A Unifying Framework for Some Directed Distances in Statistics

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Abstract. Density-based directed distances — particularly known as divergences — between probability distributions are widely used in statistics as well as in the adjacent research fields of information theory, artificial intelligence and machine learning. Prominent examples are the Kullback-Leibler information distance (relative entropy) which e.g. is closely connected to the omnipresent maximum likelihood estimation method, and Pearson’s $\chi^2$-distance which e.g. is used for the celebrated chisquare goodness-of-fit test. Another line of statistical inference is built upon distribution-function-based divergences such as e.g. the prominent (weighted versions of) Cramer-von Mises test statistics respectively Anderson-Darling test statistics which are frequently applied for goodness-of-fit investigations; some more recent methods deal with (other kinds of) cumulative paired divergences and closely related concepts. In this paper, we provide a general framework which covers in particular both the above-mentioned density-based and distribution-function-based divergence approaches; the dissimilarity of quantiles respectively of other statistical functionals will be included as well. From this framework, we structurally extract numerous classical and also state-of-the-art (including new) procedures. Furthermore, we deduce new concepts of dependence between random variables, as alternatives to the celebrated mutual information. Some variational representations are discussed, too.

1 Divergences, Statistical Motivations and Connections to Geometry

1.1 Basic Requirements on Divergences (Directed Distances)

For a first view, let $P$ and $Q$ be two probability distributions (probability measures). For those, we would like to employ real-valued indices $D(P, Q)$ which quantify the “distance” (respectively dissimilarity, proximity, closeness, discrepancy, discrimination) between $P$ and $Q$. Accordingly, we require $D(\cdot, \cdot)$ to have the following reasonable “minimal/coarse/wide” properties

(D1) $D(P, Q) \geq 0$ for all $P, Q$ under investigation (nonnegativity),
and such \(D(\cdot, \cdot)\) is then called a divergence (in the narrow sense) or disparity or contrast function. Basically, the divergence \(D(P, Q)\) of \(P\) and \(Q\) can be interpreted as a kind of “directed distance from \(P\) to \(Q\)”; the corresponding directness stems from the fact that in general one has the asymmetry \(D(P, Q) \neq D(Q, P)\). This can turn out to be especially useful in contexts where the first distribution \(P\) is always/principally of “more importance” or of “higher attention” than the second distribution \(Q\); moreover, it can technically happen that \(D(P, Q) < \infty\) but \(D(Q, P) = \infty\), for instance in practically important applications within a (say) discrete context where \(P\) and \(Q\) have different zero-valued probability masses (e.g. zero observations), see e.g. the discussion in Subsection 1.3 below.

Notice that we don’t assume that the triangle inequality holds for \(D(\cdot, \cdot)\).

1.2 Some Statistical Motivations

To start with, let us consider probability distributions \(P\) and \(Q\) having strictly positive density functions (densities) \(f_P\) and \(f_Q\) with respect to some measure \(\lambda\) on some (measurable) space \(\mathcal{X}\). For instance, if \(\lambda := \lambda_L\) is the Lebesgue measure on (some subset of) \(\mathcal{X} = \mathbb{R}\) then \(f_P\) and \(f_Q\) are “classical” (e.g. Gaussian) density functions; in contrast, in the discrete setup where \(\mathcal{X} := \mathcal{X}_\#\) has countably many elements and is equipped with the counting measure \(\lambda := \lambda_\# := \sum_{z \in \mathcal{X}_\#} \delta_z\) (where \(\delta_z\) is Dirac’s one-point distribution \(\delta_z[A] := 1_A(z)\) (where here and in the sequel \(1_A(\cdot)\) which stands for the indicator function of a set \(A\), and thus \(\lambda_\#([z]) = 1\) for all \(z \in \mathcal{X}_\#\)), then \(f_P\) and \(f_Q\) are probability mass functions (counting-density functions, relative-frequency functions, frequencies).

For such kind of probability measures \(P\) and \(Q\), let us start with the widely used class \(D_\phi(\cdot, \cdot)\) of Csiszar-Ali-Silvey-Morimoto (CASM) divergences (see [48], [6], [133]) which are usually abbreviatorily called \(\phi\)–divergences and which are defined by

\[
0 \leq D_\phi(P, Q) := \int_{\mathcal{X}} f_Q(x) \cdot \phi\left(\frac{f_P(x)}{f_Q(x)}\right) \, d\lambda(x) ,
\]

\[
= \int_{\mathcal{X}} \phi\left(\frac{f_P(x)}{f_Q(x)}\right) \, dQ(x) ,
\]

where \(\phi : [0, \infty[ \to [0, \infty[\) is a convex function which is strictly convex at 1 and which satisfies \(\phi(1) = 0\). It can be easily seen that this \(D_\phi(\cdot, \cdot)\) satisfies the above-mentioned requirements/properties/axioms (D1) and (D2). In the above-mentioned discrete setup with \(\mathcal{X} = \mathcal{X}_\#,\) (1) turns into

\[
0 \leq D_\phi(P, Q) = \sum_{x \in \mathcal{X}_\#} f_Q(x) \cdot \phi\left(\frac{f_P(x)}{f_Q(x)}\right) ,
\]

\[\text{see e.g. Weller-Fahy et al. [202]}\]
whereas in the above-mentioned real-valued absolutely-continuous case, the integral in (1) reduces (except for rare cases) to a classical Riemann integral with integrator \( d\lambda_L(x) = dx \). Notice that — depending on \( \mathcal{F} \), \( \phi \) etc. — the divergence \( D_\phi(P, Q) \) in (1) may become \( \infty \). For comprehensive treatments of \( \phi \)-divergences (CASM divergences), the reader is referred to e.g. Liese & Vajda [109], Read & Cressie [160], Vajda [196], Liese & Vajda [110], Pardo [151]. Important prominent special cases of \( D_\phi \) are the omnipresent Kullback-Leibler divergence/distance (relative entropy) with \( \phi_{KL}(t) := t \log(t) + 1 - t \) and thus

\[
D_{\phi_{KL}}(P, Q) = \int_{\mathcal{X}} f_P(x) \cdot \log \left( \frac{f_P(x)}{f_Q(x)} \right) d\lambda(x) ,
\]

the reverse Kullback-Leibler divergence/distance with \( \phi_{RKL}(t) := -\log(t) + t - 1 \) and hence

\[
D_{\phi_{RKL}}(P, Q) = \int_{\mathcal{X}} f_Q(x) \cdot \log \left( \frac{f_Q(x)}{f_P(x)} \right) d\lambda(x) = D_{\phi_{KL}}(Q, P) ,
\]

(half of) Pearson’s \( \chi^2 \)-distance with \( \phi_{PC}(t) := \frac{(t-1)^2}{2} \) and consequently

\[
D_{\phi_{PC}}(P, Q) = \frac{1}{2} \int_{\mathcal{X}} \frac{(f_P(x) - f_Q(x))^2}{f_Q(x)} d\lambda(x) ,
\]

(half of) Neyman’s \( \chi^2 \)-distance with \( \phi_{NC}(t) := \frac{(t-1)^2}{2} \) and thus

\[
D_{\phi_{PC}}(P, Q) = \frac{1}{2} \int_{\mathcal{X}} \frac{(f_P(x) - f_Q(x))^2}{f_P(x)} d\lambda(x) ,
\]

the (double of squared) Hellinger distance — also called (half of) Freeman-Tukey divergence — with \( \phi_{HD}(t) := 2(\sqrt{t} - 1)^2 \) and hence

\[
D_{\phi_{PC}}(P, Q) = 2 \int_{\mathcal{X}} \left( \sqrt{f_P(x)} - \sqrt{f_Q(x)} \right)^2 d\lambda(x) ,
\]

the total variation distance with \( \phi_{TV}(t) := |t - 1| \) and consequently

\[
D_{\phi_{TV}}(P, Q) = \int_{\mathcal{X}} |f_P(x) - f_Q(x)| d\lambda(x) ,
\]

and the power divergences \( D_\phi(P, Q) \) (also known as alpha-divergences, Cressie-Read measures/distances, and Tsallis cross-entropies) with \( \phi_\alpha(t) := \frac{t^\alpha - 1}{\alpha} \) \((\alpha \in \mathbb{R} \backslash \{0, 1\})\). Notice that (in the current setup of probability distributions with zero-free density functions) \( D_{\phi_{PC}}(P, Q) \) resp. \( D_{\phi_{NC}}(P, Q) \) resp. \( D_{\phi_{HD}}(P, Q) \) are equal to \( D_\phi(P, Q) \) with \( \alpha = 2 \) resp. \( \alpha = -1 \) resp. \( \alpha = 2 \), and that one can prove \( D_{\phi_{KL}}(P, Q) = \lim_{\alpha \to 1} D_\phi_\alpha(P, Q) =: D_\phi_1(P, Q) \) as well as \( D_{\phi_{KL}}(P, Q) = \lim_{\alpha \to 0} D_\phi_\alpha(P, Q) =: D_\phi_0(P, Q) \); henceforth, we will use this comfortable continuous embedding to a divergence family \( \{D_\phi_\alpha(P, Q)\}_{\alpha \in \mathbb{R}} \) which covers important special cases.
From a statistical standpoint, the definition \(^1\) finds motivation in the far-reaching approach by Ali \& Silvey \[^3\]: by noting that in a simple model — where a random variable \(X\) takes values on a finite discrete set \(\mathcal{X} = \mathcal{X}_\#\) and its distribution is either \(P\) or \(Q\) having probability mass function \(f_P\) or \(f_Q\) — the statistics \(f_P(X)\) is a sufficient statistics (meaning that \(P(X = x) = f_P(X) = t\) = \(Q(X = x) = f_Q(X) = t\)) for all \(x\) and \(t\) they argue that any measurement aiming at inference on the distribution of \(X\) should be a function of the likelihood ratio \(LR := \frac{f_P(X)}{f_Q(X)}\). Thus, a real-valued coefficient \(D(P, Q)\) of closeness/dissimilarity between \(P\) and \(Q\) should be considered as an aggregation/expectation — over some measure (typically \(P\) or \(Q\) — of a function \(\phi\) of LR, hence formally leading to \(^1\) with not necessarily convex function \(\phi\). This construction is compatible with the following set of four axioms/requirements which bear some fundamentals for the construction of a discrimination index between distributions, and which (amongst other things) imply the convexity of \(\phi\):

(A1) \(D_\phi(P_1, P_2)\) should be defined for all pairs of probability distributions \(P_1, P_2\) on the same sample space \(\mathcal{X}\).

(A2) Let \(x \mapsto t(x)\) a measurable transformation from \((\mathcal{X}, \mathcal{F})\) onto a measure space \((\mathcal{Y}, \mathcal{G})\) then there should hold

\[
D_\phi(P_1, P_2) \geq D_\phi(P_1t^{-1}, P_2t^{-1}),
\]

where \(P_1t^{-1}\) denotes the induced measure on \(\mathcal{Y}\) corresponding to \(P_1\). Notice that \(^5\) is called data processing inequality or information processing inequality, and — as shown in \[^6\] — it implies that \(\phi\) should be a convex function.

(A3) \(D_\phi(P_1, P_2)\) should take its minimum value when \(P_1 = P_2\) and its maximum value when \(P_1 \perp P_2\) (i.e., \(P_1\) and \(P_2\) are singular, in the sense that the supports of the distributions \(P_1\) and \(P_2\) do not overlap (are disjoint)).

(A4) A further axiom of statistical nature should be satisfied in relation with a statistical notion of separability of two distributions in a given model. Assume that for a given family of parametric distributions \((P_\theta)_{\theta \in \Theta}\) and for any small risk \(\alpha\) the following property holds: if \(P_{\theta_1}\) is rejected vs. \(P_{\theta_2}\) with risk \(\leq \alpha\) optimally (Neyman-Pearson approach), then \(P_{\theta_1}\) is rejected vs. \(P_{\theta_2}\) with risk \(\leq \alpha\) (meaning \(P_{\theta_1}\) is further away from \(P_{\theta_2}\) than \(P_{\theta_1}\) is). Then one should have

\[
D_\phi(P_{\theta_1}, P_{\theta_2}) \geq D_\phi(P_{\theta_1}, P_{\theta_2}).
\]

Notice that in (A4) we use a slight extension of the original requirements of \[^6\] (who employ a monotone likelihood ratio concept).

As a second use-of-divergence incentive stemming from considerations in statistics (as well as in the adjacent research fields of information theory, artificial intelligence and machine learning), we mention parameter estimation in terms of \(\phi\)-divergence minimization. For this, let \(Y\) be a random variable taking values in a finite discrete space \(\mathcal{X} := \mathcal{X}_\#\), and let \(f_P(x) = P[Y = x]\) be its
strictly positive probability mass function under an unknown hypothetical law \( P \). Moreover, we assume that \( P \) lies in — respectively can be approximated by — a model \( \Omega \) := \{ \mathcal{Q}_\theta : \theta \in \Theta \} (\Theta \subset \mathbb{R}) being a class of finite discrete parametric distributions having strictly positive probability mass functions \( f_{\mathcal{Q}_\theta} \) on \( \mathcal{X} \). Moreover, let \( P_{N}^{\text{emp}} := \frac{1}{N} \cdot \sum_{i=1}^{N} \delta_{Y_i} \) be the well-known data-derived empirical distribution/measure of an \( N \)-size independent and identically distributed (i.i.d.) sample/observations \( Y_1, \ldots, Y_N \) of \( Y \); the according probability mass function is \( f_{P_{N}^{\text{emp}}} \) on \( \mathcal{X} \) which reflects the underlying (normalized) histogram; here, as usual, \( \# A \) denotes the number of elements in a set \( A \). In the following, we assume that the sample size \( N \) is large enough such that \( f_{P_{N}^{\text{emp}}} \) is strictly positive (see the next subsection for a relaxation).

If the data-generating distribution \( P \) lies in \( \Omega \), i.e. \( P = Q_{\theta_{\text{tr}}} \) for some “true” unknown parameter \( \theta_{\text{tr}} \in \Theta \), then (under some mild technical assumptions) it is easy to show that the corresponding maximum likelihood estimator (MLE) \( \hat{\theta} \) is EQUAL to

\[
\hat{\theta} := \arg \min_{\theta \in \Theta} D_{\phi_{0}}(Q_{\theta}, P_{N}^{\text{emp}})
\]

where \( \phi_{0} := -\log(t) + t - 1 \) and \( D_{\phi_{0}}(\cdot, \cdot) \) is the the reverse Kullback-Leibler divergence already mentioned above. Due due its construction, \( \hat{\theta} \) is called minimum reverse-Kullback-Leibler divergence (RKLD) estimator, and \( Q_{\hat{\theta}} \) is the RKLD-projection of \( P_{N}^{\text{emp}} \) on \( \Omega \). In the other — also practically important — case where \( P \) does not lie in the model \( \Omega \) (but is reasonably “close” to it), i.e. the model is misspecified, then \( Q_{\hat{\theta}} \) is still a reasonable proxy of \( P \) if the sample size \( N \) is large enough.

In the light of the preceding paragraph, it makes sense to consider the more general minimum \( \phi \)–divergence/distance estimation problem

\[
\hat{\theta} := \arg \inf_{\theta \in \Theta} D_{\phi}(Q_{\theta}, P_{N}^{\text{emp}})
\]

where \( \phi \) is not necessarily equal to \( \phi_{0} \); for instance, through some comfortably verifiable criteria on \( \phi \) one can end up with an occurring minimum \( \phi \)–divergence/distance estimator \( \hat{\theta} \) which is more robust against outliers than the MLE \( \hat{\theta} \) (see e.g. the residual-adjustment-function approach of Lindsay [113], its comprehensive treatment in Basu et al. [25], and the corresponding flexibilizations in Kißlinger & Stummer [102], Roensch & Stummer [163]). Usually, \( \hat{\theta} \) of (6) is called minimum \( \phi \)–divergence estimator (MDE), and \( Q_{\hat{\theta}} \) is the phi–divergence-projection of \( P_{N}^{\text{emp}} \) on \( \Omega \).

A further useful generalization is the “distribution-outcome type” minimum divergence/distance estimation problem

\[
\hat{Q} := \arg \inf_{Q \in \Omega} D_{\phi}(Q, P_{N}^{\text{emp}})
\]

where \( \phi \) is not necessarily equal to \( \phi_{0} \); for instance, through some comfortably verifiable criteria on \( \phi \) one can end up with an occurring minimum \( \phi \)–divergence/distance estimator \( \hat{Q} \) which is more robust against outliers than the MLE \( \hat{\theta} \) (see e.g. the residual-adjustment-function approach of Lindsay [113], its comprehensive treatment in Basu et al. [25], and the corresponding flexibilizations in Kißlinger & Stummer [102], Roensch & Stummer [163]). Usually, \( \hat{Q} \) of (7) is called minimum \( \phi \)–divergence estimator (MDE), and \( Q_{\hat{\theta}} \) is the phi–divergence-projection of \( P_{N}^{\text{emp}} \) on \( \Omega \).
where \( P_{N}^{\text{emp}} \) stems from a general (not necessarily parametric, unknown) data generating distribution \( P \) and \( \Omega \) may be a “fairly general” model being a class of finite discrete distributions having strictly positive probability mass functions \( f_{Q} \) on \( \mathcal{X} \# \) (and, as usual, (7) can be rewritten as a minimization problem on the \((\#\Omega - 1)\)-dimensional probability simplex). The outcoming \( \hat{Q} \) of (7) is still called (distribution-type) minimum \( \phi \)-divergence estimator (MDE), and can be interpreted as \( \phi \)-divergence-projection of \( P_{N}^{\text{emp}} \) on \( \Omega \). Problem (7) is in particular beneficial in non- and semi-parametric contexts, where \( \Omega \) reflects (partially) non-parametrizable model constraints. For instance, \( \Omega \) may consist (only) of constraints on moments or on L-moments (see e.g. Broniatowski & Decurninge [37]); alternatively, \( \Omega \) may be e.g. a tubular neighborhood of a parametric model (see e.g. Liu & Lindsay [117], Ghosh & Basu [76]).

The closeness — especially in terms of the sample size \( N \) — of the data-derived empirical distribution from the model \( \Omega \) is quantified by the corresponding minimum

\[
D_{\phi}(\Omega, P_{N}^{\text{emp}}) := \inf_{Q \in \Omega} D_{\phi}(Q, P_{N}^{\text{emp}})
\]

of (7); thus, it carries useful statistical information. Moreover, under some mild assumptions, \( D_{\phi}(\Omega, P_{N}^{\text{emp}}) \) converges to

\[
D_{\phi}(\Omega, P) := \inf_{Q \in \Omega} D_{\phi}(Q, P)
\]

where \( P \) is the (unknown) data generating distribution. In case of \( P \in \Omega \) one obtains \( D_{\phi}(\Omega, P) = 0 \), whereas for \( P \notin \Omega \) the \( \phi \)-divergence minimum \( D_{\phi}(\Omega, P) \) — and thus its approximation \( D_{\phi}(\Omega, P_{N}^{\text{emp}}) \) — quantifies the adequacy of the model \( \Omega \) for modeling \( P \); a lower \( D_{\phi}(\Omega, P) \)-value means a better adequacy (in the sense of a lower departure between the model and the truth, cf. Lindsay [114], Lindsay et al. [115], Markatou & Sofikitou [120], Markatou & Chen [119]).

Hence, especially in the context of model selection/choice (and the related issue of goodness-of-fit testing) within complex big-data contexts, for the search of appropriate models \( \Omega \) and model elements/members therein, the (fast and efficient) computation of \( D_{\phi}(\Omega, P) \) respectively \( D_{\phi}(\Omega, P_{N}^{\text{emp}}) \) constitutes a decisive first step, since if the latter two are “too large” (respectively, “much larger than” \( D_{\phi}(\Omega, P) \) respectively \( D_{\phi}(\Omega, P_{N}^{\text{emp}}) \) for some competing model \( \Omega \)), then the model \( \Omega \) is “not adequate enough” (respectively “much less adequate than” (7)). For tackling the computation of \( D_{\phi}(\Omega, P) \) respectively \( D_{\phi}(\Omega, P_{N}^{\text{emp}}) \) on fairly general (e.g. high-dimensional, non-conex and even highly disconnected) constraint sets \( \Omega \), a “precise bare simulation” approach has been recently developed by Broniatowski & Stummer [43].

For the sake of a compact first glance, in this subsection we have mainly dealt with finite discrete distributions \( P \) and \( Q \) having zeros-free probability mass functions. However, with appropriate technical care, one can extend the above concepts also to general discrete distributions with zeros-carrying probability
mass functions and even to non-discrete (e.g. absolutely continuous) distributions with zeros-carrying density functions. (Only) The correspondingly necessary generalization of the basic \( \phi \)-divergence definition \(^1\) is addressed in the next subsection.

### 1.3 Incorporating density function zeros

Recall that in our first basic \( \phi \)-divergence definition \(^1\), \(^2\) we have employed probability distributions \( P \) and \( Q \) having strictly positive density functions \( f_P \) and \( f_Q \) with respect to some measure \( \lambda \) on some (measurable) space \( X \), and consequently \( P \) and \( Q \) are equivalent. However, in many applications one has to allow \( f_P \) and/or \( f_Q \) to have zero values. For instance, in the above-mentioned empirical distribution \( P_{\text{emp}}^N \) for small/medium sample size \( N \) (or even large sample size for rare-events) one may have \( f_{P_{\text{emp}}^N}(\bar{x}) = 0 \) for some \( \bar{x} \), even though the candidate-model probability mass satisfies \( f_{Q}(\bar{x}) \neq 0 \) for some \( \theta \in \Theta \).

Accordingly, we employ the following extension: for probability distributions \( P \) and \( Q \) having density functions \( f_P \) and \( f_Q \) with respect to some measure \( \lambda \) on some (measurable) space \( X \) one defines the Csiszar-Ali-Silvey-Morimoto (CASM) divergences — in short \( \phi \)-divergences — by

\[
0 \leq D_\phi(P, Q) := \int_{\{f_P, f_Q > 0\}} \phi \left( \frac{f_P(x)}{f_Q(x)} \right) dQ(x) + \phi(0) \cdot Q[f_P = 0] + \phi^*(0) \cdot P[f_Q = 0]
\]

with \( \phi(0) \cdot 0 = 0 \) and \( \phi^*(0) \cdot 0 = 0 \) (11)

(see e.g. Liese & Vajda \[110\]). Here, we have employed (as above) \( \phi : ]0, \infty[ \rightarrow ]0, \infty[ \) to be a convex function which is strictly convex at 1 and which satisfies \( \phi(1) = 0 \); moreover, we have used the (always existing) limits \( \phi(0) := \lim_{t \downarrow 0} \phi(t) \in ]0, \infty[ \) and \( \phi^*(0) := \lim_{t \downarrow 0} \phi^*(t) = \lim_{t \rightarrow \infty} \frac{\phi(t)}{t} \) of the so-called \( \ast \)-adjoint function \( \phi^*(t) := t \cdot \phi \left( \frac{1}{t} \right) \) \( (t \in ]0, \infty[) \). It can be proved that \( D_\phi(\cdot, \cdot) \) satisfies the above-mentioned requirements/properties/axioms \((D1) \) and \((D2) \); even more, one gets the following range-of-value assertion (cf. Csiszar \[48\], \[49\] and Vajda \[195\], see e.g. also Liese & Vajda \[110\]):

**Theorem 1.** There holds

\[
0 \leq D_\phi(P, Q) \leq \phi(0) + \phi^*(0)
\]

where (i) the left equality holds only for \( P = Q \), and (ii) the right equality holds always for \( P \perp Q \) (singularity, i.e. the zeros-set of \( f_P \) is disjoint from the zeros-set of \( f_Q \)) and only for \( P \perp Q \) in case of \( \phi(0) + \phi^*(0) < \infty \).

A generalization of Theorem 1 to the context of finite (not necessarily probability) measures \( P \) and \( Q \) is given in Stummer & Vajda \[187\]; for instance, in a

\(^4\) which corresponds to an empty histogram cell at \( \bar{x} \)

\(^5\) if \( f_{Q}(\theta) = 0 \) for all \( \theta \in \Theta \) one should certainly reduce the space \( X \) by removing \( \bar{x} \)
two-sample test situation \( P \) and \( Q \) may be two generalized empirical distributions which reflect non-normalized (rather than normalized) histograms.

As an example, let us illuminate the upper bounds \( \phi(0) + \phi^*(0) \) of — of the zeros-incorporating versions of — of the above-mentioned important power divergence family \( \{D_{\phi_\alpha}(P, Q)\}_{\alpha \in \mathbb{R}} \) with \( \phi_\alpha(t) := \frac{t^\alpha - \alpha t + \alpha - 1}{\alpha(\alpha-1)} \) (\( \alpha \in \mathbb{R}\{0, 1\} \)), \( \phi_1(t) := \phi_{KL}(t) = t \log(t) + 1 - t \) and \( \phi_0(t) := \phi_{RKL}(t) := -\log(t) + t - 1 \). It is easy to see that for \( P \perp Q \) one gets

\[
\phi_\alpha(0) = \phi_{1-\alpha}^*(0) = \begin{cases} 
\infty, & \text{if } \alpha \leq 0, \\
\frac{1}{\alpha}, & \text{if } \alpha > 0,
\end{cases}
\]

and hence

\[
D_{\phi_\alpha}(P, Q) = \phi_\alpha(0) + \phi_{1-\alpha}^*(0) = \begin{cases} 
\infty, & \text{if } \alpha \notin ]0, 1[, \\
\frac{1}{\alpha(1-\alpha)}, & \text{if } \alpha \in ]0, 1[.
\end{cases}
\]

Especially, for \( P \perp Q \) one gets for the Kullback-Leibler divergence \( D_{\phi_{KL}}(P, Q) = D_{\phi_1}(P, Q) = \infty \) whereas \( D_{\phi_{0,99}}(P, Q) = \frac{10000}{99} \) one achieves a finite value; thus, in order to avoid infinities it is more convenient to work with the well-approximating divergence generator \( \phi_{0,99} \) of \( \phi_1 \). Similarly, for the reverse Kullback-Leibler divergence we obtain \( D_{\phi_{RKL}}(P, Q) = D_{\phi_0}(P, Q) = \infty \) whereas \( D_{\phi_{0,99}}(P, Q) = \frac{10000}{99} \). Furthermore, for \( P \perp Q \) one gets for Pearson’s \( \chi^2 \)-divergence \( D_{\phi_2}(P, Q) = \infty \), for Neyman’s \( \chi^2 \)-divergence \( D_{\phi^{-1}}(P, Q) = \infty \) and for the (squared) Hellinger distance \( D_{\phi_{1/2}}(P, Q) = 4 \).

Returning to the general context, notice that the upper bound \( \phi(0) + \phi^*(0) \) in Theorem 1 is independent of \( P \) and \( Q \), and thus \( D_{\phi}(P, Q) \) is of no discriminative use in statistical situations where \( P \) and \( Q \) are singular (i.e. \( P \perp Q \)). This is the case, for instance, in the following commonly encountered “crossover” context:

(CO1) \( Y \) is an univariate (absolutely continuous) random variable with unknown hypothetical probability distribution \( P \) having strictly positive density function \( f_P \) with respect to the Lebesgue measure \( \lambda_L \) on \( \mathcal{X} = \mathbb{R} \) (recall that this means that \( f_P \) is a “classical” (e.g. Gaussian) probability density function),

(CO2) the corresponding model \( \Omega := \{Q_\theta : \theta \in \Theta\} (\Theta \subset \mathbb{R}) \) is a class of parametric distributions having strictly positive probability density functions \( f_{Q_\theta} \) with respect to \( \lambda_L \), and

(CO3) \( P_N^{emp} := \frac{1}{N} \cdot \sum_{i=1}^N \delta_{Y_i}[.] \) is the data-derived empirical distribution of an \( N \)-size independent and identically distributed (i.i.d.) sample/observations \( Y_1, \ldots, Y_N \) of \( Y \); recall that the according probability mass function is \( f_{P_N^{emp}}(x) = \frac{1}{N} \cdot \#\{i \in \{1, \ldots, N\} : Y_i = x\} \) which is the density function with respect to the counting measure \( \lambda_y \) on the distinct values of the sample.

This contrary density-function behaviour can be put in an encompassing framework by employing the joint density-building (i.e. dominating) measure \( \lambda := \ldots \)
\( \lambda_L + \lambda_\# \). Clearly, one always has the singularity \( P_{\text{emp}}^\theta \perp Q_\theta \) and thus, due to Theorem \( \text{I} \) one gets

\[
D_\phi(Q_\theta, P_{\text{emp}}^\theta) = \phi(0) + \phi^*(0) \quad \text{for all } \theta \in \Theta, \quad \inf_{\theta \in \Theta} D_\phi(Q_\theta, P_{\text{emp}}^\theta) = \phi(0) + \phi^*(0) \quad \text{(14)}
\]

Accordingly, in such a situation one can not obtain a corresponding minimum \( \phi \)-divergence estimator.

