On Loss Functions and f-Divergences

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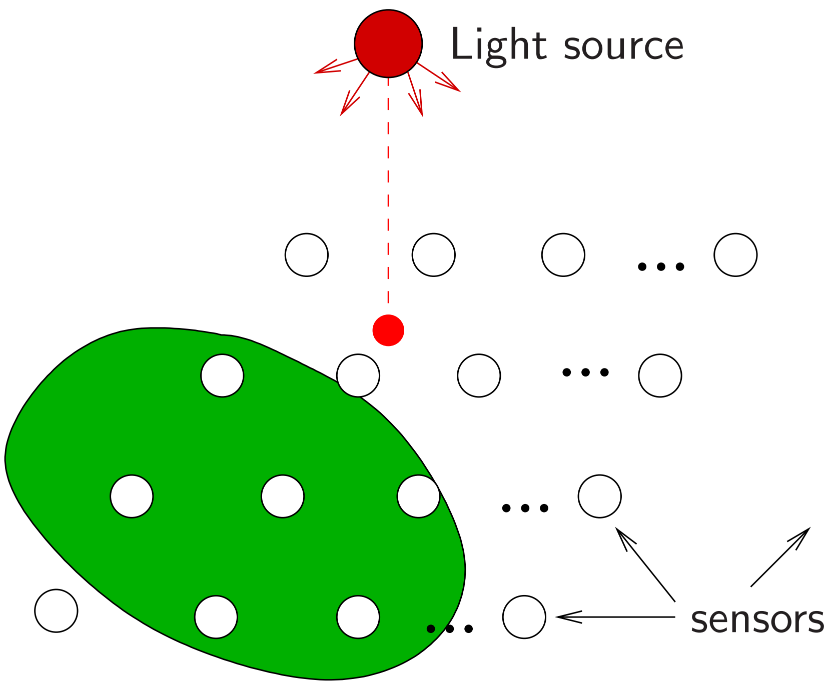
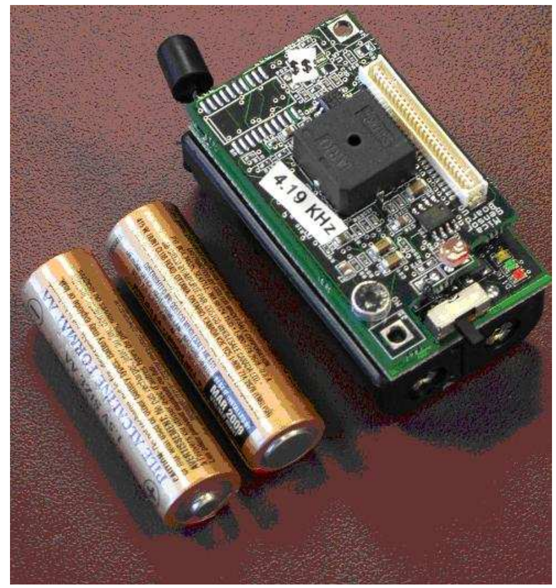
Surrogate Loss Functions

- Various losses are widely used as in the classical decision theoretic setting to evaluate procedures
- A wide range of "losses" are also used as criteria for building procedures; e.g., M-estimators, Z-estimators, empirical risk estimators, etc
- A very large literature on showing that such losses yield defensible inference
- A particularly active area: "surrogate loss functions" for discrimination
- We develop a mathematical understanding of the properties of such loss functions, via a connection to f-divergences
  - our work is based on seminal work of Blackwell (1951)

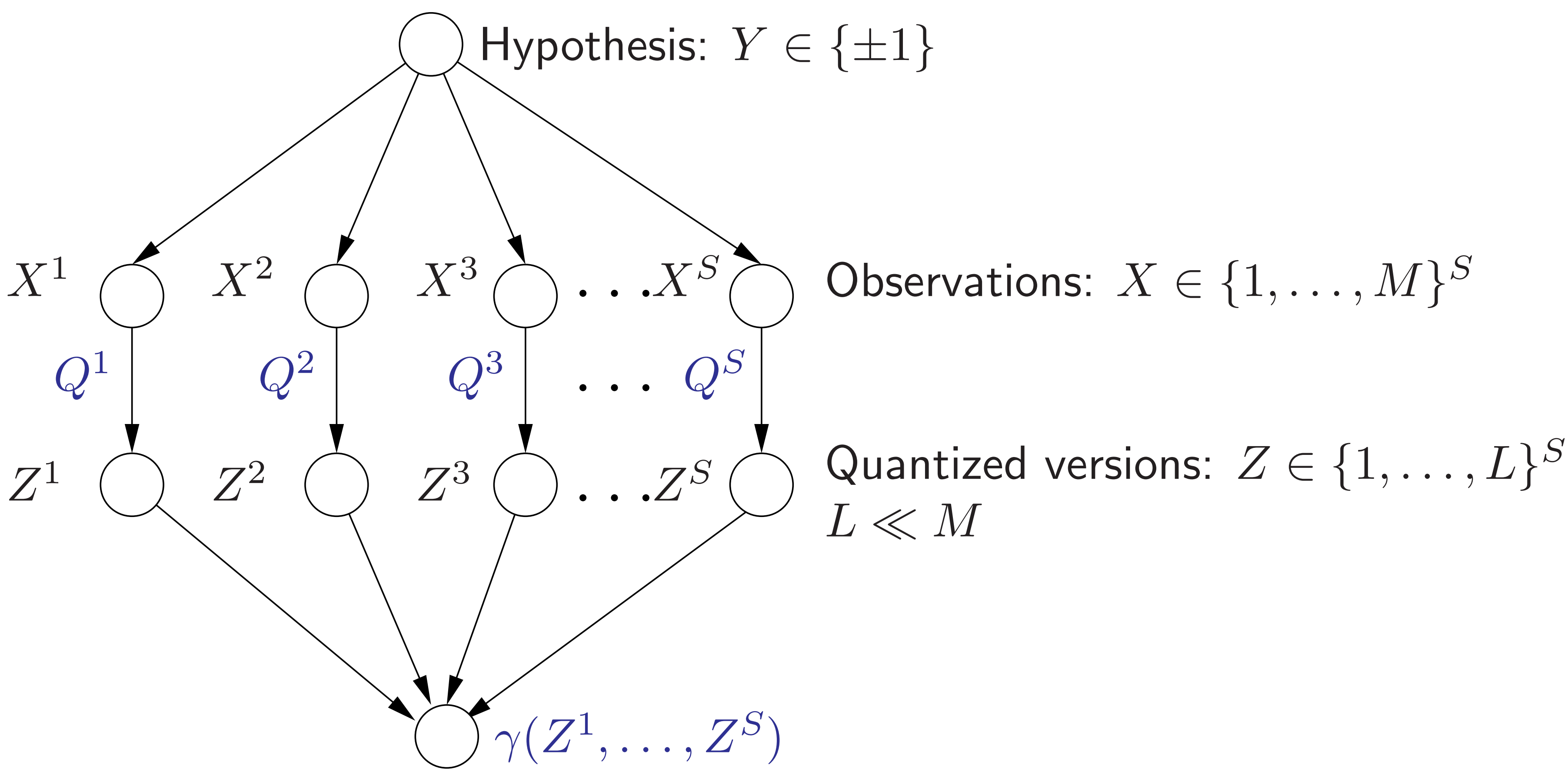
Motivating Example: Decentralized Detection





