PAC-Bayesian Theory for Transductive Learning: Supplementary Material

Lemma S9. *Let $\beta \in [0,1]$, $q \in [0,1]$ and $p \in (0,1)$. We have*

$$\mathcal{D}^{\star}_{\beta}(q,p) \;=\; \mathcal{D}_{\mathrm{KL}}(q,p) + \frac{1-\beta}{\beta}\,\mathcal{D}_{\mathrm{KL}}\Big(\frac{p-\beta\, q}{1-\beta}, p\Big)\,,$$

where $\mathcal{D}_{\mathrm{KL}}(\cdot,\cdot)$ and $\mathcal{D}^{\star}_{\beta}(\cdot,\cdot)$ are defined respectively by Equations (3) and (8) of the main paper.

Proof.

$$\begin{aligned}
&\mathcal{D}^{\star}_{\beta}(q,p)\\
={}& q\ln\beta\frac{q}{p} + (\frac{p}{\beta}-q)\ln(1-\beta\frac{q}{p}) + (1-q)\ln\beta\frac{1-q}{1-p} + (\frac{1-p}{\beta}+q-1)\ln(1-\beta\frac{1-q}{1-p}) - \ln\beta - (\frac{1}{\beta}-1)\ln(1-\beta)\\
={}& q\ln\frac{q}{p} + q\ln\beta + (\frac{p}{\beta}-q)\ln(1-\beta\frac{q}{p}) + (1-q)\ln\frac{1-q}{1-p} + (1-q)\ln\beta + (\frac{1-p}{\beta}+q-1)\ln(1-\beta\frac{1-q}{1-p}) - \ln\beta\\
&\quad - (\frac{1}{\beta}-1)\ln(1-\beta)\\
={}& q\ln\frac{q}{p} + (\frac{p}{\beta}-q)\ln(1-\beta\frac{q}{p}) + (1-q)\ln\frac{1-q}{1-p} + (\frac{1-p}{\beta}+q-1)\ln(1-\beta\frac{1-q}{1-p}) - (\frac{1}{\beta}-1)\ln(1-\beta)\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + (\frac{p}{\beta}-q)\ln(1-\beta\frac{q}{p}) + (\frac{1-p}{\beta}+q-1)\ln(1-\beta\frac{1-q}{1-p}) - (\frac{1}{\beta}-1)\ln(1-\beta)\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + (\frac{p}{\beta}-q)\ln(1-\beta\frac{q}{p}) + (\frac{1-p}{\beta}+q-1)\ln(1-\beta\frac{1-q}{1-p}) - \left[(\frac{p}{\beta}-q) + (\frac{1-p}{\beta}+q-1)\right]\ln(1-\beta)\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + (\frac{p}{\beta}-q)\left[\ln(1-\beta\frac{q}{p}) - \ln(1-\beta)\right] + (\frac{1-p}{\beta}+q-1)\left[\ln(1-\beta\frac{1-q}{1-p}) - \ln(1-\beta)\right]\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + (\frac{p}{\beta}-q)\ln\frac{1-\beta\frac{q}{p}}{1-\beta} + (\frac{1-p}{\beta}+q-1)\ln\frac{1-\beta\frac{1-q}{1-p}}{1-\beta}\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + \frac{1-\beta}{\beta}\left[\frac{p-\beta q}{1-\beta}\ln\frac{1-\beta\frac{q}{p}}{1-\beta} + \left(1-\frac{p-\beta q}{1-\beta}\right)\ln\frac{1-\beta\frac{1-q}{1-p}}{1-\beta}\right]\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + \frac{1-\beta}{\beta}\left[\frac{p-\beta q}{1-\beta}\ln\frac{\frac{p-\beta q}{1-\beta}}{p} + \left(1-\frac{p-\beta q}{1-\beta}\right)\ln\frac{1-\frac{p-\beta q}{1-\beta}}{1-p}\right]\\
={}& \mathcal{D}_{\mathrm{KL}}(q,p) + \frac{1-\beta}{\beta}\,\mathcal{D}_{\mathrm{KL}}\Big(\frac{p-\beta\, q}{1-\beta}, p\Big)\,.
\end{aligned}$$