Also notice that for power divergences \( D_{\phi, \alpha}(P, Q) \) with \( \alpha \neq 0, 1 \) it can happen that \( D_{\phi, \alpha}(P, Q) = \infty \) even though \( P \) and \( Q \) are not singular (which due to (13) is consistent with Theorem \( \text{I} \)). For instance, consider a situation with two different i.i.d. samples \( Y_1, \ldots, Y_N \) having distribution \( P \) and \( \bar{Y}_1, \ldots, \bar{Y}_M \) of \( \bar{Y} \) having distribution \( Q \) with (say) \( Q \sim P \) (equivalence): in terms of the corresponding empirical distributions \( P_{\text{emp}}^N := \frac{1}{N} \cdot \sum_{i=1}^N \delta_{Y_i} \) and \( \bar{P}_{\text{emp}}^M := \frac{1}{M} \cdot \sum_{j=1}^M \delta_{\bar{Y}_j} \) one obtains \( D_{\phi, \alpha}(P_{\text{emp}}^N, \bar{P}_{\text{emp}}^M) = \infty \) if the set of zeros of the corresponding probability mass function \( f_{P_{\text{emp}}^N} \) is strictly larger (for \( \alpha \leq 0 \)) respectively smaller (for \( \alpha > 1 \)) than the set of zeros of \( f_{\bar{P}_{\text{emp}}^M} \) (i.e. \( \bar{P}_{\text{emp}}^M[f_{\bar{P}_{\text{emp}}^M} = 0] > 0 \) respectively \( P_{\text{emp}}^N[f_{P_{\text{emp}}^N} = 0] > 0 \)), to be seen by applying (10), (11), (12).

As above, in such a non-singular situation it is e.g. better to use the (in fact, even sample-dependent !) power divergence \( D_{\phi, \alpha}(P_{\text{emp}}^N, \bar{P}_{\text{emp}}^M) \) instead of the Kullback-Leibler divergence \( D_{\phi, 1}(P_{\text{emp}}^N, \bar{P}_{\text{emp}}^M) = \infty \). Similar infinity-effects can be constructed for the above-mentioned other important special cases \( \alpha = 0 \) (reverse Kullback-Leibler divergence), \( \alpha = 2 \) (Pearson’s \( \chi^2 \)-divergence), \( \alpha = -1 \) (Neyman’s \( \chi^2 \)-divergence) whereas for the case \( \alpha = 1/2 \) (square Hellinger distance) everything works out well. Such an approach serves as an alternative to the approach of “lifting/unzeroing/adjusting” (from sampling randomly appearing) zero probability masses\(^6\) by pseudo-counts or “smoothing (in a discrete sense)”, see e.g. Fienberg & Holland \([69]\), as well as e.g. Section 4.5 (respectively Section 3.5) in Jurafsky & Martin \([93]\) and the references therein.

Next, we briefly indicate two ways to circumvent the problem described in the above-mentioned crossover context (CO1),(CO2),(CO3):

(GR) grouping (partitioning, quantization) of data: convert\(^7\) the model \( \Omega \) into a purely discrete context, by subdivinding the data-point-set \( \mathcal{X} = \bigcup_{j=1}^s A_j \) into countably many \(- \) (say) \( s \in \mathbb{N} \cup \{ \infty \} \) \(- \) (measurable) disjoint classes \( A_1, \ldots, A_s \) with the property \( \lambda_L[A_j] > 0 \) (“essential partition”); proceed as in above general discrete subsetup with \( \mathcal{X}^{\text{new}} := \{ A_1, \ldots, A_s \} \) and thus the \( i \)-th data observation \( Y_i(\omega) \) and the corresponding running variable \( x \) manifest (only) the corresponding class-membership (see e.g. Vajda & van...
der Meulen [197] for a survey on different choices). Some corresponding thorough statistical investigations (such as efficiency, robustness, types of grouping, grouping-error sensitivity, etc.) of the corresponding minimum-φ—divergence-estimation can be found e.g. in Victoria-Feser & Ronchetti [199], Menendez et al. [124,125,126], Morales et al. [131,132], Lin & He [111].

(SM) smoothing of the empirical density function: convert everything to a purely continuous context, by keeping the original data-point-set \( \mathcal{X} \) and by “continuously modifying” (e.g. with the help of kernels) the empirical density function \( f_{P_{N}^{\text{emp}}} (\cdot) \) to a function \( f_{P_{N}^{\text{emp}},\text{smo}} (\cdot) > 0 \) (a.s.) such that \( \int_{\mathcal{X}} f_{P_{N}^{\text{emp}},\text{smo}} (x) \, d\lambda (x) = 1 \). Some corresponding thorough statistical investigations (such as efficiency, robustness, information loss, etc.) of the corresponding minimum-φ—divergence-estimation can be found e.g. in Beran [26], Basu & Lindsay [23], Park & Basu [154], Chapter 3 of Basu et al. [25], Kuchibhotla & Basu [107], Al Mohamad [7], and the references therein.

In contrast to the above, let us now encounter a crossover situation where (CO1) and (CO3) still hold, but the parametric-model-assumption (CO2) is replaced by

\[
\text{(CO2')} \quad \text{the corresponding model } \Omega := \{ Q : Q \text{ satisfies some nonparametric constraints} \}
\]
is a class of distributions \( Q \) which contains both (i) distributions \( Q \) having strictly positive probability density functions \( f_{Q} \) with respect to \( \lambda_{L} \), as well as (ii) all “context-specific appropriate” finite discrete distributions \( Q \) (having ideally the same (or at least, smaller or equal) support as \( P_{N}^{\text{emp}} \)).

The subclasses of \( Q \in \Omega \) which satisfy (i) respectively (ii) are denoted by \( \Omega^{\text{ac}} \) respectively \( \Omega^{\text{dis}} \). Widely applied special cases of (CO2’) are nonparametric contexts where \( \Omega \) is the class of all distributions on \( \mathcal{X} = \mathbb{R} \) satisfying pregiven moment conditions. Suppose, that we are interested in the corresponding model-adequacy problem (cf. (9))

\[
D_{\phi} (\Omega^{\text{ac}}, P) := \inf_{Q \in \Omega^{\text{ac}}} D_{\phi} (Q, P)
\]

where \( P \) is the (unknown) data generating distribution (cf. (CO1)). Recall that in case of \( P \in \Omega^{\text{ac}} \) one obtains \( D_{\phi} (\Omega^{\text{ac}}, P) = 0 \), whereas for \( P \notin \Omega^{\text{ac}} \) the \( \phi \)—divergence minimum \( D_{\phi} (\Omega^{\text{ac}}, P) \) quantifies the adequacy of the model \( \Omega^{\text{ac}} \) for modeling \( P \); a lower \( D_{\phi} (\Omega^{\text{ac}}, P) \)—value means a better adequacy. Since in the current setup the empirical distribution \( P_{N}^{\text{emp}} \) of (CO3) satisfies \( P_{N}^{\text{emp}} \perp Q \) for all \( Q \in \Omega^{\text{ac}} \) we obtain (analogously to (14))

\[
\begin{align*}
D_{\phi} (Q, P_{N}^{\text{emp}}) &= \phi(0) + \phi^{*}(0) \quad \text{for all } Q \in \Omega^{\text{ac}}, \\
D_{\phi} (\Omega^{\text{ac}}, P_{N}^{\text{emp}}) &= \inf_{Q \in \Omega^{\text{ac}}} D_{\phi} (Q, P_{N}^{\text{emp}}) \\
&= \phi(0) + \phi^{*}(0).
\end{align*}
\]
Hence, statistically it makes no sense to approximate \( (15) \) by \( (16) \). Let us discuss an appropriate alternative, e.g. for the case of the reverse Kullback-Leibler divergence \( D_{\phi_0}(Q, P) \) with generator \( \phi_0(t) = \phi_{RKL}(t) = -\log(t) + t - 1 \) (cf. (3)). By (12), we have \( \phi_0(0) = \infty \) as well as \( \phi^*_0(0) = 1 \) and thus \( \phi_0(0) + \phi^*_0(0) = \infty \) as well as (by (10), (11))

\[
D_{\phi_0}(Q, P_{\text{emp}}^N) = \int_{\{f_Q : f_{P_{\text{emp}}^N} > 0\}} \phi_0 \left( \frac{f_Q(x)}{f_{P_{\text{emp}}^N}(x)} \right) dP_{\text{emp}}^N(x) + \infty \cdot P_{\text{emp}}^N[f_Q = 0] \\
= \frac{1}{N} \sum_{i \in \{1, \ldots, N\} : f_Q(Y_i) \cdot f_{P_{\text{emp}}^N}(Y_i) > 0} \phi_0 \left( \frac{f_Q(Y_i)}{f_{P_{\text{emp}}^N}(Y_i)} \right) + \infty \cdot P_{\text{emp}}^N[f_Q = 0] < \infty
\]

for all \( Q \) in \( \Omega_{\text{dis}}^N \) which is defined as the class of distributions in \( \Omega_{\text{dis}} \) such that \( Q \ll P_{\text{emp}}^N \) (and thus \( Q[f_{P_{\text{emp}}^N} = 0] = 0 \)); also recall that the last term becomes \( \infty \cdot 0 = 0 \) in case that \( Q \) and \( P_{\text{emp}}^N \) have the same support. Hence, under the assumption that \( \Omega_{\text{dis}}^N \) is non-void, one can approximate the \( \phi = \phi_0 \)-version of \( (15) \) by

\[
D_{\phi_0}(\Omega_{\text{dis}}^N, P_{\text{emp}}^N) := \inf_{Q \in \Omega_{\text{dis}}^N} D_{\phi_0}(Q, P_{\text{emp}}^N)
\]

This is the basic idea of the divergence-minimization formulation of the so-called “empirical likelihood” principle of Owen [146], [147], [148], which leads to many variations according to the choice of the divergence generator \( \phi \); see e.g. Baggerly [15], Judge & Mittelhammer [92], Bertail et al. [27], and Broniatowski & Keziou [40], and references therein.

Other ways to circumvent the crossover problem \((\text{CO1}), (\text{CO2}), (\text{CO3})\) respectively \((\text{CO1}), (\text{CO2}'), (\text{CO3})\) can be found e.g. in Section VIII of Liese & Vajda [110] and Section 4 of Broniatowski & Stummer [42]; moreover, some variational-representation-method approaches will be discussed in Section 6 below.

As a third statistical incentive, let us mention that with the help of \( \phi \)-divergence minimization one can build generalizations of exponential families with pregiven sufficient statistics (see e.g. Pelletier [157], Gayen & Kumar [73]). In the special case of Kullback-Leiber divergence (i.e., the divergence generator \( \phi \) is taken to be \( \phi_1(t) = \phi_{KL}(t) = t \log(t) + 1 - t \)) one ends up with classical exponential families.

### 1.4 Some Motivations From Probability Theory

Another environment where \( D_\phi(Q, P) \) appears in a natural way is probability theory, in the area of the large deviation paradigm; the celebrated Sanov theorem states that, up to technicalities,

\[
\lim_{n \to \infty} \frac{1}{n} \log P \left( P_n \in \Omega \right) = -D_\phi(\Omega, P)
\]
where $P_n$ is the empirical distribution of a sample of $n$ independent copies under $P$, and $\Omega$ is a class of probability distributions on $(\mathcal{X},\mathcal{B})$, and $D_{\phi_1}(\Omega, P) := \inf_{Q \in \Omega} D_{\phi_1}(Q, P)$. Therefore, the Kullback-Leibler divergence measures the rate of decay of the chances for $P_n$ to belong to $\Omega$ as $n$ increases, in case that $P$ does not belong to $\Omega$. Other divergences inherit of the same character: assume that the function $\phi$ is the Fenchel-Legendre transform of a moment generating function $\Lambda_{P_t}$, namely

$$\phi(x) = \sup_t t x - A(t)$$

where $A(t) := \log E[e^{tW}]$ for some random variable $W$ defined on some arbitrary space. With $(X_1, ..., X_n)$ being an i.i.d. sample under $P$ and $(W_1, ..., W_n)$ being an i.i.d. sample of copies of $W$, we define the associated weighted empirical distribution as

$$P_n^W := \frac{1}{n} \sum_{i=1}^n W_i \delta_{X_i}.$$ 

The following type of conditional Sanov theorem holds:

$$\lim_{n \to \infty} \frac{1}{n} \log P\left( P_n^W \in \Omega \mid X_1, ..., X_n \right) = -D_{\phi}(\Omega, P),$$

where $\Omega$ is a class of signed measures on $(\mathcal{X},\mathcal{B})$ satisfying some regularity assumptions. This result characterizes $D_{\phi}(\Omega, P)$ as a rate of escape of $P_n^W$ from $\Omega$ when $P$ does not belong to $\Omega$. We refer to Najim [134], Trashorras & Wintenberger [194], and Broniatowski & Stummer [43] where the latter consider several applications of this result for (deterministic as well as statistical) optimization procedures by bootstrap.

Of course, there are connections between statistical inferences and $\phi$—divergence-based large deviations results. For instance, the large deviations properties of (types of) the empirical distribution of a sample from its parent distribution is the cornerstone for the asymptotic study of tests. In this realm, the $\phi$—divergences play a significant role while testing between some parametric null hypothesis $\theta \in \Theta_0$ vs. an alternative $\eta \in \Theta_1$; the corresponding Bahadur slope of a given test statistics indicates the decay of its $p$—value under the alternative. In “standard” setups, this is connected to the Kullback-Leibler divergence $\inf_{\theta \in \Theta_0} D_{\phi_1}(P_n, P_\theta)$ (between the alternative $\eta$ and the set of all null hypotheses) which qualifies the asymptotic efficiency of the statistics at use; see Bahadur [16], Hoadley [89], and also e.g. Groeneboom & Oosterhoff [78], and Nikitin [142]. As far as other setups is concerned, Efron & Tibshirani [65] generally suggest the weighted bootstrap as a valuable approach for testing. In some concrete frameworks, it can be proved that testing in parametric models based on appropriate weighted-bootstrapped $\phi$—divergence test statistics enjoys maximal Bahadur efficiency with respect to any other weighted-bootstrapped test statistics (see Broniatowski [36]; the corresponding Bahadur slope is related to the specific weighting procedure, and substitutes the Kullback-Leibler divergence by some other $\phi$—divergence, specific of the large deviation properties of the weighted empirical distribution.
1.5 Divergences and Geometry

For this section, we return to the general framework of Section 1.1 where we have defined divergences to satisfy the two properties: 

\[(D1) \quad D(P, Q) \geq 0 \text{ for all } P, Q \text{ under investigation (nonnegativity)},\]

\[(D2) \quad D(P, Q) = 0 \text{ if and only if } P = Q \text{ (reflexivity; identity of indiscernibles)}.\]

Being interpreted as “directed” distances, the divergences $D(\cdot, \cdot)$ can be connected to geometric issues in various different ways. For the sake of brevity, we mention here only a few of those.

To start with an “all-encompassing view”, following the lines of e.g. Birkhoff [29] and Millmann & Parker [130], one can build from any set $\mathcal{S}$, whose elements can be interpreted as “points”, together with a collection $\mathcal{L}$ of non-empty subsets of $\mathcal{S}$, interpreted as “lines” (as a manifestation of a principle sort of structural connectivity between points), and an arbitrary symmetric distance $d(\cdot, \cdot)$ on $\mathcal{S} \times \mathcal{S}$, an axiomatic constructive framework of geometry which can be of far-reaching nature; therein, $d(\cdot, \cdot)$ plays basically the role of a marked ruler. Accordingly, each triplet $(\mathcal{S}, \mathcal{L}, d(\cdot, \cdot))$ forms a distinct “quantitative geometric system”; the most prominent classical case is certainly $\mathcal{S} = \mathbb{R}^2$ with $\mathcal{L}$ as the collection of all vertical and non-vertical lines, equipped with the Euclidean distance $d(\cdot, \cdot)$, hence generating the usual Euclidean geometry in the two-dimensional space.

In the case that $d(\cdot, \cdot)$ is only an asymmetric distance (divergence) but not a distance anymore, we propose that some of the outcome geometric building blocks have to be interpreted in a direction-based way (e.g. the use of $d(\cdot, \cdot)$ as a marked directed ruler, the construction of points of equal divergence from a center viewed as distorted directed spheres, etc.). For $D(\cdot, \cdot)$ one has to work with $\mathcal{S}$ being a family of real-valued functions on $\mathcal{S}$.

Secondly, from any symmetric distance $d(\cdot, \cdot)$ on a “sufficiently rich” set $\mathcal{S}$ and a finite number of (fixed or adaptively flexible) distinct “reference points” $s_i$ ($i = 1, \ldots, n$) one can construct the corresponding Voronoi cells $V(s_i)$ by

\[V(s_i) := \{ z \in \mathcal{S} : d(z, s_i) \leq d(z, s_j) \text{ for all } j = 1, \ldots, n \} .\]

This produces a tessellation (tiling) of $\mathcal{S}$ which is very useful for classification purposes. Of course, the geometric shape of these tessellations is of fundamental importance. In the case that $d(\cdot, \cdot)$ is only an asymmetric distance (divergence), then $V(s_i)$ has to be interpreted as a directed Voronoi cell and then there is also the “reversely directed” alternative

\[\tilde{V}(s_i) := \{ z \in \mathcal{S} : d(s_i, z) \leq d(s_j, z) \text{ for all } j = 1, \ldots, n \} .\]

Recent applications where $\mathcal{S} \subset \mathbb{R}^d$ and $d(\cdot, \cdot)$ is a Bregman divergence or a more general conformal divergence, can be found e.g. in Boissonnat et. al [33], Nock et al. [144] (and the references therein), where they also deal with the corresponding adaption of k-nearest neighbour classification methods.

Moreover, with each (say) asymmetric distance (divergence) $d(\cdot, \cdot)$ one can associate a divergence-ball $B_d(s, \rho)$ with “center” $s \in \mathcal{S}$ and “radius” $\rho \in [0, \infty[$.
defined by $B_\rho(s, \rho) := \{ s \in \mathcal{S} : d(s, z) \leq \rho \}$, whereas the corresponding divergence-sphere is given by $S_\rho(s, \rho) := \{ s \in \mathcal{S} : d(s, z) = \rho \}$; see e.g. Csiszar & Breuer [51] for a use of some divergence balls as a constraint in financial-risk related decisions. Of course, the “geometry/topology” induced by divergence balls and spheres is generally quite non-obvious; see for instance Roensch & Stummer [163], who describe and visualize different effects in a 3D-setup of scaled Bregman divergences (which will be covered below). Moreover, the generalization of

$$D(\Omega, P^{emp}_N) := \inf_{Q \in \Omega} D(Q, P^{emp}_N), \quad \hat{Q} := \arg \inf_{Q \in \Omega} D(Q, P^{emp}_N)$$

of the above-mentioned statistical minimum divergence/distance estimation problems [7], [5] can e.g. be (loosely) achieved by blowing up the divergence sphere $S_D(s, P^{emp}_N)$ through increasing the radius $\rho$ until it first touches the model $\Omega$. Accordingly, there may be an interesting interplay between the geometric/topological properties of both $S_D(s, P^{emp}_N)$ and the (e.g. non-convex, respectively non-smooth, respectively non-intersection-of-hyperplanes type, respectively complicated-manifold-type) boundary $\partial \Omega$ of $\Omega$ (see e.g. Roensch & Stummer [163]).

Thirdly, consider a framework where $P := \tilde{P}_{\theta_1}$ and $Q := \tilde{P}_{\theta_2}$ depend on some parameters $\theta_1 \in \Theta, \theta_2 \in \Theta$. The way of dependence of the function (say) $S(\tilde{P}_\theta)$ on the underlying parameter $\theta$ from an appropriate space $\Theta$ of e.g. manifold type, may show up directly e.g. via its operation/functioning as a relevant system-indicator, or it may be manifested implicitly e.g. such that $S(\tilde{P}_\theta)$ is the solution of an optimization problem with $\theta$-involving constraints. In such a framework, one can induce divergences $D(S(\tilde{P}_{\theta_1}), S(\tilde{P}_{\theta_2})) =: f(\theta_1, \theta_2)$ and – under sufficiently smooth dependence – study their corresponding differential-geometric behaviour of $f(\cdot, \cdot)$ on $\Theta$. An example is provided by the Kullback-Leibler divergence between two distributions of the same exponential family of distributions, which defines a Bregman divergence on the parameter space. This and related issues are subsumed in the research field of “information geometry”; for comprehensive overviews see e.g. Amari [4], Amari [2], Ay et al. [14]. Moreover, for recent connections between divergence-based information geometry and optimal transport the reader is e.g. referred to Pal & Wong [149,150], Karakida & Amari [96], Amari et al. [3], Peyre & Cuturi [158], and the literature therein.

Further relations of divergences with other approaches to geometry can be overviewed e.g. from the wide-range-covering research-article collections in Nielsen & Bhatia [141], Nielsen & Barbaresco [136], [137], [138], [139], [140], [20] and Nielsen [135].

Moreover, geometry also enters as a tool for visualizing quantitative effects on divergences. A more detailed discussion (including also other approaches) on the interplay between statistics and geometry is beyond the scope of this chapter; they will appear in other parts of this book.
1.6 Some Incentives for Extensions

\(\phi\)–Divergences Between Other Statistical Objects: Recall that for probability distributions \(P\) and \(Q\) having strictly positive density functions \(f_P\) and \(f_Q\) with respect to some measure \(\lambda\) on a data space \(\mathcal{X}\) (which covers as special cases both the classical density functions respectively the probability mass functions), we have defined the \(\phi\)–divergences (Csiszar–Ali-Silvey-Morimoto (CASM) divergences) by

\[
0 \leq D_\phi(P, Q) := \int_\mathcal{X} f_Q(x) \cdot \phi\left(\frac{f_P(x)}{f_Q(x)}\right) \, d\lambda(x) =: D_{\phi, \lambda}(f_P, f_Q),
\]

where the last notation-type term in (17) indicates the interpretation as \(\phi\)–divergence between density functions, measuring their similarity. However, e.g. for \(\mathcal{X} \subset \mathbb{R}\) and the Lebesgue measure \(\lambda = \lambda_L\) (and hence almost always \(d\lambda_L(x) = dx\)), it makes also sense to quantify the dissimilarity — in terms of \(\phi\)–divergences — between other related “statistical objects”, most notably between the information-aggregating cumulative distribution functions \(F_P\) and \(F_Q\) of \(P\) and \(Q\). For instance, formally,

\[
D_{\phi_{PC,Q}}(F_P, F_Q) = \frac{1}{2} \int_\mathcal{X} \frac{(F_P(x) - F_Q(x))^2}{F_Q(x)} \, dQ(x),
\]

(cf. (11) with \(f_P, f_Q\) replaced by \(F_P, F_Q\) and \(\lambda = Q\)) is — in case of employing the empirical measure \(P = P_{emp}^N\) — a special member of the family of weighted Cramer-von Mises test statistics (in fact it is a modified Anderson-Darling test statistics of e.g. Ahmad et al. [1] and Scott [169], see also Shin et al. [174] for applications in environmental extreme-value theory).

As another incentive, let us mention the use of \(\phi\)–divergences between quantile functions respectively between “transformations” thereof. For instance, they can be employed in situations where the above-mentioned classical minimum \(\phi\)–divergence/distance estimation problem [7] and [8] — which involves \(\phi\)–divergences between density functions — is theoretically and practically intractable; this is e.g. the case when the model \(\Omega\) is defined by constraints on the expectation of a \(L\)–statistics (e.g. describing a tubular neighborhood of a distribution with prescribed number of given quantiles; such constraints are not linear with respect to the underlying distribution of the data, but merely with respect to their quantile measure). In such a situation, one can transpose everything to a minimization problem for the \(\phi\)–divergence between the corresponding empirical quantile measures where the constraint can also be stated in terms of quantile measures (see Broniatowski & Decurninge [37]).

Further examples of \(\phi\)–divergences between other statistical objects can be found in Subsection 2.5.1.2 below.

Some Non-\(\phi\)–Divergences between Probability Distributions: In contrary to the preceding subsection, instead of replacing the probability distributions \(P\) and \(Q\), let us keep the latter two but consider now some other divergences \(D(P, Q)\) (of non–\(\phi\)–divergence type) of statistical interest. For instance,
there is a substantially growing amount of applications of the so-called (ordinary/classical) Bregman distances/divergences OBD

\[ 0 \leq D_{\phi}^{OBD}(P, Q) = \int_{\mathcal{X}} \left[ \phi(f_P(x)) - \phi(f_Q(x)) - \phi'(f_Q(x)) \cdot (f_P(x) - f_Q(x)) \right] d\lambda(x), \tag{18} \]

(see e.g. Csiszar [50], Pardo & Vajda [152], [153], Stummer & Vajda [188]) where \( \phi' \) is the derivative of the supposedly differentiable \( \phi \). The class (18) includes as important special cases e.g. the density power divergences (also known as Basu-Harris-Hjort-Jones distances, cf. [22]) with the squared \( L_2 \)-norm as a subcase.

The principal types of statistical applications of OBD are basically the same as for the \( \phi \)-divergences (minimum divergence estimation, robustness etc.); however, the corresponding technical details may differ substantially.

Concerning some recent progress of divergences, Stummer [182] as well as Stummer & Vajda [188] introduced the concept of scaled Bregman divergences/distances SBD

\[ 0 \leq D_{\phi}^{SBD}(P, Q) := D_{\phi,\lambda,m}^{SBD}(P, Q) = \int_{\mathcal{X}} \left[ \phi\left( \frac{f_P(x)}{m(x)} \right) - \phi\left( \frac{f_Q(x)}{m(x)} \right) - \phi'\left( \frac{f_Q(x)}{m(x)} \right) \cdot \left( \frac{f_P(x)}{m(x)} - \frac{f_Q(x)}{m(x)} \right) \right] m(x) d\lambda(x) \]

which (by using a scaling function \( m(\cdot) \)) generalizes all the above-mentioned (nearly disjoint) density-based \( \phi \)-divergences (17) and OBD divergences (18) at once. Hence, the SBD divergence class constitutes a quite general framework for dealing with a wide range of data analyses, in a well-structured way.

Some Non-CASM Divergences between Other Statistical Objects: Of course, for statistical applications it also makes sense to combine the extension-ideas, of the two preceding subsections. For instance,

\[ 0 \leq D_{\phi_{PC},\lambda,m}^{SBD}(F_P, F_Q) = \frac{1}{2} \int_{R} \frac{(f_P(x) - f_Q(x))^2}{m(x)} dQ(x) \]

constitutes — in case of employing the empirical measure \( P = P_{\text{n}}^{\text{emp}} \) — the family of weighted Cramer-von Mises test statistics (see [37], [200], as well as Smirnov [176]).

In the following, for the rest of the paper we work out an extensive toolkit of divergences between statistical objects, which goes far beyond the above-mentioned concepts.
2 The Framework

2.1 Statistical functionals $S$ and their dissimilarity

Let us assume that the modeled respectively observed random data take values in a state space $\mathcal{Y}$ (with at least two distinct values), which is equipped with a system $\mathcal{A}$ of admissible events ($\sigma$–algebra). On this, we consider two probability distributions (probability measures) $P$ and $Q$ of interest. By appropriate choices of $(\mathcal{Y}, \mathcal{A})$, such a general context also covers modeling of series of observations, functional data as well as stochastic process data (the latter by choosing $\mathcal{Y}$ as an appropriate space of paths, i.e., whole scenarios along a set of times).

In this paper, we deal with situations where – e.g. in face of the dichotomous nature – one can distinguish between “dissimilarity-expressing relations” $\mathfrak{R}(S(P), S(Q))$ between univariate real-valued “statistical functionals” $S(\cdot)$ of the form $S(P) := \{S_x(P)\}_{x \in \mathcal{X}}$ and $S(Q) := \{S_x(Q)\}_{x \in \mathcal{X}}$ for the two distributions $P$ and $Q$.

Where $\mathcal{X}$ is a set of (at least two different) “functional indices”. As corresponding preliminaries, in this section we broadly discuss examples of statistical functionals which we shall employ later on to recover known — respectively create new — divergences between them.

In principal, one can distinguish between unit-free (e.g. “percentage-type”) functionals $S(\cdot)$ and unit-dependent (e.g. monetary) functionals $S(\cdot)$. For the real line $\mathcal{Y} = \mathcal{X} = \mathbb{R}$, the most prominent examples for the former are the cumulative distribution functions (cdf) $\{S_x(P)\}_{x \in \mathbb{R}} := \{F_P(x)\}_{x \in \mathbb{R}} =: S^{ed}(P)$, the survival functions (suf) $\{S_x(P)\}_{x \in \mathbb{R}} := \{1 - F_P(x)\}_{x \in \mathbb{R}} =: S^{su}(P)$; the “classical” probability density functions (pdf) $\{S_x(P)\}_{x \in \mathbb{R}} := \{f_P(x)\}_{x \in \mathbb{R}}$.

$S^{ed}(P)$, the moment generating functions (mgf) $\{S_x(P)\}_{x \in \mathbb{R}} := \{M_P(x)\}_{x \in \mathbb{R}} := \{\mathbb{E} e^{xy} dP(y)\}_{x \in \mathbb{R}} =: S^{mg}(P)$, and for finite/countable $\mathcal{Y} = \mathcal{X} \subset \mathbb{R}$ the probability mass functions (pmf) $\{S_x(P)\}_{x \in \mathcal{X}} := \{pp(x)\}_{x \in \mathcal{X}} := \{P\{\{x\}\}_{x \in \mathcal{X}} =: S^{pm}(P)$; furthermore, we also cover the centered rank function (cf. e.g. Serfling 172, Serfling & Zuo 173), also called “center-outward distribution functions” in e.g. Hallin 84, Hallin et al. 86) $\{S_x(P)\}_{x \in \mathbb{R}} := \{2 \cdot F_P(x) - 1\}_{x \in \mathbb{R}} =: S^{cr,1}(P)$.

