Theory and Applications of Proper Scoring Rules

A. Philip Dawid, University of Cambridge

and

Monica Musio, Università di Cagliari

Abstract

We give an overview of some uses of proper scoring rules in statistical inference, including frequentist estimation theory and Bayesian model selection with improper priors.

1 Introduction

The theory of proper scoring rules (PSRs) originated as an approach to probability forecasting [Dawid 1986], the general enterprise of forming and evaluating probabilistic predictions. The fundamental idea is to develop ways of motivating a forecaster to be honest in the predictions he announces, and of assessing the performance of announced probabilities in the light of the outcomes that eventuate. The early applications of this methodology were to meteorology [Brier 1950] and subjective Bayesianism [Good 1952 de Finetti 1975]. However, it is becoming clear that the mathematical theory of PSRs has a wide range of other applications in Statistics generally. The aim of this paper is to give a brief outline of some of these. Some further details will appear in [Dawid et al. (2014)].

After setting out the basic ideas and properties of PSRs in §2, in §3 we describe a number of important special cases. Section 4 describes how a PSR supplies an alternative to the likelihood function of a statistical model, and how this can be used to develop new estimators that may have useful properties of robustness and/or computational feasibility. In particular, in §5 we show that, by using an appropriate PSR, it is possible to avoid difficulties associated with intractable normalising constants. In §6 the same ability to ignore a normalising constant is shown to supply an approach to Bayesian model selection with improper priors. Some concluding comments are made in §7.

2 Proper scoring rules

The most natural context in which to introduce the idea of a proper scoring rule is that of a game between a decision-maker (henceforth “You”) and Nature. Let $X$ be a random variable with values in $\mathcal{X}$, and let $\mathcal{P}$ be a family of distributions over $\mathcal{X}$. In due course, Nature will reveal the value, $x$, of $X$. Ahead of that, Your task is to quote a distribution $Q \in \mathcal{P}$, intended to represent Your uncertainty about how $X$ might turn out. Later, after Nature has revealed $x$, You will suffer a penalty $S(x,Q)$, depending on both Your quoted distribution $Q$, and Nature’s chosen value $x$, for $X$. The function $S$ is a scoring rule.

Suppose Your actual beliefs about $X$ are represented by the distribution $P \in \mathcal{P}$. If Your quoted distribution is $Q$, You assess Your expected penalty as

$$S(P,Q) := E_{X \sim P} S(X,Q).$$

(1)

According to the principles of decision theory, You should choose Your quote $Q$ to minimise Your expected score $S(P,Q)$. However, this might or might not coincide with Your true belief $P$. A proper scoring rule (PSR) is one that encourages You to be honest:
Definition 1 The scoring rule $S$ is proper with respect to $\mathcal{P}$ if, for $P, Q \in \mathcal{P}$, the expected score $S(P, Q)$ is minimised in $Q$ at $Q = P$. Further $S$ is strictly proper if this is the unique minimum: $S(P, Q) > S(P, P)$ for $Q \neq P$.

2.1 General construction

We have introduced proper scoring rules in the context of a special kind of decision problem, where Your decision has the form of a quoted distribution $Q$. But virtually any decision problem gives rise to an associated PSR.

Thus consider a decision problem, with state space $X$ and arbitrary action space $A$. Again Your task is to choose a decision, this time of the form $a \in A$, after which Nature will reveal the value $x$ of $X$, and You will be subject to a loss $L(x, a)$. The loss function $L$ is, again, essentially arbitrary.

Let $P$ be a family of distributions over $X$ such that for each $P \in \mathcal{P}$ there exists a Bayes act:

$$a_P := \arg\min_{a \in A} L(P, a)$$

where $L(P, a) := E_{X \sim P} L(X, a)$. If the Bayes act is not unique, we arbitrarily nominate one such act as $a_P$. Now define a scoring rule $S$ by:

$$S(x, Q) = L(x, a_Q) \quad (x \in X, Q \in \mathcal{P}).$$

Then $S(P, Q) = L(P, a_Q) \geq L(P, a_P) = S(P, P)$. Thus $S$ is a PSR with respect to $P$.

In this way the theory of proper scoring rules subsumes a large part of statistical decision theory.

2.2 Related concepts

Let $S$ be a PSR with respect to a large convex family $\mathcal{P}$ over $X$. Starting from $S$, we can define a collection of useful statistical functions:

Entropy The minimised value $H(P) := S(P, P)$ is the (generalised) entropy of $P \in \mathcal{P}$.

Discrepancy The excess score $D(P, Q) := S(P, Q) − H(P)$ is the discrepancy or divergence of $Q \in \mathcal{P}$ from $P \in \mathcal{P}$.

Metric Locally, $D(P, P + dP)$ defines a Riemannian Metric on $\mathcal{P}$.

Dependence Function The dependence of $X$ on a random variable $U$ jointly distributed with $X$ is

$$C(X, U) := H(P_X) − E_U\{H(P_{X|U})\}.$$ 

We note without proof the following properties of these associated functions [Dawid 1998]:

Theorem 1

1. $H(P)$ is a concave functional of $P$ (strictly concave if $S$ is strictly proper).
2. $D(P, Q) \geq 0$, and $D(P, Q) − D(P, Q_0)$ is an affine function of $Q$.
3. For a parametric model $\{P_\theta : \theta \in \Theta \subseteq \mathbb{R}^p\}$, the metric takes the form

$$D(P_\theta, P_{\theta + d\theta}) = d\theta' g(\theta) d\theta,$$

where the $(p \times p)$ matrix $g(\theta)$ satisfies

$$\partial g_{ab}(\theta)/\partial \theta_c = \partial g_{ac}(\theta)/\partial \theta_b.$$ 

4. $C(X, U) \geq 0$ and vanishes if $X \perp \perp U$ (and, when $S$ is strictly proper, only in this case.)

