A. Proofs

A.1. Proof of Theorem 1

If the composite loss $\tilde{\ell}(z)$ is convex, it is linear.

Proof: The composite loss is an odd function:

$$\widetilde{\ell}(-z) = \ell(-z) - \ell(z) = -\widetilde{\ell}(z),$$

Therefore, $\frac{d^2}{dz^2}\tilde{\ell}(z) = -\frac{d^2}{dz^2}\tilde{\ell}(-z)$. If the composite loss $\tilde{\ell}(z)$ is convex, $\frac{d^2}{dz^2}\tilde{\ell}(z) \ge 0$ holds for all z. Since the convexity of $\tilde{\ell}(z)$ implies the convexity of $\tilde{\ell}(-z)$, $\frac{d^2}{dz^2}\tilde{\ell}(-z) \ge 0$ should also hold for all z. However, if $\frac{d^2}{dz^2}\tilde{\ell}(z) > 0$, then $\frac{d^2}{dz^2}\tilde{\ell}(-z) < 0$ holds, which is contradictory to the convexity of $\tilde{\ell}(-z)$. Therefore, $\frac{d^2}{dz^2}\tilde{\ell}(z) = 0$ should hold, which is satisfied only when $\tilde{\ell}(z)$ is linear.

A.2. Proof of Lemma 2

 $J_{\rm S}(\alpha)$ is strongly convex in α with parameter at least λ , and thus

$$J_{\mathbf{S}}(\boldsymbol{\alpha}) \geq J_{\mathbf{S}}(\boldsymbol{\alpha}_{\mathbf{S}}^{*}) + \nabla J_{\mathbf{S}}(\boldsymbol{\alpha}_{\mathbf{S}}^{*})^{\top}(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\mathbf{S}}^{*}) + \lambda \|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\mathbf{S}}^{*}\|_{2}^{2}$$
$$\geq J_{\mathbf{S}}(\boldsymbol{\alpha}_{\mathbf{S}}^{*}) + \lambda \|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\mathbf{S}}^{*}\|_{2}^{2},$$

where we use the optimality condition $\nabla J_{S}(\alpha_{S}^{*}) = 0$. Similarly, we can prove the other two inequalities.

A.3. Proof of Lemma 3

The difference function can be written as

$$J_{\mathbf{S}}(\boldsymbol{lpha},\boldsymbol{u}) - J_{\mathbf{S}}(\boldsymbol{lpha}) = rac{1}{4} \boldsymbol{lpha}^{ op} \boldsymbol{u}_1 \boldsymbol{lpha} + rac{1}{2} \boldsymbol{u}_2^{ op} \boldsymbol{lpha} - \pi \boldsymbol{u}_3^{ op} \boldsymbol{lpha},$$

with a partial gradient

$$rac{\partial}{\partial oldsymbollpha}(J_{\mathrm{S}}(oldsymbollpha,oldsymbol u)-J_{\mathrm{S}}(oldsymbollpha))=rac{1}{2}oldsymbol u_1oldsymbollpha+rac{1}{2}oldsymbol u_2-\pioldsymbol u_3.$$

Given the δ -ball of α_{s}^{*} , i.e., $B_{\delta}(\alpha_{s}^{*}) = \{ \alpha \mid \|\alpha - \alpha_{s}^{*}\|_{2} \leq \delta \}$, it is easy to see that for any $\alpha \in B_{\delta}(\alpha_{s}^{*})$,

$$\|\boldsymbol{\alpha}\|_{2} \leq \|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\mathbf{S}}^{*}\|_{2} + \|\boldsymbol{\alpha}_{\mathbf{S}}^{*}\|_{2} \leq 1 + M_{\alpha},$$

and then

$$\frac{\partial}{\partial \boldsymbol{\alpha}} (J_{\mathsf{S}}(\boldsymbol{\alpha}, \boldsymbol{u}) - J_{\mathsf{S}}(\boldsymbol{\alpha})) \Big\|_{2} \leq \frac{1}{2} (1 + M_{\alpha}) \|\boldsymbol{u}_{1}\|_{\mathrm{Fro}} + \frac{1}{2} \|\boldsymbol{u}_{2}\|_{2} + \pi \|\boldsymbol{u}_{3}\|_{2}.$$

This means that $J_{S}(\cdot, \boldsymbol{u}) - J_{S}(\cdot)$ is Lipschitz continuous on $B_{\delta}(\boldsymbol{\alpha}_{S}^{*})$ with a Lipschitz constant of order $\mathcal{O}(\|\boldsymbol{u}_{1}\|_{\text{Fro}} + \|\boldsymbol{u}_{2}\|_{2} + \|\boldsymbol{u}_{3}\|_{2})$.

A.4. Proof of Lemma 5

The difference function can be written as

$$J_{\mathrm{LL}}(\boldsymbol{lpha}, \boldsymbol{u}) - J_{\mathrm{LL}}(\boldsymbol{lpha}) = -\pi \boldsymbol{u}_3^\top \boldsymbol{lpha} + u_4(\boldsymbol{lpha}).$$

Given $\alpha \in B_{\delta}(\alpha_{LL}^*)$, we have known that $-\pi u_3^\top \alpha$ is Lipschitz continuous with a Lipschitz constant of order $\mathcal{O}(||u_3||_2)$ in the proof of Lemma 3. Consequently, $J_{LL}(\cdot, u) - J_{LL}(\cdot)$ is Lipschitz continuous on $B_{\delta}(\alpha_{LL}^*)$ with a Lipschitz constant of order $\mathcal{O}(||u_3||_2 + \text{Lip}(u_4))$.

