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Analytical Expressions to Compute the Continuous Ranked Probability Score (CRPS)

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1 Purpose of this document

The main purpose of this report is to describe the detailed individual steps used to derive analytical expressions for the continuous ranked probability score (CRPS). In addition, it can serve also as a reference for others working on similar problems.

2 The continuous ranked probability score (CRPS)

The continuous ranked probability score (CRPS) is a skill score used primarily for the evaluation of predictive models which provide a predicted distribution of a measured variable. In contrast to more widespread criteria for prediction quality, e.g. root mean square error/residual, mean absolute deviation/error, the CRPS quantifies quality by incorporating information about both *(i)* the closeness to the measured variable and *(ii)* the spread of the predicted distribution around the measured variable. Most typically, the CRPS is used for univariate predictions, i.e. the prediction is a univariate distribution and the measured variable is a scalar.
The predictive distributions considered in this report are:

- Finite mixture of univariate Gaussian densities
- Univariate Gaussian densities

Analytical expressions for these cases are developed in this order.

3 Definitions

All symbols used in this work are defined in Table 1. In addition, the following definitions are applied below:

$$\psi_{kl} := \psi_k \, \psi_l \tag{1} \quad \{\texttt{def11}\}$$

$$\mu_{kl} := \mu_k - \mu_l \tag{2} \quad \{\texttt{def12}\}$$

$$\sigma_{kl} := \sqrt{{\sigma_k}^2 + {\sigma_l}^2} \tag{3} \quad \{\texttt{def13}\}$$

$$A(\mu, \sigma) := \left(2\,\sigma\,\phi\left(\frac{\mu}{\sigma}\right) + \mu\,\left(2\,\Phi\left(\frac{\mu}{\sigma}\right) - 1\right)\right) \tag{4} \quad \{\texttt{def14}\}$$

Table 1: Symbols.

{tab:symbols}

Symbol	Description
δ	Direct δ function
$\Phi(y)$	Cumulative density function (CDF) of the standard normal distribution
$\phi(y)$	Probability density function (PDF) of the standard normal distribution
$\boldsymbol{\psi}$	K-dimensional vector of probabilities
μ (μ_k)	Mean parameter (of the kth mixture component)
σ (σ_k)	Standard deviation parameter (of the kth mixture component)
$F(y)$	Cumulative density function (CDF) evaluated in y
$f(y)$	Probability density function (PDF) evaluated in y
$H(y)$	Heaviside function
$\mathcal{I}(\boldsymbol{\psi})$	Categorical distribution with parameter vector $\boldsymbol{\psi}$
k, l	Mixture component indices
T_1	Term 1 in the continuous ranked probability score (CRPS)
T_2	Term 2 in the continuous ranked probability score (CRPS)
Y, Y^*	Measured variable
y	Measurement (realization of Y)

4 General expressions for continuous ranked probability score (CRPS)

By definition, the CRPS is [1]:

$$CRPS(y) := \int_{-\infty}^{+\infty} \left(F\left(\frac{x-\mu}{\sigma}\right) - H(x-y) \right)^2 dx \qquad (5)$$ {crps11}

In [1], it is shown that the CRPS can be reformulated as follows:

$$CRPS(y) := \mathrm{E}\{|Y-y|\} - \frac{1}{2}\,\mathrm{E}\{|Y-Y^*|\} \qquad (6)$$ {crps12}

with Y and Y^* random variables drawn independently from the same distribution (independently and identically distributed). Most typically, the analytical expression for a specific distribution is derived from this second equation. This is also the case in this report.

5 Continuous ranked probability score (CRPS) for a finite mixture of univariate Gaussian densities.

An analytic expression for the CRPS is derived for the case where Y is distributed according to $f(y)$, where $f(y)$ is a finite mixture of K univariate Gaussian densities and y a realization of Y.

5.1 Case definition

In the studied case, Y is distributed as follows:

$$j \sim \mathcal{I}(\boldsymbol{\psi}) \quad (7) \quad \{\texttt{mix11}\}$$

$$Y_k \sim \mathcal{N}(\mu_k, \sigma_k) \quad (8) \quad \{\texttt{mix12}\}$$

$$Y \sim \sum_k^K \delta(j-k)\, Y_k \quad (9) \quad \{\texttt{mix13}\}$$

where $\mathcal{I}(\boldsymbol{\psi})$ is a categorical distribution defined with the K-dimensional vector $\boldsymbol{\psi}$ of probabilities ψ_k ($\sum_k^K \psi_k = 0$). μ_k and σ_k are the mean and standard deviation of the kth component in the mixture ($k = 1, \ldots, K$). $\delta(z)$ is the indicator function (also: Dirac δ function), which equals 1 when z is zero and equals zero otherwise. It follows that:

$$f(y) = \sum_k \frac{\psi_k}{\sigma_k}\, \phi\left(\frac{y-\mu_k}{\sigma_k}\right) \quad (10) \quad \{\texttt{mix21}\}$$

$$F(y) = \sum_k \psi_k\, \Phi\left(\frac{y-\mu_k}{\sigma_k}\right) \quad (11) \quad \{\texttt{mix22}\}$$