We could alternatively start with an entropy function $H$, a discrepancy function $D$, or a metric $g$, having the additional properties described above. In each case we can (under some technical conditions) construct a PSR $S$ from which it can be derived [Dawid 1998].
3 Some special proper scoring rules

Since every decision problem induces a PSR, there is a very great variety of these: the set of
PSRs has essentially the same cardinality as the set of concave functionals (serving as associated
generalised entropy functions) on $P$. Here we discuss some cases of special interest. For further
special cases, see among others [Dawid (1998)] [Dawid (2007)] [Dawid and Sebastiani (1999)]. Where
appropriate, we equip $X$ with an underlying measure $µ$ dominating $P$, and write $p(·)$ for the density
(Radon-Nikodym derivative) $dP/du$, etc.

3.1 Log score

The log score (Good 1952) is just negative log likelihood:

$$S(x, Q) = - \ln q(x).$$  \hspace{1cm} (3)

For this case we find:

- $H(P) = - \int dp(y) \cdot p(y) \ln p(y)$ is the Shannon Entropy of $P$.
- $D(P, Q) = \int dp(y) \cdot p(y) \ln \{p(y)/q(y)\}$ is the Kullback-Leibler Discrepancy $K(P, Q)$.
- $C(X, U) = E[\ln \{p(X, U)/p(X)p(U)\}]$ is the mutual Information $I(X; U)$.
- $g(θ)$ is the Fisher Information matrix.

The well-known property that $K(P, Q) \geq 0$, with equality if and only if $Q = P$, shows that
the log score is strictly proper.

It is interesting to see so many fundamental ingredients of statistical theory and information
theory flowing naturally from the log score. But it is equally true that many of the important
properties for which these are renowned remain valid for the more general constructions of § 2.2.
In particular, the whole theory of information geometry, which subsumes but goes beyond the
information metric on $P$, can be generalised to yield the decision geometry associated with a given
PSR (Dawid and Lauritzen 2003) [Dawid 2007].

3.2 Tsallis score

The Tsallis score (Tsallis 1988) is given by:

$$S(x, Q) = (\gamma - 1) \int dp(y) \cdot p(y)\gamma - \gamma q(x)\gamma - 1 \quad (\gamma > 1).$$  \hspace{1cm} (4)

With minor notational modifications, this is the same as the density power score of [Basu et al. (1998)]

We compute

$$H(P) = - \int dp(y) \cdot p(y)\gamma$$  \hspace{1cm} (5)

and

$$D(P, Q) = \int dp(y) \cdot p(y)\gamma + (\gamma - 1) \int dp(y) \cdot q(y)\gamma - \gamma \int dp(y) \cdot p(y)q(y)\gamma - 1.$$

(6)

It can be shown that $D(P, Q) > 0$ for $Q \neq P$, demonstrating the strict propriety of the Tsallis
score.
3.3 Brier score

Setting $\gamma = 2$ in the Tsallis score yields the quadratic score. For the special case of a binary sample space $X = \{0, 1\}$, an essentially equivalent scoring rule is the Brier score \cite{Brier1950}. Defining $q := Q(X = 1)$ etc., this has

\[
\begin{align*}
S(0, Q) &= q^2 \\
S(1, Q) &= (1 - q)^2 \\
H(P) &= p(1 - p) \\
D(P, Q) &= (p - q)^2.
\end{align*}
\]

3.4 Bregman score

Let $\psi : \mathbb{R}^+ \to \mathbb{R}$ be convex and differentiable. The associated Bregman score is given by:

\[
S(x, Q) = -\psi'\{q(x)\} - \int d\mu(y) \cdot [\psi\{q(y)\} - q(y) \psi'(q(y))].
\]  

(7)

Then with $p = p(y), q = q(y)$, we get

\[
\begin{align*}
H(P) &= -\int d\mu(y) \cdot \psi(p),
D(P, Q) &= \int d\mu(y) \cdot [\psi(p) - \{\psi(q) + \psi'(q) (p - q)\}].
\end{align*}
\]

(8)

By convexity of $\psi$, the integrand of (9) is non-negative, so $S$ is proper (and strictly proper if $\psi$ is strictly convex).

The log, Tsallis and Brier scores are all special cases of the Bregman score with, respectively,

$\psi(p) = p \ln p$,  $\psi(p) = p^\gamma$,  $\psi(p) = (2p^2 - 1)/4$.

3.5 Survival score

A variant of the Bregman score, but now applied to the hazard function $\lambda_Q(x) := q(x)/\{1 - F_Q(x)\}$ (where $F_Q(x) = Q(X \leq x)$), is useful for scoring a possibly censored survival time $X$.

