sup}_{u \in [m, M]} |f^{(k+1)}(u)| \) is the Lebesgue \( L_\infty \)-norm (and \( f^{(k+1)} \in L_\infty [m, M] \)). Furthermore, we have \( \chi_{k+1}(p : q) \leq (M - m)^{k+1} \).

Observe that for bounded ratio densities, we have

\[
(-1)^i(1 - m)^i \leq \chi_i^\pm(p : q) \leq (M - 1)^i,
\]

and

\[
\chi_i(p : q) \leq \min((M - 1)^i, (1 - m)^i).
\]

Let us get a better upper bound: We have \( \frac{|q(x) - p(x)|^i}{p(x)^i} = \frac{|q(x) - p(x)|^i}{p(x)^i} \) and \( m - 1 \leq \frac{q(x)}{p(x)} - 1 \leq M - 1 \). Therefore \( \left| \frac{q(x)}{p(x)} - 1 \right| \leq \min(M - 1, 1 - m) \leq M - m \). It follows that \( \chi_1(p : q) \leq (M - m) \chi_1(p : q) \) and \( \chi_2(p : q) \leq (M - m) \int |q(x) - p(x)| \, d\mu(x) \leq (M - m)^2 \). Therefore \( \chi_1(p : q) \leq (M - m) \). Thus when \( M < m + 1 \), we have \( \lim_{i \to \infty} \chi_i(p : q) = 0 \).
To ensure that the Taylor remainder of the power chi series converge to zero, we need to have
\[
\lim_{k \to \infty} \frac{1}{(k+1)!} \| f^{(k+1)} \|_\infty (M - m)^{k+1} = 0.
\]

This is a sufficient (but not necessary) condition.

Notice that using Stirling approximation formula we have \((k+1)! \simeq \sqrt{2\pi(k+1)} \exp((k+1) \log(k+1))\) for large values of \(k\).

This theorem does not apply to Gaussian distributions because we cannot bound the density ratio of two Gaussians. However, we can truncate the Gaussians distributions on a compact support \(D \subset \mathcal{X}\), and define the extrema of the density ratio of two Gaussians as follows:

\[
m(\theta_1 : \theta_2) = \inf_{x \in D} \frac{p_D(x; \theta_2)}{p_D(x; \theta_1)},
\]

\[
M(\theta_1 : \theta_2) = \sup_{x \in D} \frac{p_D(x; \theta_2)}{p_D(x; \theta_1)},
\]

where \(p_D\) is the truncated distribution \([1]\):

\[
p_D(x; \theta) = \frac{p(x; \theta)}{W_D(\theta)} = \frac{\exp(t(x)\theta + k(x))}{\int_D \exp(t(x)\theta + k(x))} 1_D(x),
\]

where \(W_D(\theta)\) denotes the probability mass inside the domain \(D\): \(W_D(\theta) = \int_D p(x; \theta) d\mu(x)\). The truncation of a regular (i.e., topologically open natural parameter space) and steep exponential family (i.e. mean parameter space coinciding with the interior of the closed convex hull of the support of the distributions, like the exponential family of Gaussian distributions) may not yield a regular and steep exponential family, see \([9]\).

Sufficient conditions to apply Theorem 3 in order to get an analytic formula are to check that

1. the remainder tends to zero when \(k \to 0\), and
2. the power chi series converges when \(k \to 0\).

Notice that these two requirements are always fulfilled for finite discrete distributions for bounded \(|f^{(i)}|\)'s.

### 3.1 Vanilla case study: The Bernoulli distributions

Let \(p = (\lambda_p, 1 - \lambda_p)\) and \(q = (\lambda_q, 1 - \lambda_q)\) be two Bernoulli distributions (i.e., categorical distributions with two choices) with parameters \(\lambda_p, \lambda_q \in (0, 1)\). The \(f\)-divergence between \(p\) and \(q\) is

\[
I_f(p : q) = \lambda_p f \left( \frac{\lambda_q}{\lambda_p} \right) + (1 - \lambda_p) f \left( \frac{1 - \lambda_q}{1 - \lambda_p} \right).
\]

Let \(m(\lambda_p : \lambda_q) = \min(\lambda_q, 1 - \lambda_q)\) and \(M(\lambda_p : \lambda_q) = \max(\lambda_q, 1 - \lambda_q)\).