5.2 Formula derivation

Starting from 6, one obtains:

$$CRPS(y) := T_1 + \frac{1}{2} T_2 \quad (12) \quad \{\texttt{mixdrv11}\}$$

with T_1 and T_2 developed as follows:

$$T_1 := \mathrm{E}\{|Y - y|\} \quad (13) \quad \{\texttt{mixdrv21}\}$$

(Rule 1)

$$= P((Y-y)\leq 0)\,\mathrm{E}\{(Y-y)_-\} + P((Y-y)>0)\,\mathrm{E}\{(Y-y)_+\} \tag{14}$$ {mixdrv22}

$$= -\sum_k^K \psi_k\, P((Y_k-y)\leq 0)\,\mathrm{E}\{|Y_k-y|_-\}$$

$$+\sum_k^K \psi_k\, P((Y_k-y)>0)\,\mathrm{E}\{|Y_k-y|_+\} \tag{15}$$ {mixdrv23}

(Rule 1)

$$= \sum_k^K \psi_k\,\mathrm{E}\{|Y_k-y|\} \tag{16}$$ {mixdrv24}

(Rule 2)

$$= \sum_k^K \psi_k\,\left(\sigma_k\, 2\,\phi\left(\frac{y-\mu_k}{\sigma_k}\right) + (y-\mu_k)\,\left(2\,\Phi\left(\frac{y-\mu_k}{\sigma_k}\right)-1\right)\right) \tag{17}$$ {mixdrv25}

$$= \sum_k^K \psi_k\, A\,(y-\mu_k,\sigma_k) \tag{18}$$ {mixdrv26}

$$T_2 := \mathrm{E}\{|Y-Y^*|\} \tag{19}$$ {mixdrv31}

(Rule 1)

$$= P((Y-Y^*)\leq 0)\,\mathrm{E}\{(Y-Y^*)_-\} + P((Y-Y^*)>0)\,\mathrm{E}\{(Y-Y^*)_+\} \tag{20}$$ {mixdrv32}

$$= -\sum_k^K\sum_l^K \psi_k\,\psi_l\, P((Y_k-Y_l)\leq 0)\,\mathrm{E}\{|Y_k-Y_l|_-\}$$

$$+\sum_k^K\sum_l^K \psi_k\,\psi_l\, P((Y_k-Y_l)>0)\,\mathrm{E}\{|Y_k-Y_l|_+\} \tag{21}$$ {mixdrv33}

(Rule 1)

$$= \sum_k^K\sum_l^K \psi_k\,\psi_l\,\mathrm{E}\{|Y_k-Y_l^*|\} \tag{22}$$ {mixdrv34}

(Rule 2)

$$= \sum_k^K\sum_l^K \psi_k\,\psi_l\,\left(2\,\sqrt{{\sigma_k}^2+{\sigma_l}^2}\,\phi\left(\frac{\mu_k-\mu_l}{\sqrt{{\sigma_k}^2+{\sigma_l}^2}}\right)\right.$$

$$\left. +(\mu_k-\mu_l)\,\left(2\,\Phi\left(\frac{\mu_k-\mu_l}{\sqrt{{\sigma_k}^2+{\sigma_l}^2}}\right)-1\right)\right) \tag{23}$$ {mixdrv35}

$$= \sum_k^K\sum_l^K \psi_{kl}\, A\,(\mu_{kl},\sigma_{kl}) \tag{24}$$ {mixdrv36}

where the applied rules of integration are:

- Rule 1.

$$\begin{aligned} \mathrm{E}\{x\} &= \int_a^c x\, f(x)dx = \int_a^b x\, f(x)dx + \int_b^c x\, f(x)dx \\ &= \frac{\int_a^b x\, f(x)dx}{\int_a^b f(x)dx} \left(\int_a^b f(x)dx \right) + \frac{\int_b^c x\, f(x)dx}{\int_b^c f(x)dx} \left(\int_b^c f(x)dx \right) \\ &= \mathrm{E}\{x_{x\leq b}\}\, P(x \leq b) + \mathrm{E}\{x_{x>b}\}\ P(x > b) \end{aligned} \quad (25) \quad \{\texttt{rule1}\}$$