Continuing on the real line, in contrast to the above discussion on unit-free statistical functionals, let us now turn our intention to unit-dependent statistical functionals. For the latter, in case of $\mathcal{Y} = \mathbb{R}$ and $\mathcal{X} = [0, 1]$, the most prominent

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8 the statistical functional $S(\cdot)$ can also be thought of as a function-valued “plug-in statistics” respectively as a real-valued function on $\mathcal{X}$ which carries a probability-distribution-valued parameter $\cdot$; accordingly $S(P), S(Q)$ are two different functions corresponding to the two different parameter constellations $P, Q$; accordingly $S_x(P), S_x(Q)$ are the corresponding function values at $x \in \mathcal{X}$.
examples are the univariate quantile functions
\[
\{S_x(P)\}_{x \in [0,1]} := \{F_P^{-1}(x)\}_{x \in [0,1]} := \{\inf\{z \in \mathbb{R} : F_P(z) \geq x\}\}_{x \in [0,1]} =: S^{qu}(P);
\]
for \(\mathcal{Y} = [0, \infty)\) we take
\[
\{S_x(P)\}_{x \in [0,1]} := \{F_P^{-1}(x)\}_{x \in [0,1]} := \{\inf\{z \in [0, \infty) : F_P(z) \geq x\}\}_{x \in [0,1]} =: S^{qu}(P).
\]
Of course, if the underlying cdf \(z \rightarrow F_P(z)\) is strictly increasing, then \(x \rightarrow F_P^{-1}(x)\) is nothing but its “classical” inverse function. Let us also mention that in quantitative finance and insurance, the quantile \(F_P^{-1}(x)\) (e.g. quoted in US dollars units) is called the value-at-risk for confidence level \(x \cdot 100\%\). A detailed discussion on properties and pitfalls of univariate quantile functions can be found e.g. in Embrechts & Hofert [66]; see also e.g. Gilchrist [77] for a comprehensive survey on quantile functions for practitioners of statistical modelling.

Similarly, the generalized inverse of the centered rank function amounts to so-called median-oriented quantile function (cf. Serfling [171])
\[
\{\tilde{S}_x(P)\}_{x \in \mathbb{R}} := \left\{\int_{-\infty}^x \tilde{S}_z(P) \, d\lambda(z)\right\}_{x \in \mathbb{R}} =: S^\lambda \tilde{S}(P)
\]
where \(\tilde{\lambda}\) is a \(\sigma\)-finite measure on \(\mathbb{R}\) and \(\tilde{S}(P) := \left\{\tilde{S}_z(P)\right\}_{z \in \mathbb{R}}\) is a non-negative respectively \(\tilde{\lambda}\)-integrable statistical functional. For special cases \(S^{Q,Q_{cd}}(P)\) (i.e. \(\tilde{\lambda} = Q\) and \(\tilde{S} = S_{cd}\)) as well as \(S^{Q,S_{cd}}(Q)\) in a goodness-of-fit testing context, see e.g. Henze & Nikitin [88].

For the multidimensional Euclidean space \(\mathcal{Y} = \mathcal{X} = \mathbb{R}^d\) (\(d \in \mathbb{N}\)), unit-free-type examples are the “classical” cumulative distribution functions (cdf) \(\{S_x(P)\}_{x \in \mathbb{R}^d} := \{F_P(x)\}_{x \in \mathbb{R}^d} =: S^{cd}(P)\) (which are based on marginal orderings), the “classical” probability density functions (pdf) \(\{S_x(P)\}_{x \in \mathbb{R}^d} := \{f_P(x)\}_{x \in \mathbb{R}^d} =: S^{pd}(P)\) (such that \(P[\cdot] := \int f_P(x) \, d\lambda_L(x)\) with \(d\)-dimensional Lebesgue measure \(\lambda_L\), the moment generating functions (mgf) \(\{S_x(P)\}_{x \in \mathbb{R}^d} := \{M_P(x)\}_{x \in \mathbb{R}^d} := \{\int_{\mathbb{R}^d} e^{<x,y>} \, dP(y)\}_{x \in \mathbb{R}^d} =: S^{mg}(P)\), and for finite/countable \(\mathcal{Y} = \mathcal{X} \subset \mathbb{R}^d\) the probability mass functions (pmf) \(\{S_x(P)\}_{x \in \mathcal{X}} := \{p_P(x)\}_{x \in \mathcal{X}} =: S^{pm}(P)\). Furthermore, we cover statistical depth functions \(\{S_x(P)\}_{x \in \mathbb{R}^d} := \{D_P(x)\}_{x \in \mathbb{R}^d} =: S^{dc}(P)\) and statistical outlyingness functions \(\{S_x(P)\}_{x \in \mathbb{R}^d} := \{O_P(x)\}_{x \in \mathbb{R}^d} =: S^{ou}(P)\) e.g. in the sense of Zuo & Serfling [210] (see also Chernozhukov et al. [40]): basically, \(x \rightarrow D_P(x) \geq 0\) provides a \(P\)-based center-outward ordering of points \(x \in \mathbb{R}^d\) (in other words, it measures

9 there are also version allowing for negative values, not discussed here
how deep (central) a point \( x \in \mathbb{R}^d \) is with respect to \( P \), where the point \( M_P \) of maximal depth (deepest point, if unique) is interpreted as multidimensional median and the depth decreases monotonically as \( x \) moves away from \( M \) along any straight line running through the deepest point; moreover, \( D_P(\cdot) \) should be affine invariant (in particular, independent on the underlying coordinate system) and vanishing at infinity; in practice, \( D_P(\cdot) \) is typically bounded. In essence, higher depth values represent greater “centrality”. A corresponding outlyingness function \( O_P(\cdot) \) is basically \( O_P(\cdot) := f_{OD}(D_P(\cdot)) \) for some strictly decreasing (but not necessarily bounded) nonnegative function \( f_{OD} \) of \( D_P(\cdot) \), such as \( O_P(\cdot) := \frac{1}{D_P(\cdot)} - 1 \) or \( O_P(\cdot) := c \cdot \left(1 - \frac{D_P(\cdot)}{\sup_{z \in \mathbb{R}^d} D_P(z)}\right) \) for some constant \( c > 0 \) (in case that \( D_P(\cdot) \) is bounded). Accordingly, \( O_P(\cdot) \) provides a \( P \)-based center-inward ordering of points \( x \in \mathbb{R}^d \); higher values represent greater “outlyingness”. Since \( f_{OD} \) is invertible, one can always “switch equivalently” between \( D_P(\cdot) \) and \( O_P(\cdot) \). Several examples for \( D_P(\cdot) \) respectively \( O_P(\cdot) \) can be found e.g. in Liu et al. [118], Zuo & Serfling [210,211], Serfling [170].

According to the “D-O-Q-R paradigm” of Serfling [172], one can link to the univariate/one-dimensional \( P \)-characteristics \( D_P(\cdot), O_P(\cdot) \) two multivariate/dimensional \( P \)-characteristics, namely a centered rank function \( R_P(\cdot) \) (also called center-outward distribution function in Hallin [54], Hallin et al. [86]) and a quantile function (also called center-outward quantile surface in Liu et al. [118], and center-outward quantile function in Hallin [54], Hallin et al. [86]), which are inverses of each other. Such a linkage works e.g. basically as follows: firstly, one chooses some bounded set \( B \subset \mathbb{R}^d \) of “indices”, often the \( d \)-dimensional unit ball \( B := B_d(0) \) which we henceforth use for the following explanations. Secondly, a \( P \)-based quantile function \( \Omega_P : B_d(0) \rightarrow \mathbb{R}^d \) with “full” range \( \mathcal{A}(\Omega_P) = \mathbb{R}^d \) is such that it generates contour sets (level sets) \( \mathcal{C}_c := \{ \Omega_P(u) : \|u\| = c \} \), \( 0 \leq c < 1 \) (where \( \| \cdot \| \) denotes the Euclidean norm on \( \mathbb{R}^d \) which are nested (as \( c \) varies increasingly). The most central point \( M_P := \Omega_P(0) \) is interpreted as \( d \)-dimensional median. The magnitude \( c \) represents a degree of outlyingness for all data points in \( \mathcal{C}_c \), and higher \( c \)-values corresponding to “more extreme data points” \( \mathcal{C}_c \). Thirdly, \( R_P \) is taken to be the (possibly multi-valued) inverse of \( \Omega_P \). For technical purposes, one attempts to use quantile functions \( \Omega_P \) such that the contour sets \( \mathcal{C}_c \) are “strictly nested” (in the sense that the do not intersect for different \( c \)'s) such that the inverse function \( R_P : \mathbb{R}^d \rightarrow B_d(0) \) is determined by uniquely solving the equation \( y = \Omega_P(u) \) for \( u \in B_d(0) \), for all \( y \in \mathbb{R}^d \). Finally, as a naturally corresponding outlyingness function one can e.g. take the magnitude \( O_P(y) := \|R_P(y)\| \) (i.e. the \( c \) for which \( y \in \mathcal{C}_c \)) and derive the associated depth function \( D_P(y) = f_{OD}(O_P(y)) \). Since our divergence framework deals with univariate statistical functionals, we shall work

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Notice that this kind of outlyingness concept is intrinsic (with respect to \( P \)), as opposed to the “relative outlyingness” defined as a degree of mismatch between the frequency of certain data-observation points compared to the corresponding (very much lower) modelling frequency; see e.g. Lindsay [113], Basu et al. [25], and the corresponding flexibilization in Kiflinger & Stummer [102].
with the \(i\)-th components \(\{S_x(P)\}_{x \in \mathbb{R}^d} = \left\{ \Omega^{(i)}_P(x) \right\}_{x \in \mathbb{R}} =: S^{\text{cr},i}(P) \) and 
\(\{S_x(P)\}_{x \in \mathbb{R}^d} = \left\{ R^{(i)}_P(x) \right\}_{x \in \mathbb{R}^d} =: S^{\text{ru},i}(P) \) \(i \in \{1, \ldots, d\}\) and finally aggregate the results by adding up the correspondingly occurring \(d\) divergences over \(i\) (see e.g. [70] and [78] below).

There are several ways to build up concrete “D-O-Q-R” setups. A recent one which generates centered \(d\)-dimensional analogues of the univariate quantile-transform mapping and the reciprocal probability-integral transformation – and which uses Brenier-McCann techniques connected to the Monge-Kantorovich theory of optimal mass transporation – is constructed by Chernozhukov et al. [46] and Hallin [84] Hallin et al. [86] (see also Figalli [70], Faugeras & Rüschendorf [67]): indeed, for absolutely continuous distributions \(P\) on \(\mathbb{R}^d\) with nonvanishing (Lebesgue) density functions they define \(R_P\) as the unique gradient \(\nabla \psi\) of a convex function \(\psi\) – mapping \(\mathbb{R}^d\) to \(\mathbb{B}_d(0)\) and – “pushing forward” the uniform measure \(\mathcal{U}(\mathbb{B}_d(0))\) on \(\mathbb{B}_d(0)\) (i.e., the distribution of \(\nabla \psi\) under \(P\) is \(\mathcal{U}(\mathbb{B}_d(0))\): as corresponding quantile function they take the inverse \(\Omega_P := R_P^{-1}\) of \(R_P\). As indicated above, this implies the transformations \(Z \sim P\) if and only if \(R_P(Z) \sim \mathcal{U}(\mathbb{B}_d(0))\) as well as \(U \sim \mathcal{U}(\mathbb{B}_d(0))\) if and only if \(\Omega_P(U) \sim P\). Depth functions for \(P\) can be generated from depth functions \(D_{\mathcal{U}(\mathbb{B}_d(0))}(\cdot)\) by \(D_P(x) := D_{\mathcal{U}(\mathbb{B}_d(0))}(R_P(x))\) \(x \in \mathbb{R}^d\). For \(d = 1\), one arrives at the univariate \(R_P(x) = R_P^{(1)}(x) = 2 \cdot F_P(x) - 1, \Omega_P^{(1)}(x) = F_P^{-1}\left(\frac{1+x}{2}\right)\), and thus there are the consistencies \(S^{\text{cr},1}(P) := \left\{ R^{(1)}_P(x) \right\}_{x \in \mathbb{R}} = S^{\text{cr}}(P), S^{\text{ru},1}(P) := \left\{ \Omega^{(1)}_P(x) \right\}_{x \in [-1,1]} = S^{\text{ru}}(P)\).

There are also several other different approaches to define multidimensional analogues of quantile functions, see e.g. Serfling [170,172], Galichon & Henry [71], Faugeras & Rüschendorf [67]. All those multivariate quantile functions are also covered by our divergence toolkit, componentwise.

Let us finally mention that for general state space \(\mathcal{Y}\), as unit-free statistical functionals one can also take for instance families \(\{S_x(P)\}_{x \in \mathcal{X}} := \{P[E_x]\}_{x \in \mathcal{X}}\) of probabilities of some particularly selected concrete events \(E_x \in \mathcal{A}\) of purpose-driven interest, where \(\mathcal{X}\) is some set of indices.

As needed later on, notice that these statistical functionals \(S(P) = \{S_x(P)\}_{x \in \mathcal{X}} \) have the following different ranges \(\mathcal{R}(S(P)) = \mathcal{R}(S^{\text{ru}}(P)) = \mathcal{R}(S^{\text{cr}}(P)) = \mathcal{R}(S^{\text{ru},i}(P)) \subset [0,1]\), \(\mathcal{R}(S^{\text{ru}}(P)) \subset [0, \infty]\), \(\mathcal{R}(S^{\text{cr}}(P)) \subset ]-\infty, \infty[\) (respectively \(\mathcal{R}(S^{\text{ru},i}(P)) \subset [0, \infty]\) for non-negative random variable \(Y \geq 0\), \(\mathcal{R}(S^{\text{de}}(P)) \subset [0, \infty]\), \(\mathcal{R}(S^{\text{ra}}(P)) \subset [0, \infty]\), \(\mathcal{R}(S^{\text{cr},i}(P)) \subset [-1,1]\), \(\mathcal{R}(S^{\text{ru},i}(P)) \subset ]-\infty, \infty[\) \((i \in \{1, \ldots, d\})\), and \(\mathcal{R}(S^{\tilde{\lambda},\tilde{S}}(P))\) depends on the choice of \(\tilde{\lambda}\) and \(\tilde{S}\).

The above-mentioned “dissimilarity-expressing functional relations” \(\mathcal{R}(S(P),S(Q))\) can be typically of (i) numerical nature or (ii) graphical/plotting
nature, or hybrids thereof. As far as (i) is concerned, for fixed \( x \in \mathcal{X} \) the dissimilarity between the real-valued \( S_x(P) \) and \( S_x(Q) \) can be expressed by (weighted) ratios close to 1, (weighted) differences close to 0, and combinations thereof; these informations on “pointwise” dissimilarities can then be compressed to a single real number e.g. by means of aggregation (weighted summation, weighted integration, etc.) over \( x \) or by taking the maximum respectively minimum value with respect to \( x \). In contrast, for \( \mathcal{X} = \mathbb{R} \) one widespread tool for (ii) is to draw a two-dimensional scatterplot \( (S_x(P), S_x(Q))_{x \in \mathcal{X}} \) and evaluate – visually by eyeballing or quantitatively – the dissimilarity in terms of sizes of deviations from the equality-expressing diagonal \( (t, t) \). In the above-mentioned special case of \( S_x(P) = F_P(x) = F(]-\infty, x]\), \( S_x(Q) = F_Q(x) = Q(]-\infty, x]\) this leads to the well-known “Probability-Probability-Plot” \((PP – Plot)\), whereas the choice \( S_x(P) = F_P^{-}(x) = \inf\{z \in \mathbb{R} : F_P(z) \geq x\}, \ S_x(Q) = F_Q^{-}(x) = \inf\{z \in \mathbb{R} : F_Q(z) \geq x\}\) amounts to the very frequently used “Quantile-Quantile-Plot” \((QQ – Plot)\). Moreover, the choice \( S_x(P) = \mathcal{D}_P(x) \) and \( S_x(Q) = \mathcal{D}_Q(x) \) for some \( P \)-based respectively \( Q \)-based depth function generates the \( DD – Plot \) in the sense of Liu et al. [118].

2.2 The divergences (directed distances) \( D \)

Let us now specify the details of the divergences (directed distances) \( D(S(P), S(Q)) \) which we are going to employ henceforth as dissimilarity measures between the statistical functionals \( S(P) := \{S_x(P)\}_{x \in \mathcal{X}} \) and \( S(Q) := \{S_x(Q)\}_{x \in \mathcal{X}} \). To begin with, we equip the index space \( \mathcal{X} \) with a \( \sigma \)-algebra \( \mathcal{F} \) and a \( \sigma \)-finite measure \( \lambda \) (e.g. a probability measure, the Lebesgue measure, a counting measure, etc.); furthermore, we assume that \( x \to S_x(P) \in []-\infty, \infty] \) and \( x \to S_x(Q) \in []-\infty, \infty] \) are correspondingly measurable functions which satisfy \( S_x(P) \in ]-\infty, \infty[ \) for \( \lambda \)-almost all (abbreviated as \( \lambda \)-a.a.) \( x \in \mathcal{X} \). For such a context, we quantify the (aggregated) divergence \( D(S(P), S(Q)) := D_\beta^\lambda(S(P), S(Q)) \) between the two statistical functionals \( S(P) \) and \( S(Q) \) in terms of the “parameters” \( \beta = (\phi, m_1, m_2, m_3, \lambda) \) and \( \epsilon \) by

\[
0 \leq D_\beta^\lambda m_1, m_2, m_3, \lambda(S(P), S(Q)) := \int_{\mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{m_1(x)} \right) - \phi \left( \frac{S_x(Q)}{m_2(x)} \right) - \phi_+ \left( \frac{S_x(Q)}{m_2(x)} \right) \cdot \frac{S_x(P) - S_x(Q)}{m_1(x) - m_2(x)} \right] m_3(x) d\lambda(x),
\]

(19)

where the meaning of the integral symbol \( \int \) – as a shortcut of the integral over an appropriate extension of the integrand – will become clear in (21) below. Here, in accordance with the \( BS \) distances of Broniatowski & Stummer [142] — who flexibilized/widened the concept of scaled Bregman distances of Stummer [152] and Stummer & Vajda [188] — we use the following ingredients:
(11) (measurable) scaling functions \( m_1 : \mathcal{X} \rightarrow (-\infty, \infty) \) and \( m_2 : \mathcal{X} \rightarrow (-\infty, \infty) \) as well as a nonnegative (measurable) aggregating function \( m_3 : \mathcal{X} \rightarrow [0, \infty] \) such that \( m_1(x) \in (-\infty, \infty), m_2(x) \in (-\infty, \infty), m_3(x) \in [0, \infty] \) for \( \lambda \)-a.a. \( x \in \mathcal{X} \). In analogy with the above notation, we use the symbols \( m_i := \{ m_i(x) \}_{x \in \mathcal{X}} \) to refer to the whole functions. Let us emphasize that we also allow for adaptive situations in the sense that all three functions \( m_1(x), m_2(x), m_3(x) \) (evaluated at \( x \)) may also depend on \( S_x(P) \) and \( S_x(Q) \), see below. In the following, \( \mathcal{R}(G) \) denotes the range (or image) of a function \( G := \{ G(x) \}_{x \in \mathcal{X}} \).

(12) the so-called “divergence-generator” \( \phi \) which is a continuous, convex (finite) function \( \phi : E \rightarrow (-\infty, \infty] \) on some appropriately chosen open interval \( E = [a, b] \) such that \( [a, b] \) covers (at least) the union of both ranges \( \mathcal{R} \left( \frac{S(P)}{m_1} \right) \) of \( \left\{ \frac{S(P)}{m_1(x)} \right\}_{x \in \mathcal{X}} \) and \( \mathcal{R} \left( \frac{S(Q)}{m_2} \right) \) of \( \left\{ \frac{S(Q)}{m_2(x)} \right\}_{x \in \mathcal{X}} \); for instance, \( E = [0, 1], E = [0, \infty] \) or \( E = (-\infty, \infty] \); the class of all such functions will be denoted by \( \Phi([a, b]) \). Furthermore, we assume that \( \phi \) is continuously extended to \( \varphi : [a, b] \rightarrow (-\infty, \infty] \) by setting \( \varphi(t) := \phi(t) \) for \( t \in [a, b] \) as well as \( \varphi(a) := \lim_{t \uparrow a} \phi(t), \varphi(b) := \lim_{t \downarrow b} \phi(t) \) on the two boundary points \( t = a \) and \( t = b \). The latter two are the the only points at which infinite values may appear (e.g. because of division by \( m_1(x) = 0 \) for some \( x \)). Moreover, for any fixed \( c \in [0, 1] \) the (finite) function \( \phi'_{+} : [a, b] \rightarrow (-\infty, \infty] \) is well-defined by \( \phi'_{+}(t) := c \cdot \phi_{+}(t) + (1 - c) \cdot \phi_{-}(t) \), where \( \phi_{+}(t) \) denotes the (always finite) right-hand derivative of \( \phi \) at the point \( t \in [a, b] \) and \( \phi_{-}(t) \) the (always finite) left-hand derivative of \( \phi \) at \( t \in [a, b] \). If \( \phi \in \Phi([a, b]) \) is also continuously differentiable – which we denote by \( \phi \in \Phi_{\text{C}}([a, b]) \) – then for all \( c \in [0, 1] \) one gets \( \phi'_{+} = \phi'_{-} \) \((t \in [a, b]) \) and in such a situation we also suppress + as well as c in all the following expressions. We also employ the continuous continuation \( \bar{\phi}'_{+} : [a, b] \rightarrow (-\infty, \infty] \) given by \( \bar{\phi}'_{+}(t) := \phi'_{+}(t) \) \((t \in [a, b]) \), \( \bar{\phi}'_{+}(a) := \lim_{t \uparrow a} \phi'_{+}(t) \), \( \bar{\phi}'_{+}(b) := \lim_{t \downarrow b} \phi'_{+}(t) \). To explain the precise meaning of \((19)\), we also make use of the (finite, nonnegative) function \( \psi_{\phi,c} : [a, b] \times [a, b] \rightarrow [0, \infty] \) given by \( \psi_{\phi,c}(s, t) := \phi(s) - \phi(t) - \phi'_{+}(c)(s - t) \geq 0 \) \((s, t \in [a, b]) \). To extend this to a lower semi-continuous function \( \psi_{\phi,c} : [a, b] \times [a, b] \rightarrow [0, \infty] \) we proceed as follows: firstly, we set \( \psi_{\phi,c}(s, t) := \psi_{\phi,c}(s, t) \) for all \( s, t \in [a, b] \). Moreover, since for fixed \( t \in [a, b] \), the function \( s \rightarrow \psi_{\phi,c}(s, t) \) is convex and continuous, the limit \( \lim_{s \uparrow a} \psi_{\phi,c}(s, t) := \lim_{s \uparrow a} \psi_{\phi,c}(s, t) \) always exists and (in order to avoid overlines in \((19)\)) will be interpreted/abbreviated as \( \phi(a) - \phi(t) - \phi'_{+}(c)(a - t) \). Analogously, for fixed \( t \in [a, b] \) we set \( \bar{\psi}_{\phi,c}(b, t) := \lim_{s \downarrow b} \bar{\psi}_{\phi,c}(s, t) \) with corresponding short-hand notation \( \phi(b) - \phi(t) - \phi'_{+}(c)(b - t) \). Furthermore, for fixed \( s \in [a, b] \) we interpret \( \bar{\phi}(s) - \phi(a) - \phi'_{+}(c)(s - a) \) as

\[
\bar{\psi}_{\phi,c}(s, a) := \left\{ \phi(s) - \phi'_{+}(c)(a) \cdot s + \lim_{\tau \uparrow a} \left( \tau \cdot \bar{\phi}'_{+}(c)(a) - \phi(t) \right) \right\} \cdot 1_{-\infty, \infty}[\bar{\phi}'_{+}(c)(a)] + \infty \cdot 1_{(-\infty, \infty]}(\bar{\phi}'_{+}(c)(a)),
\]
where the involved limit always exists but may be infinite. Analogously, for
fixed \( s \in]a, b[ \) we interpret \( \phi(s) - \phi(b) - \phi'(s,b) \cdot (s - b) \) as

\[
\psi_{\phi,c}(s, b) := \left\{ \phi(s) - \frac{\phi'}{\phi'(s,b)}(b) \cdot s + \lim_{t \to b^-} \left\{ t \cdot \frac{\phi'}{\phi'(s,b)}(b) - \phi(t) \right\} \right\} \cdot 1_{]-\infty, \infty[} \left( \frac{\phi'}{\phi'(s,b)}(b) \right)
\]

where again the involved limit always exists but may be infinite. Finally, we
always set \( \psi_{\phi,c}(a, a) := 0 \), \( \psi_{\phi,c}(b, b) := 0 \), and \( \psi_{\phi,c}(a, b) := \lim_{s \to a} \psi_{\phi,c}(s, b) \),
\( \psi_{\phi,c}(b, a) := \lim_{s \to b} \psi_{\phi,c}(s, a) \). Notice that \( \psi_{\phi,c} \) is lower-semicontinuous but
not necessarily continuous. Since ratios are ultimately involved, we also con-
sistently take \( \psi_{\phi,c} \left( \frac{a}{b}, \frac{c}{b} \right) := 0 \).

With (I1) and (I2), we define the BS divergence (BS distance) of \( \mathbf{[19]} \) precisely as

\[
0 \leq D_{\phi, m_1, m_2, m_3, \lambda}^c(S(P), S(Q)) = \int_{\mathcal{X}} \psi_{\phi,c} \left( \frac{S_2(P)}{m_1(x)}, \frac{S_2(Q)}{m_2(x)} \right) \cdot m_3(x) \, d\lambda(x) \quad (20)
\]

or

\[
\int_{\mathcal{X}} \psi_{\phi,c} \left( \frac{S_2(P)}{m_1(x)}, \frac{S_2(Q)}{m_2(x)} \right) \cdot m_3(x) \, d\lambda(x),
\]

but mostly use the less clumsy notation with \( \int \) given in \( \mathbf{[19]}, \mathbf{[20]} \) henceforth,
as a shortcut for the implicitly involved boundary behaviour. \( \square \)

As a side remark let us mention that, we could further generalize \( \mathbf{[19]} \) by adapting
a wider divergence (e.g. non-convex generators \( \phi \) covering) concept of Stummer
& Kißlinger \( \mathbf{[184]} \) who also deal even with nonconvex nonconcave divergence
generators \( \phi \); for the sake of brevity, this is omitted here.

Notice that by construction one has the following important assertion (cf. Broniatski\wsk & Stummer \( \mathbf{[12]} \)):

**Theorem 2.** Let \( \phi \in \Phi([a, b[) \) and \( c \in [0, 1] \).
Then there holds \( D_{\phi, m_1, m_2, m_3, \lambda}^c(S(P), S(Q)) \geq 0 \) (i.e. the above-mentioned de-
sired property (D1) is satisfied).
Moreover, \( D_{\phi, m_1, m_2, m_3, \lambda}^c(S(P), S(Q)) = 0 \) if \( \frac{S_2(P)}{m_1(x)} = \frac{S_2(Q)}{m_2(x)} \) for \( \lambda \)-almost all
\( x \in \mathcal{X} \).
Depending on the concrete situation, \( D_{\phi, m_1, m_2, m_3, \lambda}^c(S(P), S(Q)) \) may take in-
finite value.

To get a “sharp identifiability”, i.e. the correspondingly adapted version of the
above-mentioned desired reflexivity property (D2) in the form of

\[
D_{\phi, m_1, m_2, m_3, \lambda}^c(S(P), S(Q)) = 0 \quad \text{if and only if} \quad \frac{S_2(P)}{m_1(x)} = \frac{S_2(Q)}{m_2(x)} \quad \lambda-\text{a.a.} \, x \in \mathcal{X},
\]

(22)
one needs further requirements on $\phi \in \Phi([a, b])$ and $c \in [0, 1]$; for the rest of the paper, we assume the validity of (22) holds.

For instance, the latter is satisfied in a setup where $m_3(x) = w \left(x, \frac{S_1(P)}{m_1(x)}, \frac{S_2(Q)}{m_2(x)}\right)$ for some (measurable) function $w : \mathcal{X} \times [a, b] \times [a, b] \to [0, \infty]$, and the (correspondingly adapted) Assumptions 2 respectively Assumptions 3 of Broniatowski & Stummer hold (cf. Theorem 4 respectively Corollary 1 therein); in particular, this means that $\mathcal{R}\left(\frac{S_1(P)}{m_1}\right) \cup \mathcal{R}\left(\frac{S_2(Q)}{m_2}\right) \subset [a, b]$ and that for all $s \in \mathcal{R}\left(\frac{S_1(P)}{m_1}\right)$ and all $t \in \mathcal{R}\left(\frac{S_2(Q)}{m_2}\right)$ the following conditions hold:
- $\phi$ is strictly convex at $t$;
- if $\phi$ is differentiable at $t$ and $s \neq t$, then $\phi$ is not affine-linear on the interval $[\min(s, t), \max(s, t)]$ (i.e. between $t$ and $s$);
- if $\phi$ is not differentiable at $t$, $s > t$ and $\phi$ is affine linear on $[t, s]$, then we exclude $c = 1$ for the ("globally/universally chosen") subderivative $\phi'_{t, c}(\cdot) = c \cdot \phi'_t(\cdot) + (1 - c) \cdot \phi'_s(\cdot)$;
- if $\phi$ is not differentiable at $t$, $s < t$ and $\phi$ is affine linear on $[s, t]$, then we exclude $c = 0$ for $\phi'_{t, c}(\cdot)$.

In the following, we discuss several important (classes of) special cases of $\beta = (\phi, m_1, m_2, m_3, \lambda)$ in a well-structured way. Let us start with the latter.