We have

\[
\chi_i^\pm(\lambda_p : \lambda_q) = \frac{(\lambda_q - \lambda_p)^{i-1}}{\lambda_p^{i-1}} + \frac{(\lambda_p - \lambda_q)^{i-1}}{(1 - \lambda_p)^{i-1}}
\]

That is, we do not use the binomial expansion for computing the chi pseudo-distances.
We consider the $f$-divergence for the exponential generator $f_{\text{exp}}(u) = e^x - ex$ with the $k$-th power chi expansion: $I_{f_{\text{exp}, k}}^\chi(\lambda_p : \lambda_q) = \sum_{i=2}^{k} \frac{\epsilon}{i!} \lambda_i^\pm(\lambda_p : \lambda_q)$.

When $k \to \infty$, the remainder tends to zero, and the power chi expansions converge to $I_{f_{\text{exp}}}(\lambda_p : \lambda_q)$: $I_{f_{\text{exp}}}(\lambda_p : \lambda_q) = \sum_{i=2}^{\infty} \frac{\epsilon}{i!} \lambda_i^\pm(\lambda_p : \lambda_q)$.

Let $\lambda_p = \epsilon \leq \frac{1}{2}$ and $\lambda_q = 1 - \epsilon$. Then $m = \frac{\epsilon}{1-\epsilon}$ and $M = \frac{1-\epsilon}{1-\epsilon}$ so that $M - m = \frac{1-2\epsilon}{1-\epsilon}$.

We have

$$
\chi_i^\pm(p : q) = \frac{(1 - 2\epsilon)^i}{\epsilon^i-1} + \frac{(2\epsilon - 1)^i}{(1-\epsilon)^{i-1}}.
$$

Since we have $\|f^{(k+1)}\|_{\infty} = \exp(\frac{1}{1-\epsilon})$, it follows that the remainder is upper bounded by

$$
\frac{\exp(\frac{1-\epsilon}{1-\epsilon})}{(k+1)!} \left( \frac{1 - 2\epsilon}{\epsilon(1-\epsilon)} \right)^{k+1}.
$$

In practice, we face numerical precision for computing the factorials $i!$ and large power of numbers close to zero. In our experiments, we compute the $k$-th power chi expansions for $k = 30$.

In our Java implementation, the run for $\lambda_p = 0.9$ and $\lambda_q = 0.3$ yields the exponential divergence $E(\lambda_p : \lambda_q) = 108.20108519696437$ (closed-form formula), and we list the experimental results obtained for the power chi pseudo-distances and approximations by power chi series in Table 2.

We report our implementation in MAXIMA\(^7\), which can use high-precision arithmetic in Appendix B.3.

For the JS generator, the series may either converge (e.g., $\lambda_p = 0.1$ and $\lambda_q = 0.05$) or diverge (e.g., $\lambda_p = 0.05$ and $\lambda_q = 0.85$).

This vanilla case study can be extended to the case of multinoulli distributions (e.g., discrete distributions with $S$ choices or multinomials with one trial).

Computing $N$ $f$-divergences (for generators $f_1, \ldots, f_n$) between two discrete distributions with $S$ choices require $O(NS)$ operations. By precomputing a base of $K$ pseudo-distances $\chi_2^\pm, \ldots, \chi_{K-1}^\pm$, we can approximate those $N$ $f$-divergences in $O(KN)$-time. This yields a fast approximation scheme for batch approximations of $f$-divergences when $K \ll S$.

### 3.2 Case study: Poisson distributions

The probability mass function (pmf) of a Poisson distribution with parameter $\lambda$ is

$$
f(x; \lambda) = \frac{\lambda^x e^{-\lambda}}{x!},
$$

for $x \in \mathbb{N}_0 = \mathbb{N} \cup \{0\} = \{0, 1, 2, \ldots\}$. The Poisson distributions form a Discrete Exponential Family (DEF) with natural parameter $\theta = \log \lambda$ (with $\theta \in \mathbb{R}$) and log-normalizer $F(\theta) = e^\theta$.

