Supplementary Material for "Evaluating infectious disease forecasts with allocation scoring rules"

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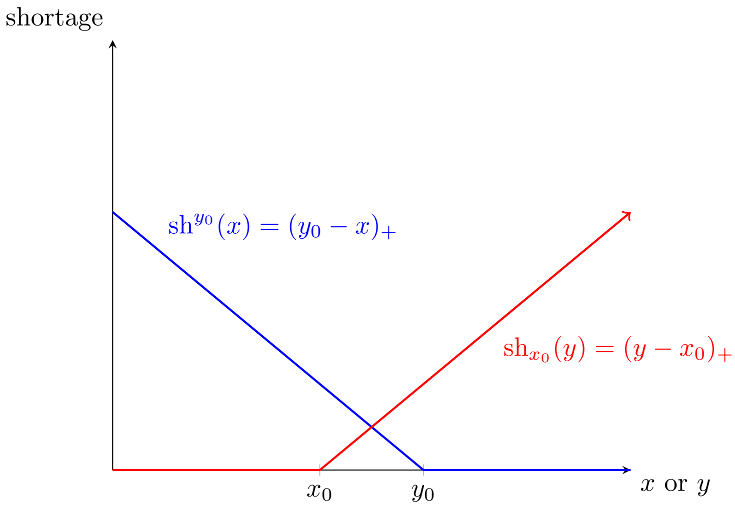
Abstract

We briefly address some technical and methodological points in the main text, referring to the forthcoming ... for more thorough discussion.

- From 2.2.1, why are Bayes act scoring rules proper?
- Explain "All proper scoring rules for probabilistic forecasts have an explicit link to a loss function" from discussion.
- DGP as optimal for any decision problem, ref Diebold, Gunther, Tay p. 866; and if forecasts are ideal, then forecasts with better information always yield better decisions, ref Holzmann and Eulert, Corr 2.
- For 2.2.2, how to get quantile representation of Bayes act using Lagrange multiplier, assuming smooth, never-zero densities well behaved at $x = 0$. Work out exponetial example. Refer to methods paper for general case.
- Derivation of quantile scoring rule with quantile as Bayes act for C/L problem, assuming never-zero densities.
- Descriptions of
  - CRPS as average quantile score across $C \in [0/L]$ decision problems
  - IS as average of two quantile scores with a prob-width penalty
  - WIS as average quantile score across 23 C/L problems.
- Sketch of scoring for decision problems involving both cost and constraint.

1 Shortages

For convenience, we write $u_+ = \max\{0, u\}$, and refer to $(y - x)_+$ as a *shortage* in accordance with our typical use of y for a demand or need and x for an available supply. To regard shortage as a function depending on only one variable x or y, with the other being a parameter describing the dependence we can write $(y - x)_+ = \mathrm{sh}^y(x) = \mathrm{sh}_x(y)$. Note that $\mathrm{sh}^y(x)$ and $\mathrm{sh}_x(y)$ are both convex functions and "mirror" each other:



Let Y be a random variable with distribution F. The random shortage $(Y - x)_+$ can be thought of as either a real-valued random variable $\mathrm{sh}_x(Y)$ for every x, or a function-valued random variable sh^Y whose value for any realization $Y = y$ is a convex function $\mathrm{sh}^y(x)$ of x. We see then that the *expected shortage*[1] $\mathbb{E}_F[(Y - x)_+] = \mathbb{E}_F[\mathrm{sh}^Y](x)$ (assuming it exists) is also convex (and therefore continuous) in x by integrating the convexity inequality for $\mathrm{sh}^y(x)$ with respect to the probability measure $dF(y)$:

$$\begin{aligned}\mathbb{E}_F[\mathrm{sh}^Y](\lambda x_1 + (1-\lambda)x_2) &= \int \mathrm{sh}^y(\lambda x_1 + (1-\lambda)x_2)dF(y) \\ &\leq \int \lambda\,\mathrm{sh}^y(x_1) + (1-\lambda)\,\mathrm{sh}^y(x_2)dF(y) \\ &= \lambda\,\mathbb{E}_F[\mathrm{sh}^Y](x_1) + (1-\lambda)\,\mathbb{E}_F[\mathrm{sh}^Y](x_2). \qquad (1)\end{aligned}$$

Convexity is also shown by directly exhibiting the the left and right derivatives of $\mathbb{E}_F[\mathrm{sh}^Y](x)$:

$$\begin{aligned}D_-\,\mathbb{E}_F[(Y-x)_+] &= \lim_{h\searrow 0}\frac{1}{h}\,\mathbb{E}_F[(Y-x)_+ - (Y-x-h)_+] &(2)\\ &= \lim_{h\searrow 0}\frac{1}{h}\int_{[x-h,x]}(x-h-y)dF(y) - \lim_{h\searrow 0}\frac{1}{h}\int_{(x,\infty)} hdF(y) &(3)\\ &= \lim_{h\searrow 0}\frac{1}{h}\int_{[x-h,x]} -hdF(y) - 1 + F(x) &(4)\\ &= -(F(x) - F(x-)) - 1 + F(x) \qquad \left(\text{where } F(x-) := \lim_{t\nearrow x} F(t)\right) &(5)\\ &= F(x-) - 1 &(6)\\ D_+\,\mathbb{E}_F[(Y-x)_+] &= \lim_{h\searrow 0}\frac{1}{h}\,\mathbb{E}_F[(Y-x+h)_+ - (Y-x)_+] &(7)\\ &= \lim_{h\searrow 0}\frac{1}{h}\int_{[x,x+h]}(x-y)dF(y) - \lim_{h\searrow 0}\frac{1}{h}\int_{(x+h,\infty)} hdF(y) &(8)\\ &= \lim_{h\searrow 0}\frac{1}{h}\int_{[x,x+h]} 0dF(y) - 1 + F(x) &(9)\\ &= F(x) - 1 &(10)\end{aligned}$$

where in (4) and (9) we are able to replace the integrands with their values at x because they are bounded over the shrinking regions of integration $[x-h, x]$ and $[x, x+h]$. Convexity follows since $D_-\,\mathbb{E}_F[\mathrm{sh}^Y](x) \leq D_+\,\mathbb{E}_F[\mathrm{sh}^Y](x)$ by the definition of $F(x)$ and $F(x-)$. This shows that if F does not

[1] A more natural sounding term for $(y - x)_+$ might have been *shortfall*. Unfortunately *expected shortfall* has long been used in finance to refer to quantities more closely related to the *conditonal* expectation $\mathbb{E}_F[Y - x \mid Y - x \geq 0] = \mathbb{E}_F[(Y - x)_+]/\mathbb{P}_F\{Y \geq x\}$.

have a point mass at x, we have

$$\frac{d}{dx}\,\mathbb{E}_F[(Y-x)_+] = F(x) - 1, \tag{11}$$

coinciding with the "Leibniz rule" calculation

$$\frac{d}{dx}\,\mathbb{E}_F[(Y-x)_+] = \frac{d}{dx}\int_x^\infty (y-x) f_Y(y)dy \tag{12}$$

$$= \int_x^\infty \frac{d}{dx}(y-x) f_Y(y)dy - (x-x)f_Y(x) = -\int_x^\infty f_Y(y)dy = F(x) - 1. \tag{13}$$

which assumes Y has an adequately well-behaved density f_Y.

2 Quantiles and Expected Shortage

We recall how quantiles arise as solutions to a probabilistic decision problem. Let Y be a random variable representing the future level of an undesirable outcome such as severe COVID incidence. Let x be a decision variable representing the possible levels of some costly counter-measure, such as procurement of monoclonal antibody treatments, that can be taken at a cost C per unit in preparation for Y. A decision maker must decide on a level x of investment in the counter-measure, and wishes to avoid excesses in either the expediture Cx or the shortage $(y-x)_+$ when $Y = y$ is realized. To formalize the trade-off between these potential excesses we quantify the loss associated with a unit of shortage by a constant $L > C$ (which assumes that the counter-measure has some economic value) and combine the total shortage loss with expenditure into a *loss function*[2]

$$l(x,y) = Cx + L(y-x)_+.$$

The decision problem is then to select a random future loss $l(x,Y)$ in a way that aligns with the preference that $l(x,y)$ be as low as possible given any realization $Y = y$.

To give the decision problem more structure we assume the decision maker either knows the distribution F of Y, or wishes to proceed as if a forecast F of Y were true. This gives us what is known in decision theory as a decision problem *under risk* (regarding the future value of Y) as opposed to one *under uncertainty* where both Y as well as F are unknown when the decision is to be made. A principle commonly invoked in this situation[3] is that the decision maker should or will seek to minimize the expected loss

$$\mathbb{E}_F[l(x,Y)] = Cx + L\mathbb{E}_F[(Y-x)_+]. \tag{14}$$

The expected loss is an affine transformation of the convex expected shortage (c.f. (1)). Therefore $\mathbb{E}_F[l(x,Y)]$ is also is convex and has right and left derivatives $D_\pm\mathbb{E}_F[l(x,Y)]$ at every x. Because these derivatives exist everywhere, a necessary condition for $x^\star$ to minimize $\mathbb{E}_F[l(x,Y)]$ is that $D_+\mathbb{E}_F[l(x^\star,Y)] \geq 0$ and $D_-\mathbb{E}_F[l(x^\star,Y)] \leq 0$, and because of convexity, this condition is also sufficient. From (6) and (10) this means that

$$D_+\mathbb{E}_F[l(x^\star,Y)] = C + L(F(x^\star)-1) \geq 0 \geq D_-\mathbb{E}_F[l(x^\star,Y)] = C + L(F(x^\star-)-1) \tag{15}$$

which rearranges with $\alpha = 1 - C/L$ to

$$F(x^\star) \geq \alpha \geq F(x^\star-). \tag{16}$$

Note that because $F(x)$ and $F(x-)$ are right and left continuous, repectively, the set $\{x \mid F(x) \geq \alpha\}$ is closed on the left and the set $\{x \mid \alpha \geq F(x-)\}$ is closed on the right. Therefore, (16) implies that

$$\min\{x \mid F(x) \geq \alpha\} \leq x^\star \leq \max\{x \mid \alpha \geq F(x-)\}. \tag{17}$$

[2] This does involve a confusing use of the word *loss* to refer to two different quantities, but this seems to be an ingrained and unavoidable habit in the literature.

