Supplementary File: Proof of Proposition 1

Tong Tong Wu[*] and Kenneth Lange[†]

The expected loss $\mathrm{E}\left(\|Y - f(X)\|_\epsilon\right)$ can be written as

$$\mathrm{E}\left[\mathrm{E}\left(\|Y - f(X)\|_\epsilon \mid X\right)\right] \;=\; \mathrm{E}\,\Big[\sum_j p_j(X)\|v_j - f(X)\|_\epsilon \mid X\Big],$$

where $p_j(x) = \Pr(Y = v_j \mid X = x)$. The optimal expected loss is achieved by minimizing $h(z) = \sum_j p_j(x)\|v_j - z\|_\epsilon$ with respect to $z = f(x)$ for each possible x. VDA makes the simplifying assumption that $f(x) = Ax + b$ is linear in x. We now drop this assumption, fix x, and show that the optimal z is closest to the vertex v_j with largest weight $p_j(x)$. For the sake of convenience, we will abbreviate $p_j(x)$ as p_j.

Let us begin with the simple case of two vertices at -1 and 1 with attached probabilities p_1 and p_2. Suppose ϵ is chosen so that the interiors of the two ϵ-insensitive intervals do not overlap. In this circumstance the objective function $h(z) = p_1|z+1|_\epsilon + p_2|z-1|_\epsilon$ is piecewise differentiable with derivative

$$h'(z) \;=\; \begin{cases} -p_1 - p_2 & z \in (-\infty, -1-\epsilon) \\ -p_2 & z \in (-1-\epsilon, -1+\epsilon) \\ p_1 - p_2 & z \in (-1+\epsilon, 1-\epsilon) \\ p_1 & z \in (1-\epsilon, 1+\epsilon) \\ p_1 + p_2 & z \in (1+\epsilon, \infty). \end{cases}$$

Examination of the sign pattern of $h'(z)$ shows that the minimum of $h(z)$ occurs at

$$\begin{cases} -1+\epsilon & \text{if } p_1 > p_2 \\ (-1+\epsilon, 1-\epsilon) & \text{if } p_1 = p_2 \\ 1-\epsilon & \text{if } p_1 < p_2. \end{cases}$$

Since $-1+\epsilon$ is closer to -1, and $1-\epsilon$ is closer to 1, Fisher consistency holds.

[*]Tong Tong Wu is an Assistant Professor in the Department of Epidemiology and Biostatistics, University of Maryland, College Park, MD 20707 (Email: ttwu@umd.edu, Phone: (301)405-3085, Fax: (301)314-9366).

[†]Kenneth Lange is Professor of Biomathematics, Human Genetics, and Statistics at the University of California, Los Angeles, CA 90095 (Email: klange@ucla.edu, Phone: (310)206-8076, Fax: (310)825-8685).

In the general case, let $v_1, \ldots, v_k$ be the vertices of a regular simplex in $\mathbb{R}^{k-1}$. We will take the vertices to be points on the unit ball. In our previous paper (Lange and Wu 2008), we found that $\|v_i - v_j\| = \sqrt{2k/(k-1)}$ for $j \neq i$. The identity

$$\begin{aligned}
\frac{2k}{k-1} &= \|v_i - v_j\|^2 \\
&= \|v_i\|^2 + \|v_j\|^2 - 2v_i^t v_j \\
&= 2 - 2v_i^t v_j
\end{aligned}$$

now yields the inner product $v_i^t v_j = -(k-1)^{-1}$ for $j \neq i$. It is clear that the objective function $h(z) = \sum_j p_j \|v_j - z\|_\epsilon$ is continuous, convex, and coercive. Thus, it attains its minimum value on a convex set C. The nature of C is not altogether obvious. A reasonable conjecture is that C is contained in the convex hull S of the vertices, that is, the regular simplex. Suppose $z \in C$, and u is the closest point in S to z. We will show that u is a better point than z. The standard characterization of the projection u requires the inner product inequality $(z-u)^t(v-u) \leq 0$ for every point $v \in S$. In other words, the three points z, u, and v form a triangle with an obtuse angle at u. The side opposite the obtuse angle is longer than either other side of the triangle. In particular, $\|v - z\| > \|v - u\|$. Taking $v = v_j$ for some v_j with $p_j > 0$ therefore implies $h(u) < h(z)$.