2.3 The reference measure $\lambda$

In (19), $\lambda$ governs the principle aggregation structure. For instance, if one chooses $\lambda = \lambda_\# = \lambda_L$ as the Lebesgue measure on $\mathcal{X} \subset \mathbb{R}$, then the integral in (19) turns out to be of Lebesgue-type and (with some rare exceptions) consequently of Riemann-type with $d\lambda(x) = dx$. In contrast, in the discrete setup where the index set $\mathcal{X}_\# = \mathcal{X}_\#$ has countably many elements and is equipped with the counting measure $\lambda_\# := \lambda_\# := \sum_{z \in \mathcal{X}_\#} \delta_z$ (where $\delta_z$ is Dirac’s one-point distribution $\delta_z[A] := 1_{A}(z)$), and thus $\lambda_\#(\{z\}) = 1$ for all $z \in \mathcal{X}_\#$, then (19) simplifies to

$$0 \leq D_{\phi, m_1, m_2, m_3, \lambda_\#}(S(P), S(Q)) := \sum_{z \in \mathcal{X}} \left[ \phi\left(\frac{S_1(P)}{m_1(z)}\right) - \phi\left(\frac{S_2(Q)}{m_1(z)}\right) - \phi'_{1, c}\left(\frac{S_2(Q)}{m_2(z)}\right) \cdot \frac{S_2(Q)}{m_2(z)} \cdot \frac{S_1(P)}{m_1(z)} - \frac{S_1(P)}{m_2(z)}\right] m_3(z),$$

(23)

which we interpret as $\sum_{z \in \mathcal{X}} \varphi_{\phi, c}\left(\frac{S_1(P)}{m_1(z)}, \frac{S_2(Q)}{m_2(z)}\right) \cdot m_3(z)$ with the same conventions and limits as in the paragraph right after (19).

2.4 The divergence generator $\phi$

We continue with the inspection of interesting special cases of $\beta = (\phi, m_1, m_2, m_3, \lambda)$ by dealing with the first component. For divergence generator $\phi \in \Phi_L([a, b])$ (recall that then we suppress the obsolete $c$ and subderivative index $+$), the formula
widths (19) turns into
\[ 0 \leq D_{\phi,m_1,m_2,m_3,\lambda}(S(P), S(Q)) \]
\[ := \int_{\mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{m_1(x)} \right) - \phi \left( \frac{S_x(Q)}{m_2(x)} \right) - \phi' \left( \frac{S_x(Q)}{m_2(x)} \right) \cdot \left( \frac{S_x(P)}{m_1(x)} - \frac{S_x(Q)}{m_2(x)} \right) \right] m_3(x) \, d\lambda(x), \tag{24} \]

whereas (23) becomes
\[ 0 \leq D_{\phi,m_1,m_2,m_3,\lambda}(S(P), S(Q)) \]
\[ := \sum_{x \in \mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{m_1(x)} \right) - \phi \left( \frac{S_x(Q)}{m_2(x)} \right) - \phi' \left( \frac{S_x(Q)}{m_2(x)} \right) \cdot \left( \frac{S_x(P)}{m_1(x)} - \frac{S_x(Q)}{m_2(x)} \right) \right] m_3(x). \]

Formally, by defining the integral functional \( g_{\phi,m_3,\lambda}(\xi) := \int_{\mathcal{X}} \phi(\xi(x)) \cdot m_3(x) \, d\lambda(x) \) and plugging in e.g. \( g_{\phi,m_3,\lambda}(S(P)/m_1) = \int_{\mathcal{X}} \phi \left( \frac{S_x(P)}{m_1(x)} \right) \cdot m_3(x) \, d\lambda(x) \), the divergence in (24) can be interpreted as
\[ 0 \leq D_{\phi,m_1,m_2,m_3,\lambda}(S(P), S(Q)) \]
\[ = g_{\phi,m_3,\lambda}(S(P)/m_1) - g_{\phi,m_3,\lambda}(S(Q)/m_2) - g'_{\phi,m_3,\lambda}(S(Q)/m_2, S(P)/m_1 - S(Q)/m_2) \tag{25} \]

where \( g'_{\phi,m_3,\lambda}(\eta, \cdot) \) denotes the corresponding directional derivative at \( \eta = \frac{S(Q)/m_2}{m_2} \).

An important special case is the following: consider the “nonnegativity-setup”
\[ (\text{NN0}) \quad \frac{S_x(P)}{m_1(x)} \geq 0 \quad \text{and} \quad \frac{S_x(Q)}{m_2(x)} \geq 0 \quad \text{for all} \quad x \in \mathcal{X}; \]
for instance, this always holds for nonnegative scaling functions \( m_1, m_2 \), in combination with \( S^{cd}, S^{pd}, S^{pm}, S^{st}, S^{mn}, S^{mc}, S^{ov}, \) and for nonnegative real-valued random variables also with \( S^{nu} \). Under (NN0), one can take \( a = 0, b = \infty \), i.e. \( E = [0, \infty[ \), and employ the strictly convex power functions
\[ \phi(t) := \phi_{\alpha}(t) := \frac{t^\alpha - 1}{\alpha(\alpha - 1)} \in ]-\infty, \infty[, \quad t \in ]0, \infty[, \quad \alpha \in \mathbb{R}\setminus\{0, 1\}, \]
\[ \phi(t) := \tilde{\phi}_{\alpha}(t) := \tilde{\phi}_{\alpha}(t) - \tilde{\phi}_{\alpha}(1) \cdot (t - 1) = \frac{t^\alpha - 1}{\alpha(\alpha - 1)} - \frac{t - 1}{\alpha - 1} \in [0, \infty[, \quad t \in ]0, \infty[, \quad \alpha \in \mathbb{R}\setminus\{0, 1\}, \] \tag{26} \]

The perhaps most important special case is \( \alpha = 2 \), for which (26) turns into
\[ \phi_2(t) := \frac{(t - 1)^2}{2}, \quad t \in ]0, \infty[ = E. \tag{27} \]
Also notice that the divergence-generator \( \phi_2 \) of \cite{42} can be trivially extended to
\[
\tilde{\phi}_2(t) := \frac{(t - 1)^2}{2}, \quad t \in \mathbb{R},
\]
which is useful in the general setup
\[
(GS) \quad \frac{S_x(P)}{m_1(x)} \in [-\infty, \infty] \quad \text{and} \quad \frac{S_x(Q)}{m_2(x)} \in [-\infty, \infty] \quad \text{for all} \ x \in \mathcal{X}^e;
\]
which appears for nonnegative scaling functions \( m_1, m_2 \) in combination with \( S^u \) for real-valued random variables.

Further examples of everywhere strictly convex divergence generators \( \phi \) for the nonnegativity-setup (NN0) (i.e. \( a = 0, b = \infty, E = ]0, \infty[ \)) can be obtained by taking the \( \alpha \)-limits
\[
\tilde{\phi}_3(t) := \lim_{\alpha \to 1} \phi_\alpha(t) = t \cdot \log t \in [-\infty, \infty], \quad t \in ]0, \infty[,
\]
\[
\phi_3(t) := \lim_{\alpha \to 1} \phi_\alpha(t) = \tilde{\phi}_3(t) - \tilde{\phi}_3'(1) \cdot (t - 1) = t \cdot \log t + 1 - t \in [0, \infty], \quad t \in ]0, \infty[,
\]
\[
\tilde{\phi}_0(t) := \lim_{\alpha \to 0} \phi_\alpha(t) = -\log t \in (-\infty, \infty], \quad t \in ]0, \infty[,
\]
\[
\phi_0(t) := \lim_{\alpha \to 0} \phi_\alpha(t) = \tilde{\phi}_0(t) - \tilde{\phi}_0'(1) \cdot (t - 1) = -\log t + t - 1 \in [0, \infty], \quad t \in ]0, \infty[.
\]

A list of extension-relevant (cf. (I2)) properties of the functions \( \phi_\alpha \) with \( \alpha \in \mathbb{R} \) can be found in Broniatowski & Stummer \cite{42}. The latter also discuss in detail the important but (in our context) technically delicate divergence generator
\[
\phi_{TV}(t) := |t - 1|
\]
which is non-differentiable at \( t = 1 \); the latter is also the only point of strict convexity.

As demonstrated in \cite{42}, \( \phi_{TV} \) can – in our context – only be potentially applied if \( \frac{S_x(Q)}{m_2(x)} = 1 \) for \( \lambda \)-a.a. \( x \in \mathcal{X}^e \), and one generally has to exclude \( c = 1 \) and \( c = 0 \) for \( \phi_{s.e}^c(\cdot) \) (i.e. we choose \( c \in ]0, 1[ \)); the latter two can be avoided under some non-obvious constraints on the statistical functionals \( S(P), S(Q) \), see for instance Subsection 2.5.1.2 below.

2.5 The scaling and the aggregation functions \( m_1, m_2, m_3 \)

In the above two Subsections 2.3 and 2.4 we have presented special cases of the first and the last component of the “divergence parameter” \( \beta = (\phi, m_1, m_2, m_3, \lambda) \), whereas now we focus on \( m_1, m_2, m_3 \). To start with, in accordance with \cite{19}, the aggregation function \( m_3 \) tunes the fine aggregation details (recall that \( \lambda \) governs the principle aggregation structure). Moreover, the function \( m_1(\cdot) \) scales the statistical functional \( S(P) \) evaluated at \( P \) and \( m_2(\cdot) \) the same statistical functional \( S(Q) \) evaluated at \( Q \). From a modeling perspective, these two scaling functions can e.g.
“purely direct” in the sense that \( m_1(x), m_2(x) \) are chosen to directly reflect some dependence on the index-state \( x \in \mathcal{X} \) (independent of the choice of \( S \)), or

“purely adaptive” in the sense that \( m_1(x) = w_1(S_x(P), S_x(Q)), m_2(x) = w_2(S_x(P), S_x(Q)) \) for some appropriate (measurable) “connector functions” \( w_1, w_2 \) on the product \( \mathcal{R}(P) \times \mathcal{R}(Q) \) of the ranges of \( \{S_x(P)\}_{x \in \mathcal{X}} \) and \( \{S_x(Q)\}_{x \in \mathcal{X}} \), or

“hybrids” \( m_1(x) = w_1(x, S_x(P), S_x(Q)), m_2(x) = w_2(x, S_x(P), S_x(Q)) \).

In the remainder of Section 2, we illuminate several important sub-setups of \( m_1, m_2, m_3 \), and special cases therein. As a side effect, this also shows that our framework \cite{19} generalizes considerably all the concrete divergences in the below-mentioned references (even for the same statistical functional such as e.g. \( S = S^{\text{cd}} \)), for the sake of brevity, we mention that only at this point, collectively.

2.5.1 \( m_1(x) = m_2(x) := m(x), m_3(x) = r(x) \cdot m(x) \in \lbrack 0, \infty \rbrack \) for some (measurable) function \( r : \mathcal{X} \rightarrow \mathbb{R} \) satisfying \( r(x) \in \lbrack -\infty, 0 \rbrack \cup \lbrack 0, \infty \rbrack \) for \( \lambda \text{-a.a.} \ x \in \mathcal{X} \).

In such a sub-setup, the scaling functions are strongly coupled with the aggregation function. In order to avoid “case-overlapping” and “uncontrolled boundary effects”, unless otherwise stated we assume here that the function \( r(\cdot) \) does not (explicitly) dependent on the functions \( m(\cdot), S(P), S(Q) \), i.e. it is not of the adaptive form \( r(\cdot) = h(\cdot, m(\cdot), S(P), S(Q)) \). From \cite{19} one can derive

\[
0 \leq D_{\phi,m,m,r,m,\lambda}(S(P), S(Q))
:= \int_{\mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{m(x)} \right) - \phi \left( \frac{S_x(Q)}{m(x)} \right) - \phi'_{+}\left( \frac{S_x(Q)}{m(x)} \right) \cdot \left( \frac{S_x(P)}{m(x)} - \frac{S_x(Q)}{m(x)} \right) \right] m(x) \cdot r(x) \, d\lambda(x),
\]

(33)

which for the discrete setup \( \mathcal{X} = (\mathcal{X}^\#, \lambda^\#) \) (recall \( \lambda^\#[\{x\}] = 1 \) for all \( x \in \mathcal{X}^\# \)) simplifies to

\[
0 \leq D_{\phi,m,m,r,m,\lambda^\#}(S(P), S(Q))
:= \sum_{x \in \mathcal{X}^\#} \left[ \phi \left( \frac{S_x(P)}{m(x)} \right) - \phi \left( \frac{S_x(Q)}{m(x)} \right) - \phi'_{+}\left( \frac{S_x(Q)}{m(x)} \right) \cdot \left( \frac{S_x(P)}{m(x)} - \frac{S_x(Q)}{m(x)} \right) \right] m(x) \cdot r(x).
\]

(34)

Remark 1. (a) In a context of \( \lambda \text{-probability-density functions} \) with general \( \mathcal{X} \) and \( P[\cdot] := \int f_P(x) \, d\lambda(x), Q[\cdot] := \int f_Q(x) \, d\lambda(x) \) satisfying \( P[\mathcal{X}] = Q[\mathcal{X}] = 1 \), one can take the statistical functionals \( S^{\text{cpd}}_x(P) := f_P(x) \geq 0, S^{\text{cpd}}_x(Q) := f_Q(x) \geq 0 \); accordingly, for \( r(x) \equiv 1 \) (abbreviated as function \( \mathbf{1} \) with constant value 1) and \( M[\cdot] := \int m(x) \, d\lambda(x) \) the divergence (33) can be
For the important special case of the above-mentioned power-function-type generator (35) reads as

\[ 0 \leq D_{\phi}^{\lambda-pd}(P, Q) = B_{\phi}^{\lambda-pd}(P, Q) \]

where the scaled Bregman divergence \( B_{\phi}^{\lambda-pd}(P, Q) \) has been first defined in Stummer [152], Stummer & Vajda [188], see also Kisslinger & Stummer [100], [101], [102] for the “purely adaptive” case \( m(x) = w(f_{P}(x), f_{Q}(x)) \) and indications on non-probability measures. Notice that this directly subsumes for the “classical density” functional \( S_{\phi}(\lambda) = S_{\phi}^{\lambda-pd}(\cdot) \) with the choice \( \lambda = \lambda_{L} \) (and the Riemann integration \( d\lambda_{L}(x) = dx \)), as well as for the discrete setup \( \mathcal{Y} = \mathcal{X} = \mathcal{X}_{\#} \), the “classical probability mass” functional \( S_{\phi}^{\lambda-pd}(\cdot) = S_{\phi}^{m}(\cdot) \) with the choice \( \lambda = \lambda_{\#} \) (recall \( \lambda_{\#}([x]) = 1 \) for all \( x \in \mathcal{X}_{\#} \)); for the latter, the divergence (35) reads as

\[ 0 \leq D_{\phi}^{\lambda-pd}(P, Q) = B_{\phi}^{\lambda-pd}(P, Q) \]

For the important special case of the above-mentioned power-function-type generator \( \phi(t) := \phi_{\alpha}(t) = t^{\frac{\alpha - 1}{\alpha}}} \) \( (\alpha \in ]0, \infty[\setminus\{1\}) \), Roenschi & Stummer [104] (see also Ghosh & Basu [75] for the unscaled special case \( m(x) = 1 \)) employed the corresponding scaled Bregman divergences (35) in order to obtain robust minimum-divergence-type parameter estimates for the setup of sequences of independent random variables whose distributions are non-identical but linked by a common (scalar or multidimensional) parameter; this is e.g. important in the context of generalized linear models (GLM) which are omnipresent in statistics, artificial intelligence and machine learning.

Returning to the general framework, for the important special case \( \alpha = 2 \) leading to the above-mentioned generator \( \phi_{2}(t) := \sqrt{t} \), the scaled Bregman divergences (35) respectively (36) turn into

\[ 0 \leq B_{\phi_{2}}(P, Q) = \sum_{x \in \mathcal{X}_{\#}} \frac{(p_{P}(x) - p_{P}(x))^{2}}{2m(x)} \mathrm{d}\lambda(x) \]

\[ 0 \leq B_{\phi_{2}}^{\lambda-pd}(P, Q) = \sum_{x \in \mathcal{X}_{\#}} \frac{(p_{P}(x) - p_{P}(x))^{2}}{2m(x)} \mathrm{d}\lambda(x) \]

in a context where \( P \) and \( Q \) are risk distributions (e.g. \( Q \) is a pre-given reference one) the SBD \( B_{\phi}(P, Q) \) can be interpreted as risk excess of \( P \) over \( Q \) (or vice versa), in contrast to Faugeras & Rüschendorf [65] who use hemimetrics rather than divergences.
For instance, in (33) and (34), if \( Y \) is a random variable taking values in the discrete space \( \mathcal{X}_\#, \) then \( p_Q(x) = Q[Y = x] \) may be its probability mass function under a hypothetical/candidate law \( Q, \) and \( p_P(x) = \frac{1}{N} \cdot \# \{ i \in \{ 1, \ldots, N \} : Y_i = x \} =: p_{emp}^\#(x) \) is the probability mass function of the corresponding data-derived "empirical distribution" \( P := P_{emp} := \frac{1}{N} \cdot \sum_{i=1}^{N} \delta_{Y_i}([\cdot]) \) of an \( N \)-size independent and identically distributed (i.i.d.) sample \( Y_1, \ldots, Y_N \) of \( Y \) which is nothing but the probability distribution reflecting the underlying (normalized) histogram; moreover, \( m(\cdot) \) is a scaling/weighting.

In contrast, within a context of clustered multinomial data, we can basically rewrite the parametric extension of the Brier’s consistent estimator of Alonso-Revenga et al. \([8]\) as \( c \cdot \sum_{\ell=1}^{L} P_{\phi,\ell}^\# \left( P_{emp,\ell}^\#, P_{emp,\ell} | P_\theta \right) \) where \( P_{emp,\ell}^\# \) is the empirical distribution of the \( \ell \)-th cluster, \( P_{emp,\ell}^\# = \frac{1}{L} \sum_{\ell=1}^{L} P_{emp,\ell}^\# \), \( P_\theta \) is a (minimum-divergence-)estimated distribution from a (log-linear) model class, and \( c \) is an appropriately chosen multiplier (under the assumption of equal cluster sizes, which can be relaxed in a straightforward manner).

(b) In contrast to (a), for the context \( \mathcal{Y} = \mathcal{X} = \mathbb{R}, \ r(x) \equiv 1, \) one obtains in terms of the cumulative distribution functions \( S^cdf_x(P) = F_P(x), \ S^cdf_Q = F_Q(x) \) the two non-probability measures \( \mu^{t,\lambda,cd}[\cdot] := \int F_P(x) \, d\lambda(x) \leq \lambda[\cdot] \) and \( \nu^{t,\lambda,cd}[\cdot] := \int F_Q(x) \, d\lambda(x) \leq \lambda[\cdot] \) with – possibly infinite – total masses \( \mu^{t,\lambda,cd}[\mathbb{R}], \nu^{t,\lambda,cd}[\mathbb{R}] \). The latter two are finite if \( \lambda \) is a probability measure or a finite measure; for the non-finite Lebesgue measure \( \lambda = \lambda_L \) and for intervals \([x_1, x_2]\) one can interpret \( \mu^{t,\lambda,cd}[x_1, x_2] \) as the corresponding area (between \( x_1 \) and \( x_2 \)) under the distribution function \( F_P(\cdot). \) Analogously to (33), one can interpret

\[
0 \leq D^c_{\phi,m,m,1-m,\lambda} \left( S^cdf_x(P), S^cdf_Q \right) \\
= \int_{\mathcal{X}} \left[ \phi \left( \frac{F_P(x)}{m(x)} \right) - \phi \left( \frac{F_Q(x)}{m(x)} \right) - \phi' \left( \frac{F_P(x)}{m(x)} \right) \cdot \left( \frac{F_P(x)}{m(x)} - \frac{F_Q(x)}{m(x)} \right) \right] m(x) \, d\lambda(x) \\
=: B_\phi \left( \mu^{t,\lambda,cd}, \nu^{t,\lambda,cd} | M \right)
\]

as scaled Bregman divergence between the non-probability measures \( \mu^{t,\lambda,cd} \) and \( \nu^{t,\lambda,cd} \).

(c) In a context of mortality data analytics (which is essential for the calculation of insurance premiums, financial reserves, annuities, pension benefits, various benefits of social insurance programs, etc.), the divergence (34) (with \( r(x) = 1 \)) has been employed by Krömer & Stummer \([106]\) in order to achieve a realistic representation of mortality rates by smoothing and error-correcting of crude rates; there, \( \mathcal{X} \) is a set of ages (in years), \( S_x(P) \) is the so-called data-based crude annual mortality rate by age \( x, \) \( S_x(Q) \) is an — optimally determinable — candidate model member (out of a parametric or nonparametric model) for the unknown true annual mortality rate by age \( x, \) and \( m(x) \) is an appropriately chosen scaling at \( x. \)

This concludes the current Remark [1].

29
In the following, we illuminate two important special cases of the scaling (and aggregation-part) function \(m(\cdot)\), namely \(m(x) := 1\) and \(m(x) := S_x(Q)\):

**2.5.1.1** \(m_1(x) = m_2(x) := 1, m_3(x) = r(x)\) for some (measurable) function \(r : X \rightarrow [0, \infty]\) satisfying \(r(x) \in ]0, \infty[\) for \(\lambda-a.a. x \in X\)

In this sub-setup, (38) becomes

\[
0 \leq D^c_{\phi, t, r, \lambda}(S(P), S(Q)) := \int_X r(x) \left[ \phi(S_x(P)) - \phi(S_x(Q)) - \phi'(c) (S_x(Q)) \cdot (S_x(P) - S_x(Q)) \right] d\lambda(x) \tag{38}
\]

which for the discrete setup \((X, \lambda) = (X^\#_{\#}, \lambda^\#)\) turns into

\[
0 \leq D^c_{\phi, t, r, \lambda}(S(P), S(Q)) := \sum_{x \in X} r(x) \left[ \phi(S_x(P)) - \phi(S_x(Q)) - \phi'(c) (S_x(Q)) \cdot (S_x(P) - S_x(Q)) \right] \lambda(x) \tag{39}
\]

For reasons to be clarified below, in case of differentiable generator \(\phi\) (and thus \(\phi'_{+,-} = \phi'\) is the classical derivative) one can interpret (38) and (39) as weighted Bregman distances between the two statistical functionals \(S(P)\) and \(S(Q)\).

Let us first discuss the important special case \(\phi = \phi_{\alpha} (\alpha \in \mathbb{R}, cf. (26), (30), (31), (28)) together with \(S_x(P) \geq 0, S_x(Q) \geq 0\) — as it is always the case for \(S^e, S^p, S_{\text{pm}}, S_{\text{mu}}, S_{\text{mq}}, S^d, S^u, \) and for nonnegative real-valued random variables also with \(S^\text{qu}\). By incorporating the above-mentioned extension-relevant (cf. (12)) properties of \(\phi_{\alpha}\) (see Broniatowski & Stummer [42]) into (38), we end up with

\[
0 \leq D_{\phi_{\alpha}, t, r, \lambda}(S(P), S(Q)) = \int_X r(x) \left[ (S_x(P))^\alpha + (\alpha - 1) \cdot (S_x(Q))^\alpha - \alpha \cdot S_x(P) \cdot (S_x(Q))^\alpha - 1 \right] d\lambda(x) \tag{40}
\]

\[
= \int_X r(x) \left[ (S_x(P))^\alpha + (\alpha - 1) \cdot (S_x(Q))^\alpha - \alpha \cdot S_x(P) \cdot (S_x(Q))^\alpha - 1 \right] \cdot 1_{[0, x]} (S_x(P) \cdot S_x(Q)) d\lambda(x)
\]

\[
+ \int_X r(x) \left[ \frac{(S_x(P))^\alpha}{\alpha(\alpha - 1)} \cdot 1_{[1, x]} [\alpha + \infty \cdot 1_{[1, \infty]}(\alpha)] \cdot 1_{[0, x]} (S_x(P) \cdot S_x(Q)) d\lambda(x)
\]

\[
+ \int_X r(x) \left[ \frac{(S_x(Q))^\alpha}{\alpha} \cdot 1_{[0, 1]} (\alpha + \infty \cdot 1_{[1, \infty]}(\alpha)) \cdot 1_{[0, x]} (S_x(Q) \cdot S_x(P)) d\lambda(x)
\]

\[
\text{for } \alpha \in \mathbb{R} \{0, 1\}, \tag{41}
\]

\[
0 \leq D_{\phi_{\alpha}, t, r, \lambda}(S(P), S(Q)) = \int_X r(x) \cdot [S_x(P) \cdot \log \left( \frac{S_x(P)}{S_x(Q)} \right) + S_x(Q) - S_x(P)] d\lambda(x) \tag{42}
\]

\[
= \int_X r(x) \cdot [S_x(P) \cdot \log \left( \frac{S_x(P)}{S_x(Q)} \right) + S_x(Q) - S_x(P)] \cdot 1_{[0, x]} (S_x(P) \cdot S_x(Q)) d\lambda(x)
\]

\[
+ \int_X r(x) \cdot \infty \cdot 1_{[0, x]} (S_x(P) \cdot 1_{[0]} (S_x(Q)) d\lambda(x)
\]

\[
+ \int_X r(x) \cdot S_x(Q) \cdot 1_{[0, x]} (S_x(Q)) \cdot 1_{[0]} (S_x(P)) d\lambda(x) \tag{43}
\]

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0 \leq D_{\phi_0,1,1,1,\lambda}(S(P), S(Q))
= \int_{\mathcal{X}} r(x) \cdot \left[- \log \left( \frac{S_x(P)}{S_x(Q)} \right) + \frac{S_x(P)}{S_x(Q)} - 1 \right] \, d\lambda(x) 
= \int_{\mathcal{X}} r(x) \cdot \left[- \log \left( \frac{S_x(P)}{S_x(Q)} \right) + \frac{S_x(P)}{S_x(Q)} - 1 \right] \cdot 1_{[0,\infty)}(S_x(P) \cdot S_x(Q)) \, d\lambda(x) 
+ \int_{\mathcal{X}} r(x) \cdot \infty \cdot 1_{[0,\infty)}(S_x(P)) \cdot 1_{[0)}(S_x(Q)) \, d\lambda(x) 
+ \int_{\mathcal{X}} r(x) \cdot \infty \cdot 1_{[0,\infty)}(S_x(Q)) \cdot 1_{[0)}(S_x(P)) \, d\lambda(x) , 
0 \leq D_{\phi_2,1,1,1,\lambda}(S(P), S(Q)) = \int_{\mathcal{X}} \frac{r(x)}{2} \cdot \left[ S_x(P) - S_x(Q) \right]^2 \, d\lambda(x) . 

as a recommendation, one should avoid \( \alpha \leq 0 \) whenever \( S_x(P) = 0 \) for all \( x \) in some \( A \) with \( \lambda[A] > 0 \), respectively \( \alpha \leq 1 \) whenever \( S_x(Q) = 0 \) for all \( x \) in some \( A \) with \( \lambda[A] > 0 \). As far as splitting of the integral e.g. in (13) resp. (15) is concerned, notice that \( \int_{\mathcal{R}} [S_x(Q) - S_x(P)] \cdot r(x) \, d\lambda(x) \) resp. \( \int_{\mathcal{X}} \frac{S_x(P)}{S_x(Q)} - 1 \cdot r(x) \, d\lambda(x) \) may be finite even in cases where \( \int_{\mathcal{X}} S_x(P) \cdot r(x) \, d\lambda(x) = \infty \) and \( \int_{\mathcal{X}} S_x(Q) \cdot r(x) \, d\lambda(x) = \infty \) (take e.g. \( \mathcal{X} = [0, \infty[, \lambda = \lambda_L, r(x) \equiv 1 \), and the exponential distribution functions \( S_x(P) = F_P(x) = 1 - \exp(-c_1 \cdot x), S_x(Q) = F_Q(x) = 1 - \exp(-c_2 \cdot x) \) with \( 0 < c_1 < c_2 \). Notice that (46) can be used also in cases where \( S_x(P) \in \mathcal{R}, S_x(Q) \in \mathcal{R} \), and thus e.g. for \( S^{ov} \) for arbitrary real-valued random variables.

As before, for the discrete setup \((\mathcal{X}, \lambda) = (\mathcal{X}_\#_{\#}, \lambda_{\#})\) all the terms \( \int_{\mathcal{X}} \ldots \, d\lambda(x) \) in (11) to (16) turn into \( \sum_{x \in \mathcal{X}} \ldots \, d\lambda(x) \).