A.5. Proof of Lemma 7

Same as the proof of Lemma 5.

A.6. Proof of Theorem 4

Let u_1 , u_2 and u_3 be defined as in Eq. (13). According to the *central limit theorem*,

$$\|\boldsymbol{u}_1\|_{\text{Fro}} = \mathcal{O}_p(n'^{-1/2}), \quad \|\boldsymbol{u}_2\|_2 = \mathcal{O}_p(n'^{-1/2}), \quad \|\boldsymbol{u}_3\|_2 = \mathcal{O}_p(n^{-1/2}),$$

as $n, n' \to \infty$. Thus, we have

$$egin{aligned} \|\widehat{m{lpha}}_{ ext{S}} - m{lpha}^*_{ ext{S}} \|_2 &\leq \lambda^{-1} \omega(m{u}) \ &= \mathcal{O}(\|m{u}_1\|_{ ext{Fro}} + \|m{u}_2\|_2 + \|m{u}_3\|_2) \ &= \mathcal{O}_p(n^{-1/2} + n'^{-1/2}) \end{aligned}$$

by Lemma 2, Lemma 3, and Proposition 6.1 in Bonnans & Shapiro (1998, p. 19). On the other hand,

$$|\widehat{J}_{\mathsf{S}}(\widehat{\alpha}_{\mathsf{S}}) - J_{\mathsf{S}}(\alpha_{\mathsf{S}}^*)| \leq |\widehat{J}_{\mathsf{S}}(\widehat{\alpha}_{\mathsf{S}}) - \widehat{J}_{\mathsf{S}}(\alpha_{\mathsf{S}}^*)| + |\widehat{J}_{\mathsf{S}}(\alpha_{\mathsf{S}}^*) - J_{\mathsf{S}}(\alpha_{\mathsf{S}}^*)|,$$

in which

$$\begin{split} \widehat{J}_{\mathrm{S}}(\widehat{\boldsymbol{\alpha}}_{\mathrm{S}}) &- \widehat{J}_{\mathrm{S}}(\boldsymbol{\alpha}_{\mathrm{S}}^{*}) = (\widehat{\boldsymbol{\alpha}}_{\mathrm{S}} + \boldsymbol{\alpha}_{\mathrm{S}}^{*})^{\top} \left(\frac{1}{4n'} \sum_{i=1}^{n'} \varphi(\boldsymbol{x}_{i}') \varphi(\boldsymbol{x}_{i}')^{\top} + \frac{\lambda}{2} I_{m} \right) (\widehat{\boldsymbol{\alpha}}_{\mathrm{S}} - \boldsymbol{\alpha}_{\mathrm{S}}^{*}) \\ &+ \left(\frac{1}{2n'} \sum_{i=1}^{n'} \varphi(\boldsymbol{x}_{i}') \right)^{\top} (\widehat{\boldsymbol{\alpha}}_{\mathrm{S}} - \boldsymbol{\alpha}_{\mathrm{S}}^{*}) - \pi \left(\frac{1}{n} \sum_{i=1}^{n} \varphi(\boldsymbol{x}_{i}) \right)^{\top} (\widehat{\boldsymbol{\alpha}}_{\mathrm{S}} - \boldsymbol{\alpha}_{\mathrm{S}}^{*}), \\ \widehat{J}_{\mathrm{S}}(\boldsymbol{\alpha}_{\mathrm{S}}^{*}) - J_{\mathrm{S}}(\boldsymbol{\alpha}_{\mathrm{S}}^{*}) = \frac{1}{4} \boldsymbol{\alpha}_{\mathrm{S}}^{*\top} \boldsymbol{u}_{1} \boldsymbol{\alpha}_{\mathrm{S}}^{*} + \frac{1}{2} \boldsymbol{u}_{2} \boldsymbol{\alpha}_{\mathrm{S}}^{*} - \pi \boldsymbol{u}_{3} \boldsymbol{\alpha}_{\mathrm{S}}^{*}. \end{split}$$

Since $0 \leq \varphi_j(\boldsymbol{x}) \leq 1$, $\|\boldsymbol{\alpha}_{\mathsf{S}}^*\|_2 \leq M_{\alpha}$ and $\|\widehat{\boldsymbol{\alpha}}_{\mathsf{S}}\|_2 \leq M_{\alpha}$,

$$\begin{aligned} |\widehat{J}_{\mathsf{S}}(\widehat{\boldsymbol{\alpha}}_{\mathsf{S}}) - J_{\mathsf{S}}(\boldsymbol{\alpha}_{\mathsf{S}}^*)| &\leq |\widehat{J}_{\mathsf{S}}(\widehat{\boldsymbol{\alpha}}_{\mathsf{S}}) - \widehat{J}_{\mathsf{S}}(\boldsymbol{\alpha}_{\mathsf{S}}^*)| + |\widehat{J}_{\mathsf{S}}(\boldsymbol{\alpha}_{\mathsf{S}}^*) - J_{\mathsf{S}}(\boldsymbol{\alpha}_{\mathsf{S}}^*)| \\ &\leq \mathcal{O}_p(\|\widehat{\boldsymbol{\alpha}}_{\mathsf{S}} - \boldsymbol{\alpha}_{\mathsf{S}}^*\|_2) + \mathcal{O}_p(\|\boldsymbol{u}_1\|_{\mathrm{Fro}} + \|\boldsymbol{u}_2\|_2 + \|\boldsymbol{u}_3\|_2) \\ &= \mathcal{O}_p(n^{-1/2} + n'^{-1/2}), \end{aligned}$$

which completes the proof.