Given that we can confine our attention to S, let us reparameterize z as a convex combination $\sum_j \alpha_j v_j$ of the vertices. The identity

$$\begin{aligned}
\Big\|\sum_j \alpha_j v_j - v_i\Big\|^2 &= \Big\|\sum_j \alpha_j (v_j - v_i)\Big\|^2 \\
&= \sum_j \sum_l \alpha_j \alpha_l (v_j - v_i)^t (v_l - v_i) \\
&= \sum_j \sum_l \alpha_j \alpha_l [v_j^t v_l - v_j^t v_i - v_i^t v_l + \|v_i\|^2] \\
&= \sum_j \sum_{l \neq j} \alpha_j \alpha_l v_j^t v_l + \sum_j \alpha_j^2 \|v_j\|^2 - \sum_j \alpha_j v_j^t v_i \\
&\quad - \sum_l \alpha_l v_i^t v_l + \Big(\sum_j \sum_l \alpha_j \alpha_l\Big) \|v_i\|^2 \\
&= -\frac{1}{k-1} \sum_j \sum_{l \neq j} \alpha_j \alpha_l + \sum_j \alpha_j^2 + \frac{1}{k-1} \sum_{j \neq i} \alpha_j \\
&\quad - \alpha_i + \frac{1}{k-1} \sum_{l \neq i} \alpha_l - \alpha_i + 1 \\
&= -\frac{1}{k-1} \sum_j \alpha_j (1 - \alpha_j) + \sum_j \alpha_j^2 + \frac{1}{k-1}(1 - \alpha_i) \\
&\quad - \alpha_i + \frac{1}{k-1}(1 - \alpha_i) - \alpha_i + 1 \\
&= \Big(1 + \frac{1}{k-1}\Big)\Big(\sum_j \alpha_j^2 + 1 - 2\alpha_i\Big) \\
&= \frac{k}{k-1}\Big[\sum_{j \neq i} \alpha_j^2 + (1 - \alpha_i)^2\Big]
\end{aligned}$$

allows us to prove that $\sum_i \alpha_j v_j$ is closest to the vertex v_i with largest coefficient α_i. Indeed, this follows from the equivalence of the inequality

$$\begin{aligned}
\sum_{j \neq i} \alpha_j^2 + (1 - \alpha_i)^2 &= \sum_{j \neq i,l} \alpha_j^2 + \alpha_l^2 + (1 - \alpha_i)^2 \\
&\leq \sum_{j \neq i,l} \alpha_j^2 + \alpha_i^2 + (1 - \alpha_l)^2 \\
&= \sum_{j \neq l} \alpha_j^2 + (1 - \alpha_l)^2
\end{aligned}$$

to the inequality $\alpha_l \leq \alpha_i$ and the equivalence of their strict analogs.

We now re-express the objective function as

$$h(z) = \sqrt{\frac{k}{k-1}} \sum_j p_j \cdot \max\left\{\sqrt{\sum_{l \neq j} \alpha_l^2 + (1 - \alpha_j)^2} - \eta, 0\right\}$$

for the convex combination $z = \sum_j \alpha_j v_j$ and $\sqrt{\frac{k}{k-1}}\eta = \epsilon$. It is convenient to minimize the equivalent objective function

$$r(\alpha) = \sum_j p_j \cdot \max\left\{\sqrt{\sum_{l \neq j} \alpha_l^2 + (1-\alpha_j)^2} - \eta, 0\right\}.$$

Since $\sum_j \alpha_j v_j \in S$ and we can choose ϵ small enough to avoid overlaps between the interiors of the balls, a minimizer $\sum_j \beta_j v_j$ lies inside at most one of the k balls. There are two possible situations: a) $\sum_j \beta_j v_j$ lies outside of all of the balls, or b) $\sum_j \beta_j v_j$ lies on the boundary or within the ball surrounding some vertex v_i. Let us consider the two cases separately.

Case a: The Euclidean distance between $\sum_j \beta_j v_j$ and any vertex is greater than ϵ since $\sum_j \beta_j v_j$ falls outside the ball centered at the vertex. In this exterior region, the objective function amounts to

$$r(\alpha) = \sum_j p_j \left\{\sqrt{\sum_{l \neq j} \alpha_l^2 + (1-\alpha_j)^2} - \eta\right\}.$$