**Distribution functions.** For \( \mathcal{Y} = \mathcal{X} = \mathcal{R} \), \( S_x(P) = S_x^d(P) = F_P(x), S_x(Q) = S_x^d(Q) = F_Q(x) \), let us illuminate the case \( \alpha = 2 \) of (10). For instance, if \( Y \) is a real-valued random variable and \( F_Q(x) = Q[Y \leq x] \) is its probability mass function under a hypothetical/candidate law \( Q \), one can take \( F_P(x) = \frac{1}{N} \cdot \# \{ i \in \{1, \ldots, N\} : Y_i \leq x \} =: F_{P_{emp}}(x) \) as the distribution function of the corresponding data-derived “empirical distribution” \( P := P_{emp} := \frac{1}{N} \cdot \sum_{i=1}^{N} \delta_{Y_i} [\cdot] \) of an \( N \)-size i.i.d. sample \( Y_1, \ldots, Y_N \) of \( Y \). In such a set-up, the choice (say) \( \lambda = Q \) in (10) and multiplication with \( 2N \) lead to the weighted Cramer-von Mises test statistics (see [17, 200, Smirnov 176], and also Darling 52 for a historic account)

\[
0 \leq 2N \cdot D_{\phi_{2,1,1,1,1}}(S^d(P_{emp}), S^d(Q)) = N \cdot \int_{\mathcal{R}} \left[ F_{P_{emp}}(x) - F_Q(x) \right]^2 \cdot r(x) \, dQ(x)
\]

(47)

which are special “quadratic EDF statistics” in the sense of Stephens [178] (who also uses the term “Cramer-von Mises family”). The special case \( r(x) \equiv 1 \) is nothing but the prominent (unweighted) Cramer-von Mises test statistics; for some recent statistical insights on the latter, see e.g. Baringhaus & Henze [21]. In contrast, if one chooses the Lebesgue measure \( \lambda = \lambda_L \) and \( r(x) \equiv 1 \) in (16), then one ends up with the \( N \)-fold of the “classical” squared \( L^2 \)-distance
between the two distribution functions \( F_{P_{emp}}(\cdot) \) and \( F_Q(\cdot) \), i.e. with

\[
0 \leq 2N \cdot D_{\phi,1,1,\lambda}(S^{cd}(P_{emp}), S^{cd}(Q)) = N \cdot \int \left[ F_{P_{emp}}(x) - F_Q(x) \right]^2 \, d\lambda_L(x)
\]

(48)

where one can typically identify \( d\lambda_L(x) = dx \) (Riemann-integral).

In a similar fashion, for the special case \( \mathcal{Y} = \mathcal{X} = \mathbb{R} \), and the above-mentioned integrated statistical functionals (cf. Section 2.1) \( S_x(P) = S_x^{Q,S^{cd}}(P) = \int_{-\infty}^{\infty} F_P(z) \, dQ(z) \), \( S_x(Q) = S_x^{Q,S^{cd}}(Q) = \int_{-\infty}^{\infty} F_Q(z) \, dQ(z) \), we get from (38) (analogously to (46))

\[
0 \leq D_{\phi,1,1,r \cdot 1,\lambda}(S^{Q,S^{cd}}(P), S^{Q,S^{cd}}(Q)) = \int \frac{r(x)}{2} \cdot \left[ S_x^{Q,S^{cd}}(P) - S_x^{Q,S^{cd}}(Q) \right]^2 \, d\lambda(x) ,
\]

for which the choice \( r(x) \equiv 2N \), \( P := P_{emp} \), \( \lambda = Q \) leads to the divergence used in a goodness-of-fit testing context by Henze & Nikitin [88].

\( \lambda \)--probability-density functions. If for general \( \mathcal{Y} \) one takes the special case \( r(x) \equiv 1 \) together with the “\( \lambda \)--probability-density functions” context (cf. Remark 1(c)) \( S_x(P) = S_x^{\lambda pd}(P) := f_P(x) \geq 0 \), \( S_x(Q) = S_x^{\lambda pd}(Q) = f_Q(x) \geq 0 \), then the divergences (38) and (39) become

\[
0 \leq D_{\phi,1,1,\lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q))
\]

\[
:= \int_{\mathcal{X}} \left[ \phi(f_P(x)) - \phi(f_Q(x)) - \phi'_+(f_Q(x)) \cdot (f_P(x) - f_Q(x)) \right] \, d\lambda(x) , \quad (49)
\]

and

\[
0 \leq D_{\phi,1,1,\lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q))
\]

\[
:= \sum_{x \in \mathcal{X}} \left[ \phi(f_P(x)) - \phi(f_Q(x)) - \phi'_+(f_Q(x)) \cdot (f_P(x) - f_Q(x)) \right] , \quad (50)
\]

In case of differentiable generator \( \phi \) (and thus \( \phi'_+ = \phi' \) is the classical derivative), the divergences in (49) and (50) are nothing but the classical Bregman distances between the two probability distributions \( P \) and \( Q \) (see e.g. Csiszar [50], Pardo & Vajda [152, 153], Stummer & Vajda [188]). If one further specializes

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\[ \phi = \phi_\alpha, \] the divergences (10), (12), (21) and (13) become

\[ 0 \leq D_{\phi, 1, 1, 1, \lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q)) \]
\[ = \int_{\mathcal{X}} \frac{1}{\alpha \cdot (\alpha - 1)} \left[ (f_P(x))^\alpha + (\alpha - 1) \cdot (f_Q(x))^\alpha - \alpha \cdot f_P(x) \cdot (f_Q(x))^{\alpha - 1} \right] d\lambda(x), \]
\[ \text{for } \alpha \in \mathbb{R} \setminus \{0, 1\}, \quad (51) \]

\[ 0 \leq D_{\phi, 1, 1, 1, \lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q)) \]
\[ = \int_{\mathcal{X}} f_P(x) \cdot \log \left( \frac{f_P(x)}{f_Q(x)} \right) + f_Q(x) - f_P(x) \right] d\lambda(x), \quad (52) \]

\[ 0 \leq D_{\phi, 1, 1, 1, \lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q)) \]
\[ = \int_{\mathcal{X}} - \log \left( \frac{f_P(x)}{f_Q(x)} \right) + \frac{f_P(x)}{f_Q(x)} - 1 \right] d\lambda(x), \quad (53) \]

\[ 0 \leq D_{\phi, 1, 1, 1, \lambda}(S^{\lambda pd}(P), S^{\lambda pd}(Q)) = \int_{\mathcal{X}} \frac{1}{2} \left[ f_P(x) - f_Q(x) \right]^2 d\lambda(x). \quad (54) \]

Analogously to the paragraph after (46), one can recommend here to exclude \( \alpha \leq 0 \) whenever \( f_P(x) = 0 \) for all \( x \) in some \( A \) with \( \lambda[A] > 0 \), respectively \( \alpha \leq 1 \) whenever \( f_Q(x) = 0 \) for all \( x \) in some \( \tilde{A} \) with \( \lambda[\tilde{A}] > 0 \). As far as splitting of the integral e.g. in (49) resp. (50) is concerned, notice that the integral \( \left( \mu^{1, \lambda, \lambda pd} - \nu^{1, \lambda, \lambda pd} \right) \) [\( \mathcal{Y} \)] = \( \int_{\mathcal{Y}} [f_Q(x) - f_P(x)] \) \( d\lambda(x) = 1 - 1 = 0 \) but \( \int_{\mathcal{Y}} \frac{f_P(x)}{f_Q(x)} - 1 \] \( d\lambda(x) \) may be infinite (take e.g. \( \mathcal{X} = [0, \infty) \), \( \lambda = \lambda_L \), and the exponential distribution density functions \( f_P(x) := c_1 \cdot \exp(-c_1 \cdot x) \), \( f_Q(x) := c_2 \cdot \exp(-c_2 \cdot x) \) with \( 0 \leq c_1 \leq c_2 \). The choice \( \alpha > 0 \) in (51) coincides with the “order-\( \alpha \)” density power divergences DPD of Basu et al. [22] for their statistical applications see e.g. Basu et al. [24], Ghosh & Basu [74], [75] and the references therein, and for general \( \alpha \in \mathbb{R} \) see e.g. Stummer & Vajda [188].

The divergence (52) is the celebrated “Kullback-Leibler information divergence KL” between \( f_P \) and \( f_Q \) (respectively between \( P \) and \( Q \)); alternatively, instead of KL one often uses the terminology “relative entropy”. The divergence (54) (cf. \( \alpha = 2 \)) is nothing but half of the squared \( L^2 \)-distance between the two \( \lambda \)-density functions \( f_P(\cdot) \) and \( f_Q(\cdot) \).

Notice that for the classical case \( \mathcal{X} = \mathcal{Y} = \mathbb{R} \), \( r(x) \equiv 1 \), \( \lambda = \lambda_L \) — where one has \( f_P(x) = f_P(x) \), \( S^{pd}(P) = S^{ed}(P) \), and \( F_P(x) = \int_{-\infty}^x f_P(z) \) \( d\lambda_L(z) \) — (51) is essentially different from (40) with \( S(P) = S^{ed}(P) \), \( S(Q) = S^{ed}(Q) \) which is explicitly of the “doubly aggregated form”

\[ 0 \leq D_{\phi, 1, 1, 1, \lambda}(S^{cd}(P), S^{cd}(Q)) \]
\[ = \int_{\mathbb{R}} \frac{1}{\alpha \cdot (\alpha - 1)} \left[ \left( \int_{-\infty}^x f_P(z) \) \( d\lambda_L(z) \) \right)^\alpha + (\alpha - 1) \cdot \left( \int_{-\infty}^x f_Q(z) \) \( d\lambda_L(z) \) \right)^\alpha - \alpha \cdot \int_{-\infty}^x f_P(z) \) \( d\lambda_L(z) \cdot \left( \int_{-\infty}^x f_Q(z) \) \( d\lambda_L(z) \) \right)^{\alpha - 1} \right] d\lambda_L(x), \quad \text{for } \alpha \in \mathbb{R} \setminus \{0, 1\}, \]

with the usual \( d\lambda_L(x) = dx \).

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In contrast, for the discrete setup \((\mathcal{X}, \lambda) = (\mathcal{X}_h, \lambda_h)\) with \(\mathcal{X}_h \subset \mathbb{R}\) (recall \(\lambda_h([x]) = 1\)) one has \(f_P(x) = p_P(x)\) for all \(x \in \mathcal{X}_h\) and the divergences \((55)\) simplify to

\[
0 \leq D_{\phi_h, 1, 1, 1, \lambda_h}(S_{sm}(P), S_{sm}(Q)) = \sum_{x \in \mathcal{X}} \frac{1}{\alpha} \cdot (\alpha - 1) \cdot (p_P(x))^{\alpha} - \alpha \cdot p_P(x) \cdot (p_Q(x))^{\alpha - 1}
\]

for \(\alpha \in \mathbb{R}\) \(\{0, 1\}\),

\[
0 \leq D_{\phi_h, 1, 1, 1, \lambda_h}(S_{sm}(P), S_{sm}(Q)) = \sum_{x \in \mathcal{X}} p_P(x) \cdot \log \left(\frac{p_P(x)}{p_Q(x)}\right) + p_Q(x) - p_P(x)
\]

and

\[
0 \leq D_{\phi_h, 1, 1, 1, \lambda_h}(S_{sm}(P), S_{sm}(Q)) = \sum_{x \in \mathcal{X}} - \log \left(\frac{p_P(x)}{p_Q(x)}\right) + \frac{p_P(x)}{p_Q(x)} - 1
\]

where again one should exclude \(\alpha \leq 0\) whenever \(p_P(x) = 0\) for all \(x\) in some \(A\) with \(\lambda_h[A] > 0\), respectively \(\alpha \leq 1\) whenever \(p_Q(x) = 0\) for all \(x\) in some \(A\) with \(\lambda_h[A] > 0\). For example, take the context from the paragraph right after \((46)\), with discrete random variable \(Y\), \(p_Q(x) = Q[Y = x]\), \(p_P(x) = p_P(x)\) (for all \(x \in \mathbb{R}\)). Then, the divergences \(2N \cdot D_{\phi_h, 1, 1, 1, \lambda_h}(S_{sm}(P_{emp}), S_{sm}(Q))\) (for \(\alpha \in \mathbb{R}\)) can be used as goodness-of-fit test statistics; see e.g. Kifflinger & Stummer \(102\) for their limit behaviour as the sample size \(N\) tends to infinity.

**Classical quantile functions.** The divergence \((58)\) with \(S(P) = S_{sm}(P), S(Q) = S_{sm}(Q)\) can be interpreted as a quantitative measure of tail risk of \(P\), relative to some preceived reference distribution \(Q\) \(12\).

Especially, for \(\mathcal{Y} = \mathbb{R}\) and \(\mathcal{X} = (0, 1)\), \(S_x(P) = S_{sm}(P) = F_P^x(x), S_x(Q) = S_{sm}(Q) = F_Q^x(x)\), and the Lebesgue measure \(\lambda = \lambda_L\) (with the usual \(d\lambda_L(x) = dx\)), we get from \((46)\) the special case

\[
0 \leq D_{\phi_x, 1, 1, 1, \lambda}(S_{sm}(P), S_{sm}(Q)) = \int_{(0, 1)} (F_P^x(x) - F_Q^x(x))^2 d\lambda_L(x) \tag{55}
\]

which is nothing but the \(2\text{-}\)Wasserstein distance between the two probability measures \(P\) and \(Q\). Corresponding connections with optimal transport are discussed in Section \(2.7\) below. Notice that \((55)\) does generally not coincide with its analogue

\[
D_{\phi_x, 1, 1, 1, \lambda}(S_{sm}(P), S_{sm}(Q)) = \int_{\mathbb{R}} (F_P(x) - F_Q(x))^2 d\lambda_L(x) \tag{56}
\]

to see this, take e.g. \(0 < c_2 < c_1\) (e.g. \(c_1 = 2, c_2 = 1\)) and the exponential quantile functions \(F_P^x(x) = -\frac{1}{c_2} \cdot \log(1 - x), F_Q^x(x) = -\frac{1}{c_1} \cdot \log(1 - x)\) for which \((55)\) becomes \(2 \cdot (\frac{1}{c_2} - \frac{1}{c_1})^2\), whereas for the corresponding exponential distribution

\(12\) hence, such a divergence represents an alternative to Faugeras & Rüschendorf \(8\) where they use hemimetrics (which e.g. have only a weak identity-property, but satisfy triangle inequality) rather than divergences.
functions $F_P(x) = 1 - \exp(-c_1 \cdot x)$, $F_Q(x) = 1 - \exp(-c_2 \cdot x)$ the divergence becomes $\frac{1}{2c_2} - \frac{2}{c_1 + c_2} + \frac{1}{2c_1}$.

**Depth, outlyingness, centered rank and centered quantile functions.**

As a special case one gets

\[
D^\phi_{\phi,S,P} (S^{de}(P), S^{de}(Q)),
\]

\[
D^\phi_{\phi,S,P} (S^{ou}(P), S^{ou}(Q)),
\]

\[
\sum_{i=1}^{d} D^\phi_{\phi,S,P} (S^{cr,i}(P), S^{cr,i}(Q)),
\]

\[
\sum_{i=1}^{d} D^\phi_{\phi,S,P} (S^{cqu,i}(P), S^{cqu,i}(Q)),
\]

all of which have not appeared elsewhere before (up to our knowledge); recall that the respective domains of $\phi$ have to take care of the ranges $R (S^{de}(P)) \subset \{0, \infty\}$, $R (S^{ou}(P)) \subset \{0, \infty\}$, $R (S^{cr,i}(P)) \subset \{-1, 1\}$, $R (S^{cqu,i}(P)) \subset \{-\infty, \infty\}$ (i.e. $\phi$). Notice that these divergences differ structurally from the Bregman distances of Hallin [85] who uses the centered rank function $\phi$ (in general not additionally separable) as a multidimensional (in general not additionally separable) generator $\phi$ and not as points between which the distance is to be measured between.

**2.5.1.2** $m_1(x) = m_2(x) := S_x(Q), m_3(x) = r(x) \cdot S_x(Q) \in [0, \infty]$ for some (measurable) function $r : \mathcal{X} \to \mathbb{R}$ satisfying $r(x) \in (-\infty, 0 \cup [0, \infty]$ for $\lambda$-a.a. $x \in \mathcal{X}$

In such a context, we require that the function $r(\cdot)$ does not (explicitly) depend on the functions $S_x(P)$ and $S_x(Q)$, i.e. it is not of the adaptive form $r(\cdot) = h(\cdot, S_x(P), S_x(Q))$. The incorporation of the zeros of $S_x(P), S_x(Q)$ can be adapted from Broniatowski & Stummer [82]: for instance, in a non-negativity set-up where for $\lambda$-almost all $x \in \mathcal{X}$ one has $r(x) \in [0, \infty]$ as well as $S_x(P) \in [0, \infty]$, $S_x(Q) \in [0, \infty]$ (as it is always the case for $S^{cd}, S^{pd}, S^{pm}, S^{ou}, S^{rng}, S^{de}, S^{ou}$, and for nonnegative real-valued random variables also with $S^{cqu}$), one can take $E = [a, b] = [0, \infty]$ to end up with the following special case of [83]

\[
0 \leq D^\phi_{\phi,S(P),S(Q),r,S(Q),\lambda}(S_x(P), S(x))
\]

\[
= \int_{\mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{S_x(Q)} \right) - \phi(1) - \phi_+ c(1) \cdot \left( \frac{S_x(P)}{S_x(Q)} - 1 \right) \right] S_x(Q) \cdot r(x) \, d\lambda(x) ,
\]

\[
= \int_{\mathcal{X}} \left[ S_x(Q) \cdot \phi \left( \frac{S_x(P)}{S_x(Q)} \right) - S_x(Q) \cdot (1 - \phi_+ c(1) \cdot (S_x(P) - S_x(Q))) \right] r(x) \, d\lambda(x) ,
\]

\[
(60)
\]
The assumption (64) together with generators \( \phi \) formulated after (22) in terms of \( s \) employ generators \( D \) with \( \phi \) and \( s \) at \( t = 1 \) together with generators \( \phi \) with \( \phi(1) = 0 \). On the other hand, c becomes obsolete.

Moreover, in case of \( \phi(1) = 0 \) and \( \int_\mathcal{X} (S_x(P) - S_x(Q)) \cdot r(x) \, d\lambda(x) \in ]-\infty, \infty[ \) (but not necessarily \( \int_\mathcal{X} S_x(P) \cdot r(x) \, d\lambda(x) < \infty, \int_\mathcal{X} S_x(Q) \cdot r(x) \, d\lambda(x) < \infty \), the divergence (61) turns into

\[
0 \leq D^{c}_{\phi, S(Q), S(Q), r-S(Q), \lambda}(S(P), S(Q))
= \int_\mathcal{X} r(x) \cdot (S_x(P) - S_x(Q)) \cdot r(x) \, d\lambda(x)
+ \phi^*(0) \cdot \int_\mathcal{X} r(x) \cdot S_x(P) \cdot 1_{[0,S_x(Q)]} \, d\lambda(x)
+ \phi(0) \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0,S_x(P)]} \, d\lambda(x)
- \phi'(1) \cdot \int_\mathcal{X} r(x) \cdot (S_x(P) - S_x(Q)) \, d\lambda(x) \tag{63}
\]

To obtain the sharp identifyability (reflexivity) of the divergence \( D^{c}_{\phi, S(Q), S(Q), r-S(Q), \lambda}(S(P), S(Q)) \) of (61), one can either use the conditions formulated after (22) in terms of \( s \in \mathcal{H}(\frac{S(P)}{S(Q)}) \) and \( t \in \mathcal{H}(\frac{S(Q)}{S(P)}) \) = \{1\}, or the strict convexity of \( \phi \) at \( t = 1 \) together with

\[
\int_\mathcal{X} (S_x(P) - S_x(Q)) \cdot r(x) \, d\lambda(x) = 0 \tag{64}
\]

\footnote{see Broniatowski & Stummer [42] for corresponding details. Additionally, in the light of [22] let us indicate that if one wants to use \( \Xi := \int_\mathcal{X} S_x(Q) \cdot \phi(\frac{S_x(P)}{S_x(Q)}) \cdot r(x) \, d\lambda(x) \) (with appropriate zero-conventions) as a divergence, then one should employ generators \( \phi \) satisfying \( \phi(1) = \phi'(1) = 0 \), or employ models fulfilling the assumption (64) together with generators \( \phi \) with \( \phi(1) = 0 \). On the other hand, c becomes obsolete.}
hand, if this integral $\Xi$ appears in your application context “naturally”, then one should be aware that $\Xi$ may become negative depending on the involved set-up; for a counter-example, see e.g. Stummer & Vajda [187].

An important generator-concerning example is the power-function (limit) case $\phi = \phi_\alpha$ with $\alpha \in \mathbb{R}$ (cf. (20), (31), (33), (28)) under the constraint $\int_\mathcal{X} (S_x(P) - S_x(Q)) \cdot r(x) \, d\lambda(x) \in [-\infty, \infty]$. Accordingly, the “implicit-boundary-describing” divergence (63) resp. the corresponding “explicit-boundary” version (65) turn into the generalized power divergences of order $\alpha$ (cf. Stummer & Vajda [187]) for $r(x) \equiv 1$

$$0 \leq D_{\phi_\alpha,S(Q),S(Q),r,S(Q),\lambda}(S(P),S(Q))$$

$$= \int_\mathcal{X} \frac{1}{\alpha(1-\alpha)} \cdot \left[ \left( \frac{S_x(P)}{S_x(Q)} \right)^\alpha - \alpha \cdot \frac{S_x(P)}{S_x(Q)} + \alpha - 1 \right] \cdot S_x(Q) \cdot r(x) \, d\lambda(x)$$

$$= \frac{1}{\alpha(1-\alpha)} \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot \left[ \left( \frac{S_x(P)}{S_x(Q)} \right)^\alpha - \alpha \cdot \frac{S_x(P)}{S_x(Q)} + \alpha - 1 \right] \cdot 1_{[0,\infty]}(S_x(P) \cdot S_x(Q)) \, d\lambda(x)$$

$$+ \phi^\alpha(0) \cdot \int_\mathcal{X} r(x) \cdot S_x(P) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x) + \phi^\alpha(0) \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0]}(S_x(P)) \, d\lambda(x)$$

$$= \frac{1}{\alpha(1-\alpha)} \cdot \int_\mathcal{X} r(x) \cdot \left[ \left( \frac{S_x(P)}{S_x(Q)} \right)^\alpha \cdot S_x(Q)^{1-\alpha} - S_x(Q) \right] \cdot 1_{[0,\infty]}(S_x(P) \cdot S_x(Q)) \, d\lambda(x)$$

$$+ \frac{1}{\alpha(1-\alpha)} \cdot 1 \cdot \int_\mathcal{X} r(x) \cdot (S_x(P) - S_x(Q)) \, d\lambda(x) + \alpha \cdot 1_{[0,\infty]}(\alpha) \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x)$$

$$+ (<\frac{1}{\alpha(1-\alpha)} \cdot 1 \cdot 1_{[0,\infty]}(\alpha) \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x)$$

$$\leq 0 \leq D_{\phi_\alpha,S(Q),S(Q),r,S(Q),\lambda}(S(P),S(Q))$$

$$= \int_\mathcal{X} \frac{S_x(P)}{S_x(Q)} \cdot \log \left( \frac{S_x(P)}{S_x(Q)} \right) + 1 - \frac{S_x(P)}{S_x(Q)} \right] \cdot S_x(Q) \cdot r(x) \, d\lambda(x)$$

$$= \int_\mathcal{X} r(x) \cdot S_x(P) \cdot \log \left( \frac{S_x(P)}{S_x(Q)} \right) \cdot 1_{[0,\infty]}(S_x(P) \cdot S_x(Q)) \, d\lambda(x)$$

$$+ \int_\mathcal{X} r(x) \cdot (S_x(Q) - S_x(P)) \, d\lambda(x) + \alpha \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x),$$

$$\leq 0 \leq D_{\phi_\alpha,S(Q),S(Q),r,S(Q),\lambda}(S(P),S(Q))$$

$$= \int_\mathcal{X} \left[ - \log \left( \frac{S_x(Q)}{S_x(Q)} \right) + \frac{S_x(P)}{S_x(Q)} - 1 \right] \cdot S_x(Q) \cdot r(x) \, d\lambda(x)$$

$$= \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot \log \left( \frac{S_x(Q)}{S_x(Q)} \right) \cdot 1_{[0,\infty]}(S_x(P) \cdot S_x(Q)) \, d\lambda(x)$$

$$+ \int_\mathcal{X} r(x) \cdot (S_x(P) - S_x(Q)) \, d\lambda(x) + \alpha \cdot \int_\mathcal{X} r(x) \cdot S_x(Q) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x),$$

$$\leq 0 \leq D_{\phi_\alpha,S(Q),S(Q),r,S(Q),\lambda}(S(P),S(Q))$$

$$= \int_\mathcal{X} \frac{1}{2} \cdot \left( \frac{S_x(P) - S_x(Q)}{S_x(Q)} \right)^2 \cdot r(x) \, d\lambda(x)$$

$$+ \alpha \cdot \int_\mathcal{X} r(x) \cdot S_x(P) \cdot 1_{[0]}(S_x(Q)) \, d\lambda(x),$$

which is an adaption of a result of Broniatowski & Stummer [12].

Another important generator-concerning example is the total variation case $\phi_{TV}(t) := |t - 1|$ (cf. (32)) together with $c = \frac{1}{2}$. Accordingly, the “implicit-boundary-describing” divergence (69) resp. the corresponding “explicit-boundary” version (65) turn into

$$0 \leq D_{1/2,\phi_{TV},S(Q),S(Q),r,S(Q),\lambda}(S(P),S(Q))$$

$$= \int_\mathcal{X} \left| S_x(P) - S_x(Q) \right| \cdot r(x) \, d\lambda(x),$$

$$= \int_\mathcal{X} |S_x(P) - S_x(Q)| \cdot r(x) \, d\lambda(x),$$

(73)
which is also an adaption of a result of Broniatowski \& Stummer \[42\]. Notice that \(\{73\}\) – which is nothing but the \(r\)–weighted \(L_1\)–distance between the two statistical functionals \(S(P)\) and \(S(Q)\) – can be used also in cases where \(S_x(P)\) is in \(\mathbb{R}\), \(S_x(Q)\) is in \(\mathbb{R}\), and thus e.g. for \(S^{\text{tu}}\) for arbitrary real-valued random variables.

As usual, for arbitrary discrete setup \((\mathcal{X}, \lambda) = (\mathcal{X}_\#, \lambda_\#)\) all the terms \(\sum_{x \in \mathcal{X}} \ldots \) in the divergences \[61\] to \[73\] turn into \(\sum_{x \in \mathcal{X}} \ldots\) (respectively \(\sum_{x \in \mathcal{X}} \ldots\)).

As far as concrete statistical functionals is concerned, let us briefly discuss several important sub-cases.

\(\lambda\)–probability-density functions. First, in the “\(\lambda\)–probability-density functions” context of Remark \[1\] one has for general \(\mathcal{X}\) the statistical functionals \(S^{\lambda\text{pd}}(P) := f_P(x) \geq 0\), \(S^{\lambda\text{pd}}(Q) := f_Q(x) \geq 0\), and under the constraints \(\phi(1) = 0\), the corresponding special case \(D_{\phi^{\lambda\text{pd}}(Q), S^{\lambda\text{pd}}(Q), \lambda}(S^{\lambda\text{pd}}(P), S^{\lambda\text{pd}}(Q))\) of \[61\] turns out to be the “\(\lambda\)–local \(\phi\)–divergence of Avlogiarias et al. \[12,13\]; in case of \(r(x) = 1\) (where \[63\] is satisfied), this reduces to the classical Csiszar-Ali-Silvey-Morimoto \[48, 6, 133\] \(\phi\)–divergence.\[15\]

\[
0 \leq D_{\phi^{\lambda\text{pd}}(Q), S^{\lambda\text{pd}}(Q), \lambda}(S^{\lambda\text{pd}}(P), S^{\lambda\text{pd}}(Q)) \\
= \int_{\mathcal{X}} f_Q(x) \cdot \phi \left( \frac{f_P(x)}{f_Q(x)} \right) \cdot 1_{[0, x]} (f_P(x) \cdot f_Q(x)) \, d\lambda(x) \\
+ \phi^*(0) \cdot \int_{\mathcal{X}} f_P(x) \cdot 1_{[0, x]} (f_P(x) \cdot f_Q(x)) \, d\lambda(x) + \phi(0) \cdot \int_{\mathcal{X}} f_Q(x) \cdot 1_{[0]} (f_P(x) \cdot f_Q(x)) \, d\lambda(x) \\
- \phi'(1) \cdot \lambda_{\mathcal{X}} (f_P(x) - f_Q(x)) \, d\lambda(x) \\
= \int_{\mathcal{X}} f_Q(x) \cdot \phi \left( \frac{f_P(x)}{f_Q(x)} \right) \cdot 1_{[0, x]} (f_P(x) \cdot f_Q(x)) \, d\lambda(x) \\
+ \phi^*(0) \cdot P[f_Q(x) = 0] + \phi(0) \cdot Q[f_P(x) = 0] \tag{74}
\]

which coincides with \[11\]; if \(\phi(1) \neq 0\) then one has to additionally subtract \(\phi(1)\) (cf. the corresponding special case of \[61\]). The corresponding special cases \(D_{\phi^{\lambda\text{pd}}(Q), S^{\lambda\text{pd}}(Q), \lambda}(S^{\lambda\text{pd}}(P), S^{\lambda\text{pd}}(Q))\) (\(\alpha \in \mathbb{R}\)) of \[65\] to \[72\] are called “power divergences” (between the \(\lambda\)–density functions \(S^{\lambda\text{pd}}(P) := f_P(\cdot)\), \(S^{\lambda\text{pd}}(Q) := f_Q(\cdot)\); if the latter two are strictly positive, the subcase \(\alpha = 1\) respectively \(\alpha = 0\) respectively \(\alpha = 2\) is nothing but the (classical) Kullback-Leibler divergence (relative entropy) respectively the reverse Kullback-Leibler divergence (reverse relative entropy) respectively the Pearson chi square divergence. The special case

\[
0 \leq D_{\phi^{\lambda\text{pd}}(Q), S^{\lambda\text{pd}}(Q), \lambda}(S^{\lambda\text{pd}}(P), S^{\lambda\text{pd}}(Q)) = \int_{\mathcal{X}} |f_P(x) - f_Q(x)| \, d\lambda(x)
\]

\[15\] see e.g. Liese \& Vajda \[109\], Vajda \[196\] on comprehensive studies thereupon

\[16\] notice that \(c\) has become obsolete

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of (73) is the total variation distance or \( L_1 \)-distance (between the \( \lambda \)-density functions \( S^{\lambda d}(P) := f_P(\cdot) \), \( S^{\lambda d}(Q) := f_Q(\cdot) \)). Analogously to Subsection 2.5.1.1, for \( \mathcal{X} = \mathcal{Y} = \mathbb{R} \) the current context subsumes the “classical density” functionals \( S^{\lambda d}(\cdot) = S^{\rho d}(\cdot) \) with the choice \( \lambda = \lambda_L \) (and the Riemann integration \( d\lambda_L(x) = dx \)). In contrast, for the discrete setup \( \mathcal{Y} = \mathcal{X}_\# \) it covers the “classical probability mass” functional \( S^{\rho m}(\cdot) = S^{\rho m}(\cdot) \) with the choice \( \lambda = \lambda_\# \) (recall \( \#(\{x\}) = 1 \) for all \( x \in \mathcal{X}_\# \)); accordingly, all the terms \( \int_{\mathcal{X}} \cdots \, d\lambda(x) \) in the divergences (71) to (74) turn into \( \sum_{x \in \mathcal{X}} \cdots \).