□

Lemma S10. *Let m, N, K be integers such that $\lambda \le m \le N-\lambda$ and $0 \le K \le N$. We have*

$$F(k) \;=\; \frac{\alpha(k,K)\,\alpha(m-k,N-K)}{\alpha(m,N)} \;\le\; e^{\frac{1}{6\lambda}}\sqrt{2\pi m(1-\tfrac{m}{N})}\,,$$

for $k = \max[0, K+m-N]$ and $k = \min[m, K]$.

Proof. First, let study the case $k = \max[0, K+m-N]$.

If $0 \ge K+m-N$, then $F(0) = \frac{\alpha(m,N-K)}{\alpha(m,N)}$ increases according to K, and its maximum is reached at $K = N-m$. We have

$$F(0) \;\le\; \frac{\alpha(m,m)}{\alpha(m,N)} \;=\; \frac{1}{\alpha(m,N)}\,.$$

If $0 \le K+m-N$, then $F(K+m-N) = \frac{\alpha(K+m-N,K)\,\alpha(N-K,N-K)}{\alpha(m,N)} = \frac{\alpha(K+m-N,K)}{\alpha(m,N)}$ decreases according to K, and its maximum is reached at $K = N-m$. Then

$$F(K+m-N) \;=\; F(0) \;\le\; \frac{1}{\alpha(m,N)}\,.$$

Now, let us study the case $k = \min[m, K]$.

If $m \le K$, then $F(m) = \frac{\alpha(m,K)}{\alpha(m,N)}$ decreases according to K, and its maximum is reached at $K = m$. We have

$$F(m) \;\le\; \frac{\alpha(m,m)}{\alpha(m,N)} \;=\; \frac{1}{\alpha(m,N)}\,.$$

If $m \ge K$, then $F(K) = \frac{\alpha(K,K)\,\alpha(m-K,N-K)}{\alpha(m,N)} = \frac{\alpha(m-K,N-K)}{\alpha(m,N)}$ increases according to K, and its maximum is reached at $K = m$. Then

$$F(K) \;=\; F(m) \;\le\; \frac{1}{\alpha(m,N)}\,.$$

Finally, by Lemma 3, we get

$$\frac{1}{\alpha(m,N)} \;\le\; \frac{1}{\sqrt{\frac{N}{2\pi m(N-m)}}e^{-\frac{1}{12m}-\frac{1}{12(N-m)}}} \;=\; \sqrt{2\pi\, m(1-\tfrac{m}{N})}e^{\frac{1}{12m}+\frac{1}{12(N-m)}} \;\le\; e^{\frac{1}{6\lambda}}\sqrt{2\pi m(1-\tfrac{m}{N})}\,.$$

$\square$

Lemma S11. *Let m, N, K be integers such that $0 \le m \le N$ and $0 \le K \le N$. We have*

$$\sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\frac{1}{k}+\frac{1}{K-k}\right)\left(\frac{1}{m-k}+\frac{1}{(N-K)-(m-k)}\right)} \;\le\; 2\sum_{k=1}^{m-1}\frac{1}{k} \tag{20}$$

$$\le\; 2\big(1+\ln(m-1)\big)\,,$$

where

$$\mathcal{K}^*_{mNK} \;=\; \big\{\max[0, K+m-N]+1, \ldots, \min[m,K]-1\big\}\,,$$

and we have an equality at Line (20) when $m = K = N-K$.