- Rule 2. Mean of folded univariate standard normal distribution [2].

$$\mathrm{E}\{|x|\} = \sigma\, 2\, \phi\left(\frac{\mu}{\sigma}\right) + \mu\, \left(2\, \Phi\left(\frac{\mu}{\sigma}\right) - 1\right) \quad (26) \quad \{\texttt{rule2}\}$$

  with $x \sim \mathcal{N}(\mu, \sigma)$

As a result, the CRPS becomes:

$$CRPS(y) = \sum_k^K \psi_k\, A\left(y - \mu_k, \sigma_k\right) - \frac{1}{2} \sum_k^K \sum_l^K \psi_{kl}\, A\left(\mu_{kl}, \sigma_{kl}\right) \quad (27) \quad \{\texttt{mixdrv41}\}$$

which equals the corresponding expression in [3].
Note that the expression for $A\left(\mu, \sigma\right)$ takes a special form when $\mu = 0$:

$$A\left(0, \sigma\right) = \left(2\, \sigma\, \phi\left(0\right) + \mu\, \left(2\, \Phi\left(0\right) - 1\right)\right) = 2\, \sigma\, \sqrt{\frac{2}{\pi}} \quad (28) \quad \{\texttt{mixdrv51}\}$$

As a result, the terms $A\left(\mu_{kk}, \sigma_{kk}\right)$ in (27) become:

$$A\left(\mu_{kk}, \sigma_{kk}\right) = A\left(0, \sigma_k\, \sqrt{2}\right) = 2\, \sigma_k\, \sqrt{2} = \sigma_k\, \frac{4}{\sqrt{\pi}} \quad (29) \quad \{\texttt{mixdrv61}\}$$

Consequently, one can write the CRPS for a finite mixture of Gaussian densities as:

$$CRPS(y) = \sum_k^K \left(\psi_k\, A\left(y - \mu_k, \sigma_k\right) - \sigma_k\, \frac{2}{\sqrt{\pi}} \right) - \frac{1}{2} \sum_{\substack{k,l=1 \\ k \neq l}}^K \psi_{kl}\, A\left(\mu_{kl}, \sigma_{kl}\right) \quad (30) \quad \{\texttt{mixdrv71}\}$$

6 Continuous ranked probability score (CRPS) for a univariate Gaussian density.

An analytic expression for the CRPS is now derived for the case where Y is distributed according to $f(y)$, where $f(y)$ is a univariate Gaussian density.

6.1 Case definition

In the studied case, Y is distributed as follows:

$$Y \sim \mathcal{N}(\mu, \sigma) \tag{31}$$ {uni11}

where μ and σ are the mean and standard deviation of the normal distribution. It follows that:

$$f(y) = \frac{1}{\sigma}\,\phi\left(\frac{y-\mu}{\sigma}\right) \tag{32}$$ {uni21}

$$F(y) = \Phi\left(\frac{y-\mu_k}{\sigma_k}\right) \tag{33}$$ {uni22}

6.2 Formula derivation

The univariate density can be interpreted as a special case of the finite mixture of Gaussian densities with $K = 1$, $\mu = \mu_1$, $\sigma = \sigma_1$, $\boldsymbol{\psi} = \psi_1 = 1$. Consequently, one can obtain the CRPS expression as a special case of (30), notably:

$$\begin{aligned} CRPS(y) &= A\,(y-\mu,\sigma) - \sigma\,\frac{2}{\sqrt{\pi}} \\ &= \sigma\,\left(2\,\phi\left(\frac{y-\mu}{\sigma}\right) + \frac{y-\mu}{\sigma}\,\left(2\,\Phi\left(\frac{y-\mu}{\sigma}\right) - 1\right) - \frac{2}{\sqrt{\pi}}\right) \end{aligned} \tag{34}$$ {unidrv31}

This expression is equal to the corresponding expression in [3].

References

[1] T Gneiting and A E Raftery. Strictly proper scoring rules, prediction, and estimation. *Journal of the American Statistical Association*, 102:359–378, 2007.

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[3] E P Grimit, T Gneiting, V J Berrocal, and N A Johnson. The continuous ranked probability score for circular variables and its application to mesoscale forecast ensemble verification. *Quarterly Journal of the Royal Meteorological Society*, 132:2925–2942, 2006.