A.7. Proof of Theorem 6

Let u_3 and $u_4(\alpha)$ be defined as in Eq. (14). The gradient of u_4 is given by

$$\nabla u_4(\boldsymbol{\alpha}) = \frac{1}{n'} \sum_{i=1}^{n'} \frac{\boldsymbol{\varphi}(\boldsymbol{x}_i')}{1 + \exp(-\boldsymbol{\varphi}(\boldsymbol{x}_i')^\top \boldsymbol{\alpha})} - \int \frac{\boldsymbol{\varphi}(\boldsymbol{x})}{1 + \exp(-\boldsymbol{\varphi}(\boldsymbol{x})^\top \boldsymbol{\alpha})} p(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}.$$

According to the central limit theorem,

$$\|\boldsymbol{u}_3\|_2 = \mathcal{O}_p(n^{-1/2}), \quad \operatorname{Lip}(u_4) = \mathcal{O}_p(n'^{-1/2}),$$

as $n, n' \to \infty$, since $\operatorname{Lip}(u_4) = \sup_{\alpha} \| \nabla u_4(\alpha) \|_2$ and

$$\sup_{\boldsymbol{\alpha} \in \mathbb{R}^m, \boldsymbol{x} \in \mathbb{R}^d} \left\| \frac{\boldsymbol{\varphi}(\boldsymbol{x})}{1 + \exp(-\boldsymbol{\varphi}(\boldsymbol{x})^\top \boldsymbol{\alpha})} \right\|_2 \le m^{1/2} < \infty.$$

Thus, we have

$$\begin{aligned} \|\widehat{\boldsymbol{\alpha}}_{\mathrm{LL}} - \boldsymbol{\alpha}_{\mathrm{LL}}^*\|_2 &\leq \lambda^{-1}\omega(\boldsymbol{u}) \\ &= \mathcal{O}(\|\boldsymbol{u}_3\|_2 + \mathrm{Lip}(\boldsymbol{u}_4)) \end{aligned}$$

$$= \mathcal{O}_p(n^{-1/2} + n'^{-1/2})$$

by Lemma 2, Lemma 5, and Proposition 6.1 in Bonnans & Shapiro (1998, p. 19). On the other hand,

$$|\widehat{J}_{\mathrm{LL}}(\widehat{\boldsymbol{\alpha}}_{\mathrm{LL}}) - J_{\mathrm{LL}}(\boldsymbol{\alpha}_{\mathrm{LL}}^*)| \leq |\widehat{J}_{\mathrm{LL}}(\widehat{\boldsymbol{\alpha}}_{\mathrm{LL}}) - \widehat{J}_{\mathrm{LL}}(\boldsymbol{\alpha}_{\mathrm{LL}}^*)| + |\widehat{J}_{\mathrm{LL}}(\boldsymbol{\alpha}_{\mathrm{LL}}^*) - J_{\mathrm{LL}}(\boldsymbol{\alpha}_{\mathrm{LL}}^*)|.$$

For the second term,

$$\begin{aligned} |\widehat{J}_{\text{LL}}(\boldsymbol{\alpha}_{\text{LL}}^*) - J_{\text{LL}}(\boldsymbol{\alpha}_{\text{LL}}^*)| &= |-\pi \boldsymbol{u}_3^\top \boldsymbol{\alpha}_{\text{LL}}^* + u_4(\boldsymbol{\alpha}_{\text{LL}}^*)| \\ &\leq \pi M_\alpha \|\boldsymbol{u}_3\|_2 + |u_4(\boldsymbol{\alpha}_{\text{LL}}^*)| \\ &= \mathcal{O}_p(n^{-1/2} + n'^{-1/2}) \end{aligned}$$

according to the central limit theorem. For the first term, it is a bit more complex:

$$\begin{aligned} |\widehat{J}_{LL}(\widehat{\alpha}_{LL}) - \widehat{J}_{LL}(\alpha_{LL}^*)| &\leq \left| \frac{\lambda}{2} (\widehat{\alpha}_{LL} + \alpha_{LL}^*)^\top (\widehat{\alpha}_{LL} - \alpha_{LL}^*) \right| + \left| \pi \left(\frac{1}{n} \sum_{i=1}^n \varphi(\boldsymbol{x}_i) \right)^\top (\widehat{\alpha}_{LL} - \alpha_{LL}^*) \right| \\ &+ \frac{1}{n'} \sum_{i=1}^{n'} |\ln(1 + \exp(\varphi(\boldsymbol{x}_i')^\top \widehat{\alpha}_{LL})) - \ln(1 + \exp(\varphi(\boldsymbol{x}_i')^\top \alpha_{LL}^*))|. \end{aligned}$$