Proof. First, examine the case where $m = K = N-K$.

$$\sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{(N-K)-(m-k)}\right)}$$

$$= \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{m-(m-k)}\right)} \;=\; \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{k}\right)}$$

$$= \sum_{k\in\mathcal{K}^*_{mNK}} \left(\tfrac{1}{k}+\tfrac{1}{m-k}\right) \;=\; \sum_{k\in\mathcal{K}^*_{mNK}} \tfrac{1}{k} + \sum_{k\in\mathcal{K}^*_{mNK}} \tfrac{1}{m-k} \;=\; 2\sum_{k\in\mathcal{K}^*_{mNK}} \tfrac{1}{k} \;=\; 2\sum_{k=1}^{m-1}\tfrac{1}{k}\,.$$

The last equality comes from the fact that when $m = K = N-K$, the set $\mathcal{K}^*_{mNK}$ equals $\{1, 2, \ldots, m-1\}$. The two sums are then equivalent.

Let us now examine all other cases. We distinguish 4 distinct cases, where each demonstration consists in using the case's inequality such that the expression's value raises.

Case 1: $m \le (N-K)$ and $m \le K$.

$$\sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{(N-K)-(m-k)}\right)}$$

$$\le \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{(N-K)-(m-k)}\right)}$$

$$\le \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{m-(m-k)}\right)} \;=\; \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{k}\right)}$$

$$= \sum_{k\in\mathcal{K}^*_{mNK}} \left(\tfrac{1}{k}+\tfrac{1}{m-k}\right) \;=\; \sum_{k\in\mathcal{K}^*_{mNK}} \tfrac{1}{k} + \sum_{k\in\mathcal{K}^*_{mNK}} \tfrac{1}{m-k} \;=\; \sum_{k=1}^{m-1}\tfrac{1}{k} + \sum_{k=1}^{m-1}\tfrac{1}{m-k} \;=\; 2\sum_{k=1}^{m-1}\tfrac{1}{k}\,.$$

Case 2: $m \le (N-K)$ and $m > K$.

$$\sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{m-k}+\tfrac{1}{(N-K)-(m-k)}\right)}$$

$$\le \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{K-k}+\tfrac{1}{(N-K)-(m-k)}\right)}$$

$$\le \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{K-k}+\tfrac{1}{m-(m-k)}\right)} \;=\; \sum_{k\in\mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right)\left(\tfrac{1}{K-k}+\tfrac{1}{k}\right)}$$

$$= \sum_{k\in\mathcal{K}^*_{mNK}} \left(\tfrac{1}{k}+\tfrac{1}{K-k}\right) \;=\; \sum_{k=1}^{K-1}\left(\tfrac{1}{k}+\tfrac{1}{K-k}\right) \;=\; \sum_{k=1}^{K-1}\tfrac{1}{k} + \sum_{k=1}^{K-1}\tfrac{1}{K-k} \;=\; 2\sum_{k=1}^{K-1}\tfrac{1}{k} \;<\; 2\sum_{k=1}^{m-1}\tfrac{1}{k}\,.$$

Case 3: $m > (N-K)$ and $m \leq K$.

$$
\begin{aligned}
&\sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k} + \tfrac{1}{K-k}\right)\left(\tfrac{1}{m-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad \leq \sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k} + \tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad \leq \sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{m-k}\right)\left(\tfrac{1}{m-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad = \sum_{k \in \mathcal{K}^*_{mNK}} \left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{m-k}\right) \;=\; \sum_{k=m-N+K+1}^{m-1} \left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{m-k}\right) \\
&\qquad = 2 \sum_{k=m-N+K+1}^{m-1} \tfrac{1}{m-k} \;<\; 2 \sum_{k=1}^{m-1} \tfrac{1}{m-k} \;=\; 2 \sum_{k=1}^{m-1} \tfrac{1}{k}\,.
\end{aligned}
$$

Case 4: $m > (N-K)$ and $m > K$.