That is, we can rewrite the pmf as

$$
f(x; \theta) = \exp(x \theta - e^\theta - \log x!),
$$

with $\theta = \log \lambda$ the natural parameter \([13]\) belonging to $\mathbb{R}$. Thus the Poisson family is a discrete affine exponential family. The power chi pseudo-distance between two Poissons distributions \([20]\)

\[^7\text{http://maxima.sourceforge.net/}\]
| \(i\) | \(\chi_i(\lambda_p = 0.9, \lambda_q = 0.3)\) | \(i\) | \(E^X(\lambda_p = 0.9, \lambda_q = 0.3)\) | \(|R^X\chi(\lambda_p = 0.9, \lambda_q = 0.3)|\) |
|-----|---------------------------------|-----|---------------------------------|-----------------|
| 2   | 4.0000000000000002             | 2   | 5.436563656918093              | 10.76452154004627 |
| 3   | 21.333333333333357            | 3   | 15.101565713661374            | 93.099519483303  |
| 4   | 129.777777777777794          | 4   | 29.800423008291787            | 78.40066218867258 |
| 5   | 777.4814814814827            | 5   | 47.412204533912885            | 60.788880663051486 |
| 6   | 4665.6790123456885          | 6   | 65.02696908486016            | 43.174116112104215 |
| 7   | 27993.547325102943         | 7   | 80.1250546023077             | 28.07603059465667 |
| 8   | 167961.6351165985          | 8   | 91.44864241519754           | 16.7524278176683  |
| 9   | 1007769.5765889378         | 9   | 98.9976992034349             | 9.203385993529466 |
| 10  | 6046617.615607398          | 10  | 103.5271339328994           | 4.673951803674427 |
| 11  | 3.627970558959522 10^7    | 11  | 105.9977385339799           | 2.203351343566382 |
| 12  | 2.176782336093753 10^8   | 12  | 107.2330340384565           | 0.968051131187188 |
| 13  | 1.306009401593817 10^9   | 13  | 107.8031726517244           | 0.3979125423997566 |
| 14  | 7.836416409603122 10^9   | 14  | 108.0475177522481           | 0.15356744471955608 |
| 15  | 4.70184984575982 10^10  | 15  | 108.14525579245294         | 0.05582940451142804 |
| 16  | 2.82110907456029 10^11  | 16  | 108.18190755753099        | 0.01917763943380023 |
| 17  | 1.6926659444736094 10^12 | 17  | 108.19484347467136         | 0.006241722347013479 |
| 18  | 1.015599566641666 10^13  | 18  | 108.19915544697947         | 0.00192949984860342 |
| 19  | 6.093597400105001 10^13  | 19  | 108.20051712246224         | 5.68074502126592 10^-4 |
| 20  | 3.6561584440063025 10^14  | 20  | 108.20092562510708         | 1.59571879257594 10^-4 |
| 21  | 2.1936950640378022 10^15  | 21  | 108.20104234014846         | 4.2856815909431134 10^-5 |
| 22  | 1.3162170384226816 10^16  | 22  | 108.20107417152339         | 1.10254408330327 10^-5 |
| 23  | 7.8973022305360928 10^16  | 23  | 108.20108247536032         | 2.721604047956112 10^-6 |
| 24  | 4.7383813383216576 10^17  | 24  | 108.201085455131955        | 6.456448176095634 10^-7 |
| 25  | 2.843028029929964 10^18   | 25  | 108.20108504954977         | 1.474145908558216 10^-7 |
| 26  | 1.7051827817957982 10^19   | 26  | 108.20108516452598         | 3.243893304801414 10^-8 |
| 27  | 1.0234903690774793 10^20  | 27  | 108.20108519007624         | 6.888129178150848 10^-9 |
| 28  | 6.140942214464877 10^20   | 28  | 108.2010851955513         | 1.4130705494608264 10^-9 |
| 29  | 3.684565328678928 10^21   | 29  | 108.20108519668408         | 2.802948984026443 10^-10 |
| 30  | 2.2107391972073577 10^22  | 30  | 108.20108519691063         | 5.37454525289398 10^-11 |

Table 2: Experimental results of the power chi expansions for the exponential \(f\)-divergence between Bernoulli distributions.
of parameters $\lambda_1$ and $\lambda_2$ is given by

$$\chi^\pm_k(\lambda_1 : \lambda_2) = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} e^{\lambda_1 \left( \frac{\lambda_2}{\lambda_1} \right)^j + (j-1)\lambda_1 - j\lambda_2}.$$ 

The ratio density between two Poisson distributions is

$$\left( \frac{\lambda_q}{\lambda_p} \right)^x \exp(\lambda_p - \lambda_q) = \exp(x(\theta_q - \theta_p) - e^{\theta_q} + e^{\theta_p}).$$

Consider $\lambda_q < \lambda_p$ so that $\frac{\lambda_q}{\lambda_p} < 1$ (or equivalently $\theta_q < \theta_p$). The ratio is then maximized at $x = 0$, and we have $M(\lambda_p : \lambda_q) = \exp(\lambda_p - \lambda_q)$. Notice that $1 < M(\lambda_p : \lambda_q) < \infty$. The ratio is lower bounded by 0 (i.e., $m(\lambda_p : \lambda_q) = 0$).