- Wireless network of motes equipped with sensors (e.g., light, heat, sound)
- Limited battery: can only transmit quantized observations
- Is the light source above the green region?

Decentralized Detection



Decentralized Detection (cont.)

- General set-up:
  - data are (X, Y) pairs, assumed sampled i.i.d. for simplicity, where $Y \in \{0, 1\}$
  - given X, let $Z = Q(X)$ denote the covariate vector, where $Q \in \mathcal{Q}$, where $\mathcal{Q}$ is some set of random mappings (can be viewed as an experimental design)
  - consider a family $\{\gamma(\cdot)\}$, where γ is a discriminant function lying in some (nonparametric) family Γ

- Problem: Find the decision $(Q; \gamma)$ that minimizes the probability of error $P(Y \neq \gamma(Z))$

- Applications include:
  - decentralized compression and detection
  - feature extraction, dimensionality reduction
  - problem of sensor placement

Perspectives

- *Signal processing literature*
  - everything is assumed known except for Q—the problem of "decentralized detection" is to find Q
  - this is done via the maximization of an "f-divergence" (e.g., Hellinger distance, Chernoff distance)
  - basically a heuristic literature from a statistical perspective (plug-in estimation)

- *Statistical literature*
  - Q is assumed known and the problem is to find γ
  - this is done via the minimization of an "surrogate loss function" (e.g., boosting, logistic regression, support vector machine)
  - decision-theoretic flavor; consistency results

f-divergences (Ali-Silvey Distances)

The f-divergence between measures μ and π is given by

$$I_f(\mu, \pi) := \sum_z \pi(z) f\left(\frac{\mu(z)}{\pi(z)}\right).$$

where $f : [0, +\infty) \to \mathbb{R} \cup \{+\infty\}$ is a continuous convex function

- Kullback-Leibler divergence: $f(u) = u \log u$.

$$I_f(\mu, \pi) = \sum_z \mu(z) \log \frac{\mu(z)}{\pi(z)}.$$

- variational distance: $f(u) = |u - 1|$.

$$I_f(\mu, \pi) := \sum_z |\mu(z) - \pi(z)|.$$

- Hellinger distance: $f(u) = \frac{1}{2}(\sqrt{u} - 1)^2$.

$$I_f(\mu, \pi) := \sum_{z \in \mathcal{Z}} (\sqrt{\mu(z)} - \sqrt{\pi(z)})^2.$$

Why the f-divergence?

- A classical theorem due to Blackwell (1951): *If a procedure A has a smaller f-divergence than a procedure B (for some fixed f), then there exist some set of prior probabilities such that procedure A has a smaller probability of error than procedure B*

- Given that it is intractable to minimize probability of error, this result has motivated (many) authors in signal processing to use f-divergences as surrogates for probability of error

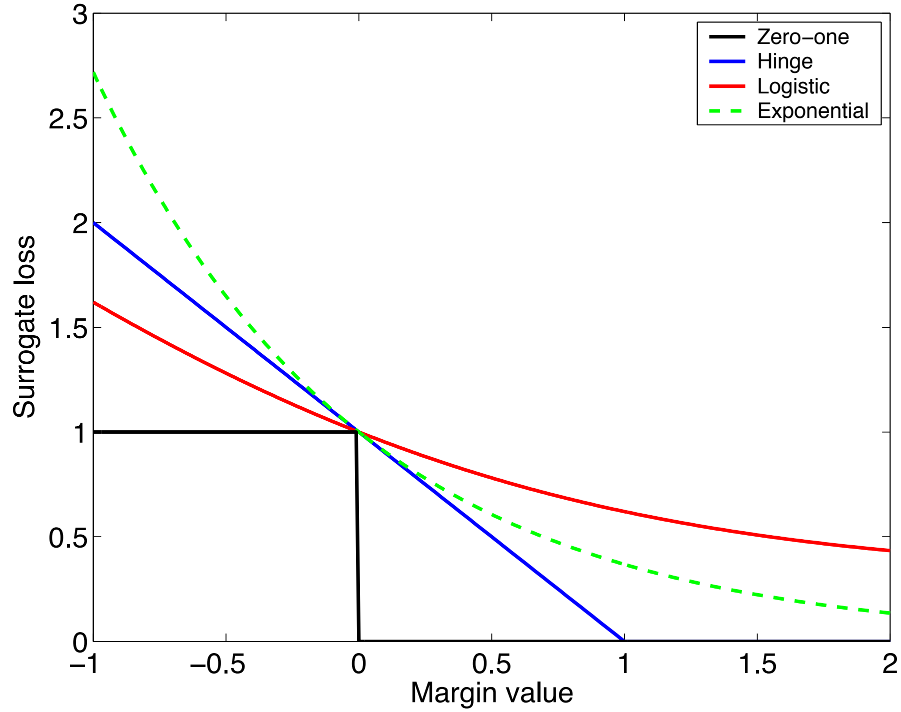
- I.e., choose a quantizer Q by maximizing an f-divergence between $P(Z|Y = 1)$ and $P(Z|Y = -1)$
  - Hellinger distance (Kailath 1967; Longo et al, 1990)
  - Chernoff distance (Chamberland & Veeravalli, 2003)