[3] Note that this priciple might be inappropriate when the decision maker is *risk averse* in some way such as having a preference for random losses with lower variance.

We call $q^-_{\alpha,F} := \min\{x \mid F(x) \geq \alpha\}$ and $q^+_{\alpha,F} := \max\{x \mid F(x-) \leq \alpha\}$ the left and right quantiles of F (for probability level α) and any element $q_{\alpha,F} \in [q^-_{\alpha,F}, q^+_{\alpha,F}]$ a quantile of F. Thus $x^\star$ minimizes the expected loss (14) and gives an optimal sultion to the decision problem if and only if it is a quantile $q_{\alpha,F}$.

Quantiles equivalently arise when the decision problem is defined in terms of the random *oportunity* loss

$$l_o(x, Y) := l(x, Y) - l(Y, Y) = Cx + L(Y - x)_+ - CY \tag{18}$$

which expresses how much more loss is realized by the decision x than an oracle would have incurred, knowing to invest exactly the future value of Y. The optimal decision for $\mathbb{E}_F[l_o(x, Y)]$ is the same as for $\mathbb{E}_F[l(x, Y)]$ since the term $-C\,\mathbb{E}_F[Y]$ is constant in x, leading again to the inequalities (15).

Opportunity loss (18) rearranges to

$$\begin{aligned} l_o(x, Y) &= C(x - Y)_+ + (L - C)(Y - x)_+ && (19)\\ &= L(1 - \alpha)(x - Y)_+ + L\alpha(Y - x)_+, && (20) \end{aligned}$$

a form in which it is often called *pinball* loss, despite its graph being an unlikely pinball trajectory for $\alpha \neq 1/2$.

3 Allocation Bayes acts as vectors of marginal quantiles.

Here we explain why the Bayes act $x_i^{F,K}$ for the allocation problem (4) can be represented as a vector of quantiles for the marginal forecast distributions F_i at a single probability level $\tau^{F,K}$, that is, $x_i^{F,K} = F_i^{-1}(\tau^{F,K})$.

For an arbitrary allocation vector $x \in \mathbb{R}^N_+$ the expected loss

$$\mathbb{E}_F[s_A(x, Y)] = \sum_{i=1}^{N} L \cdot \mathbb{E}_{F_i}[(Y_i - x_i)_+] \tag{21}$$

is the sum of expected shortages (scaled by L) under the allocations x_i in each location. We therefore have the following necessary condition for $x^\star \in \mathbb{R}^N_+$ to be an optimal allocation for $\mathbb{E}_F[s_A(x, Y)]$ under the constraint $\sum_{i=1}^N x_i = K$: if $\delta > 0$ of the $x_i^\star$ units of resource allocated to location i are reallocated to location j, expected shortage will increase in location i by at least as much as it decreases in location j. That is,

$$\mathbb{E}_{F_i}[(Y_i - x_i^\star - \delta)_+] - \mathbb{E}_{F_i}[(Y_i - x_i^\star)_+] \geq \mathbb{E}_{F_j}[(Y_j - x_j^\star)_+] - \mathbb{E}_{F_j}[(Y_j - x_j^\star + \delta)_+]. \tag{22}$$

Since the expected shortages in i and j have right and left derivatives at any x_i and x_j (see Section 1), we can divide (22) by δ and take limits for $\delta \searrow 0$ to get

$$-D_-\mathbb{E}_F[(Y_i - x_i^\star)_+] \geq -D_+\mathbb{E}_F[(Y_j - x_j^\star)_+]. \tag{23}$$

Note that the minus signs appear because our optimality condition addresses how a *decrease* in resources will *increase* the expected shortage in i and vice versa in j. Scaling by L to match the right and left partial derivatives of $\mathbb{E}_F[s_A(x, Y)]$ and using formulae (6) and (10), (23) becomes

$$L(1 - F_i(x_i^\star-)) \geq L(1 - F_j(x_j^\star)). \tag{24}$$

Inequalities (23) and (24) remain true with i and j reversed. They hold with $i = j$ as well by the definition of $F_i(x_i^\star-)$. Therefore, a single number λ (a *Lagrange multiplier*) exists such that

$$L(1 - F_i(x_i^\star-)) \geq \lambda \geq L(1 - F_i(x_i^\star)), \quad \text{for all } i \in 1, \ldots, N \tag{25}$$

that is,

$$F_i(x_i^\star) \geq 1 - \lambda/L \geq F_i(x_i^\star-), \tag{26}$$

which says (c.f. discussion after (16) and (17)) that $x_i^\star$ is a quantile q_{τ,F_i} for $\tau = 1 - \lambda/L$.

4 Properties and Properness

For a prediction to be useful, it must **proper**ly describe a **proper**ty.