Let $f(z,t) = \ln(1 + \exp(z+t))$, then $\lim_{t\to 0} f(z,t) = f(z,0)$ and

$$\lim_{t\to 0}\frac{f(z,t)-f(z,0)}{t}=\lim_{t\to 0}\frac{\partial}{\partial t}f(z,t)=\frac{1}{1+\exp(-z-t)}<\infty,$$

where we use *L'Hôpital's rule*. In other words, f(z, t) approaches f(z, 0) in $\mathcal{O}(t)$ as $t \to 0$. Subsequently, for any $x \in \mathbb{R}^d$, by $z = \varphi(x)^\top \alpha_{LL}^*$ and $t = \varphi(x)^\top \widehat{\alpha}_{LL} - \varphi(x)^\top \alpha_{LL}^*$ we can obtain

$$\begin{split} |\ln(1 + \exp(\boldsymbol{\varphi}(\boldsymbol{x})^{\top} \widehat{\boldsymbol{\alpha}}_{\text{LL}})) - \ln(1 + \exp(\boldsymbol{\varphi}(\boldsymbol{x})^{\top} \boldsymbol{\alpha}_{\text{LL}}^{*}))| &= \mathcal{O}(|\boldsymbol{\varphi}(\boldsymbol{x})^{\top} \widehat{\boldsymbol{\alpha}}_{\text{LL}} - \boldsymbol{\varphi}(\boldsymbol{x})^{\top} \boldsymbol{\alpha}_{\text{LL}}^{*}|) \\ &= \mathcal{O}(m^{1/2} \|\widehat{\boldsymbol{\alpha}}_{\text{LL}} - \boldsymbol{\alpha}_{\text{LL}}^{*}\|_{2}), \end{split}$$

which results in $|\widehat{J}_{LL}(\widehat{\alpha}_{LL}) - \widehat{J}_{LL}(\alpha^*_{LL})| = \mathcal{O}_p(n^{-1/2} + n'^{-1/2}).$

A.8. Proof of Theorem 8

The proof goes along the same line as that of Theorem 6. Let u_3 and $u_5(\alpha)$ be defined as in Eq. (15). Note that the function $\max\{0, (1+z)/2, z\}$ is piecewise linear in z, differentiable almost everywhere, and $0 \le (d/dz) \max\{0, (1+z)/2, z\} \le 1$. As a result,

$$\|\boldsymbol{u}_3\|_2 = \mathcal{O}_p(n^{-1/2}), \quad \operatorname{Lip}(u_5) = \mathcal{O}_p(n^{\prime - 1/2}),$$

as $n, n' \to \infty$, and

$$\begin{split} \|\widehat{\boldsymbol{\alpha}}_{\text{DH}} - \boldsymbol{\alpha}_{\text{DH}}^*\|_2 &\leq \lambda^{-1}\omega(\boldsymbol{u}) \\ &= \mathcal{O}(\|\boldsymbol{u}_3\|_2 + \text{Lip}(u_5)) \\ &= \mathcal{O}_p(n^{-1/2} + n'^{-1/2}) \end{split}$$

by Lemma 2, Lemma 7, and Proposition 6.1 in Bonnans & Shapiro (1998, p. 19).

On the other hand,

$$\begin{split} |\widehat{J}_{\mathsf{DH}}(\widehat{\boldsymbol{\alpha}}_{\mathsf{DH}}) - J_{\mathsf{DH}}(\boldsymbol{\alpha}_{\mathsf{DH}}^*)| &\leq |\widehat{J}_{\mathsf{DH}}(\widehat{\boldsymbol{\alpha}}_{\mathsf{DH}}) - \widehat{J}_{\mathsf{DH}}(\boldsymbol{\alpha}_{\mathsf{DH}}^*)| + |\widehat{J}_{\mathsf{DH}}(\boldsymbol{\alpha}_{\mathsf{DH}}^*) - J_{\mathsf{DH}}(\boldsymbol{\alpha}_{\mathsf{DH}}^*)| \\ &\leq \frac{1}{n'} \sum_{i=1}^{n'} |\max\{0, (1 + \boldsymbol{\varphi}(\boldsymbol{x}_i')^\top \widehat{\boldsymbol{\alpha}}_{\mathsf{LL}})/2, \boldsymbol{\varphi}(\boldsymbol{x}_i')^\top \widehat{\boldsymbol{\alpha}}_{\mathsf{LL}}\} \end{split}$$

$$-\max\{0, (1+\varphi(\mathbf{x}_{i}')^{\top}\boldsymbol{\alpha}_{\mathrm{LL}}^{*})/2, \varphi(\mathbf{x}_{i}')^{\top}\boldsymbol{\alpha}_{\mathrm{LL}}^{*}\}| + \mathcal{O}_{p}(n^{-1/2}+n'^{-1/2}).$$

Let $f(z,t) = \max\{0, (1+z+t)/2, z+t\}$, then $\lim_{t\to 0} f(z,t) = f(z,0)$ and for $z \in \mathbb{R} \setminus \{0,1\}$,
$$\lim_{t\to 0} \frac{f(z,t) - f(z,0)}{t} = \lim_{t\to 0} \frac{\partial}{\partial t} f(z,t) \in \left\{0, \frac{1}{2}, 1\right\}.$$