Suppose that $X$, non-negative, might be right-censored, at a random time $C \leq \infty$. Thus we observe $M = \min\{C, X\}$ and $\Delta = 1(X \leq C)$. Again let $\psi : \mathbb{R}^+ \to \mathbb{R}$ be convex and differentiable, and consider the scoring rule:

\[
S\{(m, \delta), Q\} = \int_0^m du \cdot \gamma \{\lambda_Q(u)\} - \psi' \{\lambda_Q(m)\} \delta
\]

where $\gamma(\lambda) := \lambda\psi'(\lambda) - \psi(\lambda)$. It can be shown that this is a PSR for the distribution of $X$, even though observation of $X$ may be subject to an unspecified non-informative censoring process.

3.6 Hyvärinen score

Let $X$ be a variable taking values in $X = \mathbb{R}^k$. What we term the Hyvärinen score \cite{Hyvarinen2005} is defined by:

\[
S(x, Q) = \Delta \ln q(x) + \frac{1}{2} |\nabla \ln q(x)|^2 = \frac{\Delta \sqrt{q(x)}}{\sqrt{q(x)}}
\]

(10)

where $\nabla$ denotes gradient, and $\Delta$ the Laplacian operator $\sum_{i=1}^k \partial^2/(\partial x_i)^2$, on $X$. With extended interpretations of these operators, the same expression can be used to define a proper scoring rule on a general Riemannian space \cite{DawidLauritzen2005}.
Under conditions that justify ignoring boundary terms when integrating by parts, we obtain:

\[
S(P, Q) = \frac{1}{2} \int d\mu(y) \cdot \langle \nabla \ln q(y) - 2\nabla \ln p(y), \nabla \ln q(y) \rangle \\
H(P) = -\frac{1}{2} \int d\mu(y) \cdot |\nabla \ln p(y)|^2 \\
D(P, Q) = \frac{1}{2} \int d\mu(y) \cdot |\nabla \ln p(y) - \nabla \ln q(y)|^2.
\]

Since \(D(P, Q) > 0\) for \(Q \neq P\), the Hyvärinen score is strictly proper. This score also has other important properties that we highlight in §5.1 below.

### 3.7 Composite score

Consider a model for a multidimensional variable \(X\). Let \(\{X_k\}\) be a collection of marginal and/or conditional variables, and let \(S_k\) be a PSR for \(X_k\). Then we can construct a composite score for \(X\) as

\[
S(x, Q) = \sum_k S_k(x_k, Q_k)
\]

where \(X_k \sim Q_k\) when \(X \sim Q\). It is easy to see that this defines a PSR. It will be strictly proper when every \(S_k\) is strictly proper and the joint distribution for \(X\) is determined by the collection of distributions for the \(\{X_k\}\).

The form \(\text{(11)}\) localises the problem to the \(\{X_k\}\), which can often simplify computation. In the special case that each \(S_k\) is the log score, \(\text{(11)}\) defines a negative log composite likelihood (see e.g. [Statistica Sinica (2011)]). We can thus treat composite likelihood in its own right, as supplying a proper scoring rule, rather than as an approximation (generally poor) to true likelihood. Most of the extensive theory and many applications of composite likelihood apply virtually unchanged to the more general composite score \(\text{(11)}\).

### 3.8 Pseudo score

A pseudo score is a special case of a composite score.

Consider a spatial process \(X = (X_v : v \in V)\), where \(V\) is a set of lattice sites. For a joint distribution \(Q\) for \(X\), let \(Q_v\) be the conditional distribution for \(X_v\), given the values of \(X\setminus v\), the variables at all other sites. Many interesting spatial processes are defined locally, by specifying \(\{Q_v, v \in V\}\) (which however can not be done arbitrarily, but is subject to consistency constraints). In particular, if \(Q\) is Markov, \(Q_v\) only depends on the values of \(X_{ne(v)}\), the variables at the sites neighbouring \(v\).

We can construct a proper scoring rule as

\[
S(x, Q) = \sum_v S_0(x_v, Q_v),
\]

where \(S_0\) is a PSR for the state at a single site. This avoids the need to evaluate the normalising constant of the full joint distribution \(Q\).

When \(S_0\) is the log score, \(\text{(12)}\) defines the negative log pseudo-likelihood of [Besag (1975)] Again, pseudo-likelihood has generally been considered as an approximation to the full likelihood, but can stand in its own right, as a proper scoring rule. For binary \(X_v\), taking \(S_0\) to be the Brier score forms the basis of the ratio matching method of [Hyvärinen (2007)]. Some comparisons can be found in [Dawid and Musio (2013)].
4 Statistical inference

4.1 Estimation

Let \( \{P_\theta : \theta \in \Theta\} \), where \( \Theta \) is an open subset of \( \mathbb{R}^p \), be a parametric family of distributions for \( X \in \mathcal{X} \). We suppose given a PSR \( S \) on \( \mathcal{X} \), and write \( S(x, \theta) \) for \( S(x, P_\theta) \), and \( s(x, \theta) \) for its gradient vector (assumed henceforth to exist) with respect to \( \theta \):

\[
s(x, \theta) := \nabla_\theta S(x, \theta) = \left( \frac{\partial S(x, \theta)}{\partial \theta_j} : j = 1, \ldots, p \right).
\]

