I. Formulations

A. Basics

$$\overline{o}^{(i,j)}(x) = \sum_{o\in\mathcal{O}} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o'\in\mathcal{O}}\exp(\alpha_o^{(i,j)})} o(x) \tag{1}$$

Find at Equation (1)

$$\min_{\alpha} \quad \mathcal{L}_{val}(w^*(\alpha),\alpha) \tag{2}$$
$$s.t. \quad w^*(\alpha) = \arg\min_{w} \mathcal{L}_{train}(w(\alpha),\alpha) \tag{3}$$

$$\begin{aligned} \min_{\alpha} \quad & \mathcal{L}_{val}(w^*(\alpha),\alpha) \\ s.t. \quad & w^*(\alpha) = \arg\min_{w} \mathcal{L}_{train}(w(\alpha),\alpha) \\ & p(\alpha) \leqslant P && (4) \\ & r(\alpha) \leqslant T && (5) \end{aligned}$$

$$r(\alpha) \propto \frac{p(\alpha)}{C} \tag{6}$$
$$r(\alpha) = k\frac{p(\alpha)}{C} \leq T \tag{7}$$
$$k\frac{P}{C} = T \tag{8}$$
$$\overline{o}^{(i,j)}(x) = \sum_{o\in\mathcal{O}} \frac{\exp(\alpha_o^{(i,j)}/p_o)}{\sum_{o'\in\mathcal{O}}\exp(\alpha_{o'}^{(i,j)}/p_{o'})} o(x) \tag{9}$$

And we can simplify our constrained bi-level optimization problem as:

$$\begin{aligned} \min_{\alpha} \quad & \mathcal{L}_{val}(w^*(\alpha),\alpha) \\ s.t. \quad & w^*(\alpha) = \arg\min_{w} \mathcal{L}_{train}(w(\alpha),\alpha) \\ & p(\alpha) \leqslant P = \frac{CT}{k} && (10) \end{aligned}$$

$$\begin{aligned} \min_{\alpha} \quad & \mathcal{L}_{val}(w^*(\alpha),\alpha)\cdot e^{(ReLu(p(\alpha)-P))} && (11) \\ s.t. \quad & w^*(\alpha) = \arg\min_{w} \mathcal{L}_{train}(w(\alpha),\alpha) \end{aligned}$$

$$\nabla_\alpha \mathcal{L}_{val}(w^*(\alpha),\alpha)\cdot e^{(ReLu(p(\alpha)-P))} \tag{12}$$
$$\approx \nabla_\alpha \mathcal{L}_{val}(w-\xi\nabla_w\mathcal{L}_{train}(w,\alpha),\alpha)\cdot e^{(ReLu(p(\alpha)-P))} \tag{13}$$

B. Formula deduction

$$\nabla_\alpha \mathcal{L}_{val}(w^*(\alpha),\alpha) \tag{14}$$
$$\approx \nabla_\alpha \mathcal{L}_{val}(w-\xi\nabla_w\mathcal{L}_{train}(w,\alpha),\alpha) \tag{15}$$
$$= \nabla_\alpha \mathcal{L}_{val}(w',\alpha) - \xi\nabla^2_{\alpha,w}\mathcal{L}_{train}(w,\alpha)\cdot\nabla_{w'}\mathcal{L}_{val}(w',\alpha) \tag{16}$$

where $w' = w - \xi\nabla_w\mathcal{L}_{train}(w,\alpha)$.

Details: denote Equation (15) as $\nabla_\alpha f(g_1(\alpha), g_2(\alpha))$, where $f(\cdot,\cdot) = \mathcal{L}_{train}(\cdot,\cdot)$, $g_1(\alpha) = w-\xi\nabla_w\mathcal{L}_{train}(w,\alpha)$, $g_2(\alpha) = \alpha$. Then, it can be deducted that:

$$\begin{aligned} & \nabla_\alpha f(g_1(\alpha), g_2(\alpha)) \\ = & \nabla_\alpha g_1(\alpha)\cdot D_1 f(g_1(\alpha), g_2(\alpha)) + \nabla_\alpha g_2(\alpha)\cdot D_2 f(g_1(\alpha), g_2(\alpha)) \end{aligned}$$

Since,

$$\begin{aligned} \nabla_\alpha g_1(\alpha) &= -\xi\nabla^2_{\alpha,w}\mathcal{L}_{train}(w,\alpha) \\ \nabla_\alpha g_2(\alpha) &= 1 \\ D_1 f(g_1(\alpha), g_2(\alpha)) &= \nabla_{w'}\mathcal{L}_{val}(w',\alpha) \\ D_2 f(g_1(\alpha), g_2(\alpha)) &= \nabla_\alpha\mathcal{L}_{val}(w',\alpha) \end{aligned}$$

Then apply the finite difference approximation, we get:

$$\begin{aligned} & \nabla^2_{\alpha,w}\mathcal{L}_{train}(w,\alpha)\cdot\nabla_{w'}\mathcal{L}_{val}(w',\alpha) \\ \approx & \frac{\nabla_\alpha\mathcal{L}_{train}(w^+,\alpha) - \nabla_\alpha\mathcal{L}_{train}(w^-,\alpha)}{2\epsilon} \end{aligned}$$

where $w^{\pm} = w \pm \epsilon\nabla_{w'}\mathcal{L}_{val}(w',\alpha)$. The following first-order Taylor expansion was adopted actually:

$$f'(x_0)\cdot A \approx \frac{f(x_0+hA) - f(x_0-hA)}{2h}$$