Thus the exponential $f$-divergence $E(p : q)$ can be expressed by a series when $\lambda_q < \lambda_p$:

$$E^X_k(\lambda_p : \lambda_q) = \sum_{i=2}^{k} \frac{e}{i!} \chi^\pm_i(\lambda_p : \lambda_q), \quad \lambda_q < \lambda_p,$$

and the remainder is $R^X_{E,k}(p : q) \leq \frac{1}{(k+1)!} \|f^{(k+1)}(u)\| \infty M(\lambda_p : \lambda_q)^{k+1}$. Here, the problem is that $\|f^{(k+1)}(u)\| \infty$ is not bounded since $f^{(k+1)}(u) = \exp(u)$.

However, if we truncate the support to $[a, a + 1, \ldots, b - 1, b]$, we can bound $\|f^{(k+1)}(u)\| \infty$ and calculate the $\chi^\pm_i$ pseudo-distances because we deal with the case of finite distributions.

### 3.3 Case study: The truncated exponential distributions

Consider the double-sided truncated exponential distributions: The density of an exponential distribution is $CDF(x; \lambda) = 1 - e^{-\lambda x}$. The exponential distributions form an exponential family with log-normalizer $\chi^\pm = \sum_{i=0}^{k} \frac{e}{i!} \lambda^i$. The mass function is $W_D(\theta) = e^{-a\theta} - e^{-b\theta}$ for an interval domain $D = [a, b]$. The double-sided truncated exponential distributions has density:

$$\exp \left( -\theta x - \log \frac{e^{-a\theta} - e^{-b\theta}}{\theta} \right).$$

When $b = \infty$, we get singly truncated exponential distributions: We have $W_D(\theta) = e^{-a\theta}$ and

$$p_D(x; \theta) = \theta \exp(-\theta x + a\theta).$$

This is an exponential family with log-normalizer $F_D(\theta) = a\theta - \log \theta$.

Symbolic computations yield closed-form solutions for the $\chi^\pm_i$ divergences (see Appendix). For example, we have when $\theta_2 > \frac{2}{3} \theta_1$:

$$\chi^\pm(\theta_2(x; \theta_1) : p_D(x; \theta_2)) = \frac{2\theta_2^4 - 10\theta_1 \theta_2^3 + 18\theta_1^2 \theta_2^2 - 14\theta_1^3 \theta_2 + 4\theta_1^4}{\theta_1^2 (6\theta_2^2 - 7\theta_1 \theta_2 + 2\theta_1^2)}.$$
Table 3: Examples of finite power chi expansions for common divergences.

| $I_f$ divergence name | generator $f$ | $k$-order power chi expansion |
|-----------------------|---------------|-----------------------------|
| generic $I_f$         | generic convex generator $f$ | $I_{f,k}^\chi(p : q) = \sum_{i=2}^{k} \frac{i^{i-1}}{i!} \chi_i^\pm (p : q)$ |
| polynomial            | $f_P(u) = \sum_{j=0}^{d} a_j u^j$ | $I_{f_P,k}^\chi(p : q) = \sum_{i=2}^{d} \left( \sum_{j=i}^{d} \frac{a_j (i)}{i!} \right) \chi_i^\pm (p : q)$ |
| KL                    | $f_{KL}(u) = - \log u$ | $\text{KL}_k^\chi(p : q) = \sum_{i=2}^{k} \frac{(-1)^i}{i!} \chi_i^\pm (p : q)$ |
| reverse KL            | $f_{KL'}(u) = u \log u$ | $\text{KL'}_k^\chi(p : q) = \sum_{i=2}^{k} (-1)^i \left( \frac{1}{i!} \right) \chi_i^\pm (p : q)$ |
| $\alpha$-divergence   | $f_\alpha(u) = \frac{4}{1-\alpha} (1 - u^{\frac{1+\alpha}{\alpha}})$ | $I_{\alpha,k}^\chi(p : q) = \sum_{i=2}^{k} \frac{2}{1-\alpha} \frac{1}{i!} \left( \frac{1}{\alpha} \right) \chi_i^\pm (p : q)$ |
| Jeffreys              | $f_J(u) = (u - 1) \log u$ | $J_{\alpha,k}^\chi(p : q) = \sum_{i=2}^{k} (-1)^i \frac{1}{i!} \chi_i^\pm (p : q)$ |
| Jensen-Shannon        | $f_{JS}(u) = -(u + 1) \log \frac{u}{2} + u \log u$ | $JS_{\alpha,k}^\chi(p : q) = \sum_{i=2}^{k} (-1)^{i-2} \frac{1}{i!(i-1)!} (1 - \frac{1}{2^i}) \chi_i^\pm (p : q)$ |
| Harmonic              | $f_H(u) = \frac{2u}{u+1}$ | $H_{\alpha,k}^\chi(p : q) = 1 + \sum_{i=2}^{k} (-1)^{i+1} \frac{1}{i!} \chi_i^\pm (p : q)$ |
| Exponential           | $f_{exp}(u) = e^x - x$ | $E_{\alpha,k}^\chi(p : q) = \sum_{i=2}^{k} \frac{i^{i-1}}{i!} \chi_i^\pm (p : q)$ |
4 Conclusion and discussion