$$
\begin{aligned}
&\sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k} + \tfrac{1}{K-k}\right)\left(\tfrac{1}{m-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad \leq \sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{k} + \tfrac{1}{K-k}\right)\left(\tfrac{1}{K-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad \leq \sum_{k \in \mathcal{K}^*_{mNK}} \sqrt{\left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{K-k}\right)\left(\tfrac{1}{K-k} + \tfrac{1}{(N-K)-(m-k)}\right)} \\
&\qquad = \sum_{k \in \mathcal{K}^*_{mNK}} \left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{K-k}\right) \;=\; \sum_{k=m-N+K+1}^{K-1} \left(\tfrac{1}{(N-K)-(m-k)} + \tfrac{1}{K-k}\right) \\
&\qquad = 2 \sum_{k=m-N+K+1}^{K-1} \tfrac{1}{K-k} \;\leq\; 2 \sum_{k=1}^{K-1} \tfrac{1}{K-k} \;=\; 2 \sum_{k=1}^{K-1} \tfrac{1}{k} \;\leq\; 2 \sum_{k=1}^{m-1} \tfrac{1}{k}\,.
\end{aligned}
$$

For each case, we showed that the expression is lower or equal than $2\sum_{k=1}^{m-1} \frac{1}{k}$. Using the approximation by definite integral technique, we obtain as needed

$$
2 \sum_{k=1}^{m-1} \frac{1}{k} \;\leq\; 2\left(1 + \int_1^{m-1} \frac{1}{x}\, dx\right) \;=\; 2\Big(1 + \ln(m-1)\Big)\,.
$$

□

Theorem S12 (Fixed version of Derbeko et al. [2004], Theorem 18)**.** *For any set Z of N examples, for any set $\mathcal{H}$ of classifiers, for any prior distribution P on $\mathcal{H}$, for any $\delta \in (0,1]$, with a probability at least $1-\delta$ over the choice S of m examples among Z,*

$$\forall Q \text{ on } \mathcal{H}: \quad R_Z(G_Q) \;\le\; R_S(G_Q) + \sqrt{\frac{1-\frac{m}{N}}{2(m-1)}\left[\mathrm{KL}(Q\|P) + \ln\tfrac{m}{\delta} + 7\ln(N{+}1)\right]}.$$

Proof. Let us use the shortcut notations $R_S = R_S(G_Q)$ and $R_Z = R_Z(G_Q)$. We start from Equation (17) of Derbeko et al. [2004]:

$$\mathcal{D}_{\mathrm{KL}}(R_S, R_Z) + \frac{1-\frac{m}{N}}{\frac{m}{N}}\,\mathcal{D}_{\mathrm{KL}}\Big(\frac{R_Z - \frac{m}{N}R_S}{1-\frac{m}{N}}, R_Z\Big) - \frac{7}{m}\log(N+1) \;\le\; \frac{\mathrm{KL}(Q\|P) + \ln\frac{m}{\delta}}{m-1}\,.$$

Applying Pinsker's inequality ($\mathcal{D}_{\mathrm{KL}}(q,p) \ge 2(q-p)^2$) twice, we get

$$\begin{aligned}\mathcal{D}_{\mathrm{KL}}(R_S, R_Z) + \frac{1-\frac{m}{N}}{\frac{m}{N}}\,\mathcal{D}_{\mathrm{KL}}\Big(\frac{R_Z - \frac{m}{N}R_S}{1-\frac{m}{N}}, R_Z\Big) \quad &\ge \quad 2(R_S - R_Z)^2 + 2(\tfrac{N}{m}-1)\Big(\tfrac{R_Z-\frac{m}{N}R_S}{1-\frac{m}{N}} - R_Z\Big)^2\\ &= \quad \frac{2(R_S-R_Z)^2}{1-\frac{m}{N}}.\end{aligned}$$

Hence, the result is obtained by isolating R_Z in

$$\frac{2(R_S-R_Z)^2}{1-\frac{m}{N}} - \frac{7}{m}\log(N+1) \;\le\; \frac{\mathrm{KL}(Q\|P) + \ln\frac{m}{\delta}}{m-1}\,.$$