Let \((x_1, \ldots, x_n)\) be a random sample from \( P_\theta \), and denote by \( \hat{P} \) the empirical distribution of the sample, which puts mass \( 1/n \) at each of its (possibly repeated) values. We might estimate \( \theta \) by that value minimising \( D(\hat{P}, P_\theta) \), where \( D \) is the discrepancy associated with \( S \). Equivalently, since \( D(\hat{P}, P_\theta) = S(\hat{P}, P_\theta) - S(\hat{P}, \hat{P}) \), we minimise \( nS(\hat{P}, P_\theta) \), which is just the total empirical score, \( \sum_{i=1}^n S(x_i, \theta) \). That is, our estimate is

\[
\hat{\theta}_S = \arg \min_\theta \sum_{i=1}^n S(x_i, \theta),
\]

which (if it exists, which we here assume) will be a root of the score equation:

\[
s(\theta) := \sum_{i=1}^n s(x_i, \theta) = 0. \tag{13}
\]

We call \( \hat{\theta}_S \) the minimum score estimator of \( \theta \). Note that when \( S \) is the log score the score equation is just the (negative of) the likelihood equation, and the minimum score estimate is just the maximum likelihood estimate.

Generalising a familiar property of the likelihood equation, the following theorem \cite{Dawid and Lauritzen 2005} shows that, for any proper scoring rule, and any family of distributions, the score equation \eqref{eq:score_equation} constructed as above will yield an unbiased estimating equation:

**Theorem 2**

\[
E_\theta s(X, \theta) = 0.
\]

As a consequence of this theorem we have that equation \eqref{eq:score_equation} delivers an M-estimator \cite{Huber and Ronchetti 2009}. We can thus apply standard results on unbiased estimating equations to describe the properties of the minimum score estimator \( \hat{\theta}_S \). In particular, this estimator is consistent in repeated independent and identically distributed sampling.

Define

\[
J(\theta) = E_\theta \left\{ s(X, \theta)s(X, \theta)^T \right\}, \tag{14}
\]

\[
K(\theta) = E_\theta \left\{ \nabla_\theta s(X, \theta)^T \right\}, \tag{15}
\]

with entries

\[
J(\theta)_{ab} = E_\theta \left\{ \frac{\partial S(X, \theta)}{\partial \theta_a} \frac{\partial S(X, \theta)}{\partial \theta_b} \right\}, \tag{16}
\]

\[
K(\theta)_{ab} = E_\theta \left\{ \frac{\partial^2 S(X, \theta)}{\partial \theta_a \partial \theta_b} \right\}, \tag{17}
\]

and introduce the Godambe information matrix:

\[
G(\theta) := K(\theta)J(\theta)^{-1}K(\theta).
\]
Then under regularity conditions on the model [Barndorff-Nielsen and Cox 1994], our estimator is asymptotically normal, with asymptotic covariance matrix given by the inverse Godambe information matrix:

$$\hat{\theta}_S \approx \mathcal{N}(\theta, \{nG(\theta)\}^{-1})$$

when $X_1, X_2, \ldots, X_n$ are independent and identically distributed as $P_{\theta}$.

### 4.2 Robust estimation

The influence function (IF) of the estimator $\hat{\theta}_S$, the solution of the unbiased estimating equation (13) deriving from the PSR $S$, measures the effect on the estimator of adding an infinitesimally small amount of contamination at the point $x$. It is given by (Huber and Ronchetti 2009):

$$IF_S(x; \theta) = K(\theta)^{-1} s(x, \theta). \quad (18)$$

Of particular importance is the supremum of the influence function over all $x$, a measure of the worst-case influence on $\hat{\theta}_S$ of contamination in the data. For a robust estimator, this supremum should be finite, i.e., for fixed $\theta$, $IF_S(x; \theta)$ should be bounded — this property defines $B$-robustness.

From (18) we see that this will obtain if and only if the function $s(x; \theta)$ is bounded in $x$ for each $\theta$.

The influence function can also be used to evaluate the asymptotic variance, $\{nG(\theta)\}^{-1}$, of $\hat{\theta}_S$:

$$G(\theta)^{-1} = E_{\theta} \{IF_S(X; \theta) IF_S(X; \theta)^T \}.$$ 

### 4.2.1 Example: location model

Suppose $\mathcal{X} = \Theta = \mathbb{R}$, and the Lebesgue density $p_{\theta}(\cdot)$ of $P_{\theta}$ is given by

$$p_{\theta}(x) = f(x - \theta),$$

where the function $f$ is positive and differentiable on $\mathbb{R}$. We consider estimation based on the Bregman score (7) for given function $\psi$. We find

$$s(x, \theta) = \psi'' \{f(u)\} f'(u) \quad (19)$$

where $u = x - \theta$. In particular, for the Tsallis score, with $\psi(t) = t^\gamma$, the necessary and sufficient condition for B-robustness is that $f(u)^{\gamma-2} f'(u)$ be a bounded function of $u$ [Basu et al. 1998]. This condition is satisfied for the normal location model.

Expression (19), together with the fact that boundedness of $f'$ implies boundedness of $f$ (see Dawid et al. (2014)), suggest the following sufficient conditions for B-robustness:

**Condition 1**

1. $f'(u)$ is bounded.
2. $\psi''(t)$ is bounded on $(0, M]$ for any $M \in (0, \infty)$.

Condition 1 holds, for example, for $f$ the normal, the logistic, the Cauchy or the extreme value distribution. In typical cases, Condition 1 will hold so long as $\psi''(0) < \infty$.