- Supporting arguments from asymptotics
  - Kullback-Leibler divergence in the Neyman-Pearson setting
  - Chernoff distance in the Bayesian setting

Statistical Perspective

- *Decision-theoretic*: based on a loss function $\phi(Y, \gamma(Z))$
- E.g., 0-1 loss:
$$\phi(Y, \gamma(Z)) = \begin{cases} 1 & \text{if } Y \neq \gamma(Z) \\ 0 & \text{otherwise} \end{cases}$$
which can be written in the binary case as $\phi(Y, \gamma(Z)) = \mathbb{I}(Y\gamma(Z) < 0)$
- The main focus is on estimating γ; the problem of estimating Q by minimizing the loss function is only occasionally addressed
- It is intractable to minimize 0-1 loss, so consider minimizing a surrogate loss functions that is a convex upper bound on the 0-1 loss

Margin-Based Surrogate Loss Functions



- Define a convex surrogate in terms of the margin $u = y\gamma(z)$
  - hinge loss: $\phi(u) = \max(0, 1 - u)$ support vector machine
  - exponential loss: $\phi(u) = \exp(-u)$ boosting
  - logistic loss: $\phi(u) = \log[1 + \exp(-u)]$ logistic regression

Estimation Based on a Convex Surrogate Loss

- Estimation procedures used in the classification literature are generally M-estimators ("empirical risk minimization")

- Given i.i.d. training data $(x_1, y_1), \ldots, (x_n, y_n)$

- Find a classifier γ that minimizes the empirical expectation of the surrogate loss:

$$\hat{\mathbb{E}}\phi(Y\gamma(X)) := \frac{1}{n}\sum_{i=1}^{n}\phi(y_i\gamma(x_i))$$

  where the convexity of ϕ makes this feasible in practice and in theory

Some Theory for Surrogate Loss Functions

(Bartlett, Jordan, & McAuliffe, JASA 2005)

- ϕ must be classification-calibrated, i.e., for any $a, b \geq 0$ and $a \neq b$,

$$\inf_{\alpha:\alpha(a-b)<0} \phi(\alpha)a + \phi(-\alpha)b > \inf_{\alpha\in\mathbb{R}} \phi(\alpha)a + \phi(-\alpha)b$$

  (essentially a form of Fisher consistency that is appropriate for classification)

- This is necessary and sufficient for Bayes consistency; we take it as the definition of a "surrogate loss function" for classification

- In the convex case, ϕ is classification-calibrated *iff* differentiable at 0 and $\phi'(0) < 0$

Outline

- A precise link between surrogate convex losses and f-divergences
  - we establish a constructive and many-to-one correspondence
- A notion of universal equivalence among convex surrogate loss functions
- An application: Proof of consistency for the choice of a (Q, γ) pair using any convex surrogate for the 0-1 loss

Setup

- We want to find (Q, γ) to minimize the ϕ-*risk*

$$R_\phi(\gamma, Q) = \mathbb{E}\phi(Y\gamma(Z))$$

- Define:

$$\begin{aligned} \mu(z) &= P(Y = 1, z) = p \int_x Q(z|x) dP(x|Y = 1) \\ \pi(z) &= P(Y = -1, z) = q \int_x Q(z|x) dP(x|Y = -1). \end{aligned}$$

- ϕ-risk can be represented as:

$$R_\phi(\gamma, Q) = \sum_z \phi(\gamma(z))\mu(z) + \phi(-\gamma(z))\pi(z)$$

Profiling

- Optimize out over γ (for each z) and define:

$$R_\phi(Q) := \inf_{\gamma\in\Gamma} R_\phi(\gamma, Q)$$

- For example, for 0-1 loss, we easily obtain $\gamma(z) = \text{sign}(\mu(z) - \pi(z))$. Thus:

$$\begin{aligned} R_{\text{0-1}}(Q) &= \sum_{z\in\mathcal{Z}} \min\{\mu(z), \pi(z)\} \\ &= \frac{1}{2} - \frac{1}{2}\sum_{z\in\mathcal{Z}} |\mu(z) - \pi(z)| \\ &= \frac{1}{2}(1 - V(\mu, \pi)) \end{aligned}$$

  where $V(\mu, \pi)$ is the variational distance.

- I.e., optimizing out a ϕ-risk yields an f-divergence. Does this hold more generally?