□

Remark. Note that Derbeko et al. [2004] state their result as bound on $R_U(G_Q)$, *i.e.*, a bound on the risk on the unlabeled examples. As

$$R_Z(h) \;=\; \frac{1}{N}\Big(mR_S(h) + (N{-}m)R_U(h)\Big),$$

the statement of Theorem S12 above can be directly converted from a bound on $R_Z(G_Q)$ to a bound of $R_U(G_Q)$. We then have

$$\frac{1}{N}\Big(mR_S(h) + (N{-}m)R_U(h)\Big) \quad\le\quad R_S(G_Q) + \sqrt{\frac{1-\frac{m}{N}}{2(m-1)}\left[\mathrm{KL}(Q\|P) + \ln\tfrac{m}{\delta} + 7\ln(N{+}1)\right]},$$

and

$$R_U(h) \quad\le\quad R_S(G_Q) + \sqrt{\frac{1}{2(m-1)(1-\frac{m}{N})}\left[\mathrm{KL}(Q\|P) + \ln\tfrac{m}{\delta} + 7\ln(N{+}1)\right]}.$$

More Empirical Study of different $\mathcal{D}$-functions

We show results similar to Figure 1, this time considering $R_S(G_Q) = 0.1$ and $R_S(G_Q) = 0.01$ in Figures 2 and 3. As these figures are generated in exactly the same fashion than Figure 1, we omit unnecessary explanation.