In other words, f(z,t) approaches f(z,0) in $\mathcal{O}(t)$ as $t \to 0$ almost surely. Subsequently, for any $x \in \mathbb{R}^d$, by z = $\varphi(x)^{\top} \alpha_{\rm DH}^*$ and $t = \varphi(x)^{\top} \widehat{\alpha}_{\rm DH} - \varphi(x)^{\top} \alpha_{\rm DH}^*$ we can obtain

$$\begin{aligned} |\max\{0, (1+\varphi(\boldsymbol{x})^{\top}\widehat{\boldsymbol{\alpha}}_{LL})/2, \varphi(\boldsymbol{x})^{\top}\widehat{\boldsymbol{\alpha}}_{LL}\} - \max\{0, (1+\varphi(\boldsymbol{x})^{\top}\boldsymbol{\alpha}_{LL}^{*})/2, \varphi(\boldsymbol{x})^{\top}\boldsymbol{\alpha}_{LL}^{*}\}| &= \mathcal{O}(|\varphi(\boldsymbol{x})^{\top}\widehat{\boldsymbol{\alpha}}_{LL} - \varphi(\boldsymbol{x})^{\top}\boldsymbol{\alpha}_{LL}^{*}|) \\ &= \mathcal{O}(m^{1/2} \|\widehat{\boldsymbol{\alpha}}_{LL} - \boldsymbol{\alpha}_{LL}^{*}\|_{2}) \\ &= \mathcal{O}_{p}(n^{-1/2} + n'^{-1/2}), \end{aligned}$$
which completes the proof

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B. Optimization problems

In this section, we give exact optimization problems for the optimization methods presented in the paper. The logistic regression and logistic loss method is solved with a quasi-Newton method, and therefore we provide the derivatives in Sec. B.1.

The Hinge loss and Double Hinge loss result in quadratic problems. The ramp-loss is solved via a sequence of quadratic problems. All quadratic problems are expressed in the form

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2} \boldsymbol{\alpha}^{\top} H \boldsymbol{\alpha} + \boldsymbol{f}^{\top} \boldsymbol{\alpha} \\ \text{s.t.} \qquad L \boldsymbol{\alpha} \leq \boldsymbol{k} \\ \boldsymbol{l} \leq \boldsymbol{\alpha}$$

This standard form can then just be plugged into an off-the-shelf optimization package such as Gurobi, IBM CPLEX or MATLAB's internal 'quadprog' function.

B.1. Logistic loss

The gradient for the objective function in Eq. (8) is

$$egin{aligned} & \partial J_{ ext{LL}}(oldsymbollpha,b) \ & \partial oldsymbollpha \ & = -rac{\pi}{n} \Phi_{ ext{P}}^{ op} \mathbf{1} + \lambda oldsymbollpha \ & -rac{1}{n'} \sum_{j=1}^{n'} \ell_{ ext{LL}}' \left(-oldsymbollpha^{ op} oldsymbolarphi(oldsymbol x_j') - b
ight) oldsymbolarphi(oldsymbol x_j'), \end{aligned}$$

where $\ell'_{LL}(z)$ is the derivative of $\ell_{LL}(z)$:

$$\ell'_{\rm LL}(z) = -\frac{\exp(-z)}{1 + \exp(-z)}.$$

The derivative with respect to the unregularized constant b is

$$\frac{\partial \widehat{J}_{\text{LL}}(\boldsymbol{\alpha}, b)}{\partial b} = -\pi - \frac{1}{n'} \sum_{j=1}^{n'} \ell'_{\text{LL}} \left(-\boldsymbol{\alpha}^{\top} \boldsymbol{\varphi}(\boldsymbol{x}'_j) - b \right).$$

B.2. Double Hinge Loss - PU Learning

The objective function can be expressed as

,

$$-\frac{\pi}{n}\sum_{i=1}^{n}g(\boldsymbol{x}_{i})+\frac{1}{n'}\sum_{j=1}^{n'}\max\left(0,\max\left(g(\boldsymbol{x}_{j}'),\frac{1}{2}+\frac{1}{2}g(\boldsymbol{x}_{j}')\right)\right)+\frac{\lambda}{2}\|g\|_{2}^{2}$$

Convex Formulation for Learning from Positive and Unlabeled Data

$$= -\frac{\pi}{n}\sum_{i=1}^{n}\left(\sum_{\ell=1}^{m}\alpha_{\ell}\varphi_{\ell}(\boldsymbol{x}_{i}) + b\right) + \frac{1}{n'}\sum_{j=1}^{n'}\max\left(0, \max\left(\sum_{\ell=1}^{m}\alpha_{\ell}\varphi_{\ell}(\boldsymbol{x}_{j}') + b, \frac{1}{2} + \frac{1}{2}\left(\sum_{\ell=1}^{m}\alpha_{\ell}\varphi_{\ell}(\boldsymbol{x}_{j}') + b\right)\right)\right) + \frac{\lambda}{2}\sum_{\ell=1}^{m}\alpha_{\ell}^{2}\varphi_{\ell}(\boldsymbol{x}_{j}') + b_{\ell}^{2}\sum_{\ell=1}^{m}\alpha_{\ell}^{2}\varphi_{\ell}(\boldsymbol{x}_{j}') + b_{\ell}^{2}\sum_{\ell=1}^{m}\alpha_{\ell}^{2$$

The objective function can then be expressed as

$$\begin{array}{ll} \min_{\boldsymbol{\alpha},b,\boldsymbol{\xi}} & -\frac{\pi}{n} \mathbf{1}^{\top} \Phi_{\mathbf{P}} \boldsymbol{\alpha} - \pi b + \frac{1}{n'} \mathbf{1}^{\top} \boldsymbol{\xi} + \frac{\lambda}{2} \boldsymbol{\alpha}^{\top} \boldsymbol{\alpha} \\ \text{s.t.} & \boldsymbol{\xi} \succeq \mathbf{0}, \\ & \boldsymbol{\xi} \succeq \frac{1}{2} \mathbf{1} + \frac{1}{2} \Phi_{\mathbf{U}} \boldsymbol{\alpha} + \frac{1}{2} b \mathbf{1}, \\ & \boldsymbol{\xi} \succeq \Phi_{\mathbf{U}} \boldsymbol{\alpha} + b \mathbf{1}, \end{array}$$