Some Examples

- **hinge loss**:

$$R_{hinge}(Q) = 1 - V(\mu, \pi) \qquad \text{(variational distance)}$$

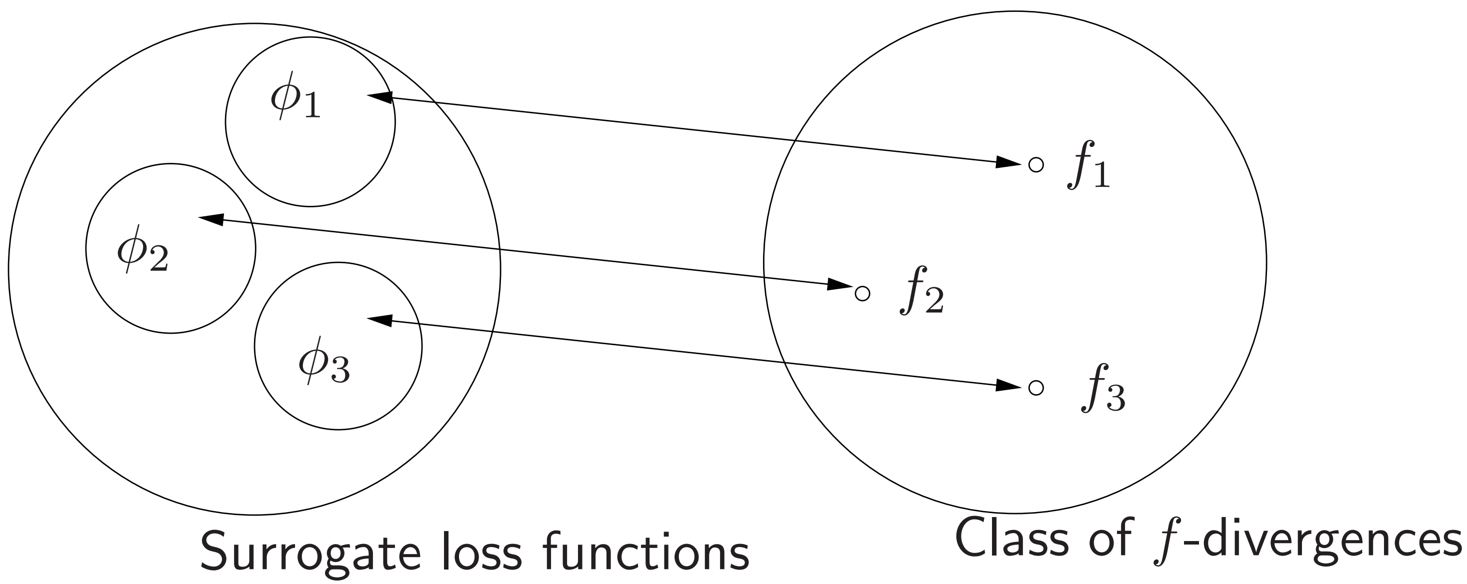
- **exponential loss**:

$$R_{exp}(Q) = 1 - \sum_{z \in \mathcal{Z}} (\sqrt{\mu(z)} - \sqrt{\pi(z)})^2 \qquad \text{(variational distance)}$$

- **logistic loss**:

$$R_{log}(Q) = \log 2 - D(\mu \| \frac{\mu + \pi}{2}) - D(\pi \| \frac{\mu + \pi}{2}) \qquad \text{(capacitory discrimination)}$$

Link between ϕ-losses and f-divergences



Conjugate Duality

- Recall the notion of *conjugate duality* (Rockafellar): For a lower-semicontinuous convex function $f : \mathbb{R} \longrightarrow \mathbb{R} \cup \{\infty\}$, the conjugate dual $f^* : \mathbb{R} \longrightarrow \mathbb{R} \cup \{\infty\}$ is defined as

$$f^*(u) = \sup_{v \in \mathbb{R}} \{uv - f(v)\},$$

which is necessarily a convex function.

- Define

$$\Psi(\beta) = f^*(-\beta)$$

Link between ϕ-losses and f-divergences

Theorem 1. *(a) For any margin-based surrogate loss function ϕ, there is an f-divergence such that $R_\phi(Q) = -I_f(\mu, \pi)$ for some lower-semicontinuous convex function f.*

In addition, if ϕ is continuous and satisfies a (weak) regularity condition, then the following properties hold:

(i) Ψ *is a decreasing and convex function.*

(ii) $\Psi(\Psi(\beta)) = \beta$ *for all* $\beta \in (\beta_1, \beta_2)$.

(iii) There exists a point u^* *such that* $\Psi(u^*) = u^*$.

(b) Conversely, if f is a lower-semicontinuous convex function satisfying conditions (i–iii), there exists a decreasing convex surrogate loss ϕ that induces the corresponding f-divergence

The Easy Direction: $\phi \to f$

- Recall

$$R_\phi(\gamma, Q) = \sum_{z \in \mathcal{Z}} \phi(\gamma(z))\mu(z) + \phi(-\gamma(z))\pi(z)$$

- Optimizing out $\gamma(z)$ for each z:

$$R_\phi(Q) = \sum_{z \in \mathcal{Z}} \inf_\alpha \phi(\alpha)\mu(z) + \phi(-\alpha)\pi(z) = \sum_z \pi(z) \inf_\alpha \left(\phi(-\alpha) + \phi(\alpha)\frac{\mu(z)}{\pi(z)} \right)$$

- For each z let $u = \frac{\mu(z)}{\pi(z)}$, define:

$$f(u) := -\inf_\alpha (\phi(-\alpha) + \phi(\alpha)u)$$

  - f is a convex function
  - we have

$$R_\phi(Q) = -I_f(\mu, \pi)$$

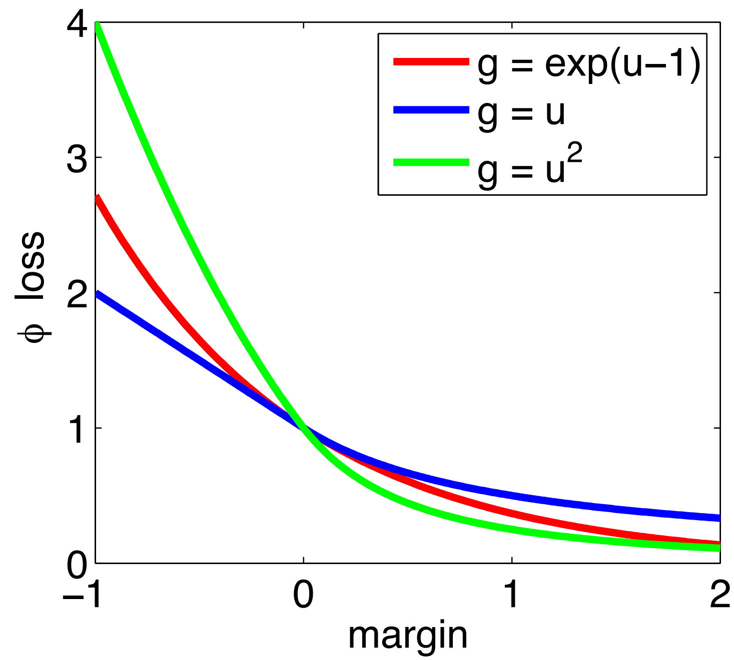
The $f \to \phi$ Direction Has a Constructive Consequence