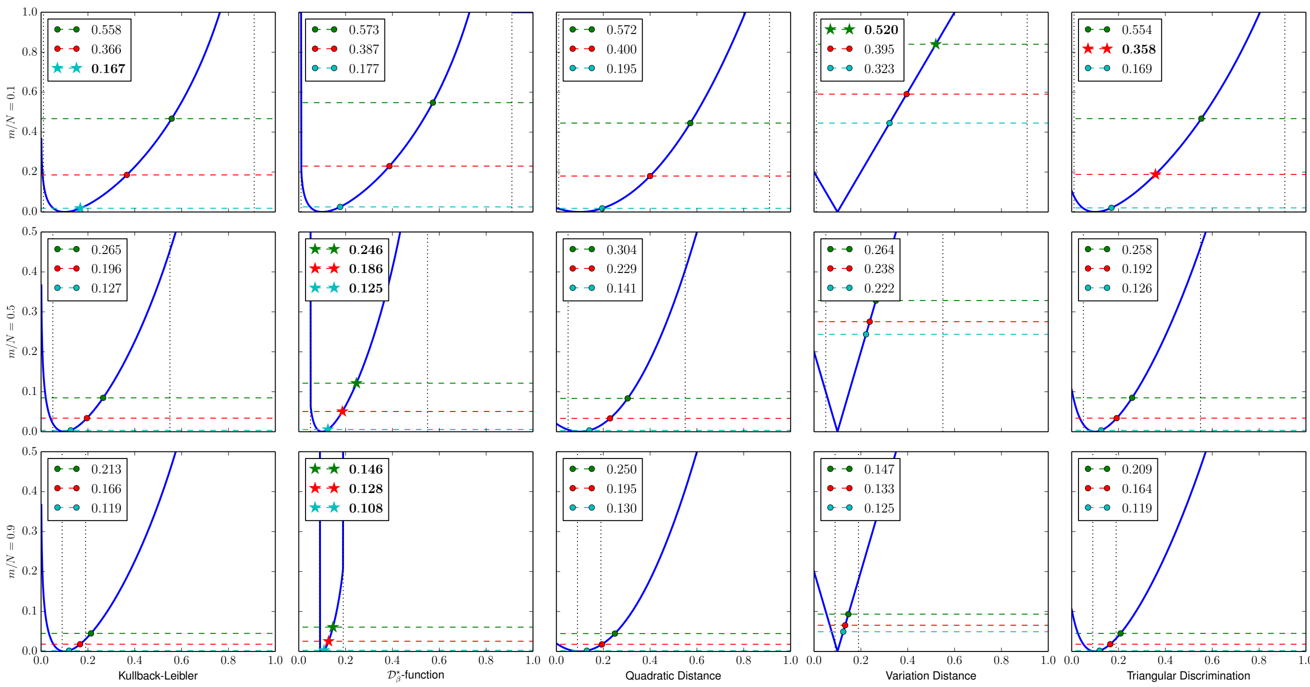

Figure 2: Study of the behavior of bounds obtained by Theorem 5. All graphics consider $R_S(G_Q) = 0.1$, $\mathrm{KL}(Q\|P) = 5$ and $\delta = 0.05$.

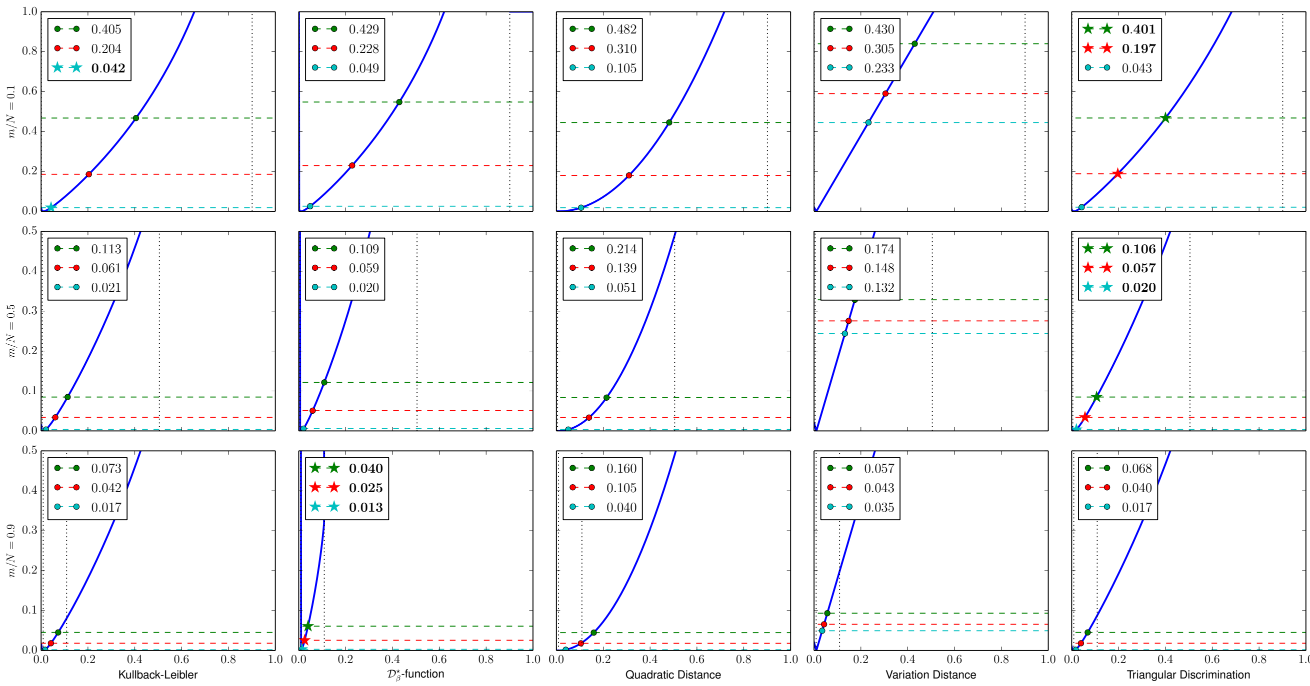

Figure 3: Study of the behavior of bounds obtained by Theorem 5. All graphics consider $R_S(G_Q) = 0.01$, $\mathrm{KL}(Q\|P) = 5$ and $\delta = 0.05$.