On one hand, it has been proven that the Kullback-Leibler divergence between Gaussians mixture models is in general not analytic [28]. On the other hand, we can express the \( f \)-divergences using power chi expansions [20] yielding to power chi series when these expansions converge. When the \( f \)-divergence generator is a polynomial, we obtain a closed-form formula for the \( f \)-divergence between members of the same exponential families with affine natural parameter space (e.g., isotropic Gaussian, Poisson, von Mises-Fisher, etc.) by using the finite power chi expansions. This polynomial case includes the \( \alpha \)-divergences for \( \alpha = 2k - 1 \) where \( k \) is an integer greater than 2.

Table 3 summarizes the power chi expansions of some common \( f \)-divergences. Observe that when we precompute or approximate the first \( k \) power chi pseudo-distances, we can calculate or approximate quickly the \( k \)-order power chi expansions of \( f \)-divergences using the basis of \( \chi^\pm_1 \) pseudo-distances (see Table 3). Thus, we can efficiently approximate a batch of \( f \)-divergences using \( \chi^\pm_1 \) look-up tables.

Truncating distributions [11, 9] on a finite compact domain let us bound both the ratio of densities and the chi pseudo-distances, potentially yielding approximation formulæ for the \( f \)-divergences. Another direction is to approximate the \( f \)-generator by a polynomial [25] and then to apply the finite chi expansion of the \( f \)-divergence induced by that polynomial approximation of the generator.

Finally, to conclude, let us mention that it is interesting to find examples where the entropy of mixture distributions is analytic (besides the case of multinomial distributions) since this would also yield analytic formula for the Jensen-Shannon divergence according to Eq. 14.

Additional materials are available online at:

https://franknielsen.github.io/PowerChiExpansionsFdiv/

A Information geometry and \( f \)-divergences

Since \( I_{\beta f} = \beta I_f \) for \( \beta > 0 \), we fix the scale of the \( f \)-divergence by choosing \( \beta \) that \( \beta f''(1) = 1 \). Indeed, theory and applications usually consider relative distances instead of absolute distances. Thus we select the representative \( f \)-divergence in the family \( \{ f_{\alpha,\beta}(u) = \beta(f(u) + \alpha(u - 1)) \} \) of generators (with \( f(1) = 0 \)) such that \( f'(1) = 0 \) and \( f''(1) = 1 \). Such a \( f \)-divergence is called a standard \( f \)-divergence in Amari’s textbook [2] (p. 56): The standard \( f \)-divergences are invariant divergences ([2], p. 54) which satisfies the property of information monotonicity by coarse-graining. At infinitesimal scale, a first-order Taylor expansion of the standard \( f \)-divergence between distributions belonging to a parametric family \( \{ p(x; \theta) \} \) yields half of the squared Mahalanobis distance\(^8\) for the Fisher information matrix \( G_\theta \) ([2], p. 62):

\[
I_f(p(x; \theta) : p(x; \theta + d\theta)) = \frac{1}{2} M_{G_\theta}^2(d\theta, d\theta) = \frac{1}{2} d\theta^\top G_\theta d\theta = \frac{1}{2} \sum_{i,j} g_{ij}(\theta) d\theta_i d\theta_j,
\]

where

\[
G_\theta = [g_{ij}(\theta)], \quad g_{ij}(\theta) = E_{p(x; \theta)} \left[ \frac{\partial}{\partial \theta_i} \log p(x; \theta) \frac{\partial}{\partial \theta_j} \log p(x; \theta) \right].
\]