The Brier score, with $\psi(t) = (2t^2 - 1)/4$, satisfies Condition 1 indeed, $\psi''(t) \equiv 1$ is bounded on the whole of $(0, \infty)$. For $\gamma > 2$ the Tsallis score satisfies Condition 1 with $\psi''(0) = 0$. However for the log score, having $\psi(t) \equiv t \ln(t)$, $\psi''(t) \equiv 1/t$ is not bounded at 0, so this particular Bregman scoring rule violates Condition 1. This is reflected in the fact that the maximum likelihood estimator is typically not B-robust.
5 Evading the normalising constant

When we use the log score, (13) is just the likelihood equation, and we obtain the maximum likelihood estimator.

Often we will know the density \( p_\theta \) only up to a multiplier:

\[
p(x \mid \theta) \propto f(x \mid \theta)
\]

where the omitted normalising constant, \( Z(\theta) := \int d\mu(\mathbf{y}) \cdot f(\mathbf{y} \mid \theta) \), may depend on \( \theta \), but not on \( x \). In this case to solve (13) we generally need to be able to compute and differentiate \( Z(\theta) \), but often this cannot be done explicitly. The identical problem affects estimates based on Bregman scores and many others.

One solution to this problem proposed in the literature is to use a composite likelihood approach, which will often avoid the requirement to evaluate and manipulate \( Z(\theta) \). We will see below that an alternative escape route is possible by using a suitable local PSR.

5.1 Locality

To evaluate the log score we only need to know the value of Your forecast density function, \( q(\cdot) \), at the value \( x \) of \( X \) that Nature in fact produces. It is thus termed a strictly local proper scoring rule. It can be shown that this property essentially characterises the log score. However, we can slightly weaken the locality requirement to admit further PSRs. For the case of a sample space that is a real interval, we ask that \( S(x,Q) \) should depend on \( q(\cdot) \) only through its value and the value of a finite number of its derivatives at \( x \). \cite{Parry2012} have characterised all such local PSRs as a linear combination of the log score and what they term a key local scoring rule, having the form

\[
S(x,Q) = \sum_{k=0}^{t} (-1)^k \frac{d^k}{dx^k} \phi_{[k]} \left\{ x, q(x), q'(x), \ldots, q^{(t)}(x) \right\},
\]

where \( \phi(x,q_0,\ldots,q_t) \) is 1-homogeneous (i.e., \( \phi(x,\lambda q_0,\ldots,\lambda q_t) = \lambda \phi(x,q_0,\ldots,q_t) \) for all \( \lambda > 0 \)) and concave in \( (q_0,\ldots,q_t) \) for each fixed \( x \), and \( \phi_{[k]} \) denotes \( \partial^k \phi / \partial q_k \). Some multivariate extensions are considered by \cite{Parry2013}.

The simplest key local scoring rule is the Hyvärinen score, given by (10) with \( k = 1 \), which arises on taking \( \phi = -q_1^2/q_0 \) in (20).

An important property of every key local scoring rule is homogeneity: it is unchanged if \( q(\cdot) \) is scaled by a positive constant. In particular, \( S(x,Q) \) can be computed without knowledge of the normalising constant of the distribution \( Q \). Thus if the main computational challenge is to compute this normalizing constant, it can be tackled by applying a homogeneous scoring rule to the full joint distribution.

5.2 Example: Markov process

Consider the following Gaussian dispersion model for a vector \( \mathbf{Y} \) taking values in \( \mathbb{R}^N \):

\[
\mathbf{Y} \sim \mathcal{N}(0, \Phi^{-1})
\]

with

\[
\Phi (N \times N) = \begin{pmatrix}
\alpha & \beta & 0 & 0 & \cdots & 0 \\
\beta & \alpha & \beta & 0 & \cdots & 0 \\
0 & \beta & \alpha & \beta & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & \beta & \alpha
\end{pmatrix}
\]

where, to ensures that \( \Phi \) is positive definite, we take the parameter space to be

\[
\Omega = \{ (\alpha, \beta) : \alpha > 2|\beta| \}.\]
Note that $\alpha^{-1}$ is the residual variance of each $Y_i$, given its neighbours. This model describes a Gaussian time series that is Markov and approximately stationary.

The determinant of $\Phi$ is

$$
\det (\Phi) = \beta^N \rho^{N+1} - \rho^{-N+1} - \rho \rho^{-1}
$$

where $\rho$ is determined by

$$
\rho + \rho^{-1} = \alpha / \beta.
$$

For an observed data-sequence $Y = y$, the likelihood is proportional to

$$
\det (\Phi)^{1/2} \exp \left( -\frac{1}{2} y' \Phi y \right)
$$

with $\det(\Phi)$ given by (22) and (23). This will be hard to maximise directly.

The Hyvärinen score (10) eliminates the problematic normalising constant, and yields a simple quadratic:

$$
S(\alpha, \beta) = -N \alpha + \frac{1}{2} \sum_{i=1}^{N} (\alpha y_i + \beta z_i)^2
$$

(24)

where $z_i := y_{i-1} + y_{i+1}$ (taking $y_{N+1} = y_1 = 0$). So it is easy to minimise directly. (Note however that the unconstrained minimum might not belong to $\Omega$, in which case the minimum score estimate does not exist).