- Any continuous loss function ϕ that induces an f-divergence must be of the form

$$\phi(\alpha) \quad = \quad \begin{cases} u^* & \text{if } \alpha = 0 \\ \Psi(g(\alpha + u^*)) & \text{if } \alpha > 0 \\ g(-\alpha + u^*) & \text{if } \alpha < 0, \end{cases}$$

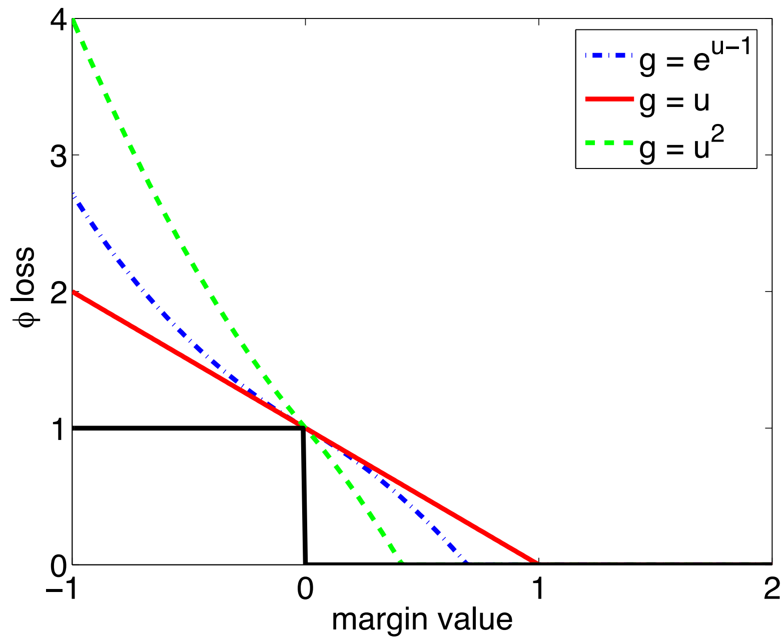
  where $g : [u^*, +\infty) \to \overline{\mathbb{R}}$ is some increasing continuous and convex function such that $g(u^*) = u^*$, and g is right-differentiable at u^* with $g'(u^*) > 0$.

Example – Hellinger distance



- Hellinger distance corresponds to an f-divergence with $f(u) = -2\sqrt{u}$
- Recover immediate function $\Psi(\beta) = f^*(-\beta) = \begin{cases} 1/\beta & \text{when } \beta > 0 \\ +\infty & \text{otherwise.} \end{cases}$
- Choosing $g(u) = e^{u-1}$ yields $\phi(\alpha) = \exp(-\alpha)$ $\Rightarrow$ exponential loss

Example – Variational distance

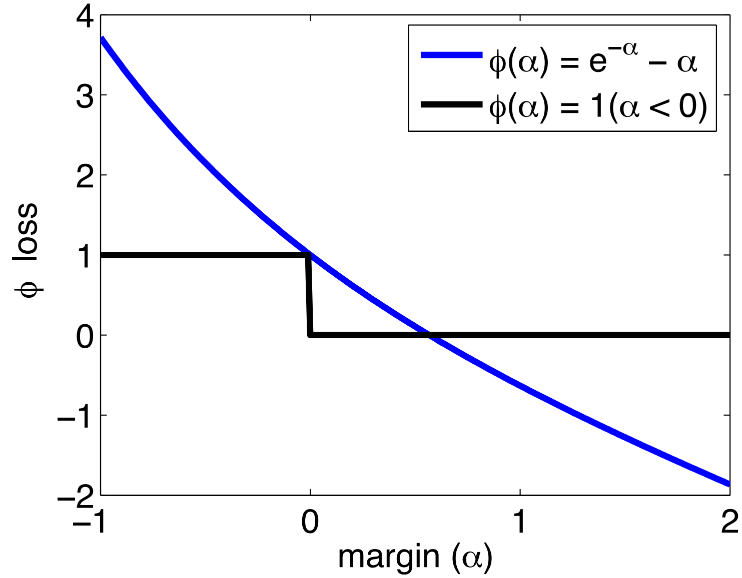


- Variational distance corresp. to an f-divergence with $f(u) = -2\min\{u, 1\}$

- Recover immediate function $\Psi(\beta) = f^*(-\beta) = \begin{cases} (2-\beta)_+ & \text{when } \beta > 0 \\ +\infty & \text{otherwise.} \end{cases}$

- Choosing $g(u) = u$ yields $\phi(\alpha) = (1-\alpha)_+$ $\Rightarrow$ hinge loss

Example – Kullback-Leibler divergence



- There is no corresponding ϕ loss for either $D(\mu\|\pi)$ or $D(\pi\|\mu)$
- But the *symmetrized* KL divergence $D(\mu\|\pi) + D(\pi\|\mu)$ is realized by

$$\phi(\alpha) = e^{-\alpha} - \alpha$$

Bayes Consistency for Choice of (Q, λ)

- Recall that from the 0-1 loss, we obtain the variational distance as the corresponding f-divergence, where $f(u) = \min\{u, 1\}$.