If v_i is a closest vertex to $\sum_j \beta_j v_j$, then $\beta_i \geq \beta_l$ for every l. The first claim of Proposition 1 is true unless there exists a vertex $v_l \neq v_i$ with $p_l > p_i$. Assume this condition is true, and define a new vector α whose entries equal those of β except for a switch of their entries in positions i and l. Thus, $\alpha_i = \beta_l$ and $\alpha_l = \beta_i$. A brief calculation shows that

$$\begin{aligned} r(\alpha) - r(\beta) &= p_l\sqrt{c + \alpha_i^2 + (1-\alpha_l)^2} + p_i\sqrt{c + \alpha_l^2 + (1-\alpha_i)^2} \\ &\quad - p_l\sqrt{c + \alpha_l^2 + (1-\alpha_i)^2} - p_i\sqrt{c + \alpha_i^2 + (1-\alpha_l)^2} \\ &= (p_i - p_l)\Big[\sqrt{c + \alpha_l^2 + (1-\alpha_i)^2} - \sqrt{c + \alpha_i^2 + (1-\alpha_l)^2}\Big], \end{aligned} \tag{1}$$

where $c = \sum_{j \neq i,l} \beta_j^2$. The difference $r(\alpha) - r(\beta)$ is negative if and only if

$$\sqrt{c + \alpha_l^2 + (1-\alpha_i)^2} > \sqrt{c + \alpha_i^2 + (1-\alpha_j)^2},$$

which is true if and only if $\alpha_i < \alpha_l$, or equivalently $\beta_i > \beta_l$. Thus, the value $r(\alpha)$ represents an improvement over the value $r(\beta)$ when strict inequality holds in $\beta_i \geq \beta_l$. This contradiction almost proves the first contention of Proposition 1.

Unfortunately, our argument does not eliminate the possibility $\beta_i = \beta_l$. When this is the case, we define a vector-valued function $\alpha(t)$ with entries the same as those of β except for $\alpha_i(t) = \beta_i - t$ and $\alpha_l(t) = \beta_l + t$. For $t > 0$ the sum $\sum_j \alpha_j(t) v_j$ remains in the exterior region. Now calculate the derivative

$$\begin{aligned} \frac{d}{dt} r[\alpha(0)] &= p_i \frac{(1-\beta_i) + \beta_l}{\sqrt{c + (\beta_l)^2 + (1-\beta_i)^2}} + p_l \frac{-(1-\beta_l) - \beta_i}{\sqrt{c + (\beta_i)^2 + (1-\beta_l)^2}} \\ &= \frac{(p_i - p_l)}{\sqrt{c + (\beta_i)^2 + (1-\beta_l)^2}}. \end{aligned}$$

Because this derivative is negative, $\alpha(t)$ improves on β for $t > 0$ small.

Case b: We first show that if a minimizer $\sum_j \beta_j v_j$ lies on the boundary or within a ball, then the vertex at the center of the ball has the highest probability. Suppose the vertex v_i lies closest to the minimizer, but $p_l > p_i$ for some $l \neq i$. The vector β defining the minimizer satisfies $\| \sum_j \beta_j v_j - v_i\| \leq \epsilon$. If we define α to equal β except for the switch of entries β_i and β_l, then $\| \sum_j \alpha_j v_j - v_l\| \leq \epsilon$. After some simple algebra, we obtain

$$r(\alpha) - r(\beta) \;\; = \;\; (p_i - p_l)\sqrt{c + \alpha_l^2 + (1-\alpha_i)^2},$$

where $c = \sum_{j \neq i,l} \alpha_j^2$. Now the difference $r(\alpha) - r(\beta)$ is negative unless the equality $\alpha_i = 1$ holds, which is inconsistent with the inequalities $\beta_i \geq \beta_j$ for all j. Hence, α represents an improvement of β. This contradiction again demonstrates that $p_i = \max_j p_j$.

We next show that the minimizer lies on the boundary of the ball with center v_i. Suppose $\sum_j \beta_j v_j$ lies inside the ball. Define the vector-valued function $\alpha(t)$ with entries $\alpha_i(t) = \beta_i - t > 0$ and $\alpha_j(t) = \beta_j + t/(k-1)$ for $j \neq i$, where $t > 0$ is restricted by the requirement that $\sum_j \alpha_j(t) v_l$ remain inside the given ball. For sufficiently small t, we will show that $r[\alpha(t)] < r(\beta)$. In fact, the identities