Defining $\lambda = -\beta / \alpha$, (24) is

$$
- N \alpha + \frac{1}{2} \alpha^2 \sum_{i=1}^{N} (y_i - \lambda z_i)^2.
$$

(25)

The unconstrained minimum is given by

$$
\hat{\lambda} = \frac{c_{yz}}{c_{zz}}
$$

(26)

$$
\hat{\alpha}^{-1} = \frac{c_{yyz}}{N}
$$

(27)

(and then $\hat{\beta} = -\hat{\alpha} \hat{\lambda}$), where $c_{yz} := \sum_{i=1}^{N} y_i z_i$ etc., and $c_{yyz} := c_{yy} - (c_{yz})^2 / c_{zz}$. These will be the minimum score estimates so long as they lie in $\Omega$, which holds when $c_{yz}^2 < c_{zz} / 4$.

Alternatively we can apply pseudo-likelihood. The full conditionals are given by

$$
Y_i | (Y_{-i} = y_{-i}) \sim \mathcal{N} \left( \lambda z_i, \alpha^{-1} \right) \quad (i = 1, \ldots, N),
$$

and the log pseudo-likelihood is thus, up to a constant:

$$
\frac{1}{2} N \log \alpha - \frac{1}{2} \alpha \sum_{i=1}^{N} (y_i - \lambda z_i)^2.
$$

(28)

Maximising this gives the same estimates as for the Hyvärinen score.

5.2.1 Multiple observations

Now suppose we have $\nu$ independent vectors $Y_1, \ldots, Y_\nu$, all distributed as $\mathcal{N}(0, \Phi^{-1})$. We could form an estimating equation by summing those derived for the individual vectors, using either the Hyvärinen or the log pseudo-likelihood score. This leads again to equations (26) and (27), with $c_{yz}$ redefined as $\sum_{n=1}^{\nu} \sum_{i=1}^{N} y_{ni} z_{ni}$ etc., and $N$ replaced by $\nu N$ in (27).

However, we note that a sufficient (albeit not minimal sufficient) statistic in this problem is the sum-of-squares-and-products matrix $S = \sum_{n=1}^{\nu} Y_n Y_n'$, which has a Wishart distribution:
$S \sim W_N(\nu; \Phi^{-1})$. And the above estimates are not a function of $S$. To construct more efficient estimators, we take $S$ as our basic observable.

It is not clear how pseudo-likelihood could be applied to this problem. However, we can still apply a homogeneous scoring rule. Assume $\nu \geq N$, so that the Wishart density exists, and consider the multivariate Hyvärinen score (10) based on variables $(t_{ij} : 1 \leq i \leq j \leq N)$, where $t_{ii} = s_{ii}$, and $t_{ij} = s_{ij}/\sqrt{2}$ for $i < j$. The associated estimate of $\Phi$ is obtained by minimising

$$
\sum_{i,j} \left\{ (\nu - N - 1) s^{ij} - \phi_{ij} \right\}^2
$$

where $s^{ij}$ denotes the $(i, j)$ entry of $S^{-1}$. If $\Phi$ is totally unrestricted, this yields the unbiased estimate

$$
\hat{\Phi} = (\nu - N - 1) S^{-1}.
$$

Taking $\Phi$ to have the tridiagonal form (21), we get

$$
\hat{\alpha} = \frac{\nu - N - 1}{N} \sum_{i=1}^{N} s_{ii},
$$

$$
\hat{\beta} = \frac{\nu - N - 1}{N - 1} \sum_{i=1}^{N-1} s_{i,i+1},
$$

(so long as these estimates satisfy $(\hat{\alpha}, \hat{\beta}) \in \Omega$).

## 6 Bayesian Model Selection

Suppose that the distribution of an observable $X$ is drawn from one of a discrete collection $\mathcal{M}$ of competing parametric models, where under $M$ the density at $X = x$ is $p_M(x | \theta_M)$, with unknown parameter $\theta_M \in \mathbb{R}^{d_M}$.

The Bayesian approach requires us to specify, for each $M \in \mathcal{M}$, a prior density function $\pi_M(\theta_M)$ for its parameter $\theta_M$. Of central importance is the marginal density of $X$ under model $M$, given by:

$$
p_M(x) = \int d\theta_M \cdot p_M(x | \theta_M) \pi_M(\theta_M).
$$

On observing $X = x_0$, the various models can be compared by means of the marginal likelihood function, $L(M) \propto p_M(x_0)$. In particular, the posterior odds in favour of model $M$ as against model $M'$ are obtained on multiplying the corresponding prior odds by the Bayes factor, $BF_{M'}^{M} = L_M/L_{M'}$.

The marginal density (30), and hence the marginal likelihood, is sensitive to the choice of the prior distribution $\pi_M$. Unfortunately this problem is not solved by using so-called non informative or objective priors. These priors are typically improper and specified in the form $\pi_M(\theta_M) \propto h_M(\theta_M)$. That is to say, $\pi_M(\theta_M) = c_M h_M(\theta_M)$, where $c_M$ is an unspecified constant. The same arbitrary scale factor $c_M$ will then appear in the formal expression (30) for the marginal density. The Bayes Factor $BF_{M'}^{M}$, computed using such priors is then not defined, since it will depends on the ratio $c_M/c_{M'}$, of arbitrary positive constants. A variety of ad hoc methods have been suggested to evade this problem (see, among others, O’Hagan (1995); Berger and Pericchi (1996)). Here we propose a different solution, using proper scoring rules.