Let

$$oldsymbol{\gamma} = \left[egin{array}{c} oldsymbol{lpha}_{b imes 1} \ b \ oldsymbol{\xi}_{n' imes 1} \end{array}
ight].$$

Then H is defined as

$$H = \left[\begin{array}{ccc} \lambda I_{m \times m} & O_{m \times 1} & O_{m' \times n'} \\ O_{1 \times m} & 0 & O_{1 \times n'} \\ O_{n' \times m} & O_{n' \times 1} & O_{n' \times n'} \end{array} \right],$$

where $O_{n \times m}$ is a zero matrix of n rows and m columns. The linear part of the objective is

$$oldsymbol{f} = \left[egin{array}{c} -rac{\pi}{n} \Phi_{
m P}^{ op} \mathbf{1} \ -\pi \ rac{1}{n'} \mathbf{1}_{n' imes 1} \end{array}
ight]$$

The lower-bound is

$$m{l} = \left[egin{array}{c} -\infty_{m imes 1} \ -\infty \ m{0}_{n' imes 1} \end{array}
ight].$$

The first linear constraint is

$$\boldsymbol{\xi} \succeq \frac{1}{2} \mathbf{1} + \frac{1}{2} \Phi_{\mathrm{U}} \boldsymbol{\alpha} + \frac{1}{2} b \mathbf{1}$$
$$\frac{1}{2} \Phi_{\mathrm{U}} \boldsymbol{\alpha} + \frac{1}{2} b \mathbf{1} - \boldsymbol{\xi} \preceq -\frac{1}{2} \mathbf{1}$$
$$\begin{bmatrix} \frac{1}{2} \Phi_{\mathrm{U}} & \frac{1}{2} \mathbf{1}_{n' \times 1} & -I_{n' \times n'} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ u \\ \boldsymbol{\xi} \end{bmatrix} \preceq -\frac{1}{2} \mathbf{1}_{n' \times 1}.$$

The second linear constraint is

$$\begin{split} \boldsymbol{\xi} \succeq \Phi_{\mathrm{U}} \boldsymbol{\alpha} + b \mathbf{1} \\ \Phi_{\mathrm{U}} \boldsymbol{\alpha} + b \mathbf{1} - \boldsymbol{\xi} \preceq \mathbf{0}_{n' \times 1} \\ \begin{bmatrix} \Phi_{\mathrm{U}} & \mathbf{1}_{n' \times 1} & -I_{n' \times n'} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ b \\ \boldsymbol{\xi} \end{bmatrix} \preceq \mathbf{0}_{n' \times 1}. \end{split}$$

Combining the two sets of inequalities, we get

$$L = \begin{bmatrix} \frac{1}{2} \Phi_{\mathrm{U}} & \frac{1}{2} \mathbf{1}_{n' \times 1} & -I_{n' \times n'} \\ \Phi_{\mathrm{U}} & \mathbf{1}_{n' \times 1} & -I_{n' \times n'} \end{bmatrix},$$

and

$$m{k} = \left[egin{array}{c} -rac{1}{2} m{1}_{n' imes 1} \ m{0}_{n' imes 1} \end{array}
ight].$$

B.3. Weighted hinge loss classifier

We want a cost-sensitive classifier with a per-sample weighting. Using the model

$$g(\boldsymbol{x}) = \sum_{\ell=1}^{m} \alpha_{\ell} \varphi_{\ell}(\boldsymbol{x}) + b,$$

where

$$\{\boldsymbol{c}_1,\ldots,\boldsymbol{c}_m\}:=\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n\},$$

we wish to minimize

$$J(g) = \frac{1}{n} \sum_{i=1}^{b} w_i \ell_{\mathrm{H}} \left(y_i \sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b \right) + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha},$$

$$= \frac{1}{2n} \sum_{i=1}^{n} w_i \max\left(0, 1 - y_i \sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b \right) + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha}.$$

This gives a QP of

$$\begin{array}{ll} \min_{\boldsymbol{\alpha},b,\boldsymbol{\xi}} & \frac{1}{2n} \boldsymbol{w}^{\top} \boldsymbol{\xi} + \frac{\lambda}{2} \boldsymbol{\alpha}^{\top} R \boldsymbol{\alpha} \\ \text{s.t.} & \boldsymbol{\xi}_i \geq 0, \quad \forall i = 1, \dots, n \\ & \boldsymbol{\xi}_i \geq 1 - y_i \sum_{\ell=1}^b \alpha_\ell k(\boldsymbol{x}_i, \boldsymbol{c}_\ell) + u \qquad \forall i = 1, \dots, n. \end{array}$$

We then set

$$oldsymbol{\gamma} = \left[egin{array}{c} oldsymbol{lpha} \ b \ oldsymbol{\xi} \end{array}
ight].$$

H is then

$$H = \begin{bmatrix} \lambda I & O_{m \times 1} & O_{m \times n} \\ O_{1 \times n} & 0 & O_{1 \times n} \\ O_{n \times n} & O_{n \times 1} & O_{n \times n} \end{bmatrix}.$$