**Distribution and survival functions.** Let us first consider the context \( \mathcal{Y} = \mathcal{X} = \mathbb{R} \), \( S_\#(P) = S^{\# d}(P) = F_P(x) \), \( S_\#(Q) = S^{\# d}(Q) = F_Q(x) \), and the Lebesgue measure \( \lambda = \lambda_L \) (with the usual \( d\lambda_L(x) = dx \)), and \( r(x) \equiv 1 \). Therein, the special case

\[
0 \leq D_{1/2}^{\phi_{TV}, S^{\# d}(Q), S^{\# d}(Q), 1} \lambda_L (S^{\# d}(P), S^{\# d}(Q)) = \int_{\mathbb{R}} |F_P(x) - F_Q(x)| \, d\lambda_L(x)
\]

of (75) is the well-known Kantorovich metric (between the distribution functions \( F_P(\cdot), F_Q(\cdot) \)). It is known that the integral in (75) is finite provided that \( \int_{\mathcal{X}} x \, dF_P(x) \in ]-\infty, \infty[ \) and \( \int_{\mathcal{X}} x \, dF_Q(x) \in ]-\infty, \infty[ \) (if the distribution \( P \) resp. \( Q \) is generated by some real-valued random variable, say \( X \) resp. \( Y \), this means that \( E[X] \) resp. \( E[Y] \) exists and is finite). To proceed, let us discuss the special case

\[
0 \leq D_{\phi_{1}, S^{\# d}(Q), S^{\# d}(Q), 1} \lambda_L (S^{\# d}(P), S^{\# d}(Q)) = \int_{\mathbb{R}} \left[ f_P(x) \cdot \log \left( \frac{f_P(x)}{f_Q(x)} \right) + 1 - \frac{f_P(x)}{f_Q(x)} \right] \cdot F_Q(x) \, d\lambda_L(x)
\]

of (76). For the special subsetup of nonnegative random variables (and thus \( \mathcal{Y} = \mathcal{X} = [0, \infty[ \) with finite expectations and strictly positive cdf, (76) simplifies to the so-called “cumulative Kullback-Leibler information” of Park et al. (150) (see also Park et al. (153) for an extension to the whole real line, Di Crescenzo & Longobardi (59) for an adaption to possibly smaller support as well as for an adaption to a dynamic form analogously to the explanations in the following lines). In contrast, we illuminate the special case

\[
0 \leq D_{\phi_{1}, S^{\#}(Q), S^{\#}(Q), 1} \lambda_L (S^{\#}(P), S^{\#}(Q)) = \int_{\mathbb{R}} \left[ \frac{1-F_P(x)}{1-F_Q(x)} \cdot \log \left( \frac{1-F_P(x)}{1-F_Q(x)} \right) + 1 - \frac{1-F_P(x)}{1-F_Q(x)} \right] \cdot (1 - F_Q(x)) \, d\lambda_L(x)
\]

of (67), (68). This has been employed by Liu (116) for the special case of \( P = F_N^{\text{emp}} \) and \( Q = Q_\theta \) in order to obtain corresponding minimum-divergence parameter estimator of \( \theta \) (see e.g. also Yari & Saghaﬁ (205), Yari et. al. (204), and Mehrali & Asadi (123) for follow-up papers). For the general context of non-negative, absolutely continuous random variables (and thus \( \mathcal{Y} = \mathcal{X} = [0, \infty[ \) with finite expectations and strictly positive cdf, (74) simplifies to the so-called “cumulative (residual) Kullback-Leibler information” of Baratpour & Habibi.
Rad [19] (see also Park et al. [150] for further properties and Park et al. [155] for an extension to the whole real line); the latter has been adapted to a dynamic form by Champaney & Baratpour [44] as follows (adapted to our terminology): take arbitrarily fixed “instance” $t \geq 0$, $\mathcal{Y} = \mathcal{X} = [t, \infty[$ and replace in (77) the survival function $S_{x}^{\nu}(P) := \{1 - F_{P}(x)\}_{x \in \mathbb{R}}$ by $S_{x}^{\nu,t}(P) := \{1 - F_{P}(x)\}_{x \in [t, \infty]}$ being essentially the survival function of a random variable (e.g. residual lifetime) $[X - t, X > t]$ under $P$, and analogously for $Q$; accordingly, the integral range is $[t, \infty[$. We can generalize this by simply plugging in $S_{x}^{\nu}(P)$, $S_{x}^{\nu}(Q)$ into our general divergences [59] and [38] — and even [19] — and thus covering the corresponding dynamic Kullback-Leibler divergence of Di Crescenzo & Longobardi [58] as well as the more general $\phi$—divergences between residual lifetimes of Vonta & Karagrigoriou [201] as special cases; notice that $S_{x}^{\nu,t}$ is essentially the density function of the random variable $X_{t} := [X - t, X > t]$ under $P$, where e.g. $X$ is typically a (non-negative) absolutely continuous random variable which describes the residual lifetime of a person or an item or a “process” and hence, $X_{t}$ is called residual lifetime (at $t$) which is fundamentally used in survival analysis and systems reliability engineering. In risk management and extreme value theory, $X_{t}$ describes the important notion of random excess (e.g. of a loss $X$) over the threshold $t$, which is e.g. employed in the well-known peaks-over-threshold method.

Analogously, we can plug in $S_{x}^{\nu,t}$ := $\{f_{P}(x)\}_{x \in [t, \infty]}$ instead of $S_{x}^{\nu} = \{f_{P}(x)\}_{x \in \mathbb{R}}$ [59] and [38] — and even [19] — and thus covering the corresponding dynamic Kullback-Leibler divergence of Di Crescenzo & Longobardi [58] as well as the more general $\phi$—divergences between past lifetimes of Vonta & Karagrigoriou [201] as special cases; notice that $S_{x}^{\nu,t}$ is essentially the density function of the random variable $[X - \infty, X \leq t]$ under $P$.

**Classical quantile functions.** The divergence [59] with $S(P) = S^{\nu}(P)$, $S(Q) = S^{\nu}(Q)$ can be interpreted as a quantitative measure of tail risk of $P$, relative to some pregiven reference distribution Q [18]

For $\mathcal{Y} = \mathcal{X}$ and $\mathcal{X} = (0, 1)$, we get for the quantiles context

\[
0 \leq D^{1/2}_{\phi_{tv},S^{\nu}(Q),S^{\nu}(Q),1,\phi_{tv}(Q),\lambda_{L}}(S^{\nu}(P), S^{\nu}(Q)) = \int_{\mathcal{X}} |F_{P}^{-}(x) - F_{Q}^{-}(x)| \, d\lambda_{L}(x)
\] (78)

which is nothing but the $1$—Wasserstein distance between the two probability measures $P$ and $Q$. It is well-known that the right-hand sides of [75] and [78]

\footnote{In this setup, they also introduce an alternative with $\tilde{\phi}_{1}(t)$ of [20] together with $S_{x}^{\nu,\varphi_{1}(P)} := \frac{1 - F_{P}(x)}{\varphi_{1}(F_{P}(x))}$ rather than with $\phi_{1}(t)$ of [30] together with $S_{x}^{\nu}(P) := 1 - F_{P}(x)$ — and analogously for $Q$}

\footnote{Hence, such a divergence represents an alternative to Faugeras & R"uschendorf [65] where they use hemimetrics rather than divergences}
coincide, in contrast to the discussion on the “$L_2$-case” right after \[56\]. Corresponding connections with optimal transport are discussed in Section 2.7 below.

Let us briefly discuss some other connections between $\phi-$divergences and quantile functions. In the above-mentioned setup of Baratpour & Habibi Rad [19] (under the existence of strictly positive probability density functions), Sunoj et al. [188] rewrite the cumulative Kullback-Leibler information (cf. the special case of \[73\]) equivalently in terms of quantile functions. In contrast, in a context of absolutely continuous probability distributions $P$ and $Q$ on $\mathcal{X} = \mathbb{R}$ with strictly positive density functions $f_P$ and $f_Q$, Sankaran et al. [167] rewrite the classical Kullback-Leibler divergence \[\int_{\mathcal{X}} \left( f_P(x) \cdot \log \left( \frac{f_P(x)}{f_Q(x)} \right) + f_Q(x) - f_P(x) \right) \, \text{d}\lambda_L(x) = D_{\phi_1, s_N}^*(P, Q) \] as \[\int_{\mathcal{X}} \left( \frac{f_p(x)}{f_q(x)} \right)^\alpha - \alpha \frac{f_p(x)}{f_q(x)} + \alpha - 1 \right) f_Q(x) \, \text{d}\lambda(x) = D_{\phi_1, s_N}^*(P, Q) \] for any probability measure $\lambda$ on $\mathcal{X}$. Such tasks have numerous applications in climate sciences or hydrology. As a side remark, let us mention that for the general context of quantile measures $\Omega_Q$ and $\Omega_P$ being absolutely continuous (with respect to the Lebesgue measure $\lambda_L$ on $[0, 1]$), the $\phi-$divergence $D_{\phi}(\Omega_Q, \Omega_P)$ turns into to the divergence $D_{\phi, s_N}^*(p, q) \cdot \lambda_L \left( S_{\phi, s_N}^d(Q), S_{\phi, s_N}^d(P) \right)$ (cf. \[59\]) between the quantile density functions $S_{\phi, s_N}^d(P) := \left\{ S_{\phi, s_N}^d(x) \right\}_{x \in [0, 1]} := \left\{ \left( F_P^{-1}(x) \right) \right\}_{x \in [0, 1]}$ and $S_{\phi, s_N}^d(Q)$. Thus, by applying our general divergences \[19\] to $S_{\phi, s_N}^d(Q)$ and $S_{\phi, s_N}^d(P)$ we end up with a completely new framework $D_{\phi, m_1, m_2, m_3, \lambda}^c \left( S_{\phi, s_N}^d(Q), S_{\phi, s_N}^d(P) \right)$.
(and many interesting special cases) for quantifying dissimilarities between quantile density functions.

**Depth, outlyingness, centered rank and centered quantile functions.**

As a special case one gets $D_{\phi,S^c(Q),S^c_i(Q),r,S^c_i(Q),\lambda_L}(S^c(P),S^c(Q))$, $D_{\phi,S^c(S^\text{ou}(Q)),S^c(S^\text{ou}(Q)),r,S^c(S^\text{ou}(Q)),\lambda_L}(S^\text{ou}(P),S^\text{ou}(Q))$, 

$$\sum_{i=1}^d D_{\phi,S^\text{cr}^i(Q),S^\text{cr}^i(Q),r,S^\text{cr}^i(Q),\lambda_L}(S^\text{cr}^i(P),S^\text{cr}^i(Q)),$$

all of which have not appeared elsewhere before (up to our knowledge); recall that the respective domains of $\phi$ have to take care of the ranges $\mathcal{R}(S^c(P)) \subset [0,\infty]$, $\mathcal{R}(S^\text{ou}(P)) \subset [0,\infty]$, $\mathcal{R}(S^\text{cr}^i(P)) \subset [-1,1]$, $\mathcal{R}(S^\text{equ}^i(P)) \subset -\infty, \infty$ (i \in \{1,\ldots,d\}).

**2.5.1.3** $m_1(x) = m_2(x) := w(S_x(P),S_x(Q))$, $m_3(x) = r(x) \cdot w(S_x(P),S_x(Q)) \in [0,\infty[$ for some (measurable) functions $w : \mathcal{H}(P) \times \mathcal{H}(Q) \rightarrow \mathbb{R}$ and $r : \mathcal{X} \rightarrow \mathbb{R}$.

Such a choice extends the contexts of the previous Subsections 2.5.1.1 resp. 2.5.1.2 (where the “connector function” $w$ took the simple form $w(u,v) = 1$ resp. $w(u,v) = v$). This introduces a wide adaptive modeling flexibility, where $\phi$ specializes to

$$0 \leq D^c_{\phi,w(S(P),S(Q)),w(S(P),S(Q)),r-w(S(P),S(Q)),\lambda}(S(P),S(Q))$$

$$\text{:=} \int_{\mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{w(S_x(P),S_x(Q))} \right) - \phi \left( \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \right]$$

$$-\phi^c \left( \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \cdot \left( \frac{S_x(P)}{w(S_x(P),S_x(Q))} - \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \cdot w(S_x(P),S_x(Q)) \cdot r(x) \, d\lambda(x) ,$$

which for the discrete setup $(\mathcal{X},\lambda) = (\mathcal{X}_#,\lambda_#)$ (recall $\lambda_#(\{x\}) = 1$ for all $x \in \mathcal{X}_#$) simplifies to

$$0 \leq D^c_{\phi,w(S(P),S(Q)),w(S(P),S(Q)),r-w(S(P),S(Q)),\lambda}(S(P),S(Q))$$

$$\text{=} \sum_{x \in \mathcal{X}} \left[ \phi \left( \frac{S_x(P)}{w(S_x(P),S_x(Q))} \right) - \phi \left( \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \right]$$

$$-\phi^c \left( \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \cdot \left( \frac{S_x(P)}{w(S_x(P),S_x(Q))} - \frac{S_x(Q)}{w(S_x(P),S_x(Q))} \right) \cdot w(S_x(P),S_x(Q)) \cdot r(x) .$$

As a side remark, let us mention that by appropriate choices of $w(\cdot,\cdot)$ and $\phi$ in [63] we can even derive divergences of the form [63] but with non-convex non-concave $\phi$: see e.g. the “perturbed” power divergences of Roensch & Stummer [163].
In the following, let us illuminate the important special case of \( \mathcal{X} \) with \( \phi = \phi_{\alpha} \) (\( \alpha \in \mathbb{R} \), cf. \([20], [30], [31], [28]\)) together with \( S_x(P) \geq 0, S_x(Q) \geq 0 \) (as it is always the case for \( S^\text{cd}, S^\text{pd}, S^\text{pm}, S^\text{su}, S^\text{mg}, S^\text{de}, S^\text{ouv} \), and for nonnegative real-valued random variables also with \( S^\text{ouv} \)):

\[
0 \leq D_{\phi_{\alpha}, w(S(P), S(Q)), w(S(P), S(Q)), r-w(S(P), S(Q)), \lambda(S(P), S(Q))}
= \int_{\mathcal{X}} r(x) \cdot \left[ \frac{S_x(P)}{S_x(Q)} \right]^{1-\alpha} (\alpha - 1) \cdot (S_x(Q))^{\alpha}
\]

\[
- \alpha \cdot S_x(P) \cdot (S_x(Q))^{\alpha-1} \right] \, d\lambda(x) , \quad \text{for } \alpha \in \mathbb{R} \setminus \{0, 1\}, \quad (81)
\]

\[
0 \leq D_{\phi_{\alpha}, w(S(P), S(Q)), w(S(P), S(Q)), r-w(S(P), S(Q)), \lambda(S(P), S(Q))}
= \int_{\mathcal{X}} r(x) \cdot \left[ S_x(P) \cdot \log \left( \frac{S_x(P)}{S_x(Q)} \right) + S_x(Q) - S_x(P) \right] \, d\lambda(x), \quad (82)
\]

\[
0 \leq D_{\phi_{0}, w(S(P), S(Q)), w(S(P), S(Q)), r-w(S(P), S(Q)), \lambda(S(P), S(Q))}
= \int_{\mathcal{X}} r(x) \cdot w(S_x(P), S_x(Q)) \cdot \left[ - \log \left( \frac{S_x(P)}{S_x(Q)} \right) + S_x(P) - S_x(Q) \right] \, d\lambda(x), \quad (83)
\]

\[
0 \leq D_{\phi_{2}, w(S(P), S(Q)), w(S(P), S(Q)), r-w(S(P), S(Q)), \lambda(S(P), S(Q))}
= \int_{\mathcal{X}} r(x) \cdot \left( S_x(P) - S_x(Q) \right)^2 \, d\lambda(x) . \quad (84)
\]

\( \lambda \)-probability-density functions. For general \( \mathcal{X}, r(x) = 1 \), and (cf. Remark \([11] \)) \( S_x(P) = S^\text{pd}_x(P) := f_P(x) \geq 0, S_x(Q) = S^\text{pd}_x(Q) = f_Q(x) \geq 0 \), the divergences \([29], [30], [31] \) to \([33] \) are due to Kissinger \& Stummer \([100], [101], [102] \) (where they also gave indications on non-probability measures). Recall that this directly subsumes for \( \mathcal{X} = \mathcal{Y} = \mathbb{R} \) the “classical density” functional \( S^\text{pd} (\cdot) = S^\text{pd} (\cdot) \) with the choice \( \lambda = \lambda_L \) (and the Riemann integration \( d\lambda(x) = dx \)), as well as for the discrete setup \( \mathcal{Y} = \mathcal{X} = \mathbb{N} \) the “classical probability mass” functional \( S^\text{pd} (\cdot) = S^\text{pm} (\cdot) \) with the choice \( \lambda = \lambda_{\mathbb{N}} \).

Distribution functions. Recall that \( \mathcal{Y} = \mathcal{X} = \mathbb{R}, S_x(P) = S^\text{cd}_x(P) = F_P(x), S_x(Q) = S^\text{cd}_x(Q) = F_Q(x) \). Let us illuminate \([34] \) for the setup of a real-valued random variable \( Y, F_Q(x) = Q[Y \leq x] \) under a hypothetical/candidate law \( Q, F_P(x) = \frac{1}{N} \cdot \#\{ i \in \{1, \ldots, N\} : Y_i \leq x \} =: F_{P^\text{emp}}(x) \) as the distribution function of the corresponding data-derived “empirical distribution” \( P := P^\text{emp} \) := \( \frac{1}{N} \cdot \sum_{i=1}^{N} \delta_{Y_i}[.] \) of an \( N \)-size i.i.d. sample \( Y_1, \ldots, Y_N \) of \( Y \). In such a set-up, the choice \( \lambda = Q \) in \([34] \) and multiplication with \( 2N \) lead to

\[
0 \leq 2N \cdot D_{\phi_{\alpha}, w(S^\text{cd}(P^\text{emp}), S^\text{cd}(Q)), r-w(S^\text{cd}(P^\text{emp}), S^\text{cd}(Q)), \lambda(S^\text{cd}(P^\text{emp}), S^\text{cd}(Q))}
= \frac{1}{2N} \int_{\mathcal{Y}} r(x) \cdot \left( \frac{F_{P^\text{emp}}(x) - F_Q(x)}{F_{P^\text{emp}}(x) \cdot F_Q(x)} \right)^2 \, dQ(x) . \quad (85)
\]

The special case \( w(u, v) = 1 \) reduces to the Cramer-von Mises (test statistics) family \([17] \) and the choice \( r(x) = 1, w(u, v) = v \cdot (1 - v) \) gives the Anderson-Darling \([22] \) test statistics. With \([35] \), we can also imbed as special cases (together with \( r(x) = 1 \)) some other known divergences which emphasize the upper tails:
w(u, v) = 1 - v \quad (\text{cf. Ahmad et al. [11]}, w(u, v) = 1 - v^2 \quad (\text{cf. Rodriguez \& Viollaz [162]}, see also Shin et al. [173] for applications in environmental extreme-value theory), w(u, v) = (1 - v)^\beta \quad \text{with } \beta > 0 \quad (\text{cf. Deheuvels \& Martynov [56], see also Chernobai et al. [134] for the case } \beta = 2 \text{ together with a left-truncated version of the empirical distribution function). Moreover, [55] covers as special cases (together with } r(x) = 1 \text{ some other known divergences which emphasize the lower tails: } w(u, v) = v \quad (\text{cf. Ahmad et al. [11], Scott [109]}, w(u, v) = v^\beta \quad \text{with } \beta > 0 \quad (\text{cf. Deheuvels \& Martynov [56], w(u, v) = v \cdot (2 - v) \quad (\text{cf. Rodriguez \& Viollaz [162], see also Shin et al. [174] in contrast, in a two-sample-test situation where } Q \text{ is replaced by the empirical distribution } F_{\text{emp}} \quad \text{interpreted as a quantitative measure of tail risk of } P \text{ which has first been given in Stummer [183] in an even more flexible form – can be reference distribution } Q; \text{ corresponding connections with optimal transport are)})

Depth, outlyingness, centered rank and centered quantile functions.

As a special case of [79] one gets

\[ D_{\phi, \omega, \nu, \sigma}^c \left( S^\nu, S^\sigma \right), \left( D_{\phi, \omega, \nu, \sigma}^c \left( S^\nu, S^\sigma \right), r \right) \left( S^\nu, S^\sigma \right), \left( \lambda \right) \left( S^\nu, S^\sigma \right) \]

\[ = \sum_{i=1}^d D_{\phi, \omega, \nu, \sigma}^c \left( S^{\nu,i}, S^{\sigma,i} \right), r \left( S^{\nu,i}, S^{\sigma,i} \right), \left( \lambda \right) \left( S^{\nu,i}, S^{\sigma,i} \right) \]

all of which have not appeared elsewhere before (up to our knowledge); recall that the respective domains of \( \phi \) have to take care of the ranges \( \mathcal{R} \left( S^{\nu} \right) \subset [0, \infty], \mathcal{R} \left( S^{\sigma} \right) \subset [0, \infty], \mathcal{R} \left( S^{\nu,i} \right) \subset [-1, 1], \mathcal{R} \left( S^{\sigma,i} \right) \subset [-1, 1], \mathcal{R} \left( S^{\nu,i} \right) \subset \mathbb{R} \).

\[ 2.5.2 \quad \text{Recall } S(P) := \{ S_x(P) \}_{x \in \mathcal{X}}, S(Q) := \{ S_y(Q) \}_{y \in \mathcal{Y}}, \text{ and let } \hat{S}(P) := \{ \hat{S}_x(P) \}_{x \in \mathcal{X}} \]

\[ \hat{S}(Q) := \{ \hat{S}_y(Q) \}_{y \in \mathcal{Y}} \quad \text{for (typically) } \hat{S} \text{ being “essentially different” to } S \text{ (e.g., take } \hat{S} \text{ and } S \text{ as different choices from } S^{cd}, S^{pd}, S^{pm}, S^{en}, S^{mg}, S^{nu}, S^{de}, S^{ou}). \]
In quite some meaningful situations, (86) turns into which for the discrete setup $(\mathcal{X}, \lambda) = (\mathcal{X}_\# + \mathcal{X}_\#)$ simplifies to

\[
0 \leq D_{\phi, S(P), S(Q), m_3, \lambda}(S(P), S(Q)) = \sum_{x \in \mathcal{X}} \left[ \phi\left( \frac{S_x(P)}{S_x(P)} \right) - \phi\left( \frac{S_x(Q)}{S_x(Q)} \right) - \phi'_{\lambda, c}\left( \frac{S_x(Q)}{S_x(Q)} \right) \cdot \left( \frac{S_x(P)}{S_x(P)} - \frac{S_x(Q)}{S_x(Q)} \right) \right] m_3(x) dx.
\]

As an example, take $\mathcal{Y} = \mathcal{X} = [0, \infty]$, $\lambda = \lambda_L$, the probability (Lebesgue-) density functions $S = S_{pd}$, i.e. $S(P) = \{S_x(P)\}_{x \in [0, \infty]} = \{f_P(x)\}_{x \in [0, \infty]} = \{dF(x)\}_{x \in [0, \infty]}$, as well as the survival (reliability, tail) functions $S = S_{\nu}$, i.e. $S(P) = \{S_x(P)\}_{x \in [0, \infty]} = \{1 - F_P(x)\}_{x \in [0, \infty]} = \{P(x, \infty)\}_{x \in [0, \infty]}$. Accordingly, the function $x \rightarrow \frac{S_x(P)}{S_x(P)} = \frac{F_P(x)}{1 - F_P(x)}$ – with the convention $\xi = \infty$ for all $c \in \mathbb{R}$ – can be interpreted as the hazard rate function (failure rate function, force of mortality) under the model distribution $P$ (and analogously under the alternative model distribution $Q$) of a nonnegative random variable $Y$. Hence, (86) turns into

\[
0 \leq D_{\phi, S_{pd}(P), S_{\nu}(Q), m_3, \lambda_{\nu}}(S_{pd}(P), S_{\nu}(Q)) = \int_{\mathcal{X}} \left[ \phi\left( \frac{f_P(x)}{1 - F_P(x)} \right) - \phi\left( \frac{f_Q(x)}{1 - F_Q(x)} \right) \right.
\]

\[-\phi'_{\lambda, c}\left( \frac{f_Q(x)}{1 - F_Q(x)} \right) \cdot \left( \frac{f_P(x)}{1 - F_P(x)} - \frac{f_Q(x)}{1 - F_Q(x)} \right) \left] m_3(x) dx, \right. \]

which can be interpreted as divergence between the two modeling hazard rate functions at stake.

### 2.6 Auto-Divergences

The main-stream of this paper deals with divergences/distances between (families of) real-valued “statistical functionals” $S(\cdot)$ of the form $S(P) := \{S_x(P)\}_{x \in \mathcal{X}}$ and $S(Q) := \{S_x(Q)\}_{x \in \mathcal{X}}$ stemming from two different distributions $P$ and $Q$. In quite some meaningful situations, $P$ and $Q$ can stem from the same fundamental underlying random mechanism $\hat{P}$. Take for instance the situation where $\mathcal{Y} = \mathcal{X} = \mathbb{R}$, $\lambda = \lambda_L$ and $Y_1, \ldots, Y_N$ are i.i.d. observations from a random variable $Y$ with distribution $\hat{P}$ having (with a slight abuse of notation $\hat{P} = \hat{P} \circ Y^{-1}$)
distribution function \( F_{\rho}(x) = \bar{P}[Y \leq x] \) which is differentiable with a density \( f_{\rho}(x) = \frac{dF_{\rho}(x)}{dx} \) being positive in an interval and zero elsewhere. The corresponding order statistics are denoted by \( Y_{1:N} < Y_{2:N} < \ldots < Y_{N:N} \) where \( Y_{k:N} \) is the \( k \)-th largest observation and in particular \( Y_{1:N} := \min\{Y_1, \ldots, Y_N\}; Y_{N:N} := \max\{Y_1, \ldots, Y_N\} \); the distribution \( \bar{P}_k \) of \( Y_{k:N} \ (k \in \{1, \ldots, N\}) \) has distribution function \( f_{\bar{P}_k}(x) := \bar{P}[Y_{k:N} \leq x] \) with well-known density function

\[
f_{\bar{P}_k}(x) := \frac{N!}{(N-k)! \cdot (k-1)!} \cdot (F_{\rho}(x))^{k-1} \cdot (1 - F_{\rho}(x))^{n-k} \cdot f_{\rho}(x). \tag{87}
\]

(see e.g. Reiss \[161\], Arnold et al. \[10\], David & Nagaraja \[53\] for comprehensive treatments of order statistics). In such a context, it makes sense to take \( P := \bar{P}_j, Q := \bar{P}_k \ (j, k \in \{1, \ldots, N\}) \) respectively \( P := \bar{P}, Q := \bar{P}_k \) (or vice versa) and study the divergences

\[
0 \leq D_{\phi, m_1, m_2, m_3, \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right) \\
:= \int_{\mathcal{X}} \left[ \phi \left( \frac{f_\rho(x)}{m_1(x)} \right) - \phi \left( \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) - \phi'_{+c} \left( \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) \cdot \left( \frac{f_\rho(x)}{m_1(x)} - \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) \right] m_3(x) \, d\lambda_L(x) 
\]

respectively

\[
0 \leq D_{\phi, m_1, m_2, m_3, \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right) \\
:= \int_{\mathcal{X}} \left[ \phi \left( \frac{f_\rho(x)}{m_1(x)} \right) - \phi \left( \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) - \phi'_{+c} \left( \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) \cdot \left( \frac{f_\rho(x)}{m_1(x)} - \frac{f_{\bar{P}_k}(x)}{m_2(x)} \right) \right] m_3(x) \, d\lambda_L(x), 
\tag{88}
\]

or deterministic transformations thereof.

For instance, (some of) the divergences in Ebrahimi et al. \[64\], Asadi et al. \[11\] can be imbedded here as the special cases \( D_{\phi, 1, 1, 1, \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right); D_{\phi, 1, 1, 1, \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right); \quad \frac{1}{\alpha-1} \log \left[ 1 + \alpha \cdot (\alpha - 1) \cdot \left( D_{\phi, S^{pd}(\bar{P}_k), S^{pd}(\bar{P}_k), \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right) \right) \right], \\
\frac{1}{\alpha-1} \log \left[ 1 + \alpha \cdot (\alpha - 1) \cdot \left( D_{\phi, S^{pd}(\bar{P}_k), S^{pd}(\bar{P}_k), \lambda_L} \left( S^{pd}(\bar{P}), S^{pd}(\bar{P}_k) \right) \right) \right], \\
\alpha \in \mathbb{R} \setminus \{0, 1\} \). 

