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1: hyper-parameter  $\{\beta_t\}_{t=1 \dots \infty}$   $\triangleright$  exploration-exploitation trade-off values
2: hyper-parameter  $n_p$   $\triangleright$  random samples used to pre-train the model
3: hyper-parameter  $r$   $\triangleright$  Hessian approximation rank
4: hyper-parameter  $n_H$   $\triangleright$  samples used for training Hessian approximation
5: hyper-parameter  $n_I$   $\triangleright$  samples used for computing influence

6: procedure NNINF( $f, \mathcal{X}, T, g_\theta$ )
   $\blacktriangleright$  Minimize  $f$  over  $\mathcal{X}$  for  $T$  steps using the network  $g_\theta$ .

7:    $D \leftarrow \{(x, f(x)) : x \in \text{SAMPLE}(\mathcal{X}, n_p)\}$   $\triangleright$  samples for pre-training
8:    $|\theta| \leftarrow$  number of parameters in  $\theta$ 
9:    $P \leftarrow \text{MATRIX}(|\theta|, r)$   $\triangleright$  for low rank Hessian approximation

10:  for  $t \leftarrow 1 \dots T$  do
11:     $\text{TRAINNETWORK}(g_\theta, D)$ 
12:     $P, \mathcal{I} \leftarrow \text{IHVP}(g_\theta, D, P)$ 
13:     $x_t \leftarrow \arg \min_{x \in \mathcal{X}} \text{ACQUISITION}(x, g_\theta, \mathcal{I}, \beta_t)$ 
14:     $D \leftarrow D \cup \{(x_t, f(x_t))\}$ 
15:  end for

16:  return  $\arg \min_{(x, y) \in D} y$ 
17: end procedure

18: procedure IHVP( $g_\theta, D, P$ )
   $\blacktriangleright$  Compute  $H_\theta^{-1} \nabla_\theta L(z, \theta)$  for  $z \in D$ .

19:   $\pi_P \leftarrow \text{FULLYCONNECTEDNETWORK}(P, P^T)$ 
20:   $S_H \leftarrow \text{SAMPLE}(D, n_H)$ 
21:   $L_H \leftarrow \{\nabla_\theta L(z, \theta) : z \in S_H\}$ 
22:   $J_\theta \leftarrow (1/n_H) \sum_{z \in S_H} L(z, \theta)$ 
23:   $\nu_J \leftarrow \nabla_\theta J_\theta$ 
24:   $D_H \leftarrow \{(v, \nabla_\theta v^T \nu_J) : v \in L_H\}$ 

25:   $\text{TRAINNETWORK}(\pi_P, D_H)$ 
26:   $U, \Sigma, V \leftarrow \text{SVD}(P)$ 
27:   $W \leftarrow U \Sigma^{\dagger^2}$ 

28:   $\mathcal{I} \leftarrow \{WU^T v : v \in \text{SAMPLE}(L_H, n_I)\}$ 
29:  return  $P, \mathcal{I}$ 
30: end procedure

31: procedure ACQUISITION( $x, g_\theta, \mathcal{I}, \beta$ )
   $\blacktriangleright$  compute the acquisition function at  $x$ 

32:   $\mu \leftarrow g_\theta(x)$ 
33:   $\nu_\mu \leftarrow \nabla_\theta \mu$ 
34:   $\sigma \leftarrow \sqrt{\frac{1}{n_I} \sum_{\iota \in \mathcal{I}} (\nu_\mu^T \iota)^2}$ 
35:  return  $\mu - \beta^{1/2} \sigma$ 
36: end procedure

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