The linear term is

$$oldsymbol{f} = \left[egin{array}{c} oldsymbol{0}_{m imes 1} \ 0 \ rac{1}{2n}oldsymbol{w} \end{array}
ight]$$

The lower bound is

$$\boldsymbol{l} = \begin{bmatrix} -\infty_{m \times 1} \\ -\infty \\ \boldsymbol{0}_{n \times 1} \end{bmatrix}$$

Define $\bar{\Phi}$ as

$$\Phi_{i\ell} = y_i \varphi_\ell(\boldsymbol{x}_i).$$

The constraint can be written in matrix form as

$$oldsymbol{\xi} \succeq \mathbf{1}_{n imes 1} - ig(ar{\Phi} oldsymbol{lpha} + b oldsymbol{y} ig) \ - ar{\Phi} oldsymbol{lpha} - b oldsymbol{y} - oldsymbol{\xi} \preceq - \mathbf{1}_{n imes 1}$$

The matrix is then

 $L = \begin{bmatrix} -\Phi & -\boldsymbol{y} & -I_{n \times n} \end{bmatrix},$

and \boldsymbol{k} is

$$\boldsymbol{k} = [-\boldsymbol{1}_{n imes 1}].$$

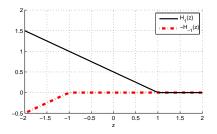


Figure 6. Decomposition of the ramp-loss into convex and concave parts.

B.4. Weighted ramp-loss classifier (CCCP)

Classification with the ramp-loss is difficult, due to the the non-convexity of the loss function. One popular method to perform optimization is to split the non-convex function into a convex and concave part. The concave part is then upperbounded by a linear function, and optimization is iteratively performed: minimization of the upper-bound, and tightening of the upper-bound around the new minima. We minimize the ramp-loss problem here using this approach. This is a straightforward application of the convex-concave procedure (CCCP) in Yuille & Rangarajan (2002) and is essentially the same as Collobert et al. (2006).

We wish to minimize the following non-convex objective function:

$$J(\boldsymbol{\alpha}, b) = \frac{1}{n} \sum_{i=1}^{n} w_i \ell_{\mathrm{R}} \left(y_i \sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b \right) + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha},$$
(16)

where the ramp loss $\ell_{\rm R}(z)$ is defined as

$$\ell_{\rm R}(z) = \max\left(0, \min\left(1, \frac{1}{2} - \frac{1}{2}z\right)\right) = \frac{1}{2}\max\left(0, \min(2, 1 - z)\right).$$

By defining the following (slightly more general) hinge loss

$$H_{\epsilon}(z) = \frac{1}{2}\max(0, \epsilon - z),$$

the ramp loss $\ell_{\rm R}(z)$ can be decomposed as:

$$\ell_{\rm R}(z) = H_1(z) - H_{-1}(z).$$

This is illustrated in Fig. 6. The objective Eq. (16) can therefore be decomposed as

$$J(\boldsymbol{\alpha}, b) = J_{\text{vex}}(\boldsymbol{\alpha}, b) + J_{\text{cave}}(\boldsymbol{\alpha}, b),$$

$$J_{\text{vex}}(\boldsymbol{\alpha}, b) = \frac{1}{n} \sum_{i=1}^{n} w_i H_1\left(\sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b\right) + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha},$$

$$J_{\text{cave}}(\boldsymbol{\alpha}, b) = -\frac{1}{n} \sum_{i=1}^{n} w_i H_{-1}\left(\sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b\right)$$

The following self-evident relation can be used to upper-bound the concave part

$$tz - f(z) \le \sup_{y \in \mathbb{R}} yt - f(y)$$

$$\Rightarrow f(z) \ge tz - f^*(t), \tag{17}$$

where

$$f^*(t) = \sup_{y \in \mathbb{R}} yt - f(y)$$

The inequality in Eq.(17) is known as the *Fenchel inequality* and the function $f^*(z)$ is known as the *Fenchel dual* or *convex conjugate*. Applying the above inequality to $H_{\epsilon}(z)$, we can obtain a bound as

$$H_{\epsilon}(z) \ge zt - H_{\epsilon}^{*}(t), -H_{\epsilon}(z) \le H_{\epsilon}^{*}(t) - zt,$$

where $H_{\epsilon}^{*}(t)$ is the Fenchel dual of $H_{\epsilon}(z)$. The Fenchel dual of $H_{-1}(t)$ is (the full calculation is given in Appendix B.4.3)

$$H_{-1}^*(t) = \begin{cases} -t & -\frac{1}{2} \le t \le 0, \\ \infty & \text{otherwise.} \end{cases}$$

We can minimize the upper-bound as

$$\underset{t}{\arg\min} H^*_{-1}(t) - tz = \begin{cases} t = 0 & z > -1.\\ t = -\frac{1}{2} & z \le -1. \end{cases}$$

The concave part is then bounded, with the parameter a as

$$\bar{J}_{\text{cave}}(\boldsymbol{\alpha}, b, \boldsymbol{a}) = \frac{1}{n} \sum_{i=1}^{n} w_i \left(H_1^*(a_i) - a_i y_i \left(\sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b \right) \right),$$

where $J_{\text{cave}}(\boldsymbol{\alpha}, u) \leq \overline{J}_{\text{cave}}(\boldsymbol{\alpha}, b, \boldsymbol{a})$, for any \boldsymbol{a} .