- Consider a broader class of f-divergences defined by:

$$f(u) = -c \min\{u, 1\} + au + b$$

- And consider the set of (continuous, convex and classification-calibrated) ϕ-losses that can be obtained (via Theorem 1) from these f-divergences

- We will provide conditions under which such ϕ-losses yield Bayes consistency for procedures that jointly choose (Q, λ)

- (And later we will show that *only* such ϕ-losses yield Bayes consistency)

Setup

- Consider sequences of increasing compact function classes $\mathcal{C}_1 \subseteq \ldots \subseteq \Gamma$ and $\mathcal{D}_1 \subseteq \ldots \subseteq \mathcal{Q}$

- Assume there exists an oracle that outputs an optimal solution to:

$$\min_{(\gamma,Q)\in(\mathcal{C}_n,\mathcal{D}_n)} \hat{R}_\phi(\gamma, Q) = \min_{(\gamma,Q)\in(\mathcal{C}_n,\mathcal{D}_n)} \frac{1}{n} \sum_{i=1}^{n} \sum_{z\in\mathcal{Z}} \phi(Y_i\gamma(z))Q(z|X_i)$$

  and let (γ_n^*, Q_n^*) denote one such solution.

- Let R^*_{Bayes} denote the minimum Bayes risk:

$$R^*_{Bayes} := \inf_{(\gamma,Q)\in(\Gamma,\mathcal{Q})} R_{Bayes}(\gamma, Q).$$

- Excess Bayes risk: $R_{Bayes}(\gamma_n^*, Q_n^*) - R^*_{Bayes}$

Setup

- *Approximation error*:

$$\mathcal{E}_0(\mathcal{C}_n, \mathcal{D}_n) = \inf_{(\gamma, Q) \in (\mathcal{C}_n, \mathcal{D}_n)} \{R_\phi(\gamma, Q)\} - R_\phi^*$$

where $R_\phi^* := \inf_{(\gamma, Q) \in (\Gamma, \mathcal{Q})} R_\phi(\gamma, Q)$

- *Estimation error*:

$$\mathcal{E}_1(\mathcal{C}_n, \mathcal{D}_n) = \mathbb{E} \sup_{(\gamma, Q) \in (\mathcal{C}_n, \mathcal{D}_n)} \left| \hat{R}_\phi(\gamma, Q) - R_\phi(\gamma, Q) \right|$$

where the expectation is taken with respect to the measure $\mathbb{P}^n(X, Y)$

Bayes Consistency for Choice of (Q, λ)

Theorem 2.

Under the stated conditions:

$$R_{Bayes}(\gamma_n^*, Q_n^*) - R_{Bayes}^* \leq \frac{2}{c}\left\{2\mathcal{E}_1(\mathcal{C}_n, \mathcal{D}_n) + \mathcal{E}_0(\mathcal{C}_n, \mathcal{D}_n) + 2M_n\sqrt{2\frac{\ln(2/\delta)}{n}}\right\}$$

- Thus, under the usual kinds of conditions that drive approximation and estimation error to zero, and under the additional condition on ϕ:

$$M_n := \max_{y\in\{-1,+1\}} \sup_{(\gamma,Q)\in(\mathcal{C}_n,\mathcal{D}_n)} \sup_{z\in\mathcal{Z}} |\phi(y\gamma(z))| < +\infty,$$

  we obtain Bayes consistency (for the class of ϕ obtained from $f(u) = -c\min\{u, 1\} + au + b$)

Universal Equivalence of Loss Functions

- Consider two loss functions ϕ_1 and ϕ_2, corresponding to f-divergences induced by f_1 and f_2

- ϕ_1 and ϕ_2 are **universally** equivalent, denoted by

$$\phi_1 \stackrel{u}{\approx} \phi_2$$

if for **any** $P(X, Y)$ and quantization rules Q_A, Q_B, there holds:

$$R_{\phi_1}(Q_A) \leq R_{\phi_1}(Q_B) \Leftrightarrow R_{\phi_2}(Q_A) \leq R_{\phi_2}(Q_B).$$

An Equivalence Theorem

Theorem 3.

$$\phi_1 \overset{u}{\approx} \phi_2$$

if and only if

$$f_1(u) = c f_2(u) + au + b$$

for constants $a, b \in \mathbb{R}$ *and* $c > 0$.

- $\Leftarrow$ is easy; $\Rightarrow$ is not
- In particular, surrogate losses universally equivalent to 0-1 loss are those whose induced f divergence has the form:

$$f(u) = -c \min\{u, 1\} + au + b$$

- Thus we see that *only* such losses yield Bayes consistency for procedures that jointly choose (Q, λ)

Estimation of Divergences

- Given i.i.d. $\{x_1, \ldots, x_n\} \sim \mathbb{Q}$, $\{y_1, \ldots, y_n\} \sim \mathbb{P}$
  - $\mathbb{P}, \mathbb{Q}$ are unknown multivariate distributions with densities p_0, q_0 wrt Lesbegue measure μ on $\mathbb{R}^d$

- Consider the problem of estimating a divergence; e.g., KL divergence:
  - Kullback-Leibler (KL) divergence functional

$$D_K(\mathbb{P}, \mathbb{Q}) = \int p_0 \log \frac{p_0}{q_0} \, d\mu$$

Existing Work

- Relations to entropy estimation
  - large body of work on functional of one density (Bickel & Ritov, 1988; Donoho & Liu 1991; Birgé & Massart, 1993; Laurent, 1996 and so on)
- KL is a functional of two densities
- Very little work on nonparametric divergence estimation, especially for high-dimensional data
- Little existing work on estimating density ratio per se

Main Idea

- Variational representation of f-divergences:

  Lemma 4. *Letting $\mathcal{F}$ be any function class in $\mathcal{X} \to \mathbb{R}$, there holds:*

  $$D_\phi(\mathbb{P}, \mathbb{Q}) \geq \sup_{f \in \mathcal{F}} \int f \, d\mathbb{Q} - \phi^*(f) \, d\mathbb{P},$$

  with equality if $\mathcal{F} \cap \partial\phi(q_0/p_0) \neq \emptyset$.