$$\begin{aligned}
& r[\alpha(t)] - r(\beta) \\
= & \sum_{j \neq i} p_j \left\{ \sqrt{\sum_{l \neq j} \alpha_l^2(t) + [1-\alpha_j(t)]^2} - \sqrt{\sum_{l \neq j} \beta_l^2 + (1-\beta_j)^2} \right\} \\
= & \sum_{j \neq i} p_j \left\{ \sqrt{\sum_{l \neq i,j} \left(\beta_l + \frac{t}{k-1}\right)^2 + (\beta_i - t)^2 + \left(1 - \beta_j - \frac{t}{k-1}\right)^2} \right. \\
& \qquad \left. - \sqrt{\sum_{l \neq j} \beta_l^2 + (1-\beta_j)^2} \right\} \\
= & \sum_{j \neq i} p_j \left\{ \sqrt{\sum_{l \neq j} \beta_l^2 + (1-\beta_j)^2 - \frac{2k\beta_i t}{k-1} + \frac{kt^2}{k-1}} \right. \\
& \qquad \left. - \sqrt{\sum_{l \neq j} \beta_l^2 + (1-\beta_j)^2} \right\},
\end{aligned}$$

make this obvious. Hence, we can improve the current point by moving along the trajectory $\alpha(t)$. It follows that the minimizer lies on the boundary of the ball surrounding v_i.

We now turn to proving the uniqueness of the minimizer assuming all of the p_j are distinct. In support of this conjecture, consider the function $q(z) = \sum_j p_j \|v_j - z\|$ with Euclidean distance substituted for ϵ-insensitive distance. Except at the vertices v_j, one can calculate the gradient

$$\nabla q(z) \;\; = \;\; \sum_j \frac{p_j}{\|z - v_j\|}(z - v_j)$$

and second differential

$$d^2q(z) \;=\; \sum_j \frac{p_j}{\|z-v_j\|^3}\Big[\|z-v_j\|^2 I-(z-v_j)(z-v_j)^t\Big].$$

Based on the second differential, it is possible to demonstrate that $q(z)$ is strictly convex for $k>2$. This result is not true when $k=2$. For strict convexity, it suffices to prove that $d^2q(z)$ determines a positive definite quadratic form. The validity of this claim for all points z except the vertices allows one to assert global strict convexity of $q(z)$. Here one can fall back on the chord above the graph definition of convexity. If a line segment passes through a vertex, then we split the segment into two subsegments at the vertex. The subchord lies strictly above the graph on each subsegment, and the chord above the full segment lies strictly above the two subchords.

Consider therefore the quadratic form defined by a nontrivial vector u. It is clear that

$$u^t d^2q(z)u \;=\; \sum_j \frac{p_j}{\|z-v_j\|^3}\Big\{\|u\|^2\|z-v_j\|^2-[u^t(z-v_j)]^2\Big\}$$

for z distinct from all v_j. The Cauchy-Schwarz inequality implies that each contribution to this sum is nonnegative. A contribution is 0 if and only if $z-v_j$ is a multiple $c_j u$ of u. Thus, the quadratic form vanishes only if $v_j=z-c_ju$ for all j. This says all vertices lie on the same line. Now any line intersects the ball where the v_j reside in at most 2 points. When there are 3 or more vertices, we get a contradiction. Hence, the quadratic form is positive.

With these facts in mind, we now demonstrate that the minimizer of $h(z)=\sum_j p_j\|v_j-z\|_\epsilon$ is unique when the probabilities are unique. The proof is by induction on the number of dimensions k. The case $k=2$ has already been proved, so take $k>2$. Suppose an optimal point occurs at an interior point of the regular simplex where the objective function reduces to the function $q(z)-k\epsilon$. If there is a second optimal point, then the entire line segment between the two points is optimal. This forces points near z to be optimal, contradicting the local strict convexity of $q(z)$. The other possibility is that all optimal points occur on one of the faces of the unit simplex where some $\alpha_j=0$ or on the boundary of one of the ϵ-insensitive balls. We now argue that there can be at most one optimal point per face or ball. The case of a face corresponds to reducing the problem from dimension $k-1$ to dimension $k-2$. Uniqueness now follows by induction and the validity of the hypothesis when $k=2$. For a boundary point, suppose there is a second optimal point. The line segment from the original optimal point to this second optimal point passes through the interior of the ball. Since the entire segment is optimal, there must be optimal points interior to the ball. However, we have excluded such a possibility.

Now consider two optimal points on different faces, different balls, or on a combination of a ball and a face. The line segment connecting the points is optimal. It cannot pass through a ball or along a face because this would contradict the fact just established. It therefore passes through the interior of the simplex possibly tangent to a ball. Our earlier reasoning showing the strict convexity of the function $q(z)$ excludes this possibility. Thus, the optimal point is unique. $\square$

References

Lange, K. and Wu, T. T. (2008), “An MM algorithm for multicategory vertex discriminant analysis,” *J. Computational and Graphical Statistics*, 17, 527–544.