B.4.1. TIGHTENING OF THE UPPER-BOUND

The upperbound is minimized (tightened) when

$$a_i = \begin{cases} -\frac{1}{2} & y_i \left(\sum_{\ell=1}^m \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b \right) \le -1, \\ 0 & \text{otherwise.} \end{cases}$$

B.4.2. MINIMIZING THE OBJECTIVE

We wish to minimize the convex part and the upper bound $\bar{J}(\alpha, u, a) = J_{vex}(\alpha, u) + \bar{J}_{cave}(\alpha, u, a)$ with respect to a. This gives an objective of

$$\bar{J}(\boldsymbol{\alpha}, b, \boldsymbol{a}) = \frac{1}{n} \sum_{i=1}^{n} w_i H_1\left(y_i\left(\sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b\right)\right) + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha} - \frac{1}{n} \sum_{i=1}^{n} w_i a_i y_i\left(\sum_{\ell=1}^{m} \alpha_\ell \varphi_\ell(\boldsymbol{x}_i) + b\right).$$

We define the following matrices:

$$\Phi_{i,\ell} = y_i k(\boldsymbol{x}_i, \boldsymbol{c}_\ell),$$

$$\bar{\Phi}_{i,\ell} = w_i a_i y_i k(\boldsymbol{x}_i, \boldsymbol{c}_\ell),$$

The QP for this is then

$$\min_{\boldsymbol{\alpha}, b, \boldsymbol{\xi}} \quad \frac{1}{2n} \boldsymbol{w}^{\top} \boldsymbol{\xi} + \frac{\lambda}{2} \boldsymbol{\alpha}^{\top} \boldsymbol{\alpha} - \frac{1}{n} \mathbf{1}^{\top} \bar{\Phi} \boldsymbol{\alpha} - b \frac{1}{n} \sum_{i=1}^{n} w_{i} a_{i} y_{i}.$$
s.t. $\xi_{i} \geq 0 \quad \forall i = 1, \dots, n$
 $\xi_{i} \geq 1 - y_{i} \left(\sum_{\ell=1}^{b} \alpha_{\ell} \varphi_{\ell}(\boldsymbol{x}_{i}) + b \right) \quad \forall i = 1, \dots, n$

We define again

$$\gamma = \left[egin{array}{c} lpha \ b \ oldsymbol{\xi} \end{array}
ight].$$

The quadratic term is

$$H = \begin{bmatrix} \lambda I_{m \times m} & O_{m \times 1} & O_{n \times n} \\ O_{1 \times n} & 0 & O_{1 \times n} \\ O_{n \times n} & O_{n \times 1} & O_{n \times n} \end{bmatrix}$$

The linear term is

$$\boldsymbol{f} = \left[\begin{array}{c} -\frac{1}{n} \bar{\boldsymbol{\Phi}}^{\top} \boldsymbol{1} \\ -\frac{1}{n} \sum_{i=1}^{n} w_{i} a_{i} y_{i} \\ \frac{1}{2n} \boldsymbol{w} \end{array} \right]$$

The lower-bound is

$$lb = \begin{bmatrix} -\infty_{m \times 1} \\ -\infty \\ \mathbf{0}_{n \times 1} \end{bmatrix}.$$

The linear term is

$$-\Phi \boldsymbol{\alpha} - b \boldsymbol{y} - \boldsymbol{\xi} \preceq -\mathbf{1}_{n \times 1}.$$

This gives a matrix of

$$L = \begin{bmatrix} -\Phi & -\boldsymbol{y} & -I_{n \times n} \end{bmatrix},$$

and \boldsymbol{k} is

 $\boldsymbol{k} = \left[-\boldsymbol{1}_{n \times 1}\right].$

B.4.3. Calculation of the Fenchel dual of $H_\epsilon(z)$

In this section, we briefly give the derivation of the Fenchel dual of $H_\epsilon(z)$

$$H_{\epsilon}^{*}(t) = \sup_{v} tv - H_{\epsilon}(v)$$
$$= \sup_{v} tv - \frac{1}{2} \max(0, \epsilon - v).$$

To make the above easier, we split the domain of the v:

$$\begin{aligned} H_{\epsilon}^{*}(t) &= \max\left(\sup_{v \leq \epsilon} tv - \frac{1}{2}\max\left(0, \epsilon - v\right), \sup_{v > \epsilon} tv - \frac{1}{2}\max\left(0, \epsilon - v\right)\right), \\ &= \max\left(\sup_{v \leq \epsilon} tv - \frac{1}{2}\left(\epsilon - v\right), \sup_{v > \epsilon} tv\right). \end{aligned}$$

For the first part:

$$\begin{split} \sup_{v \le \epsilon} tv - \frac{1}{2} \left(\epsilon - v \right) &= \sup_{v \le \epsilon} v \left(t + \frac{1}{2} \right) - \frac{1}{2} \epsilon, \\ &= \begin{cases} \epsilon t & t \ge -\frac{1}{2}, \\ \infty & t < \frac{1}{2} \end{cases} \end{split}$$

The second part is

$$\sup_{t>\epsilon} tv = \begin{cases} \epsilon v & t \le 0, \\ \infty & t > 0. \end{cases}$$

Putting these two together gives:

$$H^*_{\epsilon}(t) = \begin{cases} \epsilon t & -\frac{1}{2} \leq t \leq 0, \\ \infty & \text{otherwise.} \end{cases}$$