For other (non-auto type) scaled Bregman divergences involving distributions of certain transforms of spacings between observations (i.e., differences of order statistics), the reader is e.g. referred to Roensh & Stummer \[165\].

Vaughan & Venables \[198\], Bapat & Beg \[18\] and Hande \[87\] give some extensions of (87) for random observations \( Y_1, \ldots, Y_N \) which are independent but non-identically distributed, e.g. their distributions may be linked by a common
(scalar or multidimensional) parameter; this is a common situation in contemporary statistical applications e.g. in data analytics, artificial intelligence and machine learning (which employ GLM models, etc.). By employing \( \mathbb{S} \) for these extensions of \( (87) \), we end up with an even wider new toolkit for auto-divergences.

### 2.7 Connections with optimal transport and coupling

In this section we consider the context of Subsection 2.5.1.3 with \( \mathcal{X} = [0, 1] \). Lebesgue measure \( \lambda = \lambda_L \) as well \( r(x) = 1 \) for all \( x \in \mathcal{X} \), and apply this to the quantile functions \( S^{\nu}(P) = \{ S_x(P) \}_{x \in [0, 1]} := \{ F^{-1}_P(x) \}_{x \in [0, 1]} \) respectively \( S^{\nu}(Q) \) of two random variables \( X \) respectively \( Y \) on \( \mathcal{Y} = \mathbb{R} \) having distribution \( P \) respectively \( Q \); recall from Section 2.1 that for \( \mathcal{Y} = [0, \infty) \) we take \( S^{\nu}(P) = \{ S_x(P) \}_{x \in [0, 1]} := \{ F^{-1}_P(x) \}_{x \in [0, 1]} \) instead. Accordingly, we quantify the corresponding dissimilarity as the divergence (directed distance)

\[
D^\phi_{\phi, w}(S^{\nu}(P), S^{\nu}(Q)) := \int_{[0, 1]} \frac{F^{-1}_P(x)}{w(F^{-1}_P(x), F^{-1}_Q(x))} - \frac{F^{-1}_Q(x)}{w(F^{-1}_P(x), F^{-1}_Q(x))} \cdot \left( \frac{F^{-1}_P(x)}{w(F^{-1}_P(x), F^{-1}_Q(x))} - \frac{F^{-1}_Q(x)}{w(F^{-1}_P(x), F^{-1}_Q(x))} \right) \cdot r(x) \, d\lambda_L(x)
\]

\[
= \int_{[0, 1]} \psi(F^{-1}_P(x), F^{-1}_Q(x)) \, d\lambda_L(x)
\]

with \( \psi : \mathcal{X} \times \mathcal{X} \to [0, \infty] \) defined by (cf. (12) and (21))

\[
\psi(u, v) := W(u, v) \cdot \psi_{\phi, c}(\frac{u}{W(u, v)}, \frac{v}{W(u, v)}) \geq 0 \quad \text{with} \quad \psi_{\phi, c}(\frac{u}{W(u, v)}, \frac{v}{W(u, v)}) := \left[ \phi\left( \frac{u}{W(u, v)} \right) - \phi\left( \frac{v}{W(u, v)} \right) \right] \cdot \left[ \psi_{\phi, c}\left( \frac{u}{W(u, v)} \right) - \psi_{\phi, c}\left( \frac{v}{W(u, v)} \right) \right].
\]

Under Assumption 1 (and hence under the more restrictive Assumption 2) of Stummer [183] – who deals even with a more general context where the scaling and the aggregation function need not coincide – one can adapt Theorem 4 and Corollary 1 of Broniatowski & Stummer [12] to obtain the desired basic divergence properties (D1) and (D2) in the form of

\[
(NN) D^\phi_{\phi, w}(S^{\nu}(P), S^{\nu}(Q)) \geq 0 \quad \text{and} \quad (RE) D^\phi_{\phi, w}(S^{\nu}(P), S^{\nu}(Q)) = 0 \quad \text{if and only if} \quad F^{-1}_P(x) = F^{-1}_Q(x) \quad \text{for} \lambda\text{-a.a.} \ x \in \mathcal{X}.
\]

In order to establish a connection between the divergence \( \mathbb{S} \) and optimal transport problems, we impose for the rest of this section the additional requirement that the function \( \psi \) is continuous (except for the point \( (u, v) = (0, 0) \)) and
other names are: supermodular, Lattice-superadditive, 2-increasing, 2-positive, 2-monotone, 2-antitone, supernegative, “satisfying the (continuous) Monge property/condition”

other names are: submodular, Lattice-subadditive, 2-anti tone, 2-negative, Δ-antitone, supernegative, “satisfying the (continuous) Monge property/condition”

a comprehensive discussion on general quasi-monotone functions can be found e.g. in Chapter 6.C of Marshall et al. [121]
Remark 2(ii) generally contrasts to those prominently used KTP whose cost function is a power \(d(u, v)^p\) of a metric \(d(u, v)\) (denoted as POM-type cost function) which leads to the well-known Wasserstein distances. (Apart from technicalities) There are some overlaps, though:

**Example 1.** (i) Take \(\mathcal{Y} \subset [0, \infty)\) (and thus the support of \(P\) and \(Q\) is contained in \([0, \infty]\)) together with the non-smooth \(\phi(t) := \phi_{TV}(t) := |t - 1| (t \in [0, \infty])\),

\[
c = \frac{1}{2}, W(u, v) := v \in [0, \infty[ \text{ to obtain } \psi(u, v) = |u - v| = d(u, v) (u, v \in [0, \infty[).
\]
For an extension to \(\mathcal{Y} = \mathbb{R}\) see Stummer \[183\].

(ii) Take \(\mathcal{Y} = \mathbb{R}\), \(\phi(t) := \phi_{2}(t) := \frac{(t - 1)^2}{2} (t \in \mathbb{R}, \text{ with obsolescent } c)\), \(W(u, v) := 1\) to end up with \(\psi(u, v) = \frac{(u - v)^2}{2} = \frac{d(u, v)^2}{2}\).

(iii) The symmetric distances \(d(u, v)\) and \(d(u, v)^2\) are convex functions of \(u - v\) and thus continuous quasi-antitone. The correspondingly outcoming Wasserstein distances are thus considerably flexibilized by our new much more general distance \(D_{\phi, \omega(S^{\psi}(P), S^{\psi}(Q)), \omega(S^{\psi}(P), S^{\psi}(Q))}^{\lambda}(S^{\psi}(P), S^{\psi}(Q))\) of \(\psi\).

We give some further special cases of pBS-type cost functions, which are continuous and quasi-antitone, but which are generally not symmetric and thus not of POM-type:

**Example 2.** “smooth” pointwise Csiszar-Ali-Silvey-Morimoto divergences (CASM divergences): take \(\phi : [0, \infty[ \to \mathbb{R}\) to be a strictly convex, twice continuously differentiable function on \([0, \infty[\) with continuous extension on \(t = 0\), together with \(W(u, v) := v \in [0, \infty[, \text{ and } c \text{ is obsolete}\). Accordingly, \(\psi(u, v) = v \cdot \phi\left(\frac{u}{v}\right) - v \cdot \phi(1) - \phi'(1) \cdot (u - v)\), and hence the second mixed derivative satisfies \(\frac{\partial^2\psi}{\partial u \partial v} = -\frac{v}{u} \phi''\left(\frac{u}{v}\right) < 0 (u, v \in [0, \infty[)\); thus, \(\psi\) is quasi-antitone on \([0, \infty[ \times [0, \infty[\). Accordingly, \(91\) to \(93\) applies to such kind of (cf. Section 2.5.1.2) CASM divergences concerning \(P, Q\) having support in \([0, \infty[\). As an example, take e.g. the power function \(\phi(t) := \frac{\gamma}{\gamma - 1} t^{\gamma - 1} \in \mathbb{R}\{0, 1\}\). A different connection between optimal transport and other kind of CASM divergences can be found in Bertrand et al. \[28\].

**Example 3.** “smooth” pointwise classical (i.e. unscaled) Bregman divergences (CBD): take \(\phi : \mathbb{R} \to \mathbb{R}\) to be a strictly convex, twice continuously differentiable function \(W(u, v) := 1\) and \(c\) is obsolete. Accordingly, \(\psi(u, v) = \phi(u) - \phi(v) - \phi'(v) \cdot (u - v)\) and hence \(\frac{\partial^2\psi}{\partial u \partial v} = -\phi''(v) < 0 (u, v \in \mathbb{R}\); thus, \(\gamma_{\phi, c, W, W_{\phi}}\) is quasi-antitone on \(\mathbb{R} \times \mathbb{R}\). Accordingly, the representation \(90\) to \(93\) applies to such kind of (cf. Section 2.5.1.1) CBD. The corresponding special case of \(91\) is called “a relaxed Wasserstein distance (parameterized by \(\phi\)) between \(P\) and \(Q\) in the recent papers of Lin et al. \[112\] and Guo et al. \[80\] for a restrictive setup where \(P\) and \(Q\) are supposed to have compact support; the latter two references do not give connections to divergences of quantile functions, but substantially concentrate on applications to topic sparsity for analyzing user-generated web content and social media, respectively, to Generative Adversarial Networks (GANs).
Example 4. “smooth” pointwise Scaled Bregman Distances: for instance, consider $P$ and $Q$ with support in $[0, \infty[$. One gets that $\tilde{\psi}$ is quasi-antitone on $]0, \infty[ \times ]0, \infty[$ if the generator function $\phi$ is strictly convex and thrice continuously differentiable on $]0, \infty[$ (and hence, $c$ is obsolete) and the so-called scale connector $W$ is twice continuously differentiable such that $\frac{\psi}{\phi}$ is twice continuously differentiable and $\frac{\psi}{\phi} \leq 0$ (an explicit formula of the latter is given in the appendix of Kißlinger & Stummer [103], who also give applications to robust change detection in data streams). Illustrative examples of suitable $\phi$ and $W$ can be found e.g. in Kißlinger & Stummer [102].

Returning to the general context, it is straightforward to see that if $P$ does not give mass to points (i.e. it has continuous distribution function $F_P$) then there exists even a deterministic optimal transportation plan: indeed, for the map $T_{\text{com}}: F_P \mapsto F_Q$ one has $P_{\text{com}} \circ T_{\text{com}} = P$ and thus (92) is equal to

$$\min_{T \in \hat{P}(P, Q)} \mathbb{E}
\left[
\frac{\psi}{\phi}(X, T(X))
\right]$$

where (93) is called Monge transportation problem (MTP). Here, $\hat{P}(P, Q)$ denotes the family of all measurable maps $T: \mathbb{R} \rightarrow \mathbb{R}$ such that $P[T \in \cdot] = Q[\cdot]$.

3 Aggregated/Integrated Divergences

Suppose that $\phi = \phi_z$, $P = P_z$, $Q = Q_z$, $m_1 = m_{1,z}$, $m_2 = m_{2,z}$, $m_3 = m_{3,z}$, $\lambda = \lambda_z$ depend on the same (!!!) “parameter/quantity” $z \in \mathcal{Z}$. Then it makes sense to study the aggregated/integrated divergence

$$\int_{\mathcal{Z}} D_{\phi_z, m_{1,z}, m_{2,z}, m_{3,z}, \lambda_z}(S(P_z), S(Q_z)) \, d\tilde{\lambda}(z)$$

where $\tilde{\lambda}$ is a $\sigma$–finite measure on $\mathcal{Z}$ (e.g. the Lebesgue-measure $\lambda_L$, the counting measure $\lambda_\#$, or a probability measure, where in case of the latter one also uses the terminology “expected divergence”).

Another interesting special case is the following family: recall first that for the two-element space $\mathcal{Y} = \mathcal{Z} = \{0, 1\}$ we denote the corresponding probability mass functions as $S^{\text{pm}}(P) = \{P([x])\}_{x \in \mathcal{Z}} = \{1 - P([1]), P([1])\}$; in other words, $P$ is a Bernoulli distribution $\text{Ber}(\theta)$ which is completely determined by its parameter $\theta \in [0, 1]$ with interpretation $\theta_P = P([1])$. Now suppose that $\theta_P = \theta_P(z)$ depends on a real-valued parameter $z \in \mathbb{R}$. In such a situation it makes sense to study the the aggregated (integrated) divergence for
\[ \phi \in \Phi_{C_1}(\{a, b\}) \]

\[ 0 \leq \int_{\mathbb{R}} D_{\phi, m_1, m_2, m_3, \lambda_{\#}}(S^{pm}(\text{Ber}(\theta_P(z))), S^{pm}(\text{Ber}(\theta_Q(z)))) d\tilde{\lambda}(z) \]

\[ = \int_{\mathbb{R}} \left\{ \left[ \phi \left( \frac{1 - \theta_P(z)}{m_{1,z}(0)} \right) - \phi \left( \frac{1 - \theta_Q(z)}{m_{2,z}(0)} \right) - \phi' \left( \frac{1 - \theta_Q(z)}{m_{2,z}(0)} \right) \cdot \left( \frac{1 - \theta_P(z)}{m_{1,z}(0)} - \frac{1 - \theta_Q(z)}{m_{2,z}(0)} \right) \right] \cdot m_{3,z}(0) \right\} d\tilde{\lambda}(z) \]

\[ + \left[ \phi \left( \frac{\theta_P(z)}{m_{1,z}(1)} \right) - \phi \left( \frac{\theta_Q(z)}{m_{2,z}(1)} \right) - \phi' \left( \frac{\theta_Q(z)}{m_{2,z}(1)} \right) \cdot \left( \frac{\theta_P(z)}{m_{1,z}(1)} - \frac{\theta_Q(z)}{m_{2,z}(1)} \right) \right] \cdot m_{3,z}(1) \cdot d\tilde{\lambda}(z) \]  

(95)

where \( \tilde{\lambda} \) is a \( \sigma \)-finite measure on \( \mathbb{R} \) (e.g., the Lebesgue-measure \( \lambda_L \), the counting measure \( \lambda_{\#} \) or a probability measure) and the scaling functions \( m_1, m_2 \) as well as the aggregating function \( m_3 \) are allowed to depend (in a measurable way) on \( z \) (which is denoted by extending their indices with \( z \)). For the non-differentiable case \( \phi \in \Phi_0([a, b]) \), the derivative \( \phi' \) has to be replaced by \( \phi'_{+, \cdot} \).

In adaption of the discussion after formula (25), by defining the integral functional \( g_{\phi, m_3, \lambda}(\xi):= \int_{\mathbb{R}} \left( \int_{[0, 1]} \phi(\xi(x, z)) \cdot m_3(x) d\lambda_{\#}(x) \right) d\tilde{\lambda}(z) \) and plugging in e.g.

\[ g_{\phi, m_3, \lambda}(S^{pm}(\text{Ber}(\theta_P(z)))) = \int_{\mathbb{R}} \left\{ \phi \left( \frac{1 - \theta_P(z)}{m_{1,z}(0)} \right) \cdot m_{3,z}(0) + \phi \left( \frac{\theta_P(z)}{m_{1,z}(1)} \right) \cdot m_{3,z}(1) \right\} d\tilde{\lambda}(z), \]

(96)

the divergence in (95) can be (formally) interpreted as

\[ 0 \leq 0 \leq \int_{\mathbb{R}} D_{\phi, m_1, m_2, m_3, \lambda_{\#}}(S^{pm}(\text{Ber}(\theta_P(z))), S^{pm}(\text{Ber}(\theta_Q(z)))) d\tilde{\lambda}(z) \]

\[ = g_{\phi, m_3, \lambda}(S^{pm}(\text{Ber}(\theta_P(z)))) - g_{\phi, m_3, \lambda}(S^{pm}(\text{Ber}(\theta_Q(z)))) \]

\[ - g_{\phi, m_3, \lambda}(S^{pm}(\text{Ber}(\theta_Q(z)))) - S^{pm}(\text{Ber}(\theta_P(z))) \].

As an important special case, take \( \tilde{\lambda} := \lambda_L \) (and we formally identify the Lebesgue-integral with the Riemann-integral over \( dz \), \( \theta_P(z) := F_P(z) = P([-\infty, z]) = S_{\#}^L(P), \theta_Q(z) := F_Q(z) = Q([z, \infty]) = S_{\#}^L(Q), m_{1,z}(0) = m_{2,z}(0) = m_{3,z}(1) = 1 - \theta_Q(z), m_{1,z}(1) = m_{2,z}(1) = m_{3,z}(1) = \theta_Q(z), \) and accordingly (95) simplifies to

\[ 0 \leq \int_{\mathbb{R}} D_{\phi, m_1, m_2, m_3, \lambda}(S^{pm}(\text{Ber}(\theta_P(z))), S^{pm}(\text{Ber}(\theta_Q(z)))) d\tilde{\lambda}(z) \]

\[ = \int_{\mathbb{R}} \left\{ \left[ \phi \left( \frac{1 - F_P(z)}{1 - F_Q(z)} \right) - \phi(1) - \phi' \left( \frac{1 - F_P(z)}{1 - F_Q(z)} \right) \right] \cdot (1 - F_Q(z)) \right\} \cdot dz \]

\[ + \left[ \phi \left( \frac{F_P(z)}{F_Q(z)} \right) - \phi(1) - \phi' \left( \frac{F_P(z)}{F_Q(z)} \right) \right] \cdot F_Q(z) \]

\[ =: CPD_\phi(P, Q), \]
which in case of \( \phi(1) = 0 \) becomes

\[
0 \leq CPD_\phi(P, Q) = \int_R \left\{ \phi\left( \frac{1 - F_P(z)}{1 - F_Q(z)} \right) \cdot (1 - F_Q(z)) + \phi\left( \frac{F_P(z)}{F_Q(z)} \right) \cdot F_Q(z) \right\} \, dz. \quad (97)
\]

If basically \( \phi(0) = \phi(1) = 0 \) and \( P, Q \) are generated by random variables, say \( P = \Pr[X \in \cdot], \ Q = \Pr[Y \in \cdot] \) – and thus \( F_P(z) = \Pr[X \leq z], \ F_Q(z) = \Pr[Y \leq z] \) – then according to (97) the \( CPD_\phi(P, Q) \) coincides with the cumulative paired \( \phi \)-divergence \( CPD_\phi(X, Y) \) of Klein et al. [105]; the special case \( CPD_{\phi_n}(X, Y) \) with \( \phi = \phi_n \) from [20] was employed by Jager & Wellner [91]. Notice that without the assumption \( \phi(1) = 0 = \phi'(1) \), the right-hand side of (97) may become negative and thus is not a divergence anymore.

As a side remark, notice that in the “unscaled setup” \( \bar{\lambda} := \lambda_L, \ \theta_P(z) := F_P(z), \ m_{1,z}(0) = m_{3,z}(0) = m_{1,z}(1) = m_{3,z}(1) = 1 \), the formula (97) becomes

\[
\tilde{g}_{\phi, m_3}(\frac{S_{\text{emp}}(\text{Ber}(\theta_P)))}{m_1}) = \int_R \left\{ \phi(1 - F_P(z)) + \phi(F_P(z)) \right\} \, dz
\]

which corresponds to the cumulative \( \phi \)-entropy of \( P \) introduced by Klein et al. [105].

4 Dependence expressing divergences

Let the data take values in some product space \( \mathcal{X} = \times_{i=1}^d \mathcal{Y}_i \) with product-\( \sigma \)-algebra \( \mathcal{A} = \times_{i=1}^d \mathcal{A}_i \). On this, we consider probability distributions \( P \) having marginals \( P_i \) determined by \( P_i[A_i] := P_i[A_i \times \cdots \times A_i \times \cdots A_i] \) \( (i \in \{1, \ldots, d\}, \ A_i \in \mathcal{A}_i) \). Furthermore, let \( Q := \times_{i=1}^d P_i \) be the product measure having the same marginals as \( P \). Typically, \( P_\cdot := \Pr[[Y_1, \ldots, Y_d] \in \cdot] \) is the joint distribution of some random variables \( Y_1, \ldots, Y_d \); on the other hand, the latter are independent under the (generally different) probability measure \( Q \).

As usual, we also involve statistical functionals \( S(P) := \{S_x(P)\}_{x \in \mathcal{X}} \) and \( S(Q) := \{S_x(Q)\}_{x \in \mathcal{X}} \), where \( \mathcal{X} \) is an index space equipped with a \( \sigma \)-algebra \( \mathcal{F} \) and a \( \sigma \)-finite measure \( \lambda \) (e.g. a probability measure, the Lebesgue measure, a counting measure, etc.). Accordingly, any of the above divergences (cf. (99))

\[
0 \leq D^\phi_{\phi, m_1, m_2, m_3, \lambda}(S(P), S(Q))
\]

\[
:= \int_{\mathcal{X}} \left[ \phi\left( \frac{S_x(P)}{m_1(x)} \right) - \phi\left( \frac{S_x(Q)}{m_2(x)} \right) - \phi'_+ \left( \frac{S_x(Q)}{m_2(x)} \right) \cdot \left( \frac{S_x(P)}{m_1(x)} - \frac{S_x(Q)}{m_2(x)} \right) \right] m_3(x) \, d\lambda(x)
\]

(98)

can be interpreted as a directed degree of dependence of \( P \) (e.g. of the above-mentioned random variables \( Y_1, \ldots, Y_d \)), since it measures the amount of dissimilarity between the same statistical functional of \( P \) and of the independence-expressing \( Q \). Some special cases of (98) have already appeared in literature.
(which we put into our notation):

(1) Micheas & Zografos \[129\] consider Csizsar-Ali-Silvey-Morimoto (CASM)
\(\phi\)–divergences between \(\lambda\)–density functions, i.e. they take
\(\mathcal{X} := \mathcal{Y}\), a real continuous convex function on \([0, \infty]\), a product measure \(\lambda := \otimes_{i=1}^{d} \lambda_{i}\), \(S_{x}^{\lambda \text{pd}}(Q) := f_{Q}(x) := \prod_{i=1}^{d} f_{P_{i}}(x_{i}) \geq 0\) where \(x = (x_{1}, \ldots, x_{d})\) and \(f_{P_{i}}\) is the \(\lambda_{i}\)–density function of the marginal distribution \(P_{i}\), as well as \(S_{x}^{\lambda \text{pd}}(P) := f_{P}(x) \geq 0\) to be the
\(\lambda\)–density function of \(P\), to end up with the following special case of (74):

\[
0 \leq D_{\phi,S_{x}^{\lambda \text{pd}}(Q),S_{x}^{\lambda \text{pd}}(Q),1,S_{x}^{\lambda \text{pd}}(Q),\lambda}(S_{x}^{\lambda \text{pd}}(P),S_{x}^{\lambda \text{pd}}(Q))
\]

\[
= \int_{\mathcal{X}} \prod_{i=1}^{d} f_{P_{i}}(x_{i}) \cdot \phi \left( \frac{f_{P}(x)}{\prod_{i=1}^{d} f_{P_{i}}(x_{i})} \right) \cdot 1_{[0,\infty]} \left( f_{P}(x) \cdot \prod_{i=1}^{d} f_{P_{i}}(x_{i}) \right) \, d\lambda(x)
\]

\[
+ \phi^{*}(0) \cdot P \left( \prod_{i=1}^{d} f_{P_{i}}(x_{i}) = 0 \right) + \phi(0) \cdot Q \left[ f_{P}(x) = 0 \right] - \phi(1).
\]

In applications, one often takes \(\mathcal{X} = \mathcal{Y} = \mathbb{R}^{d}\), \(\mathcal{Y} = \mathbb{R}\), \(\lambda_{i} := \lambda_{L}\) to be the
Lebesgue measure on \(\mathbb{R}\) and thus \(\lambda = \lambda_{L}\) is the Lebesgue measure on \(\mathbb{R}^{d}\) (with a slight abuse of notation), \(f_{P}\) to be the classical joint (Lebesgue) density function of \(Y_{1}, \ldots, Y_{d}\), and \(f_{P_{i}}\) to be the classical (Lebesgue) density function of \(Y_{i}\).

By plugging \(\phi(t) = \phi_{1}(t) = t \cdot \log t + t \in [0, \infty] \cdot t \in [0, \infty]\) (cf. (30)) into (99),
one obtains the prominent mutual information. References to further subcases of (99)
can be found e.g. in [129].

For \(d = 2\), \(\mathcal{X} = \mathcal{Y} = \mathbb{R}^{2}\), \(\lambda := \lambda_{L}\), continuous marginal density functions \(f_{P_{1}}, f_{P_{2}}\), by Sklar’s theorem \[175\] one can uniquely rewrite the joint distribution function \(F_{P}(x_{1}, x_{2}) = C(F_{P_{1}}(x_{1}), F_{P_{2}}(x_{1}))\) in terms of a copula \(C(\cdot, \cdot)\). Suppose further that \(C(\cdot, \cdot)\) is absolutely continuous (with respect to the Lebesgue measure on \([0, 1] \times [0, 1]\), and hence for its (Lebesgue) density function \(c(\cdot, \cdot)\) – called copula density – one gets \(c(u_{1}, u_{2}) = \frac{\partial^{2} C(u_{1}, u_{2})}{\partial u_{1} \partial u_{2}}\) for almost all \(u_{1}, u_{2} \in [0, 1] \times [0, 1]\) (see e.g. p.83 in Durante & Sempi \[61\] and the there-mentioned references). Accordingly, \(f_{P}(x_{1}, x_{2}) = f_{P_{1}}(x_{1}) \cdot f_{P_{2}}(x_{2}) \cdot c(F_{P_{1}}(x_{1}), F_{P_{2}}(x_{1}))\) and thus, in case of strictly positive \(f_{P_{1}}(\cdot) > 0\), \(f_{P_{2}}(\cdot) > 0\) the divergence (99) rewrites as

\[
0 \leq D_{\phi,S_{x}^{\lambda \text{pd}}(Q),S_{x}^{\lambda \text{pd}}(Q),1,S_{x}^{\lambda \text{pd}}(Q),\lambda}(S_{x}^{\lambda \text{pd}}(P),S_{x}^{\lambda \text{pd}}(Q))
\]

\[
= \int_{\mathcal{R}} \int_{\mathcal{R}} f_{P_{1}}(x_{1}) \cdot f_{P_{2}}(x_{2}) \cdot \phi \left( \frac{f_{P}(x_{1}, x_{2})}{f_{P_{1}}(x_{1}) \cdot f_{P_{2}}(x_{2})} \right) \, d\lambda_{L}(x_{1}) \, d\lambda_{L}(x_{2}) - \phi(1)
\]

\[
= \int_{0}^{1} \int_{0}^{1} \phi(c(u_{1}, u_{2})) \, d\lambda_{L}(u_{1}) \, d\lambda_{L}(u_{2}) - \phi(1),
\]

which solely depends on the copula (density) and not on the marginals. For
\(\phi(1) = 0\) formula (114) was established basically in Durrani & Zeng \[62\] without
assumptions and without a proof; they also give some examples including
\(\phi = \phi_{\alpha}(\alpha \in \mathbb{R}\setminus\{0, 1\})\) of (20), as well as the KL-generator \(\phi = \phi_{1}(t)\) of (29)
leading to the “copula-representation of mutual information”. The latter also
appears in the earlier work of Davy & Doucet \[54\], as well as e.g. in Zeng &
Durrani [206], Zeng et al. [207] and Tran [193]: in contrast, Tran also gives a copula-representation of the Kullback-Leibler information divergence between two general \(d\)-dimensional Lebesgue density functions \(S^{\lambda_{\ell,pd}}(P) := f_P(\cdot)\) and \(S^{\lambda_{\ell,pd}}(Q) := f_Q(\cdot)\) where \(P\) and \(Q\) are allowed to have different marginals, and \(Q\) need not be of independence-expressing product type.