### 6.1 Use of scoring rules

The negative log marginal likelihood, $- \log p_M(x_0)$, is just the log score for the predictive distribution $P_M$ at the observation $x_0$. We might now consider replacing the log score by some other proper scoring rule, $S(x, Q)$ and using that to compare the models [Musio and Dawid 2013][Dawid and Musio 2014]. That is, we replace the (negative log) marginal likelihood function by
the (marginal) score function, \( SF(M) = S(x_0, P_M) \). Correspondingly, the (negative log) Bayes factor, \( - \log BF_M \), is replaced by the score difference, 
\[
SD^M_M := S(x_0, P_M) - S(x_0, P_M').
\]
We are thus comparing different hypothesised models for \( X \) by means of their associated scores at the observation \( x_0 \).

### 6.2 Homogeneous score

In particular, if \( S \) is homogeneous, then SF and SD will be insensitive to the arbitrary choice of scale factor in an improper prior density, and will deliver a well-defined value — so long only as \( \pi \) having a proper posterior density.

For simplicity we here just consider the use of the Hyvärinen score \( SH \) of [10]. For the general case of multivariate \( X \), we find
\[
SH(x, P_M) = E \left\{ SH \left( x, P_{\theta M} \right) \bigg| X = x \right\} + \sum_i \text{var} \left\{ \frac{\partial \ln p_M(x | \theta_M)}{\partial x_i} \bigg| X = x \right\}
\]
where expectation and variance are taken under the posterior distribution of \( \theta_M \) given \( X = x \) in model \( M \). This score is thus well-defined so long as the posterior is proper (even though the prior may not be), and the required posterior expectation and variance exist.

#### Example 1
Suppose the statistical model is an exponential family with natural statistic \( T = t(X) \):
\[
p(x | \theta) = \exp \left\{ a(x) + b(\theta) + \theta' t(x) \right\}.
\]
Define \( \mu = \mu(x) \), \( \Sigma = \Sigma(x) \) to be the posterior mean-vector and dispersion matrix of \( \theta \), given \( X = x \). Then the multivariate Hyvärinen score is given by
\[
SH(x, Q) = 2\Delta a(x) + 2d' \mu + \| \nabla a(x) + J \mu \|^2 + 2 \text{tr} J \Sigma J'
\]
with \( d = d(x) := (\Delta t_j), J = J(x) := (\partial t_j(x)/\partial x_i) \).

#### Example 2
Consider the following normal linear model for a data-vector \( Y = (Y_1, \ldots, Y_N)' \):
\[
Y \sim \mathcal{N}(X\theta, \sigma^2 I),
\]
where \( X (N \times p) \) is a known design matrix of rank \( p \), and \( \theta \in \mathbb{R}^p \) is an unknown parameter vector. We take \( \sigma^2 \) as known.

We give \( \theta \) a normal prior distribution: \( \theta \sim \mathcal{N}(m, V) \). The marginal distribution \( Q \) of \( Y \) is then \( Y \sim \mathcal{N}(Xm, XVX' + \sigma^2 I) \), with precision matrix
\[
\Phi = (XVX' + \sigma^2 I)^{-1}
\]
\[
= \sigma^{-2} \left\{ I - X (X'X + \sigma^2 V^{-1})^{-1} X' \right\}
\]
on applying equation (10) of [Lindley and Smith (1972)]

An improper prior can be generated by allowing \( V^{-1} \to 0 \), yielding \( \Phi = \sigma^{-2} \Pi \), where \( \Pi := I - X (X'X)^{-1} X' \) is the projection matrix onto the space of residuals. Although this \( \Phi \) is singular, and thus can not arise from any genuine dispersion matrix, there is no problem in using it to evaluate the Hyvärinen score. We obtain
\[
SH(y, Q) = \frac{1}{\sigma^4} \{ \text{RSS} - 2\nu \sigma^2 \}
\]
where RSS is the usual residual sum-of-squares, on $\nu := N - p$ degrees of freedom. This is well-defined so long as $\nu > 0$.

When we are comparing normal linear models all with the same known variance $\sigma^2$, (34) is equivalent to $(\text{RSS}/\sigma^2) + 2p$, Akaike’s AIC for this case — which is known not to deliver consistent model selection.

An alternative to the multivariate Hyvärinen score, which avoids this problem, is the *sequential* Hyvärinen score. This is a form of composite score, obtained by cumulating the univariate Hyvärinen scores for the sequence of predictive distributions of each $X_n$, given $(X_1, \ldots, X_{n-1})$. This yields

$$S^N_H = \sum_{n=p}^{N} \frac{1}{k^2_n \sigma^4}(Z^2_n - 2\sigma^2) \quad (N \geq p)$$

(35)

where $Z_n \sim \mathcal{N}(0, \sigma^2)$ is the difference between $Y_n$ and its least-squares predictor based on $(Y_1, \ldots, Y_{n-1})$, divided by $k_n$. Without the term $k^2_n$, (35) would reduce to (34), and so be inconsistent. With it (even when $k_n \to 1$, which will typically be the case), the difference between the two expressions tends to infinity, and use of $S^N_H$ does indeed deliver consistent model selection.

\[ \square \]

7 Conclusion

Proper scoring rules, of which there is a very great variety, supply a valuable and versatile extension to standard statistical theory based on the likelihood function. Many of the standard results can be applied, with little modification, in this more general setting. Homogeneous proper scoring rules, which do not make any use of normalising constant of a distribution, prove particularly useful in cases where that constant is computationally intractable, or even non-existent. We have illustrated the application of proper scoring rules for parameter estimation and Bayesian model selection. We believe that there will be many other problems for which they will supply a valuable additional tool in the statistician’s kitbag.