\(^8\)For a positive definite matrix \( Q \succ 0 \), the Mahalanobis metric (distance) is \( M_Q(p, q) = \sqrt{(p - q)^\top Q(p - q)} \).
The $f$-divergence can be extended to positive measures\textsuperscript{9} instead of probability measures \textsuperscript{22}. The $f$-divergence is a separable divergence that can be written as:

$$I_f(p : q) = \int_X i_f(p(x) : q(x))d\mu(x),$$

with $i_f(a : b) = af\left(\frac{b}{a}\right)$ for $a, b > 0$. The function $i_f$ is called the perspective function \textsuperscript{15} of the convex function $f$.

B Some sanity checks using a computer algebra system

We use the Computer Algebra System (CAS) MAXIMA\textsuperscript{10} Some code has also been written in Python using Sympy \textsuperscript{16}.

B.1 Checking the closed-form formula for $\frac{f^{(k)}(1)}{k!}$

/* k-th order derivative of the Jensen-Shannon f-generator evaluated at one and divided by k! */

\begin{verbatim}
k:23;
fJSderivative(i) := ((-1)**(i-2))*(1-1/(2**(i-1)))*(1/((i*(i-1))));
fJSderivative(23);

fJS(u) := -(u+1)*log((1+u)/2) + u*log(u);
at(diff(fJS(u),u,k),u=1)/k!;
\end{verbatim}

We find: $f^{(23)}_{\text{JS}}(1) = -\frac{182361}{92274688}$.

B.2 Chi pseudo-distances between truncated exponential distributions

theta1 : 1;
theta2 : 2;
a : 2;
b : 3;

/* truncated exponential distribution */
p(x,theta) := theta*exp(-theta*x);
mass(theta) := exp(-a*theta)-exp(-b*theta);
q(x,theta) := theta*exp(-theta*x)/(exp(-a*theta)-exp(-b*theta));
k:10;
integrate( (q(x,theta2)-q(x,theta1))**k/(q(x,theta1))**(k-1),x,a,b);

B.3 Power chi expansions for the exponential $f$-divergence between binomials

/* Exponential f-divergence */

\textsuperscript{9}For standard $f$-divergence, we let $I_f(p^+ : q^+) = I_f(\bar{p} : \bar{q}) + q^+ - p^+$, where $\bar{p} = \frac{p^+}{\int p^+d\mu(x)}$ and $\bar{q} = \frac{q^+}{\int q^+d\mu(x)}$ are normalized probability densities.

\textsuperscript{10}http://maxima.sourceforge.net/
\( f(u) := \exp(u) - (u*%e); \)
\( \text{coeff}(i) := %e/i!; \)

\[
\text{fdiv}(p,q) := (p*f(q/p)) + ((1-p)*f((1-q)/(1-p)));
\]

\[
\text{chipm}(i,p,q) := (((q-p)**i)/(p**(i-1))) + (((p-q)**i)/(1-p)**(i-1)))
\]

\[
\text{fapprox}(p,q,max) := \text{sum(coeff(i)}*\text{chipm}(i,p,q), i, 2,max);\]

/* test */
\[ p: 0.2; q: 0.99; \]
\[ \text{result: float(fdiv(p,q));} \]

for i: 2 step 1 thru 30 do
bloc(
approx: float(fapprox(p,q,i)),
err: float(abs(result-approx)),
display(i,approx,result,err)
);

References

[1] Masafumi Akahira. Statistical Estimation for Truncated Exponential Families. Springer, 2017.

[2] Shun-ichi Amari. Information geometry and its applications, volume 194. Springer, 2016.

[3] Shun-ichi Amari and Andrzej Cichocki. Information geometry of divergence functions. Bulletin of the Polish Academy of Sciences: Technical Sciences, 58(1):183–195, 2010.

[4] George A Anastassiou. Higher order optimal approximation of Csiszár’s \( f \)-divergence. Nonlinear Analysis: Theory, Methods & Applications, 61(3):309–339, 2005.