(2) For the special case \(\mathcal{X} := \mathcal{Y} = \mathbb{R}^2\), continuous marginal distribution functions \(F_{P_1}\) and \(F_{P_2}\), product measure \(\lambda := P_1 \otimes P_2\), \(S^{\ell}(Q) := F_Q(x) = F_{P_1}(x_1) \cdot F_{P_2}(x_2)\) in \([0, 1]\), as well as joint distribution function \(S^{\ell}(P) := F_P(x)\), one gets the following special cases of (40) respectively (73):

\[
0 \leq D_{\phi_{\ell},\lambda}^{\ell}(S^{\ell}(P), S^{\ell}(Q)) = \int_\mathbb{R} \int_\mathbb{R} \frac{1}{2} \left[ \frac{F_P(x_1, x_2) - F_{P_1}(x_1) \cdot F_{P_2}(x_2)}{F_{P_1}(x_1) \cdot F_{P_2}(x_2)} \right]^2 dP_1(x_1) dP_2(x_2)
\]

As a side remark, let us mention that other interplays between divergences and copula functions can be constructed. For instance, suppose that \(P\) and \(Q\) are two probability distributions on the \(d\)-dimensional product (measurable) space \((\mathcal{Y}, \mathcal{A})\) having copula density functions \(c_P\) respectively \(c_Q\); the latter can be interpreted as special statistical functionals \(S^{\text{cop}}(P)\) of \(P\) respectively \(S^{\text{cop}}(Q)\) of \(Q\), and thus, by employing the divergences (19) we obtain

\[
0 \leq D_{\phi_{\ell},\lambda}^{\text{cop}}(S^{\text{cop}}(P), S^{\text{cop}}(Q)) = \int_\mathcal{Y} \int_\mathcal{Y} C(u_1, u_2) - u_1 \cdot u_2 \ d\lambda(u_1) d\lambda(u_2)
\]

where \(\lambda_{\ell,d}\) denotes the \(d\)-dimensional Lebesgue measure and thus the integral in (100) turns out to be (with some rare exceptions) of \(d\)-dimensional Riemann-type with \(d\lambda_{\ell,d}(x) = dx\). The (CASM \(\phi\)-divergences type) special case \(D_{\phi,\lambda}^{\text{cop}}(S^{\text{cop}}(P), S^{\text{cop}}(Q))\) leads to a divergence which has been used by Bouzebda & Keziou [34] in order to obtain new estimates and tests of independence in semiparametric copula models with the help of variational methods.
5 Bayesian contexts

There are various different ways how divergences can be used in Bayesian frameworks:

(1) as “direct” quantifiers of dissimilarities between statistical functionals of various parameter distributions:

for instance, consider a \(n\)-dimensional vector of observable random quantities \(\mathbf{z} = (Z_1, \ldots, Z_n)\) whose distribution depends on an unobservable (and hence, also random) multivariate parameter \(\Theta := (\Theta_1, \ldots, \Theta_d)\), as well as a real-valued quantity \(Z_{n+1}\) (whose distribution also depends on \(\Theta\)) to be predicted. Corresponding candidates for distributions \(P, Q\) – to be used in \(D(S(P), S(Q))\) – are for example the following: the prior distribution \(P_w[\cdot] := P(\Theta \in \cdot)\) of \(\Theta\) (under some underlying probability measure \(P\)), the posterior distribution \(P_{w|z}[\cdot] := P_{w|z}(\Theta \in \cdot | \mathbf{z} = \mathbf{z})\) of \(\Theta\) given the data observation \(\mathbf{z} = \mathbf{z}\), the predictive prior distribution \(P_{w|z}[\cdot] = P_{w|z}(Z_{n+1} \in \cdot) = \int_{\mathbb{R}^d} P_{w|z}(\Theta = \theta | \mathbf{z} = \mathbf{z}) \, dP_{\Theta}(\theta)\) of \(Z_{n+1}\), and the predictive posterior distribution \(P_{w|z}[\cdot] = P_{w|z}(Z_{n+1} \in \cdot | \mathbf{z} = \mathbf{z}) = P_{w|z}(Z_{n+1} \in \cdot | \mathbf{z} = \mathbf{z}) = \int_{\mathbb{R}^d} P_{w|z}(\Theta = \theta | \mathbf{z} = \mathbf{z}) \, dP_{\Theta}(\theta)\) of \(Z_{n+1}\). For instance, the divergence \(D(S^{\mathbf{z}}(P_{\Theta}), S^{\mathbf{z}}(P_{\Theta|\mathbf{z} = \mathbf{z}}))\) serves as “degree of informativity of the new data-point observation on the learning of the true unknown parameter”.

Analogously, one can also consider more complex setups like e.g. a continuum \(\mathbf{z} = \{Z_t : t \in [0, T]\}\) of observations, parameters \(\Theta\) of function type, and \(Z_u\) \((u > T)\) rather than \(Z_{n+1}\).

(2) as “decision risk reduction” (“model risk reduction”, “information gain”):

dichotomous Bayesian decision problem between the two alternative probability distributions \(P := P_{\mathcal{H}}\) and \(Q := P_{\mathcal{A}}\); one takes \(\Theta = \{\mathcal{H}, \mathcal{A}\}\), \(P_{w|\mathcal{H}}[\cdot] := \pi_{\mathcal{H}} \cdot \delta_{\mathcal{H}}[\cdot] + (1 - \pi_{\mathcal{H}}) \cdot \delta_{\mathcal{A}}[\cdot]\) for some \(\pi_{\mathcal{H}} \in [0, 1]\[.\]

Within this context, suppose we want to make decisions/actions \(d\) taking values in a space \(\mathbb{D}\). Furthermore, for the case that \(\mathcal{H}\) were true we attribute a real-valued loss \(L_{\mathcal{H}}(d) \geq 0\) to each \(d\); \(L_{\mathcal{A}}(d) = 0\) corresponds to a “right” decision \(d\), \(L_{\mathcal{A}}(d) > 0\) to the amount of loss taking the “wrong” decision \(d\). In the same way, for the case that \(\mathcal{A}\) were true we use \(L_{\mathcal{A}}(d) \geq 0\). Prior to random observations \(\mathbf{Z}\), the corresponding prior minimal mean decision loss (prior Bayes loss, prior Bayes risk) is given by

\[
\mathcal{R}(\pi_{\mathcal{H}}) := \inf_{d \in \mathbb{D}} \{\pi_{\mathcal{H}} \cdot L_{\mathcal{H}}(d) + (1 - \pi_{\mathcal{H}}) \cdot L_{\mathcal{A}}(d)\}.
\]

Based upon a concrete observation \(\mathbf{z}\), we decide for some “action” \(d \in \mathbb{D}\), operationalized by a decision rule \(d\) from the space of all possible observations to \(\mathbb{D}\) (i.e. \(d(\mathbf{z}) \in \mathbb{D}\). The corresponding posterior minimal mean decision loss (posterior Bayes loss, posterior Bayes risk) is defined by

\[
\mathcal{R}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{A}}) := \inf_{d} \{\pi_{\mathcal{H}} \cdot \int L_{\mathcal{H}}(d(\mathbf{z})) \, dP_{\mathcal{H}}(\mathbf{z}) + (1 - \pi_{\mathcal{H}}) \cdot \int L_{\mathcal{A}}(d(\mathbf{z})) \, dP_{\mathcal{A}}(\mathbf{z})\}
\]

where the infimum is taken amongst all “admissible” decision functions \(d\). Up to technicalities, one can show that

\[
\mathcal{R}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{A}}) = \mathcal{R}(\mathcal{H}, P_{\mathcal{H}}, P_{\mathcal{A}}) = \mathcal{R}(\mathcal{A}, P_{\mathcal{H}}, P_{\mathcal{A}}),
\]
with posterior probability (for \( \mathcal{H} \)) \( \pi_{\text{post}}(\mathcal{H}) := \frac{\pi_{\mathcal{H}} f_{P}(z)}{\pi_{\mathcal{H}} f_{P}(z) + (1-\pi_{\mathcal{H}}) f_{Q}(z)} \) in terms of the \( \lambda \)-density functions \( f_{P}(\cdot) \) and \( f_{Q}(\cdot) \) where \( \lambda \) is e.g. \( \frac{P+Q}{2} \) (or any measure such that \( P \) and \( Q \) are absolutely continuous w.r.t. \( \lambda \)). The difference \( \mathcal{J}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) := \mathcal{B}(\pi_{\mathcal{H}}) - \mathcal{B}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) \geq 0 \) can be interpreted as a statistical information measure in the sense of De Groot [55], and as degree of reduction of the decision risk due to observation. Let us first discuss the special case statistical information measure in the sense of De Groot [55], and as degree of ref

\[ \int_{0.1} \mathcal{J}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) \frac{1}{\pi_{\mathcal{H}}} \text{d}g_{\phi}(\pi_{\mathcal{H}}) = D_{\phi, S_{\lambda}^{\phi}(P_{\mathcal{S}}), S_{\lambda}^{\phi}(P_{\mathcal{H}}), 1, S_{\lambda}^{\phi}(P_{\mathcal{S}}), \lambda}(S_{\lambda}^{\phi}(P_{\mathcal{H}}), S_{\lambda}^{\phi}(P_{\mathcal{S}})) \]

(101)

where \( g_{\phi}(\pi) := -\phi'\left(\frac{1-\pi}{\pi}\right) \) is nondecreasing in \( \pi \in [0, 1] \). If \( \phi \) is twice differentiable, then one can simplify \( \int_{0.1} \mathcal{J}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) \frac{1}{\pi_{\mathcal{H}}} \text{d}g_{\phi}(\pi_{\mathcal{H}}) = \frac{1}{\pi_{\mathcal{H}}} \phi''\left(\frac{1-\pi_{\mathcal{H}}}{\pi_{\mathcal{H}}}\right) \text{d}\pi_{\mathcal{H}} \) in (101).

For the divergence generators \( \phi_{\alpha} \) with \( \alpha \in \mathbb{R} \) (cf. [20], [30], [31], [28]) one gets \( \int_{0.1} \mathcal{J}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) \frac{1}{\pi_{\mathcal{H}}} \text{d}g_{\phi}(\pi_{\mathcal{H}}) = \int_{0.1} \phi''\left(\frac{1-\pi_{\mathcal{H}}}{\pi_{\mathcal{H}}}\right) \text{d}\pi_{\mathcal{H}} \); see also Stummer [180,181,181] for an adaption to a context of path-observations of financial diffusion processes. (in our notation)

\[ \mathcal{J}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) = D_{\phi, S_{\lambda}^{\phi}(P_{\mathcal{S}}), S_{\lambda}^{\phi}(P_{\mathcal{H}}), 1, S_{\lambda}^{\phi}(P_{\mathcal{S}}), \lambda}(S_{\lambda}^{\phi}(P_{\mathcal{H}}), S_{\lambda}^{\phi}(P_{\mathcal{S}})) \]

for some appropriately chosen loss functions \( L_{\mathcal{H}}(\cdot), L_{\mathcal{S}}(\cdot) \) which depend on \( \phi \) and \( \pi_{\mathcal{H}} \); see also Stummer [180,181] for an adaption of the case \( \phi := \phi_{\alpha} \) with \( \alpha \in \mathbb{R} \) within a context of financial diffusion processes.

(3) as bounds of minimal mean decision losses:

In the context of (2), let us now discuss the binary decision space \( \mathcal{D} = \{ \mathcal{H}, \mathcal{S} \} \) where \( \mathcal{D}_{\mathcal{H}} \) stands for an action preferred in the case that \( P_{\mathcal{H}} \) were true. Furthermore, suppose that \( P_{\mathcal{H}} \) is absolutely continuous with respect to \( \lambda := P_{\mathcal{S}} \) having density function \( f_{P_{\mathcal{H}}}(\cdot) \); notice that \( f_{P_{\mathcal{S}}}(\cdot) = 1 \). For the loss functions \( L_{\mathcal{H}}(d) = c_{\mathcal{H}} \cdot 1_{\{d_{\mathcal{H}}\}}(d) \) and \( L_{\mathcal{S}}(d) = c_{\mathcal{S}} \cdot 1_{\{d_{\mathcal{S}}\}}(d) \) with some constants \( c_{\mathcal{H}} > 0, c_{\mathcal{S}} > 0 \), the posterior minimal mean decision loss (posterior Bayes loss) is

\[ \mathcal{B}(\pi_{\mathcal{H}}, P_{\mathcal{H}}, P_{\mathcal{S}}) = \int \min\{A_{\mathcal{H}} \cdot f_{P_{\mathcal{H}}}(z), A_{\mathcal{S}} \} \text{d}P_{\mathcal{S}}(z) \]

with constants \( A_{\mathcal{H}} := \pi_{\mathcal{H}} \cdot c_{\mathcal{H}} > 0, A_{\mathcal{S}} := (1 - \pi_{\mathcal{H}}) \cdot c_{\mathcal{S}} > 0 \). For this, Stummer & Vajda [180] have achieved the following bounds in terms of CASD-type power \( D := D_{\phi, S_{\lambda}^{\phi}(P_{\mathcal{S}}), S_{\lambda}^{\phi}(P_{\mathcal{H}}), 1, S_{\lambda}^{\phi}(P_{\mathcal{S}}), \lambda}(S_{\lambda}^{\phi}(P_{\mathcal{H}}), S_{\lambda}^{\phi}(P_{\mathcal{S}})) \) for

\[ \text{they also have shown some kind of “reciprocal”} \]
arbitrary $\chi \in ]0, 1[$

$$\mathcal{R}(\pi, P, P_{\text{af}}) \begin{cases} 
\geq \frac{A_{\pi}}{(A_{\pi} + A_{\text{af}}) \max\left\{ \frac{1}{1 - \chi}, \frac{1}{1 - \chi} \right\}} \cdot \left(1 - \chi \cdot (1 - \chi) \cdot D \right) \max\left\{ \frac{1}{1 - \chi}, \frac{1}{1 - \chi} \right\} \\
\leq A_{\pi} \cdot A_{\text{af}} \chi \cdot (1 - \chi \cdot (1 - \chi) \cdot D)
\end{cases}$$

(in an even slightly more general form), which can be very useful in case that the posterior minimal mean decision loss can not be computed explicitly. For instance, Stummer & Vajda [186] give applications to decision making of time-continuous, non-stationary financial stochastic processes.

(4) as auxiliary tools: for instance, in an i.i.d.-type Bayesian parametric model-misspecification context, Kleijn & van der Vaart [104] employ the reverse-Kullback-Leibler-distance minimizer

$$\hat{\theta} := \arg\inf_{\theta \in \Theta} D_{\phi}(Q_{\theta}, P_{tr}) = \arg\inf_{\theta \in \Theta} D_{\phi, S_{\lambda pd}(Q), S_{\lambda pd}(Q), 1, S_{\lambda pd}(Q), \lambda}(S_{\lambda pd}(Q_{\theta}), S_{\lambda pd}(P_{tr}))$$

(cf. (10) respectively (74) with $\phi = \phi_0$) in order to formulate and prove an asymptotic normality — under the unknown true out-of-model-lying data-generating distribution $P_{tr}$ — of the involved posterior parameter-distribution.

6 Variational Representations

Variational representations of (say) $\phi-$divergences, often referred to as dual representation, transform $\phi-$divergence estimation into an optimization problem on an infinite dimensional function space, generally, but may also lead to a simpler optimization problem when some knowledge on the class of measures $Q$ where $D_{\phi}(Q, P)$ has to be optimized is available; moreover, as already mentioned at the end of Section 1.3 above, such variational representations can also be employed to circumvent the crossover problem (CO1),(C2),(CO3).

To begin with, in the following we loosely sketch the corresponding general setting. We equip $\mathcal{M}$, the linear space of all finite signed measures (including all probability measures) on $(\mathcal{X}, \mathcal{B})$ with the so called $\tau$-topology, the coarsest one which makes the mapping $f \mapsto \int f dQ$ continuous for all measure $Q$ in $\mathcal{M}$ when $f$ runs in the class $\mathfrak{M}_b$ of all bounded measurable functions on $(\mathcal{X}, \mathcal{B})$. As an exemplary statistical incentive for the use of signed measures, let us mention the context where one wants to estimate, respectively test for, a mixture probability distribution $c \cdot Q_1 + (1 - c) \cdot Q_2$ with probability measures $Q_1, Q_2$ and $c \in [0, 1]$. In such a situation, it is sometimes technically useful to extend the range of $c$ beyond $[0, 1]$ which leads to a signed finite measure. As a next step, since the mapping $Q \mapsto D_{\phi}(Q, P)$ is convex and lower semi-continuous in the $\tau$-topology we deduce that the following result holds for all $Q$ in $\mathcal{M}$ and $P$ in $\mathcal{P}$:

$$\tilde{D}_{\phi}(Q, P) = \sup_{g \in \mathfrak{M}_b} \int_{\mathcal{X}} g(x) dQ(x) - \int_{\mathcal{X}} \phi_*(g(x)) dP(x) \quad (102)$$
where (cf. Broniatowski [35] in the Kullback-Leibler divergence case as well as Broniatowski & Keziou [38] for a general formulation)

\[ \widetilde{D}_\phi(Q, P) := \begin{cases} \int_X \phi \left( \frac{dQ}{dP}(x) \right) dP(x), & \text{for } Q << P, \\ \infty, & \text{else,} \end{cases} \]

is a slightly adopted version of the \( \phi \)-divergence defined in (10) (see also (74)) and \( \phi_a(x) := \sup_t (t \cdot x - \phi(t)) \) designates the Fenchel-Legendre transform of the generator \( \phi \), see [38] and Nguyen et al. [143]. The choice of the \( \tau \)-topology is motivated by statistical considerations, since most statistical functionals are continuous in this topology; see Groeneboom et al. [79]. This choice is in contrast with similar representations for the Kullback-Leibler divergences (see e.g. Dembo & Zeitouni [57], under the weak topology on \( \mathcal{P} \), for which the supremum in (102) is taken over all continuous bounded functions on \( (X, \mathcal{B}) \).

Representation (102) offers a useful mathematical tool to measure statistical similarity between data collections or to measure the directed distance between a distribution \( P \) (either explicit or known through sampling), and a class of distributions \( \Omega \), as well as to compare complex probabilistic models. The main practical advantage of variational formulas is that an explicit form of the probability distributions or their likelihood ratio, \( dQ/dP \), is not necessary. Only samples from both distributions are required since the difference of expected values in (102) can be approximated by statistical averages, in case both \( Q \) and \( P \) are known through sampling. In practice, the infinite-dimensional function space has to be approximated or even restricted. One attempt is the restriction of the function space to a reproducing kernel Hilbert space (RKHS) and the corresponding kernel-based approximation in Nguyen et al. [143]. In many cases of relevance, however, some information can be inserted in the description of the minimization problem of the form \( \inf \left\{ \tilde{D}_\phi(Q, P) : Q \in \Omega \right\} \) when some relation between \( P \) and all members in \( \Omega \) can be assumed. Such is the case in logistic models, or more globally in two sample problems, when it is assumed that \( dQ/dP \) belongs to some class of functions; for example we may assume that \( \Omega \) consists in all distributions such that \( x \mapsto (dQ/dP)(x) \) belongs to some parametric class. This requires some analysis around (102), which is handled now.

The supremum in equation (102) may not be reached, even in elementary cases. Consider the case when \( \phi = \phi_1 \), hence the case when \( \tilde{D}_\phi(Q, P) \) is the Kullback-Leibler divergence between \( Q \) and \( P \), and assume that both \( Q \) and \( P \) are two Gaussian probability measures on \( \mathbb{R} \) with same variance and different mean values. Then it is readily checked that the supremum in (102) is reached on a polynomial with degree 2, hence outside of \( \mathcal{M}_n \). For statistical purposes it is relevant that formula (102) holds with attainment; indeed the supremum, in case when \( \tilde{D}_\phi(Q, P) \) is finite, is reached at \( g := \phi' (dQ/dP) \), therefore, in case when \( \phi \) is differentiable, on a function which may not be bounded.

It is also of interest to consider (102) in the case when \( P \) is atomic and \( Q \) is a continuous distribution; for example let \( (X_1, \ldots, X_n) \) be an i.i.d. sample under some probability measure \( R \) on \( \mathbb{R} \), and consider \( Q \) a probability measure
In case when we define $M$ variational form of the divergence in order to circumvent this obstacle. Assuming it stands. Some more structure and information has to be incorporated in the inference can be performed about $R$ making use of the variational form as it stands. Some more structure and information has to be incorporated in the variational form of the divergence in order to circumvent this obstacle. Assuming that $\phi$ is a differentiable function in its domain, the supremum in (102) is reached at $g_s := \phi'(dQ/dP)$ as checked by substitution. Let $\mathcal{F}$ be a class of functions containing all functions $\phi'(dQ/dP)(x)$ as $Q$ runs in a given model $\Omega$. Consider the subspace $\mathcal{M}_Q$ of all finite signed measures $Q$ such that $\int |f| d|Q|$ is finite for all function $f$ in $\mathcal{F}$, then similarly as in (102) we may obtained the following variational form of $\tilde{D}_\phi(Q, P)$, which is valid when $Q$ belongs to $\mathcal{M}_Q$ and $P$ belongs to $\mathcal{F}$

$$\tilde{D}_\phi(Q, P) = \sup_{g \in \mathcal{M}_b \cup \mathcal{F}} \int_{\mathcal{X}} g(x) dQ(x) - \int_{\mathcal{X}} \phi_s(g(x)) dP(x)$$

in which we substituted $\mathcal{M}_b$ by the broader class $\mathcal{M}_b \cup \mathcal{F}$ which may contain unbounded functions; note that (103) is valid for a smaller class of measures $Q$ than (102).

For instance, in the above example pertaining to the Kullback-Leibler divergence and both $P$ is Gaussian on $\mathbb{R}$ and $Q$ belongs to the class $\Omega$ of all Gaussian distributions on $\mathbb{R}$ with same variance as $P$, then $\mathcal{F}$ consists of all polynomial functions with degree 2, and the supremum in (103) is attained. Looking at the case when $P$ is substituted by $P_n$ and $Q$ is absolutely continuous, and since $\tilde{D}_\phi(Q, P_n)$ does not convey any information from the data, we are led to define a restriction to the supremum operation on the space $\langle \mathcal{M}_b \cup \mathcal{F} \rangle$; since we assumed that $\phi'(dQ/dP) \in \mathcal{F}$ for any $Q$ in $\Omega \subset \mathcal{M}_Q$ we have

$$\tilde{D}_\phi(Q, P) = \sup_{g \in \mathcal{F}} \int_{\mathcal{X}} g(x) dQ(x) - \int_{\mathcal{X}} \phi_s(g(x)) dP(x)$$

which is valid only when $Q << P$. We thus can define a new “pseudo divergence”, say $\tilde{D}_\phi(Q, P)$ which coincides with $\tilde{D}_\phi(Q, P)$ in these cases, and which takes finite values depending on the data when $P$ is substituted by $P_{n_{emp}}$. In that case we define

$$\tilde{D}_\phi(Q, P_{n_{emp}}) := \sup_{g \in \mathcal{F}} \int_{\mathcal{X}} g(x) dQ(x) - \frac{1}{n} \sum_{i=1}^{n} \phi_s(X_i),$$

which is the starting point of variational divergence-based inference; see Broniatowski & Keziou [39]. Note that the above formula does not require any grouping

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23 In case when $\phi$ is not differentiable at some point, then the supremum in (103) should satisfy $g_s(x) \in \partial \phi(dQ/dP)(x)$ for all $x$ in $\mathcal{F}$, where $\partial \phi(t)$ is the subdifferential set of the convex function $\phi$ at point $t$, $\partial \phi(t) := \{z \in \mathbb{R} : \phi(s) \geq \phi(t) + z(s - t), \forall s \in \mathbb{R}\}$. 

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or smoothing. Also the resulting estimator of the likelihood ratio \( dQ^*/dP \) where

\[
Q^* := \arg \inf_{Q \in \Omega} \hat{D}_\phi(Q, P)
\]

results from a double optimization, the inner one pertaining to the estimation of \( g_\phi(Q) \) solving (105) for any \( Q \) in \( \Omega \). Assuming that \( \{\phi_\phi(g), g \in \mathcal{F}\} \) is a Glivenko-Cantelli class of functions in some appropriate metrics provides the ingredients to handle convergence properties of the estimators. The choice of the divergence \( \phi \) may obey robustness vs efficiency equilibrium, as exemplified in parametric models; see also Al Mohamad [7].

Formula (104) can be obtained through simple convexity considerations (see p. 172 of Liese & Vajda [109] or Theorem 17 of Liese & Vajda [110]) and is used when \( \mathcal{F} \) consists in all the functions \( \phi' (dQ/dP) \) as \( Q \) and \( P \) run in some parametric model. In a more general (semiparametric or nonparametric setting), formula (103) is adequate for inference in models consisting in probability distributions \( Q \) which integrate functions in \( \mathcal{F} \), and leads to numerical optimization making use of regularity assumptions on the likelihood ratio \( dQ/dP \).

7 Some Further Variants

Extending the (say) \( \phi \)--divergence definition outside the natural context of probability measures appear as necessary in various situations; for example models defined by conditions pertaining to expectations of order statistics (or more generally of L-statistics) are ubiquitous in meteorology, hydrology or in finance through constraints on the value at risk, for example on the Distortion Risk Measure (DRM) of index \( \alpha \), which is defined in terms of the quantile function \( F^- \) associated to the distribution function \( F \) on \( \mathbb{R}^+ \) through \( \int_0^1 F^-(u) \cdot 1_{(u>\alpha)} \, du \).

Note that this class of constraints are not linear with respect to \( F \) but with respect to \( F^- \) only; so characterization of the projection of some measure \( P \) on such sets of measures are not characterized by exponential family types of distributions. Inference on whether a distribution \( P \) satisfies this kind of constraints leads to the extension of the definition of divergences between quantile measures, which might be signed measures. Variational representations for inference can be defined and projections on linear constraints pertaining to quantile measures can be characterized; see Broniatowski & Decurninge [37]. Also in the statistical frame, testing for the number of components in a finite mixture requires the extension of the definition of divergences to not-necessarily positive argument, such as occurs for the Pearson \( \chi^2 \)--divergence; this allows to replace the non-regular statistical task of estimating (testing) a value of a parameter at the border of its domain into a regular problem, at the cost of introducing mixtures with negative weights; an attempt in this direction is made in Broniatowski et al. [41].

For large-dimensional spaces \( \mathcal{F} \), variational representations of \( \phi \)--divergences (i.e. CASM divergences) offer significant theoretical insights and practical advantages in numerous research areas. Recently, they have gained popularity in machine learning as a tractable and scalable approach for training probabilistic models and for statistically differentiating between data distributions; see e.g. Birrell et al. [31].
Explicit methods to estimate the $\phi$–divergence and likelihood ratio between two probability measures known through sampling (hence substituting $Q$ and $P$ in (104) by their empirical counterparts) have been considered making some hypothesis on its regularity, or adding some penalty term in terms of the assumed complexity of the class $\mathcal{F}$; examples include Sobolev classes of functions or Reproducing Kernel Hilbert Space approximations; see Nguyen et al. [143] for explicit methods and properties of the estimators.

Extensions of the basic divergence formula as given in (104) to include some extra inner optimization term have been proposed in by Birrell et al. [30] under the name of $(f-\Gamma)$–divergences; this new class encompasses both the $\phi$–divergence class and many integral probability metrics (see also Sriperumbudur et al. [177] on the overlap of the latter two); they provide uncertainty quantification bounds for misspecified models in terms of the $\phi$–divergence between the truth and the model, somehow in a similar way as considered in cryptology (see Arikan & Merhav [9] and subsequent extensive literature). Also, [30] apply optimization of those divergences to training Generative Adversial Networks (GAN).

Another area where extension of the $\phi$–divergences (i.e. CASM divergences) to signed measures is useful is related to general optimization problems, where one aims at projecting a vector (or a function) on a class of vectors (or a class of functions); we refer to Broniatowski & Stummer [43] for an extensive treatment of such problems in the finite dimensional case.

As already indicated above, there are also divergences between stochastic processes where $\mathcal{X}$ is the set of all possible paths (i.e. all time-evolution scenarios). By nature, the analysis of the outcoming (say) $\phi$–divergences between two distributions on the path space $\mathcal{X}$ may become very involved. For instance, power divergences between diffusion processes — and applications to finance, Bayesian decision making, etc. — were treated in Stummer [179,180,181] as well as in Stummer & Vajda [186] (see also the corresponding binomial-process-approximations in Stummer & Lao [185]); in contrast, Kammerer & Stummer [94] study power divergences between Galton-Watson branching processes with immigration and apply the outcomes to optimal decision making in the presence of a pandemics (such as e.g. COVID-19).

For continuous, convex, homogeneous functions $\phi : \mathbb{R}_+^K \rightarrow \mathbb{R}$, general multivariate $\phi$–dissimilarities of the form

$$D_\phi(Q, P) = \int_{\mathcal{X}} \phi \left( \frac{dQ_1}{dP}(x), \ldots, \frac{dQ_K}{dP}(x) \right) dP(x)$$

(which need not necessarily be divergences in the sense of a multivariate analogue of the above axioms (D1), (D2)) have been first introduced by Györfi & Nemetz [81, 82] and later on investigated by e.g. Zografos [208] for stratified random sampling, by Zografos [204] for hypothesis testing, and by Garcia-Garcia & Williamson [72] for multiclass classification problems. As noticed by [81], the multivariate $\phi$–dissimilarities cover as special cases Matusita’s affinity [122], the more general Toussaint’s affinity [191, 192] (which by nature is
a multivariate (form of a) Hellinger integral being also called Hellinger transform in Liese & Miescke [108]), and — in the bivariate case \( K = 2 \) — also the \( \phi \)-divergences (i.e the CASM divergences). Special multivariate \( \phi \)-divergences \( \mathcal{D}_{\phi}(Q, P) \) were e.g. employed by Toussaint [191] [192] (see also Menendez et al. [128]) in form of an average over all pairwise Jeffreys divergences (where the latter are sum-symmetrized Kullback-Leibler divergences), by Menendez et al. [127] in form of a convex-combination of “Kullback-Leibler divergences between each individual probability distribution and the convex-combination of all probability distributions” (i.e. multivariate extensions of the Jensen-Shannon divergence), and by Werner & Ye [203] in form of integrals over the geometric mean of all the integrands in pairwise \( \phi \)-divergences (and they even flexibilize to components of a \( \mathbb{R}_+^K \)-valued function \( \phi \), and call the outcome a mixed \( \phi \)-divergence).

A general “natural multivariate” extension of a \( \phi \)-divergence in the sense of CASM — called multidistribution \( \phi \)-divergence — has been given by Duchi et al. [60] who employed this to multiclass classification problems (see also Tan & Zhang [190] for further application to loss functions and regret bounds). The general multivariate \( \phi \)-dissimilarity between signed measures (rather than the more restrictive probability distributions) — under assumptions which imply the multivariate analogue of the above axioms \((D1), (D2)\) — has been introduced by Keziou [98] and used for the analysis of semiparametric multisample density ratio models (for the latter, see e.g. Keziou & Leoni-Aubin [99] and Kanamori et al. [95]).

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