References

Almeida, M. P. and Gidas, B. (1993). A variational method for estimating the parameters of MRF from complete or incomplete data. *Annals of Applied Probability*, 3, 103–36.

Barndorff-Nielsen, O. E. and Cox, D. R. (1994). *Inference and Asymptotics*. Chapman & Hall, London.

Basu, A., Harris, I. R., Hjort, N. L., and Jones, M. C. (1998). Robust and efficient estimation by minimising a density power divergence. *Biometrika*, 85, 549–59.

Berger, J. O. and Pericchi, L. R. (1996). The intrinsic Bayes factor for model selection and prediction. *Journal of the American Statistical Association*, 91, 109–22.

Besag, J. E. (1975). Statistical analysis of non-lattice data. *Journal of the Royal Statistical Society. Series D (The Statistician)*, 24, 179–95.

Brier, G. W. (1950). Verification of forecasts expressed in terms of probability. *Monthly Weather Review*, 78, 1–3.

Dawid, A. P. (1986). Probability forecasting. In *Encyclopedia of Statistical Sciences*, (ed. S. Kotz, N. L. Johnson, and C. B. Read), pp. 210–8. Wiley-Interscience.

Dawid, A. P. (1998). Coherent measures of discrepancy, uncertainty and dependence, with applications to Bayesian predictive experimental design. Technical Report 139, Department of Statistical Science, University College London.

[http://www.ucl.ac.uk/Stats/research/pdfs/139b.zip](http://www.ucl.ac.uk/Stats/research/pdfs/139b.zip)
Dawid, A. P. (2007). The geometry of proper scoring rules. *Annals of the Institute of Statistical Mathematics*, **59**, 77–93. [http://www.ism.ac.jp/editsec/aism/pdf/059_1_0077.pdf](http://www.ism.ac.jp/editsec/aism/pdf/059_1_0077.pdf)

Dawid, A. P. and Lauritzen, S. L. (2005). The geometry of decision theory. In *Proceedings of the Second International Symposium on Information Geometry and its Applications*, pp. 22–8. University of Tokyo.

Dawid, A. P. and Musio, M. (2013). Estimation of spatial processes using local scoring rules. *AS*TA *Advances in Statistical Analysis*, **97**, 173–9. [doi:10.1007/s10182-012-0191-8](https://doi.org/10.1007/s10182-012-0191-8)

Dawid, A. P. and Musio, M. (2014). Bayesian model selection based on proper scoring rules. Manuscript in preparation.

Dawid, A. P., Musio, M., and Ventura, L. (2014). Minimum scoring rule inference. Manuscript in preparation.

Dawid, A. P. and Sebastiani, P. (1999). Coherent dispersion criteria for optimal experimental design. *The Annals of Statistics*, **27**, 65–81.

de Finetti, B. (1975). *Theory of Probability (Volumes 1 and 2)*. John Wiley and Sons, New York. (Italian original Einaudi, 1970).

Good, I. J. (1952). Rational decisions. *Journal of the Royal Statistical Society, Series B*, **14**, 107–14.

Huber, P. J. and Ronchetti, E. M. (2009). *Robust Statistics*. John Wiley and Sons, New York.

Hyvärinen, A. (2005). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning*, **6**, 695–709.

Hyvärinen, A. (2007). Some extensions of score matching. *Computational Statistics and Data Analysis*, **51**, 2499–512.

Lindley, D. V. and Smith, A. F. M. (1972). Bayes estimates for the linear model (with Discussion). *Journal of the Royal Statistical Society, Series B*, **34**, 1–41.

Statistica Sinica (2011). Special issue on composite likelihood. *Statistica Sinica*, **21**, (1). [http://www3.stat.sinica.edu.tw/statistica/j21n1/21-1.html](http://www3.stat.sinica.edu.tw/statistica/j21n1/21-1.html)

Musio, M. and Dawid, A. P. (2013). Local scoring rules: A versatile tool for inference. In *Proceedings of the 59th ISI World Statistics Congress, Hong Kong*. [http://www.statistics.gov.hk/wsc/STS019-P3-S.pdf](http://www.statistics.gov.hk/wsc/STS019-P3-S.pdf)

O’Hagan, A. (1995). Fractional Bayes factors for model comparison. *Journal of the Royal Statistical Society, Series B*, **57**, 99–138.

Parry, M. F. (2013). Multidimensional local scoring rules. In *Proceedings of the 59th ISI World Statistics Congress, Hong Kong*. [http://www.statistics.gov.hk/wsc/STS019-P2-S.pdf](http://www.statistics.gov.hk/wsc/STS019-P2-S.pdf)

Parry, M. F., Dawid, A. P., and Lauritzen, S. L. (2012). Proper local scoring rules. *Annals of Statistics*, **40**, 561–92.

Tsallis, C. (1988). Possible generalization of Boltzmann-Gibbs statistics. *Journal of Statistical Physics*, **52**, 479–87.