[5] Neil S Barnett, Pietro Cerone, Sever Silvestru Dragomir, and Anthony Sofo. Approximating csiszár \( f \)-divergence by the use of Taylor’s formula with integral remainder. Mathematical Inequalities and Applications, 5:417–434, 2002.

[6] Manuel Bronstein. Symbolic integration I: transcendental functions, volume 1. Springer Science & Business Media, 2006.

[7] Marek Capinski and Peter E Kopp. Measure, integral and probability. Springer Science & Business Media, 2013.

[8] Imre Csiszár. Information-type measures of difference of probability distributions and indirect observation. studia scientiarum Mathematicarum Hungarica, 2:229–318, 1967.
[9] Joan Del Castillo. The singly truncated normal distribution: a non-steep exponential family. *Annals of the Institute of Statistical Mathematics*, 46(1):57–66, 1994.

[10] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In *Advances in neural information processing systems*, pages 2672–2680, 2014.

[11] Laxman M Hegde and Ram C Dahiya. Estimation of the parameters in a truncated normal distribution. *Communications in Statistics-Theory and Methods*, 18(11):4177–4195, 1989.

[12] Kurt Hornik and Bettina Grün. On conjugate families and Jeffreys priors for von Mises–Fisher distributions. *Journal of statistical planning and inference*, 143(5):992–999, 2013.

[13] Friedrich Liese and Igor Vajda. On divergences and informations in statistics and information theory. *IEEE Transactions on Information Theory*, 52(10):4394–4412, 2006.

[14] Jianhua Lin. Divergence measures based on the Shannon entropy. *IEEE Transactions on Information theory*, 37(1):145–151, 1991.

[15] Pierre Maréchal. On a functional operation generating convex functions, Part 1: Duality. *Journal of Optimization Theory and Applications*, 126(1):175–189, 2005.

[16] Aaron Meurer, Christopher P Smith, Mateusz Paprocki, Ondřej Čertík, Sergey B Kirpichev, Matthew Rocklin, AMiT Kumar, Sergiu Ivanov, Jason K Moore, Sartaj Singh, et al. SymPy: symbolic computing in Python. *PeerJ Computer Science*, 3:e103, 2017.

[17] Frank Nielsen. The statistical Minkowski distances: Closed-form formula for Gaussian mixture models. *arXiv preprint arXiv:1901.03732*, 2019.

[18] Frank Nielsen and Vincent Garcia. Statistical exponential families: A digest with flash cards. *arXiv preprint arXiv:0911.4863*, 2009.

[19] Frank Nielsen and Richard Nock. Entropies and cross-entropies of exponential families. In *2010 IEEE International Conference on Image Processing*, pages 3621–3624. IEEE, 2010.

[20] Frank Nielsen and Richard Nock. On the chi square and higher-order chi distances for approximating f-divergences. *IEEE Signal Processing Letters*, 21(1):10–13, 2014.

[21] Frank Nielsen and Ke Sun. Guaranteed bounds on information-theoretic measures of univariate mixtures using piecewise log-sum-exp inequalities. *Entropy*, 18(12):442, 2016.

[22] Tomoaki Nishimura and Fumiyasu Komaki. The information geometric structure of generalized empirical likelihood estimators. *Communications in Statistics-Theory and Methods*, 37(12):1867–1879, 2008.

[23] Sebastian Nowozin, Botond Cseke, and Ryota Tomioka. f-GAN: Training generative neural samplers using variational divergence minimization. In *Advances in neural information processing systems*, pages 271–279, 2016.
[24] Karl Pearson. On the criterion that a given system of deviations from the probable in the case of a correlated system of variables is such that it can be reasonably supposed to have arisen from random sampling. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 50(302):157–175, 1900.

[25] George M Phillips. *Interpolation and approximation by polynomials*, volume 14. Springer Science & Business Media, 2003.

[26] Steve Selvin. Maximum likelihood estimation in the truncated, single parameter, discrete exponential family. *The American Statistician*, 25(1):41–42, 1971.

[27] Karlheinz Spindler. A short proof of the formula of Faà di Bruno. *Elemente der Mathematik*, 60(1):33–35, 2005.

[28] Sumio Watanabe, Keisuke Yamazaki, and Miki Aoyagi. Kullback information of normal mixture is not an analytic function. *IEICE technical report. Neurocomputing*, 104(225):41–46, 2004.