  ϕ^* denotes the conjugate dual of ϕ

- Implications:
  - obtain an M-estimation procedure for divergence functional
  - also obtain the likelihood ratio function $d\mathbb{P}/d\mathbb{Q}$
  - how to choose $\mathcal{F}$
  - how to implement the optimization efficiently
  - convergence rate?

Kullback-Leibler Divergence

- For the Kullback-Leibler divergence:

$$D_K(\mathbb{P}, \mathbb{Q}) = \sup_{g>0} \int \log g \, d\mathbb{P} - \int g d\mathbb{Q} + 1.$$

- Furthermore, the supremum is attained at $g = p_0/q_0$.

M-Estimation Procedure

- Let $\mathcal{G}$ be a function class: $\mathcal{X} \to \mathbb{R}_+$
- $\int \, d\mathbb{P}_n$ and $\int \, d\mathbb{Q}_n$ denote the expectation under empirical measures $\mathbb{P}_n$ and $\mathbb{Q}_n$, respectively
- One possible estimator has the following form:

$$\hat{D}_K = \sup_{g \in \mathcal{G}} \int \log g \, d\mathbb{P}_n - \int g d\mathbb{Q}_n + 1.$$

- Supremum is attained at $\hat{g}_n$, which estimates the likelihood ratio p_0/q_0

Convex Empirical Risk with Penalty

- In practice, control the size of the function class $\mathcal{G}$ by using a penalty
- Let $I(g)$ be a measure of complexity for g
- Decompose $\mathcal{G}$ as follows:

$$\mathcal{G} = \cup_{1 \leq M \leq \infty} \mathcal{G}_M,$$

where $\mathcal{G}_M$ is restricted to g for which $I(g) \leq M$.

- The estimation procedure involves solving:

$$\hat{g}_n = \text{argmin}_{g \in \mathcal{G}} \int g d\mathbb{Q}_n - \int \log g \, d\mathbb{P}_n + \frac{\lambda_n}{2} I^2(g).$$

Convergence Rates

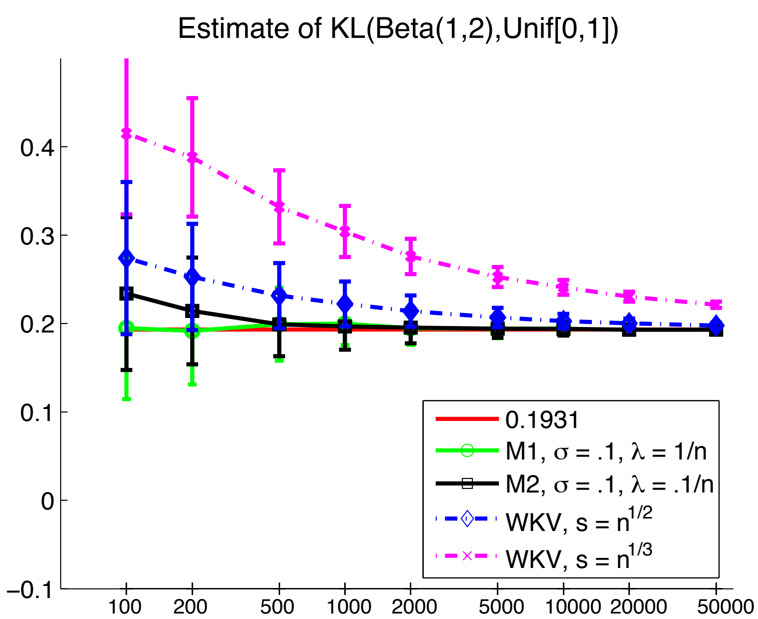
Theorem 5. *When* λ_n *vanishes sufficiently slowly:*

$$\lambda_n^{-1} = O_P(n^{2/(2+\gamma)})(1 + I(g_0)),$$

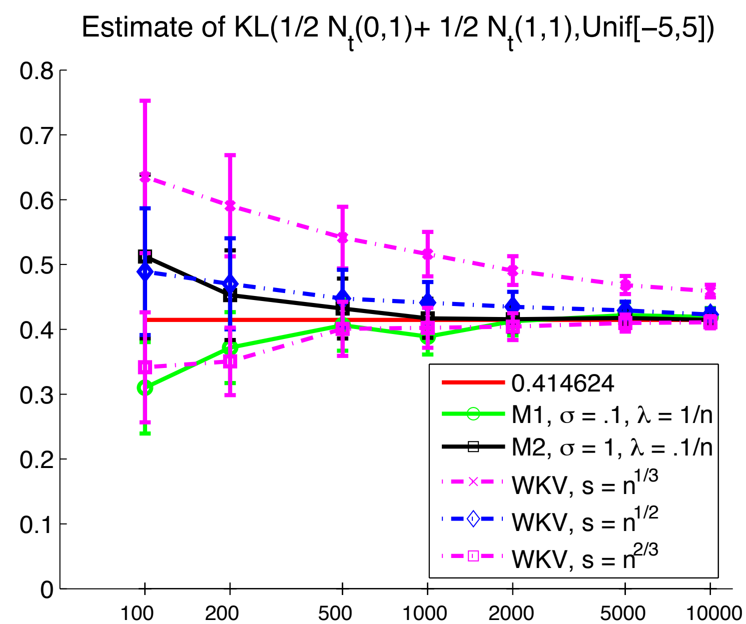
then under $\mathbb{P}$*:*

$$h_{\mathbb{Q}}(g_0, \hat{g}_n) = O_P(\lambda_n^{1/2})(1 + I(g_0))$$
$$I(\hat{g}_n) = O_P(1 + I(g_0)).$$

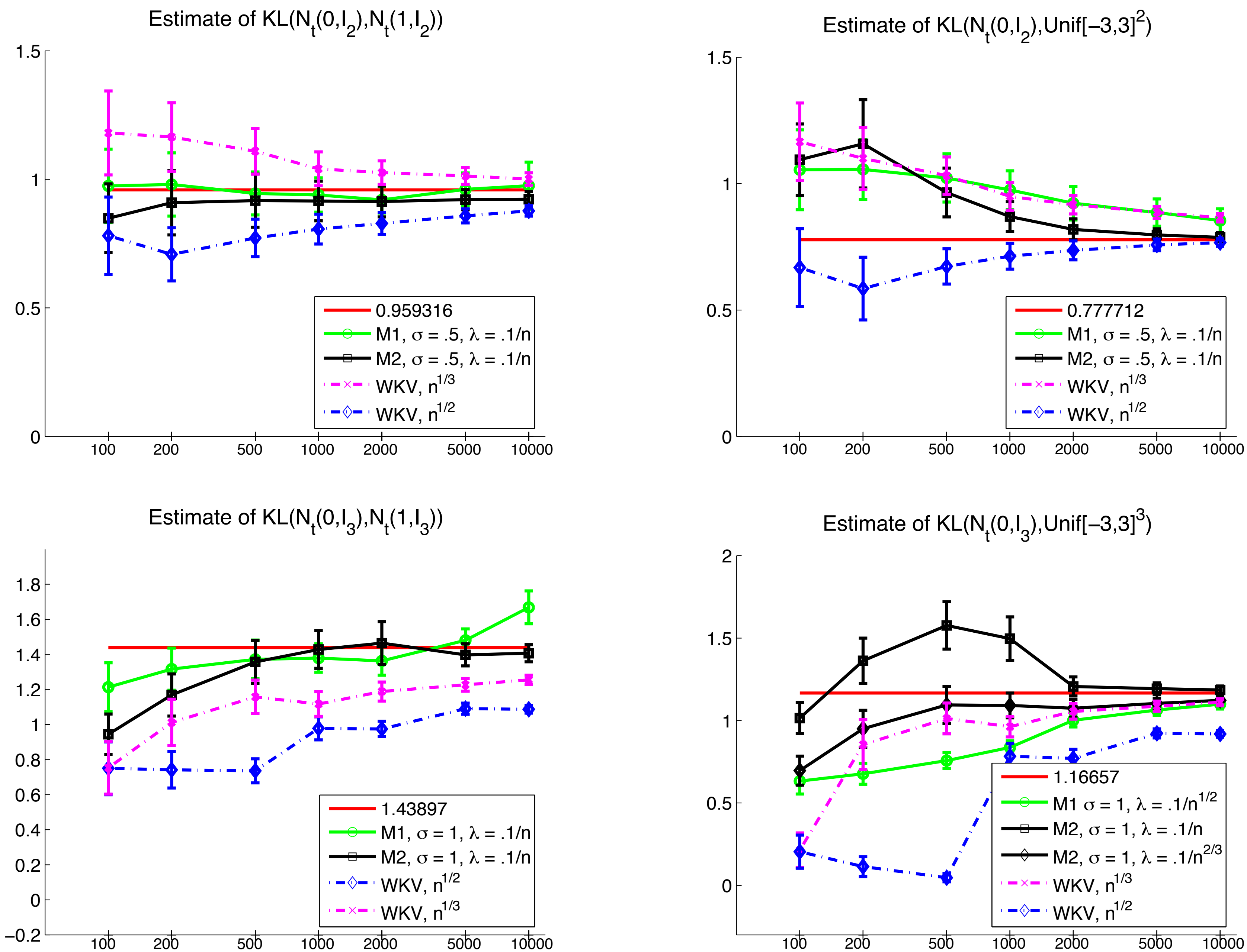
Results



Estimate of KL(Beta(1,2),Unif[0,1])
0.4
0.3
0.2
0.1
0
−0.1
100
200
500
1000
2000
5000
10000
20000
50000
0.1931
M1, σ = .1, λ = 1/n
M2, σ = .1, λ = .1/n
WKV, s = n^1/2
WKV, s = n^1/3



Estimate of KL(1/2 N_t(0,1)+ 1/2 N_t(1,1),Unif[−5,5])
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
100
200
500
1000
2000
5000
10000
0.414624
M1, σ = .1, λ = 1/n
M2, σ = 1, λ = .1/n
WKV, s = n^1/3
WKV, s = n^1/2
WKV, s = n^2/3



Estimate of KL(N_t(0,I_2),N_t(1,I_2))
1.5
1
0.5
0
100 200 500 1000 2000 5000 10000
0.959316
M1, σ = .5, λ = .1/n
M2, σ = .5, λ = .1/n
WKV, n^1/3
WKV, n^1/2
Estimate of KL(N_t(0,I_2),Unif[−3,3]^2)
1.5
1
0.5
0
100 200 500 1000 2000 5000 10000
0.777712
M1, σ = .5, λ = .1/n
M2, σ = .5, λ = .1/n
WKV, n^1/3
WKV, n^1/2
Estimate of KL(N_t(0,I_3),N_t(1,I_3))
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
100 200 500 1000 2000 5000 10000
1.43897
M1, σ = 1, λ = .1/n
M2, σ = 1, λ = .1/n
WKV, n^1/2
WKV, n^1/3
Estimate of KL(N_t(0,I_3),Unif[−3,3]^3)
2
1.5
1
0.5
0
100 200 500 1000 2000 5000 10000
1.16657
M1 σ = 1, λ = .1/n^1/2
M2, σ = 1, λ = .1/n
M2, σ = 1, λ = .1/n^2/3
WKV, n^1/3
WKV, n^1/2

Conclusions

- Formulated a precise link between f-divergences and surrogate loss functions
- Decision-theoretic perspective on f-divergences
- Equivalent classes of loss functions
- Can design new convex surrogate loss functions that are equivalent (in a deep sense) to 0-1 loss
  - Applications to the Bayes consistency of procedures that jointly choose an experimental design and a classifier
  - Applications to the estimation of divergences and entropy